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POP Model Intercomparison Study

Stage II. Comparison of mass balance estimates and sensitivity studies

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CONTENTS

Introduction 3

Chapter 1. Intercomparison programme of Stage II 5

1.1. Calculation domain 5

1.2. Input data 6

1.3. Computational experiments 7

1.4. Time table 8

Chapter 2. Description of calculation domain and input data used for modeling 9

2.1. Description of mass balance approaches used in participating models 9

2.2. Description of calculation domain 12

2.2.1. Land cover data 12

2.2.2. Leaf Area Index 14

2.2.3. Organic matter content in the soil 14

2.2.4. Parameters of the environmental compartments 15

2.2.5. Other input data 15

2.3. Physical-chemical properties and degradation rate constants 17

2.4. Description of PCB emissions 17

2.5. Initial concentrations of pollutants in media 19

Chapter 3. Comparison of results of Stage II computational experiments for PCB-153 21

3.1. Distribution of PCB-153 mass between environmental compartments 23

3.1.1.Comparison of calculated values of PCB-153 mass in the atmosphere 23

3.1.2. Comparison of calculated values of PCB-153 mass in soil 33

3.1.3. Comparison of calculated values of PCB-153 mass in water 41

3.1.4. Comparison of calculated values of PCB-153 mass in vegetation 45

3.1.5. Comparison of distribution of PCB-153 mass between environmental media 48

3.2. Masses degraded in the environmental compartments and deposited into deep sea 63

3.2.1. Comparison of calculated values of PCB-153 mass degraded in the atmosphere 63

3.2.2. Comparison of calculated values of PCB-153 mass degraded in soil 71

3.2.3. Comparison of calculated values of PCB-153 mass degraded in water` 78

3.2.4. Comparison of calculated values of PCB-153 mass degraded in vegetation 82

3.2.5. Comparison of distribution of PCB-153 mass degraded in the environment 85

3.2.6. Comparison of calculated values of PCB-153 mass deposited into deep sea 97

3.3. Mass flows transported in/out the specified domain: inflow and outflow 99

3.3.1. Comparison of calculated values of PCB-153 mass flows transported in/out the calculation domain through the atmosphere 99

3.3.2. Comparison of calculated values of PCB-153 mass flows transported in/out the calculation domain through ocean 104

3.3.3 Calculated values of PCB-153 mass flows transported in/out the calculation domain through other compartments 108

3.3.4. Comparison of calculated values of PCB-153 total mass flows transported in/out the specified domain 113

3.3.5. Comparison of PCB-153 mass flows transported in/out the specified domain 118

3.4. Mass flows transported from one compartment to another in both directions 128

3.4.1. Comparison of calculated values of PCB-153 mass flows transported from the atmosphere to soil 128
3.4.2. Comparison of calculated values of PCB-153 mass flows transported from vegetation to soil: Litterfall 142
3.4.3. Comparison of calculated values of PCB-153 mass flows transported from the atmosphere to water 146
3.4.4. Comparison of calculated values of PCB-153 mass flows transported from the atmosphere to vegetation 163
3.5. Concentrations at each interface 180
3.5.1. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with soil 180
3.5.2. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with ocean 184
3.5.3. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with vegetation 188
3. 5.4. Comparison of calculated values of PCB-153 concentration in surface ocean layer 192
3.5.5. Comparison of calculated values of PCB-153 concentration in vegetation 196
3.5.6. Comparison of calculated values of PCB-153 concentration in surface soil layer 200
3.5.7. Comparison of PCB-153 intermedia mass flows and concentrations at the interfaces of main environmental media 203
3.6. Spatial distribution of depositions and concentrations in different compartments (optional) 222
3.6.1. Comparison of results on spatial distribution of PCB-153 depositions and concentrations in different compartments obtained on the basis of “reference data set” 224
3.6.2. Comparison of results on spatial distribution of PCB-153 depositions and concentrations in different compartments obtained on the basis of “own or alternative data sets” 236
3.7. Comparison of model results with measurements 247

Chapter 4. Sensitivity study with respect to substance-specific properties used in the description of basic processes for PCB-153 251
4.1. Gas/particle partitioning 251
4.2. Wet deposition 255
4.3. Gaseous exchange between atmosphere and soil 259
4.4. Gaseous exchange between atmosphere and water 266
4.5. Gaseous exchange between atmosphere and vegetation 270

Conclusions 275

References 279

Annex A. Alternative data set of physical-chemical properties 281

Annex B. Comparison of results of Stage II computational experiments for PCB-28 283

Annex C. Comparison of results of Stage II computational experiments for PCB-180 483

Annex D. Sensitivity study with respect to substance-specific properties used in the description of basic processes for PCB-28 687

Annex E. Sensitivity study with respect to substance-specific properties used in the description of basic processes for PCB-180 707

INTRODUCTION

Following the recommendations of the Executive Body for the Convention on Long-Range Transboundary Air Pollution UN ECE [*ECE/EB.AIR/75*], the POP model intercomparison study was initiated under EMEP in 2002. Four EMEP expert meetings on intercomparison of POP models have been held since that year (Moscow, Russia, 2002; 2003; 2005).

Main aim of POP model intercomparison study is to exchange scientific experience between different groups of POP modelers. National experts from a large number of countries take part in this study, which concerns a wide spectrum of models designed for the simulation of POP behaviour in the environment and differing by their type (box or spatially resolved), resolution and scope (from regional to global scales). According to the agreed programme, the POP model intercomparison study is performed within three stages:

Stage I. Comparison of descriptions of main processes determining POP behaviour in various environmental compartments.

Stage II. Comparison of mass balance estimates and calculated deposition and concentration fields of POPs in different environmental compartments. Sensitivity study with respect to physical-chemical parameter values used in basic process descriptions and mass balance estimates.

Stage III. Comparison of calculated overall environmental persistence and long-range transport potential for evaluation of new substances

Stage I of the intercomparison study was launched in 2002 and completed last year. Fourteen scientific groups from Canada, the Czech Republic, Denmark, France, Germany, Japan, the Netherlands, Norway, Switzerland, the United Kingdom, the USA and representatives of the OECD and MSC-E took part in the first stage. At which model approaches to the description of such processes as gas/particle partitioning, dry deposition of particulate phase, wet deposition, gaseous exchange between the atmosphere and different types of underlying surface (soil, water, vegetation) and degradation processes were considered. This implied the comparison of process descriptions as well as results of relevant computation experiments. Main outcome of Stage I was published in the joint Technical Report 1/2004 “POP Model Intercomparison Study. Stage I. Comparison of descriptions of main processes determining POP behaviour in various environmental compartments” [*Shatalov et al*., 2004].

Stage II of the POP model intercomparison study has been ongoing since 2004. The third and fourth EMEP expert meetings on intercomparison of POP models (Moscow, February, 2005; October, 2005) were attended by national experts from Canada, Germany, Japan, the Netherlands, Norway, Switzerland, the United Kingdom, the USA and MSC-E. Experts and their twelve models participating in this stage of the intercomparison study are listed in Table 1. Computational experiments on calculation of mass balance, inflow/outflow, intermedia transport and spatial distribution of depositions and concentrations together with a comparison of model results with monitoring data were performed by participants in the framework of Stage II. PCB-153 (first priority), and PCB-28, PCB-180 and B[a]P (second priority) were considered within the computational experiments. Sensitivity of each model to variation in physical-chemical parameter values used in mass balance estimates as well as in descriptions of basic processes was also examined. A sensitivity study on wet deposition process included a comparative model simulation of the atmospheric scavenging of particulate B[a]P over the entire troposphere containing a precipitating cumulus cloud with different precipitation rates and was carried out by ADOM-POP and MSCE-POP models. At the fourth meeting it was agreed to proceed with the exercise on wet deposition for PCB-153 proposed by GKSS-CMAQ modeling group. Model results within the sensitivity study will be presented in the final report on the whole POP model intercomparison study.

Since the beginning of 2005 Stage III of the POP model intercomparison study has been started. This stage is aimed at the comparison of relative order in ranking a number of chemicals with respect to LRTP and P_{over} calculated by different models. An extended work-programme and time-schedule of Stage III were elaborated at the latter two meetings.

Table 1. *The list of participating models*

	Model name	Experts	Institution
1	HYSPLIT 4	P. Bartlett	CBNS, Queens College, USA
2	EVN-BETR and UK-MODEL	K. Jones, A. Sweetman	Lancaster University, UK
3	CliMoChem	M. Scheringer, J. Stocker, K. Hungerbühler, F. Wegmann	ETH Zürich, Switzerland
4	CAN/POPs	S. Gong, P. Huang	Air Quality Research Branch, Canada
5	G-CIEMS	N. Suzuki	National Institute for Environmental Studies, Japan
6	ADOM-POP	G. Petersen, A. Aulinger	GKSS, Germany
7	GKSS-CMAQ		
8	DEHM-POP	J. Christensen, K.M. Hansen	National Environmental Research Institute, Denmark
9	SimpleBox	D. van de Meent, A. Hollander	RIVM Laboratory for Ecological Risk Assessment, the Netherlands
10	LOTOS	M.G.M. Roemer	TNO-MEP, the Netherlands
11	ADEPT	A.C. Baart	Delft Hydraulics, the Netherlands
12	MSCE-POP	S. Dutchak, V. Shatalov, A. Gusev, E. Mantseva	EMEP/MSC-E
POP emissions and measurements		K. Breivik	NILU, Norway

In this Intermediate Technical Report a preliminary analysis of results obtained by participating models within Stage II for PCBs is presented. This report is organized in four chapters and five annexes. Brief outline of their contents is given below.

Chapter 1 is devoted to the description of the programme on Stage II of the POP model intercomparison study.

In Chapter 2 a brief overview of the input data used in Stage II calculation experiments is presented. Description of the calculation domain specified for the experiments (land cover data, leaf area index, organic matter content in the soil, parameters of the environmental compartments), physical-chemical properties and degradation rate constants for pollutants in question, emission scenario and measurement data is included. There is also information on initial concentrations of pollutant in main media obtained by the participating models for the end of 1999. In addition, alternative data set of physical-chemical properties for the three considered congeners is presented in Annex A.

Chapter 3 provides information on comparison of results of Stage II computational experiments for PCB-153 obtained by the participating models. Mass balance estimates, deposition and concentration fields in different environmental compartments and results of sensitivity study with respect to physical-chemical parameter values used for mass balance estimates are discussed in this chapter. The comparison of model results on POP depositions and concentrations in various environmental compartments with monitoring data is also presented. A comparison of results of Stage II computational experiments for PCB-28 and PCB-180 is given in Annexes B and C, respectively.

In Chapter 4 results of the sensitivity study with respect to substance-specific properties used in the description of basic processes are presented for PCB-153. A comparison of the similar results for PCB-28 and PCB-180 is given in Annexes D and E, respectively.

Main conclusions are drawn in the end of the Intermediate Technical Report.

As it was agreed at the fourth EMEP expert meetings on intercomparison of POP models, a mechanistic interpretation and detailed analysis of similarities and distinctions between different models' results obtained within Stage II calculations will be prepared as a scientific paper.

More detailed information on the POP model intercomparison study can be found at the MSC-E website: www.msceast.org.

Chapter 1

INTERCOMPARISON PROGRAMME OF STAGE II

This chapter is devoted to the description of the programme of Stage II of POP model intercomparison study discussed in detail at the second and third EMEP expert meetings.

Stage II is aimed at the comparison of mass balance estimates (POPs mass distribution between different environmental compartments; masses of POPs degraded in these compartments; mass fluxes of POPs transported in/out the specified domain; mass fluxes of POPs transported from one compartment to another; and POPs concentrations at each interface) and calculated deposition and concentration fields of POPs in different environmental compartments (optional). These compartments are: atmosphere, soil, water, and vegetation (optional). Calculation experiments are performed with the use of physical-chemical data set of the individual model (if possible) on the basis of agreed input data (POP emission data scenario with zero initial concentrations and with initial concentrations in media of the specified calculation domain) and a number of geophysical parameters of the calculation domain (e.g. land cover data, leaf area index, organic matter content in the soil, etc). The results of calculation experiments are compared between the models. Additionally, POP depositions and concentrations in various environmental compartments as predicted by different models are compared with monitoring data.

This stage is also focused on several sensitivity studies with respect to descriptions of basic processes and mass balance estimates. To do this, the results of calculation experiments formulated at Stage I and Stage II obtained using physical-chemical data sets of each model are compared with those obtained with the use of “reference data sets” (partly these experiments were done in the course of Stage I). For models using “reference data sets” as own sets of physical-chemical properties, it is proposed to carry out these sensitivity studies with the use of alternative data sets based on individual physical-chemical data sets of some other participating models. In addition, simulation of some precipitation episode with emphasis on comparison of modeling results with measurements is performed.

At Stage II the following pollutants selected for the intercomparison study: PCB-153 (first priority), and PCB-28, PCB-180 and B[a]P (second priority) are included into computational experiments.

As it was agreed at the fourth EMEP expert meetings on intercomparison of POP models, a mechanistic interpretation and detailed analysis of similarities and distinctions between different models’ results obtained within Stage II calculations will be prepared as a scientific paper. The timetable of the paper preparation is given in Subsection 1.4 below.

1.1. Calculation domain

To perform calculation experiments at Stage II of the intercomparison study, the European calculation domain (35° N – 70° N; 10° W – 30° E) is agreed to be used.

Description of the specified calculation domain needed for these experiments includes several environmental characteristics commonly used by all models: land cover data, leaf area index, organic matter content in the soil, and total percentage of land, water and vegetation areas.

In calculations such input parameters as volume of each environmental compartment including also air height, soil depth, water depth and meteorological data in 2000 for the specified calculation domain are used by the participants in accordance with their modelling approaches. Particular parameters of environmental compartments such as properties of atmospheric aerosol, soil properties, etc are also chosen for each model individually.

More detailed description of calculation domain is presented in Chapter 2.

1.2. Input data

"Reference" data sets of the considered PCBs presented in the report on Stage I [*Shatalov et al.,* 2004] are input data on physical-chemical properties (including degradation rate constants) harmonized for all models and proposed for the calculations within sensitivity studies to be carried out at Stage II. These data are mainly relied on the internally consistent data sets of key physical-chemical properties presented by [*Li et al*., 2003]. For the evaluation of the organic carbon/water partition coefficient, the most frequently used coefficients of regression relation with the temperature dependent octanol-water partitioning coefficient from [*Karikhoff*, 1981] are chosen. Degradation rate constants in various environmental media are assumed seasonally independent. These values were taken from [*Mackay et al.,* 1992].

To perform sensitivity studies within Stage II, alternative data sets of physical-chemical properties (see Annex A) are proposed for models carrying out calculations on the basis of "reference" data sets as own sets of physical-chemical properties. The "alternative" data sets are in general agreement with the individual physical-chemical data sets of CliMoChem and DEHM-POP models based mainly on data taken from [*Beyer et al*., 2002]. Values of subcooled liquid vapour pressure and water solubility that are not used as parameters in the models mentioned above are added from the same paper. Coefficients of regression relation of the organic carbon/water partition coefficient with the temperature dependent octanol-water coefficient are taken from [*Seth et al*., 1999] as they are in CliMoChem model's data sets. Degradation rate constants in various environmental media used in CliMoChem model in the form of temperature dependencies are transferred into seasonally independent values.

Emission scenario as one of the important harmonized input parameter for the calculations within Stage II is agreed to be common to all models. Thus, consistent global atmospheric emission estimates of PCBs presented by *Breivik et al*., 2002a] (see also http://www.nilu.no/projects/globalpcb/) have been chosen. Spatial distribution of the higher (or worst-case) emission estimate for 2000 and historical emissions is to be applied. All amount of emissions is assumed to be released into the atmosphere.

Initial concentrations of the considered pollutants in media for calculations are prepared by MSC-E.

More detailed description of input data used for computational experiments within Stage II is presented in Chapter 2.

1.3. Computational experiments

The following computational experiments are agreed to be performed at Stage II:

1. *Sensitivity study with respect to basic processes:*
    - comparison of calculation experiments formulated at Stage I carried out with the use of "reference data sets" and physical-chemical data sets of the individual model (or alternative data set);
    - additional experiments on wet deposition process of B[a]P and PCBs for some precipitation episodes.

2. *Comparison study of mass balance estimates (annual and monthly means) calculated with the use of physical-chemical data set of the individual model (or alternative data set).*

A base year for the calculations is 2000. Calculations of mass balance estimates of PCB-153 (of PCB-28 and PCB- 180 as optional) are performed for one-year period (2000) with zero initial concentrations and with initial concentrations in media with the use of two different data sets: "own or alternative" and "reference". For the sake of comparison with measurements (as optional), calculations are carried out for 20-year period (from 1981 to 2000) with zero initial data with historical emissions with the use of "own or alternative" data sets. Output parameters are:

- masses of PCB-153 in specified sub-domains in air, soil and seawater compartments:
    - the atmosphere: layers of 1 km, 5 km and 10 km height,
    - soil: 5 cm and 10 cm depth,
    - sea: 200 m depth;
- masses of PCB-153 degraded in specified sub-domains of these compartments;
- mass flow of PCB transported in/out the specified domain: inflow and outflow (for each transport media as optional);
- mass flow of PCB transported from one compartment to another in both directions (net, dry and wet deposition, gaseous exchange);
- PCB concentrations at each interface (pg/m^3, pg/l, ng/g, for air, water and soil, respectively);
- spatial distributions of PCB depositions and concentrations in different compartments (optional).

3. *Sensitivity study with respect to mass balance estimates*:
    - Comparison of the above calculations of mass balance estimates with those obtained with the use of "reference data sets".

1.4. Timetable

The timetable of activities within Stage II adopted by the participants and revised after the fourth EMEP expert meeting is presented in Table 1.1.

Table 1.1. *Timetable for Stage II*

What	Who	When	Where
Description of calculation domain (land cover data, leaf area index, organic matter content in the soil, etc)	MSC-E	April 2004	Experts
Input data for computational experiments (spatial distribution of emissions in 2000 and historical emissions with resolution 1°by 1° over all Northern Hemisphere)	K.Breivik and S.Gong	April 2004	Experts
Input data for computational experiments (initial concentration scenarios)	MSC-E	April 2004	Experts
Output protocol (templates on each experiments to be filled in)	MSC-E	April 2004	Experts
Monitoring data on air concentrations and depositions of PCBs in 2000 for the comparison with calculations	K.Breivik	May 2004	Experts
Experiment on wet deposition process of B[a]P	G.Petersen	May 2004	Experts
Descriptions of mass balance approaches used in the participating models and output of computational experiments	Experts	October 2004	MSC-E
Processing of the results	MSC-E	December 2004	Experts
Preparation of the first draft of intermediate report on Stage II	MSC-E/ Experts	January 2004	Experts
Third EMEP expert meeting on POP model intercomparison study	MSC-E	February 2005	Experts
Submission of additional data on masses contained and degraded in specified sub-domains in air, soil and seawater compartments	Experts	February 25, 2005	MSC-E
Processing results and distribution them between participants	MSC-E	end of March, 2005	Experts
Preparation of the final version of the Intermediate Technical Report on Stage II and its distribution between participants	MSC-E	end of May, 2005	Experts
Calculations of mass balance estimates for one-year period with zero initial concentrations and with the use of two different data sets: “own or alternative” and “reference” and their distribution between participants (for models, which have not submitted these calculations yet).	Experts	middle of May, 2005	MSC-E
Calculations of mass balance estimates for 20-year period with zero initial data with historical emissions (optional) and their distribution between participants	Experts	middle of May, 2005	MSC-E
Processing results obtained within long-term goal and distribution them between participants	MSC-E	end of July, 2005	Experts
Fourth EMEP expert meeting on intercomparison of POP models	MSC-E/Experts	October 2005	MSC-E/ Experts
Proposals from GKSS-CMAQ group on wet deposition exercise for PCB-153	GKSS-CMAQ	30 October 2005	Experts
List of revisions for the results presented in the report on Stage II	Experts	1 December, 2005	MSC-E
Proposals on developing of preliminary research questions on similarities and discrepancies between different models	Lead authors	1 December, 2005	Experts
Results on “long-term goals” of Stage II and on sensitivity study of process description (Stage i calculations) (for models, which have not submitted them yet)	Experts	1 December, 2005	MSC-E
Statistical processing of the model results and preparation of a final version of the report on Stage II	MSC-E	31 January, 2006	Experts
Research questions on key similarities and discrepancies between the own model and other participating models and interpretation of these points (if possible)	Experts	28 February, 2006	MSC-E
Results on wet deposition of PCB-153	Experts	28 February, 2006	MSC-E
List of priority research questions and key points in similarities and discrepancies of different model results	Lead authors	31 March, 2006	Experts
Additional calculations for a scientific paper (if necessary)	Experts	30 June, 2006	Lead authors/ MSC-E
First draft of a scientific paper	Lead authors	1 September, 2006	Experts
Fifth EMEP expert meeting on intercomparison of POP models	MSC-E/Experts	2 October, 2006	MSC-E/ Experts
Preparation of a final version of a scientific paper and its publishing	Lead authors	15 December, 2006	Experts

The fifth EMEP expert meeting on POP model intercomparison study will be held in Moscow on October 2, 2006. The intermediate informal meeting is planned to be organized on June 9, 2006.

Chapter 2

DESCRIPTION OF CALCULATION DOMAIN AND INPUT DATA USED FOR MODELING

This chapter is devoted to a brief description of model input information used by the participating models at Stage II of the intercomparison study. This description covers two types of model input information: input data common for all models and data used by each particular model individually.

To describe the European calculation domain including its total fractions of land, water and vegetation areas, several input characteristics: land cover data, leaf area index, and organic matter content in the soil are agreed to be used by all models in Stage II experiments. Besides, for the sake of comparison, calculation of mass balance estimates requires other harmonised input information among which emissions data and/or initial concentrations of PCBs in the main environmental media, and physical-chemical properties and degradation rates of the considered POPs are the most important. The common data sets used in the calculations are presented below.

In addition to them, the participating models, which differ from each other by their type, resolution, overall modelling approaches, processes description and number of environmental media considered, require also a lot of another input data, e.g. on meteorological parameters, geophysical characteristics, concentrations of different reactants, data on specific aerosol surface in air, data on sea currents, the particles settling rates in seawater and so on. Due to a large diversity, such input data used by the participating models are described very briefly in this chapter.

A brief description of measurement data on air concentrations and depositions of PCBs used for the comparison with model estimates is given in Chapter 3 (Section 3.7).

2.1. Description of mass balance approaches used in participating models

Evaluation of the mass balance for PCBs within the specified calculation domain is based on the calculations of mass balances for main environmental compartments, which are considered by the particular model. ADEPT, CAN/POPs, CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, SimpleBox, and MSCE-POP considered the dispersion of PCB emissions between the atmosphere and the underlying surfaces. Further redistribution and accumulation of PCBs in the main environmental compartments other than atmosphere (soil and water) is also included in these models, but ADEPT model is purely atmospheric. Vegetation is taken into account in CliMoChem, EVN-BETR and UK-MODEL, G-CIEMS, SimpleBox, and MSCE-POP models. EVN-BETR and UK-MODEL, SimpleBox and MSCE-POP models imply also sediments and MSCE-POP considers the exchange between the atmosphere and the cryosphere (sea ice and snow).

Most of the models describe the same main processes: gas/aerosol partitioning, degradation in various environmental media, wet and dry deposition processes, and gaseous exchange between different environmental compartments. Along with degradation and outflow from the calculation domain, CliMoChem consider also deposition of the pollutants to the deep sea as additional loss process. Model parameterizations and comparison of the results of Stage I were discussed in detail in [*Shatalov et al.,* 2004]. Sensitivity study with respect to descriptions of basic processes is given in Chapter 4 of this report.

As it was agreed at the third EMEP expert meeting on intercomparison of POP models, this Intermediate Technical Report summarizes results on calculations of PCB mass balance estimates and sensitivity studies of process description and mass balance estimates. The included mass balance estimates for 2000 were obtained by participants on the basis of one-year calculation with zero initial concentrations (ADEPT, CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, MSCE-POP, SimpleBox) and with initial concentrations in media given as input data (CAN/POPs, EVN-BETR and UK-MODEL, G-CIEMS, DEHM-POP, MSCE-POP, SimpleBox). Calculations of CliMoChem, EVN-BETR and UK-MODEL and SimpleBox carried out for 20-year period (from 1981 to 2000) with zero initial data with historical emissions are also included in this note. Calculations were performed with the use of two different data sets: "own or alternative" and "reference» and for the three considered congeners – PCB-153, PCB-28 and PCB-180 (See Table 2.1). In Table 2.1 main comments and descriptions of model approaches to the calculation of mass balance provided by the participants when they submitted their calculation results on Stage II experiments can be also found.

Table 2.1. *Calculations of the mass balance and comments to these estimates*

Models	Physical-chemical data set	PCBs	Calculations and comments
ADEPT	Reference	PCB-153	One-year calculations are made with zero initial concentrations
EVN-BETR and UK-MODEL	Reference	PCB-153, PCB-28, PCB-180	One-year calculations are carried out using both a single box version of European model and the spatially resolved version. Results are calculated on the basis of initial concentrations given as input data, zero initial concentrations for one-year period (2000) and with historical emissions for 20-year period (from 1981 to 2000). The only exception was that the initial conditions for the vegetation were set to zero.
SimpleBox	Alternative and Reference	PCB-153, PCB-28, PCB-180	One-year calculations are made with zero initial concentrations and with initial concentrations in media given as input data; calculations are also carried out for 20-year period (from 1981 to 2000) with zero initial data with historical emissions. Calculations are done with 2 versions of the SimpleBox model, SimpleBox 3.0 and SimpleBox 3.12 The difference between the models is in the definition of the soil compartment. In the old Simplebox 3.0 model we assume that chemicals are distributed equally thoughout the soil compartment (the model calculates average soil concentrations). In the new SimpleBox 3.12 model it is assumed that concentrations of chemicals in the soil compartment decline exponentially (based on the chemical specific soil penetration depth). With this model we can calculate the chemical concentration at each depth of the soil compartment, and we can calculate average concentrations over, for example, the upper 5 cm of the soil based on the concentration profile. We did this for the MSC-E calculations. **General Mass balance equation for SimpleBox** Vi * dCi/dt = Emissioni + Importi - Exporti - Degradationi + Advectionij + Diffusionij -**Mass balance equation for the air compartment**: Vair * dCair/dt = EmissionAir + ImportAir - ExportAir - Vair * DegAir * Cair - SUM(DepWater)* Cair - SUM(DepSoil)* Cair - SUM(DepVeg)* Cair - SUM(XCHairwater) * Cair - SUM(XCHairsoil)* Cair - SUM(XCHairveg)* Cair + SUM(XCHwaterair) * Cwater + SUM(XCH soilair) * Csoil + SUM(XCHvegair)* Cveg Vair = volume of air compartment (m^3) Cair = total concentration in air (mol/m^3) t = time (s) EmissionAir = Emission mass flow into air compartment (mol/s) ImportAir = Import mass flow into air (mol/s) ExportAir = Export mass flow out of air (mol/s) DegAir = pseudo first order transformation rate constant in air (s^{-1}) DepWater/DepSoil/DepVeg = transport coefficient for atmospheric deposition (wet and dry) to water, soil, veg resp. (m^3/s) XCHair-water/soil/veg = transport coefficient gas absorption to water, soil, vegetation resp. (m^3/s) XCHwater/soil/veg-air = transport coefficient volatilization from water, soil, vegetion resp. (m^3/s) Cwater = concentration in water (dissolved) (mol/m^3) Csoil = concentration in soil (mol/m^3) Cveg = concentration in vegetation (mol/m^3)

SimpleBox	Alternative and Reference	PCB-153, PCB-28, PCB-180	**SimpleBox settings:** Height air = 1 km Soil depth = 5 cm (for forest and urban soil), 20 cm for agricultural soil Water depth = 200 m in continental level of SimpleBox. For regional level only 3 and 10 m water depths exist So, we only calculated the mass and degraded mass in air for the first 1 km, in soil for a depth of 5 cm and in water for a depth of 200 m. For water we could only calculate values on a continental level. **Comments**: SimpleBox is not a spatially explicit multimedia fate model. The only possibility for incorporating some spatial variability is by nesting regional and local model scales in the larger continental and global scales. So, the regional and the continental scale together form the calculation domain. The regional level covers the cells: 3W-10E/55-57N; 2W-11E/53-54N; 1W/52N; 1E-11E/51N; 3E-11E/50N; 5E-10E/49N; 6E-10E/48N. According to SimpleBox model layout it was pointed out which cells of the calculation domain belong to the regional level and which belong to the continental level. For this study we have taken the calculation domain specified by MSC-E as the total model domain (10W-30E/35N-70N). Within this area we have distinguished a regional level that covers the river basins that flow into the Southern North Sea (North-Western Europe). The rest of the model domain belongs to the continental model scale.
CAN/POPs	Own	PCB-153; PCB-180	One-year calculations are made with initial concentrations in media given as input data.
CliMoChem	Own and Reference	PCB-153, PCB-28, PCB-180	Calculations are carried out for 20-year period (from 1981 to 2000) with zero initial data with historical emissions and for one-year of 2000 on zero initial concentrations. **Comments:** CliMoChem is a climate zone model and does not provide longitudinal resolution. It is not possible to compute masses and mass fluxes for sub-zonal regions like the EMEP region (35°N – 70°N; 10°W – 30°E). Therefore, masses and mass fluxes were converted as followed. First, calculations were done for 10 latitudinal zones of equal latitudinal width, but varying longitudinal length (zone 1: North Pole, zone 10 South Pole). The EMEP region is covered by zone 2 (72°N – 54°N) and zone 3 (55°N – 36°N). Second, the masses and mass fluxes in zone 2 and zone 3 were summarized. Third, based on CliMoChem's assumption that the mass within a zone is uniformly distributed, the summarized masses and mass fluxes were divided by 9 (360°/40°) to obtain masses and mass fluxes per EMEP region. CliMoChem does calculate masses and mass fluxes per season (three months, starting in January) and monthly values are not available. Therefore, we suggest summarizing monthly outputs calculated by other models to obtain seasonal values that can be compared to CliMoChem's results.
MSCE-POP	Own and Reference	PCB-153, PCB-28, PCB-180	One-year calculations are made with zero initial concentrations and with initial concentrations in media as input data. **Comments:** The model used is a hemispheric model spatially resolved with resolution 2.5°x2.5°. It includes the following main environmental compartments: atmosphere, soil, seawater, sea ice/snow and vegetation. Horizontal spatial resolution in the oceanic compartment is two times finer. Vertical structure of the atmosphere consists of 12 layers with bounds defined in σ-coordinates. The overall coverage is about 12 km. Soil is divided into 7 vertical layers with thickness 0.1, 0.3, 0.6, 1, 2, 5,11 cm. In the ocean depth is given by special batimetry file.
G-CIEMS	Alternative and Reference	PCB-153	One-year calculations are made with initial concentrations in media given as input data and with zero initial conditions. **Comments:** All target region was treated as one-box environment. Land, emission and relevant information are developed by average and/or sum of the provided data-set. Generic moderate, tropic and polar regions are assumed to calculate the target region. The net in/out flux of the target region between surrounding generic region are presented in the "inflor-outflow" section.
DEHM-POP	Own and Reference	PCB-153, PCB-28, PCB-180	One-year calculations are made with zero initial concentrations and with initial concentrations in media given as input data. **Comments:** Results on calculations of mass contained and degraded in different environmental compartments are given for 15 km layer of the atmosphere; for 15 cm layer of soil; for 75 m layer of water.

2.2. Description of calculation domain

The calculation domain agreed to be used in Stage II experiments covers the most part of the European region occupying also some small parts of the North Atlantic and the Arctic oceans and Northern Africa (see Fig. 2.1). In the horizontal dimensions it is confined by the surface grid (i,j) with latitude: 35° N – 70° N; and longitude:10° W – 30° E. It has spatial resolution 1°×1°, which is arranged such that i = 1 is centered at 179.5°W and I increases eastward; and j = 1 is centered at 89.5°N and J increases southward.

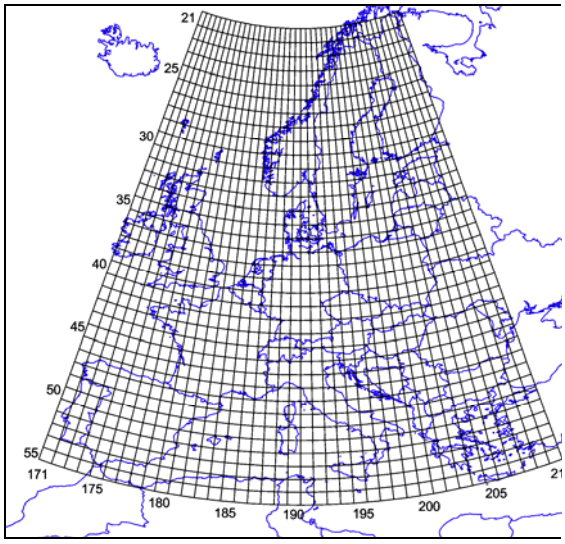


Fig. 2.1. *The European calculation domain (1°×1° grid)*

Information on land cover data, leaf area index, organic matter content in the soil and total fractions of land, water and vegetation areas in the European calculation domain were given as common input data for Stage II experiments and are described below. In addition, comments to these input data provided by the participants are also given in the appropriate subsections.

2.2.1. Land cover data

Land cover information used for the description of the European calculation domain within Stage II experiments and presented as input data is based on 25-category USGS Land Use/Land Cover dataset obtained from NCAR Mesoscale Modeling System (MM5) [*Guo and Chen*, 1994]. The original data set includes the detailed information on underlying surface types with high spatial resolution (10'x10'). Land cover data for model intercomparison study are presented in 1°×1° surface grid system. Each grid cell is characterized by several types of surface proportional their area. The USGS Land Use/Land Cover System Legend is presented in Table 2.2.

Total area of the European calculation domain is equal to 1.05E+07 km^2. Data on total fractions of land, water and vegetation areas in this calculation domain calculated by MSC-E on the basis of 25-category USGS Land Use/Land Cover dataset from [*Guo and Chen*, 1994] and presented as input data are given in Table 2.3.

Table 2.2. *USGS Land Use/Land Cover System Legend*

No	Description
1	Urban and Built-Up Land
2	Dryland Cropland and Pasture
3	Irrigated Cropland and Pasture
4	Mixed Dryland/Irrigated Cropland and Pasture
5	Cropland/Grassland Mosaic
6	Cropland/Woodland Mosaic
7	Grassland
8	Shrubland
9	Mixed Shrubland/Grassland
10	Savanna
11	Deciduous Broadleaf Forest
12	Deciduous Needleleaf Forest
13	Evergreen Broadleaf Forest
14	Evergreen Needleleaf Forest
15	Mixed Forest
16	Water Bodies
17	Herbaceous Wetland
18	Wooded Wetland
19	Barren or Sparsely Vegetated
20	Herbaceous Tundra
21	Wooded Tundra
22	Mixed Tundra
23	Bare Ground Tundra
24	Snow or Ice
25	Unidentified

Table 2.3. *Total percentage of land, water and vegetation areas in the European calculation domain*

Land Cover Categories	Fractions (%):
Water	46.9
Soil	53.1
Vegetation	52.6

Comments of CliMoChem:

Currently, land cover data in *CliMoChem* are taken from [*DeFries and Townshend*, 1994]. The resulting surface type distribution summarized for zone 2 and zone 3 can be found in Table 2.4. Table 2.4 also shows surface type distribution based on [*Guo and Chen*, 1994].

Table 2.4. *Surface fraction based on [DeFries and Townshend, 1994][1] and [Guo and Chen, 1994] [2]*

Environmental Media	Surface Fraction	
	CliMoChem zone '2+3'	European region
Bare soil	0.0166[1]	0.0120[2]
Sea	0.3952[1]	0.4687[2]
Vegetation-Covered Soil	0.5882[1]	0.5193[2]

The spatial dimensions of the specific compartments directly influences mass fluxes and bulk compartment specific parameters (i.e. bulk vegetation compartment). Thus, the use of different land cover data results in different masses in the compartments.

Therefore, along with calculations carried out on the basis of land cover data from [*DeFries and Townshend*, 1994] additional calculations were performed where the default surface type distribution in zone 2 and zone 3 was overwritten with the surface type distribution from [*Guo and Chen*, 1994] for the European region. The data for the 25 land use categories summarized in the file LandUse11_domain.xls were regrouped in the following surface types: bare soil, grassland, coniferous forest, deciduous forest and water.

Comments of MSCE-POP:

Since the formulation of MSCE-POP model does not require detailed specification of data on the underlying surface, the original 25-categories of land cover from [*Guo and Chen*, 1994] were reduced to six general categories (deciduous forests, coniferous forests, grassland, urban and built-up land, bare land and glaciers, water bodies) and redistributed over the model grid. As an example we present here the spatial distribution of two land cover categories from reduced set: deciduous forests and grassland within the Northern Hemisphere (Fig. 2.2).

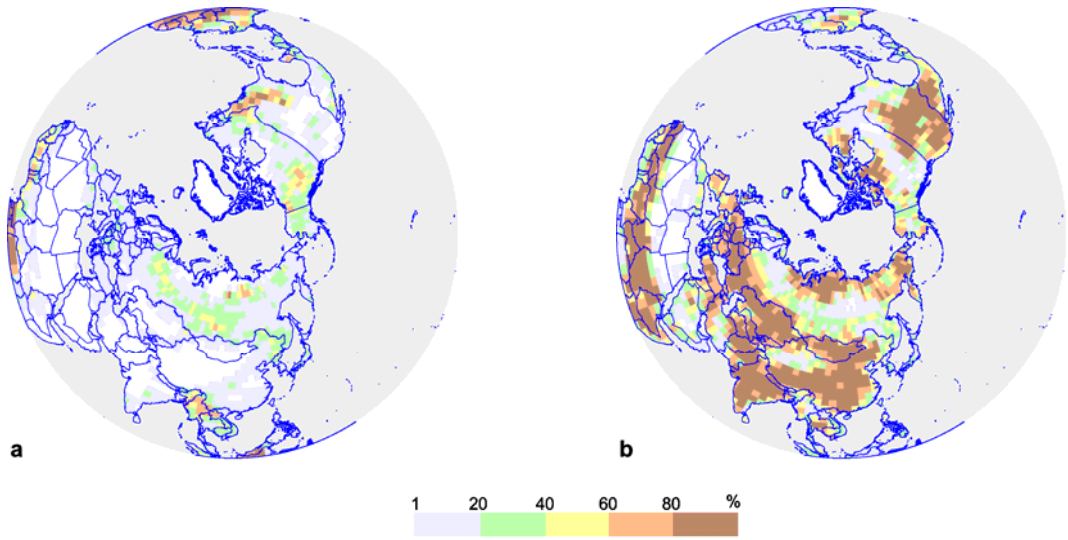


Fig. 2.2. *Fraction of the area covered by deciduous forests (a) and grassland (b) in the Northern Hemisphere used by MSCE-POP model*

2.2.2. Leaf Area Index

Leaf Area Index (LAI) data set used for the description of the European calculation domain within Stage II experiments and presented as input data includes the geographically resolved data for 1987 with monthly resolution. The Leaf Area Index for a given grid cell implies the ratio between the area of leaves in this cell to its total area (m^2/m^2). The geographically resolved leaf area index data with monthly resolution was adopted from CD-ROM of NASA Goddard Space Flight Center [*Sellers et al*., 1994, 1995] and converted to 1°×1° surface grid system. Consistency of these data in relation to the land cover information was investigated by correlation analysis.

2.2.3. Organic matter content in the soil

Data on organic matter content in the soil are taken from http://www.giss.nasa.gov/ and presented in 1°×1° surface grid system. The organic matter content in the soil for a given grid cell implies the share of organic matter in this cell relative to its total content (%).

Comments of CliMoChem:

CliMoChem's default model parameters were used to describe organic matter content in soil, as well as LAI. The reason for not using the data proposed by MSC-E is the fact that they are area specific and not – as required in *CliMoChem* – vegetation type specific. Table 2.5 gives an overview of the annually averaged organic matter content in soil and LAI for the different soil cover types. References can be found in the supporting information to [*Wegmann et al*., 2004].

Table 2.5. *Leaf area index (m^3/m^2) and fraction of organic carbon for different soil cover (%)*

Soil cover	LAI	Organic carbon content
Bare soil	none	2
Grassland	$2.77*10^{-4}$	8.5
Coniferous forest	$1.68*10^{-3}$	35.5
Deciduous forest	$7.81*10^{-4}$	22.5

2.2.4. Parameters of the environmental compartments

For calculations of mass balance estimates for the specified domain, such input parameters as volume of each environmental compartment including air height, soil depth and water depth were used by the participants in accordance with their modelling approaches. However, calculated values of mass contained and degraded in the environmental media are agreed to be submitted for the atmospheric layers of 1 km, 5 km and 10 km height, for soil layers of 5 cm and 10 cm depth; and seawater layer of 200 m depth.

Other particular geophysical parameters of environmental compartments used in the calculations such as properties of atmospheric aerosol (e.g. fraction of organic carbon content in the aerosol, specific aerosol surface, etc), soil, water and vegetation are also chosen for each model individually. Geophysical parameters of environmental compartments used by the participating models for the calculations of mass balance of PCBs in the specified calculation domain are presented in Table 2.6.

2.2.5. Other input data

The participants in accordance with their modelling approaches also use some other inputs parameters. They can include meteorological data, concentrations of OH-radical in the atmosphere, data on sea currents, concentrations of suspended particles, the particles settling rates in seawater and the content of organic carbon (OC) in these particles and so on. For example, in MSCE-POP model meteorological data provided by The System of Diagnosis of the Lower Atmosphere (SDA) developed by Hydrometeorological Centre of Russia [*Frolov et al.*, 1994; *Rubinstein et al*., 1997,1998; *Frolov et al.*, 1997 a,b,c] are used. A large set of meteorological parameters among which are data on wind velocity; precipitation rates; surface pressure; air temperature and a number of parameters of the atmospheric boundary layer (e.g. friction velocity, Monin-Obukhov length etc.) is implemented in the parameterization of the main processes of POP behavior. For the description of POP degradation in the atmosphere in MSCE-POP a spatial distribution of monthly mean concentrations of hydroxyl radical from [*Spivakovsky et al*., 2000] is used. The original data were interpolated to the calculation grid.

References to the input parameters used individually can be also found in the detailed descriptions of the participating models presented in the report on Stage I [*Shatalov et al.,* 2004].

Table 2.6. *Geophysical parameters of environmental compartments in the calculation domain used by participating models*

Media	Parameter	Dimen-sion	DEHM-POP		ADEPT		CAN/POPs		CliMoChem		G-CIEMS		EVN-BETR and UK-MODEL		SimpleBox		MSCE-POP	
			Value	Reference	Value	Reference	Value	Reference	Value	Reference	Value	Reference	Value	Reference	Value	Reference	Value	Reference
Atmosphere	Air volume	km^3			3.85E+06		3.40E+08	own model	5.57E+08 (height: 6km)		1.05E+08		1.42E+07		9.60E+06		1.26E+08 (height: 12km)	Own
	Total Suspended Matter, TSP	$\mu g/m^3$	Variable	Own			Variable		86	*Wegmann et al.*, 2004	30		30				30	
	Fraction of organic carbon content in the aerosol, foc	%	20				Variable		not used		20		20				20	
	Specific aerosol surface, θ	m^2/m^3	Not used		1.50E-04		Variable		not used						1.50E-04		1.50E-04	*Whitby*, 1978
	Others …..														1.72E-01*		[OH] spatial distribution	*Spivakovsky et al.*, 2000
Soil	Soil volume	km^3					5.95E+03	own model	4.94E+03 (depth 0.1m)		5.57E+02		8.39E+02		7.21E+02**		1.11E+03 (depth 0.2m)	Own
	Bulk soil density, ρ	kg/m^3	1.35E+03	*Jury et al.*, 1983			1.35E+03	MSC-E	2.4	*Scheringer*, 2003	1.50E+03		2.40E+03		1.70E+03		1.35E+03	
	Volumetric water content in soil	%	30	*Jury et al.*, 1983			30	MSC-E	30	*Wegmann et al.*, 2004	30		0.3		20		30	
	Volumetric air content in soil	%	20	*Jury et al.*, 1983			20	MSC-E	20		20		0.3		20		20	
	Others …..																	
Water	Water volume	km^3					1.07E+06	own model	8.71E+06 (depth: 200m)		3.35E+06		8.66E+05		8.71E+05		9.83E+05 (depth 200m)	
	Freshwater	-											1.27E+05		3.39E-02		-	
	Seawater	-							8.71E+06		1		5.78E+06		9.66E-01		9.83E+05 (depth 200m)	
	Inclusion of suspended particulate matter	-	no				N/A		yes		yes		yes				yes	
	Others…..																	
Vegetation	Specific surface area of vegetation, *aV*	m^2/m^3													1.275E+03		8.00E+03	*Duyzer and van Oss*, 1997
	grassland	m^2/m^3							2.77E-04***	*Wegmann et al.*, 2004								
	coniferous forest	m^2/m^3							1.68E-03***	*Wegmann et al.*, 2004								
	decideous forest	m^2/m^3							7.81E-04***	*Wegmann et al.*, 2004								
	Others…..																	

* - Junge constant, *Pa·m;*
** - the total value of soil volume; for natural soil it is equal to 2.42E+02 km^3; for agricultural soil it is equal to 4.76E+02km^3; for other soil it is equal to 2.90E+00 km^3;
***-annual average values.

2.3. Physical-chemical properties and degradation rate constants

The data sets of basic physical-chemical properties and degradation rates of PCBs in the main environmental media are one of the most important input data used for model calculations. The key characteristics required for POP modelling are the following:

- air-water Henry's law constant (K_H);
- subcooled liquid vapour pressure (p_{0L});
- coefficients of partitioning between different media (octanol-water partition coefficient (K_{OW}), octanol-air partition coefficient (K_{OA}), organic carbon-water partition coefficient (K_{OC}));
- water solubility;
- degradation rate constants for different environmental compartments;

Temperature dependencies of Henry's law constant, subcooled liquid-vapour pressure, octanol-air partition coefficient and degradation rate constants are also of great importance for the reliable description and parameterization of POP behaviour in the environment.

The participating models perform calculations of mass balance estimates at Stage II using individual data sets of these physical-chemical properties and degradation rates. Descriptions of individual data sets for the considered congeners of PCBs ("own data sets") presented by CAN/POPs, DEHM-POP, G-CIEMS, EVN-BETR and UK-MODEL, CliMoChem and MSCE-POP are given in the MSC-E Technical Report 1/2004 [*Shatalov et al.,* 2004]. Comparison of base values of key physical-chemical parameters and coefficients of their temperature dependencies made within Stage I of POP model intercomparison study are also presented in [*Shatalov et al.,* 2004].

To study sensitivity of participating models with respect to variability of PCB physical-chemical parameter values, Stage II experiments and partly experiments proposed in the course of Stage I are repeated with the help of common "reference data sets". The latter are internally consistent data sets of key physical-chemical properties and degradation rates of PCBs taken mostly from [*Li et al*., 2003; *Mackay et al.,* 1992] and proposed for model testing. These data sets are also presented in the report on Stage I [*Shatalov et al.,* 2004]. For models using "reference data sets" as own physical-chemical properties, "alternative data sets" based on individual data of CliMoChem and DEHM-POP models and based mainly on data taken from [*Beyer et al*., 2002] are proposed for this sensitivity study. The "alternative data sets" used for modelling of PCB-153, PCB-28 and PCB-180 are presented below in Annex A.

2.4. Description of PCB emissions

Although reliable emission data for persistent organic pollutants PCBs is essential both to understand and control the large-scale environmental distribution of these contaminants, surprisingly little is still known about their emissions on a regional and global scale. Official emission data for PCBs submitted by Parties to CLRTAP tend to have an incomplete spatial, temporal and congeneric distribution which obstructs the possibility to use them for regional / hemispheric / global modelling activities. For this reason, the model calculations presented herein rely on global emission estimates derived from a European Union research project (Global SOC ENV4 – CT97 – 0638). These estimates were developed, using a dynamic mass balance approach, aiming to quantify the global historical production, consumption and emissions of selected PCBs [*Breivik et al*. 2002a,b].

The production of PCBs was addressed by collecting data from the literature on production of total PCB as well as of technical mixtures [*Breivik et al.*, 2002a]. These data were coupled with the chemical composition of the mixtures in order to estimate the production of individual homologues and congeners. Whenever there were gaps in the data, assumptions were made to come up with quantitative estimates for the production. More than 70% of the total PCB produced was in the form of Tri-CB, Tetra-CB and Penta-CB. The estimated total production of the selected 22 congeners (ΣPCB22) adds up to 0.566 million tonnes.

The global historical consumption pattern was estimated from collected data on the import, export, usage, and restrictions of PCB import on a regional/national level, along with assumptions regarding the PCB trade between countries and regions. The homologue and congener consumption was approached by treating groups of countries as closed markets. The results indicate that near 97% of the total historical consumption of PCBs occurred in the Northern Hemisphere (Figure 2.3). The main uncertainty related to the spatial pattern, is the estimated consumption for countries where no information is available on imports, exports and consumption. However, these countries contribute very little to the overall consumption and hence the associated uncertainty on a global scale is considered relatively small.

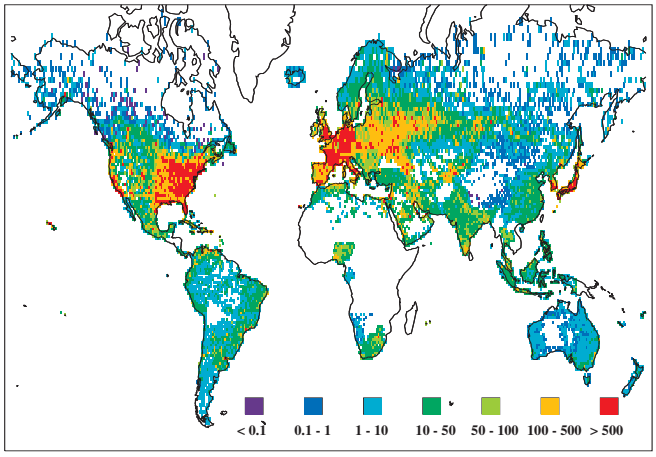


Fig. 2.3. *Estimated cumulative consumption of total PCBs on a 1˚ by 1˚ basis, using population distribution for spatial allocation [Breivik et al., 2002a]*

The diversity of PCB consumption and disposal pathways of PCB products makes the true emission pathways equally complex [*Breivik et al*., 2002b]. A lumped approach has been chosen to bridge the gap between consumption and emissions, thus clustering categories of usage, accidental releases and disposal pathways together. The crucial simplification in this approach is that any potential usage and loss process to the atmosphere is included in the selected categorisation of emission sources. Usage and disposal were further divided into four lumped sub-categories each and two accidental release pathways were addressed. Emissions were estimated through a mass balance approach.

The uncertainties in the emission estimates are predicted to be much higher than the uncertainty in the production estimates. For this reason, three different emission scenarios were elaborated (Minimum/Default/Maximum). These date are considered crucial as a research tool for mass balance studies and regional and global fate modelling. The results could also assist in the evaluation and interpretation of atmospheric levels of PCBs.

Mass balance studies as well as model studies utilising these data in combination with monitoring results have already facilitated some interpretation of the uncertainties/reliability of these estimates. *Wania and Daly* [2002] used the Globo-POP model to evaluate the global fate of PCBs. They found the maximum emission estimate to be the more reliable when comparing predicted and observed concentrations. Secondly, *Meijer et al*., [2003] studied the global occurrence of PCBs in soil. They suggested that the surface soil burden account for about 1.6% of the known historical production, and reasoned that it is likely that the true cumulative emission is toward – or above – the upper emission scenario presented by *Breivik et al*. [2002b]. For these reasons, the higher emission scenario has been used as common model input in the model calculations presented in this report.

Spatial distribution of PCB emissions in 2000 and in all years of the preceding period from 1980 up to the base year over the grid were prepared by S. Gong and P. Huang on the basis of this emission scenario in compliance with global distribution of population density. As an example, a map of gridded data of PCB-153 emissions in the Northern Hemisphere used for modeling at Stage II is presented in Fig. 2.4.

Within Stage II calculation experiments all amount of PCB emissions is assumed to be released into the atmosphere and for each year of the period the total annual emission value is continually distributed among the year.

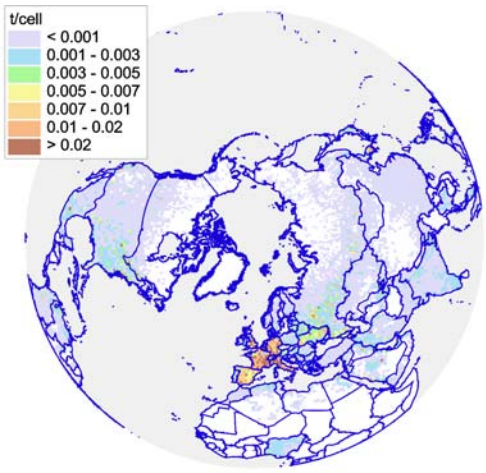


Fig. 2.4. *Spatial distribution of PCB-153 emissions in the Northern Hemisphere in 2000 prepared on the basis of data from [Breivik et al., 2002b]*

2.5. Initial concentrations of pollutants in media

For the sake of comparison of the model results vs measurements in 2000, one-year calculations of pollution levels of such persistent pollutants with significant long-range potential as PCBs requires appropriate information on their mass accumulated in the main environmental media of the European calculation domain up to the base year within rather long period of time.

Therefore, according to the agreed programme of Stage II modeling of PCB mass balance made on the basis of zero initial concentrations for one year are supplemented by the calculations for the same year but with the initial conditions of PCBs in the environmental compartments. So, calculations of PCB mass balance for one-year period (2000) with initial concentrations given as input data and for 20-year period (from 1981 to 2000) with zero initial data with historical emissions are performed. In the first case PCB initial concentrations as common input data for all participating models are calculated using hemispheric version of MSCE-POP model. In the latter case, initial conditions for PCBs in main environmental compartments are calculated by each participating model in their model runs using historical emissions from 1981 to 1999.

Input data on initial concentrations of PCB-153, 28 and 180 in the main environmental media (atmosphere, soil, water and vegetation) obtained by MSC-E for the end of 1999 and as it was agreed delivered for other models calculations are based on the data on global emission inventory from [*Breivik et al*., 2002b] taking into account long-term calculations from 1970 to 1999. These MSC-E calculations were performed under the joined EMEP, AMAP and WMO project ”Persistent toxic substances, food safety and indigenous people of the Russian North” [*Dutchak et al*., 2002]. Data for modeling within Stage II are given in the 1°×1° surface grid system. As an example, spatial distribution of initial concentrations of PCB-153 in the atmosphere (a), soil (b), seawater (c) and vegetation (d) in the Northern Hemisphere in 1999 calculated by MSC-E on the basis of emission historical scenario of 1970-1999 from [*Breivik et al*., 2002b] are shown in Fig. 2.5.

These input data on initial concentrations of the considered congeners of PCBs were used in the calculations of CAN/POPs, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS and SimleBox model. Of note, in the case of EVN-BETR and UK-MODEL model run the initial conditions for the vegetation are set to zero.

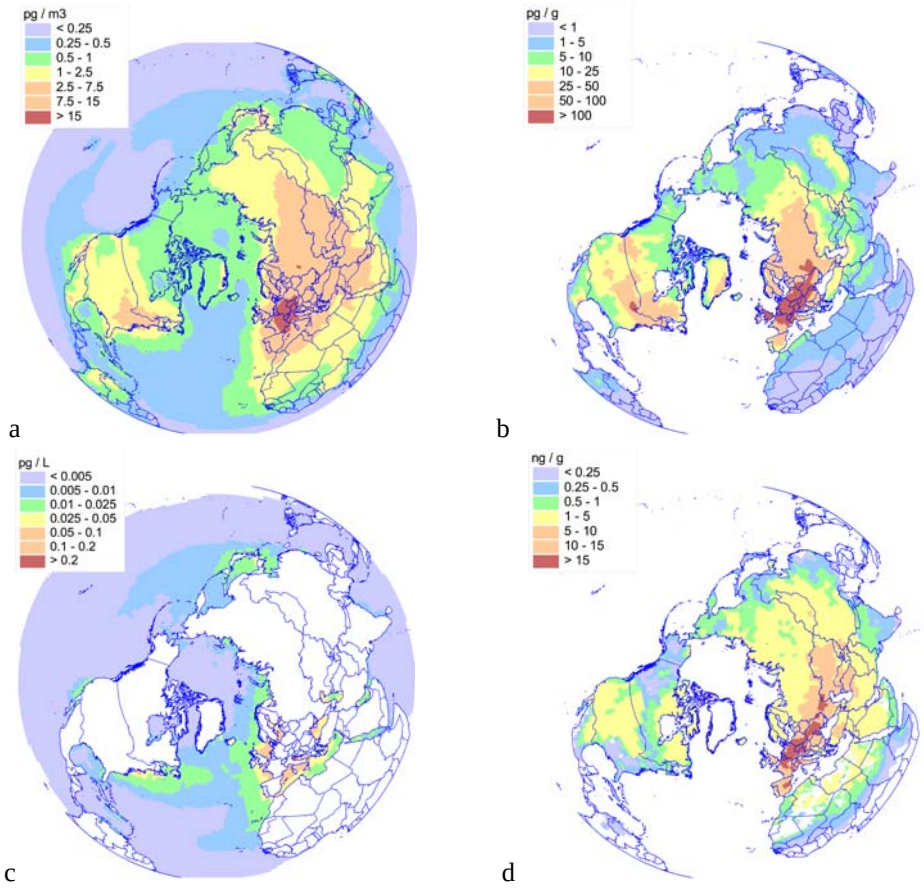


Fig. 2.5. *Spatial distribution of initial concentrations of PCB-153 in the atmosphere, (a), soil (b), seawater (c) and vegetation (d) in the Northern Hemisphere in 1999 calculated by MSC-E on the basis of historical data 1970-1999 from [Breivik et al., 2002b]*

Up to the moment of this report preparation, simulations of mass balance estimates of PCBs for 20-year period (from 1981 to 2000) with zero initial data based on a historical emission scenario run from 1981 to 1999 have been made and presented by the following models: CliMoChem, EVN-BETR and UK-MODEL, SimpleBox and MSCE-POP. Initial conditions on PCB mass contained in 1, 5 and 10 km layers of the atmosphere; 5 and 10 cm soil layers, 200m water layer and vegetation (kg) by the end of 1999 calculated by CliMoChem, SimpleBox and MSCE-POP models on the basis of "reference" and "own/alternative" physical-chemical data sets are presented in Table 2.7.

Table 2.7. *Values of PCBs mass contained in specified sub-domains in air, soil, seawater and vegetation compartments (kg) by the end of 1999*

Models	With "reference" data set							With "own/alternative" data set						
	Atmosphere			Soil		Water	Vege-tation	Atmosphere			Soil		Water	Vege-tation
	1 km	5 km	10 km	5cm	10cm	200m		1 km	5 km	10 km	5cm	10cm	200m	
PCB-153														
CliMoChem	0.466	2.330	4.660	4788.559	9577.118	162.328	111.377	1.242	6.208	12.415	7125.757	14251.513	286.554	45.659
SimpleBox	13.026	-	-	0.139	-	2.060	0.060	14.178	-	-	0.293	-	4.662	0.036
MSCE-POP	10.505	26.993	33.011	22907.554	23157.949	2.041	34.787	11.002	28.271	34.574	22930.800	23181.449	2.241	42.141
PCB-28														
CliMoChem	4.220	21.098	42.196	5239.535	10479.071	961.232	202.713	2.431	12.156	24.311	1845.345	3690.690	176.171	8.517
SimpleBox	27.195	-	-	0.052	-	1.561	0.068	23.409	-	-	0.019	-	0.292	0.018
MSCE-POP	44.296	113.819	139.194	22699.220	22947.338	10.197	97.119	40.335	103.643	126.749	22735.852	22984.370	11.596	104.608
PCB-180														
CliMoChem	0.035	0.175	0.350	1379.516	2759.032	38.735	21.214	0.243	1.214	2.428	3327.713	6655.425	60.341	16.047
SimpleBox	11.006	-	-	0.153	-	2.059	0.026	11.916	-	-	0.369	-	5.394	0.022
MSCE-POP	3.244	8.337	10.195	22829.235	23078.774	0.458	7.740	3.450	8.864	10.840	22879.179	23129.264	0.489	8.681

Chapter 3

COMPARISON OF RESULTS OF STAGE II COMPUTATIONAL EXPERIMENTS FOR PCB-153

A comparison of results on computational experiments of Stage II obtained by the participating models is presented in this Chapter. This stage is aimed at the comparison of mass balance estimates and calculated deposition and concentration fields of POPs in different environmental compartments and a sensitivity study with respect to physical-chemical parameter values used for mass balance estimates. Eight models participated in this comparison: ADEPT, CAN/POPs, CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, SimpleBox, and MSCE-POP.

Following the programme of this stage, a base year for the calculation is 2000. The results of computational experiments formulated at Stage II include annual and monthly values (quarterly data as optional) of the following mass balance estimates:

- masses of PCB-153 in specified sub-domains in air, soil and seawater compartments (see Section 3.1 below):
  - the atmosphere: layers of 1 km, 5 km and 10 km height,
  - soil: 5 cm and 10 cm depth,
  - sea: 200 m depth;
- masses of PCB-153 degraded in specified sub-domains of these compartments (see Section 3.2 below);
- mass flows of PCB-153 transported in/out the specified domain: inflow and outflow (for each transport media as optional) (see Section 3.3 below);
- mass flows of PCB-153 transported from one compartment to another in both directions (dry and wet deposition, gaseous exchange) (see Section 3.4 below);
- PCB-153 concentrations at each interface (in the atmosphere at its interface with soil, ocean and vegetation; in surface ocean layer; in vegetation; in surface soil layer) (see Section 3.5 below) and calculated annual deposition and concentration fields of PCB-153 in different environmental compartments (optional) (see Section 3.6). Besides, calculation results on masses of PCB-153 deposited into deep sea presented by CliMoChem model are also given in Section 3.2.6.

The calculation results mentioned above and presented in this Chapter are devoted to PCB-153 (a substance of the first priority); appropriate results on PCB-28 and PCB-180 are presented in Annexes B and C.

The comparison of model results on PCB depositions and air concentrations with monitoring data (optional) are presented in Section 3.7. Results on comparison of model estimates vs measurements are given here for the three considered PCB congeners.

The calculation experiments are performed with the use of physical-chemical data set of the individual model (“own” data set) on the basis of agreed input data (POP emission data scenario with zero initial concentrations and, as optional, with initial concentrations in media of the specified calculation domain for comparison of calculated and measured data) and a number of geophysical parameters of the calculation domain (e.g. land cover data, leaf area index, organic matter content in soil, etc). In order

to evaluate sensitivity of each model to variation of physical-chemical parameter values, the calculation experiments are carried out also with the use of "reference" data set common for all models. The results obtained with "own" data set are compared with this latter. For models using "reference" data set as own set of physical-chemical properties, this sensitivity study is carried out with the use of "alternative" data set based on individual physical-chemical data sets of some other participating models. G-CIEMS and SimpleBox carried out these calculations with the use of "reference" and "alternative" data sets. Results of EVN-BETR and UK-MODEL and ADEPT models were obtained only on the basis of "reference" data set; results of CAN/POPs – on the basis of "own" data set. All other models performed the calculations on the basis of "reference' and "own" data sets.

SimpleBox and EVN-BETR and UK-MODEL obtained three sets of results on the basis of initial concentrations given as input data, zero initial concentrations for one-year period (2000) and with historical emissions for 20-year period (from 1981 to 2000). The calculations of SimpleBox model are performed with two versions: SimpleBox 3.0 and SimpleBox 3.12. The latter version does not assume that the soil compartment has homogeneous concentrations, but it assumes an exponentially decline of soil concentration with depth. Results of CliMoChem model are calculated on the basis of their own Land Cover Data [*DeFries and Townshend*, 1994] (below CliMoChem_1) as well as results obtained with the help of Land Cover Data given as input data for this intercomparison study [*Guo and Chen*, 1994] (below CliMoChem_2). Of note, for CliMoChem_2, DEHM-POP, G-CIEMS and MSCE-POP models there are two sets of results obtained. In particular, CliMoChem_2 simulations for 2000 are based on both a historical emission scenario run from 1981 to 1999 and on zero initial concentrations. DEHM-POP, G-CIEMS and MSCE-POP models performed calculations both with initial concentrations given as input data and with zero initial concentrations. Results of CAN/POPs were calculated with the use of initial concentrations. Results of ADEPT model were calculated with zero initial concentrations in the main environmental media for the beginning of 2000.

In all model results emissions are based on the expert estimates of 2000 and historical emissions presented by [*Breivik et al*. 2002a,b] (see also www.nilu.no/projects/globalpcb/). Emissions are equally distributed around the year. The only exception is the simulation of PCB-153 mass deposited into deep see obtained by CliMoChem model with two different Land Cover Data (Section 3.2.6). In this calculation PCB-153 is emitted as pulse emission into air each year at the beginning of season one.

CliMoChem model calculates masses and mass fluxes per season (each three months, starting in January, April, July and October) and monthly values are not available. For comparison with these results, seasonal values of all output parameters were calculated on the basis of monthly values given by all other models.

The comparison of results on each computation experiment consists of two parts. In the first part the results of calculation experiments are compared between the models. The comparison of absolute values obtained by the models on the basis of "reference" data set as well as on the basis of "own or alternative" data sets is made. The following statistical parameters for each experiment are used:

- m - the mean values of the considered parameters averaged between participating models;
- σ – the values of square deviation between results obtained by different models.

At that, the corresponding statistical processing is made for two groups of results obtained. The first group includes results calculated on the basis of initial concentrations or historical emissions (non-zero initial conditions); in the second group results based on zero initial conditions are involved. A preliminary analysis of the results is carried out for these two groups separately.

The second part of comparison devoted to the sensitivity study of the calculation results to the variations of input parameters is based on two set of results obtained by each model on the basis of two different physical-chemical data sets ('reference" and "own/alternative"). The percentage difference in the results calculated on the basis of "own or alternative" data sets of pollutant-specific properties in comparison with those obtained with the use of "reference" data set and normalized to the "reference" results is shown. In the case of computational experiments on mass flows transported in/out of the specified domain and gaseous exchange between media, the absolute values of the calculation results are compared.

3.1. Distribution of PCB-153 mass between environmental compartments

3.1.1. Comparison of calculated values of PCB-153 mass in the atmosphere

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-153 contained in the atmosphere within layers of 1 km, 5 km and 10 km height.

Reference data set. Calculation results on PCB-153 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.1.

Monthly values of PCB-153 mass contained in 1 km layer of the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.1 a and b, respectively. Seasonal variations of low values of mass contained in 1 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. 3.1c in more detail.

Calculation results on PCB-153 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.2.

Monthly values of PCB-153 mass contained in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. 3.2.

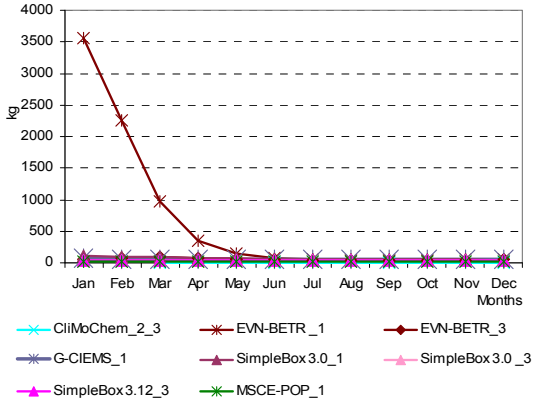


Fig. 3.1a. *PCB-153 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

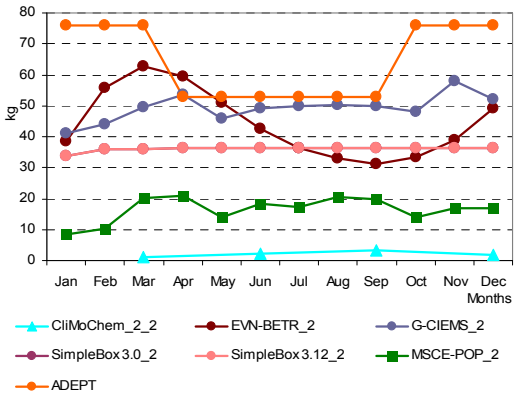


Fig. 3.1b. *PCB-153 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

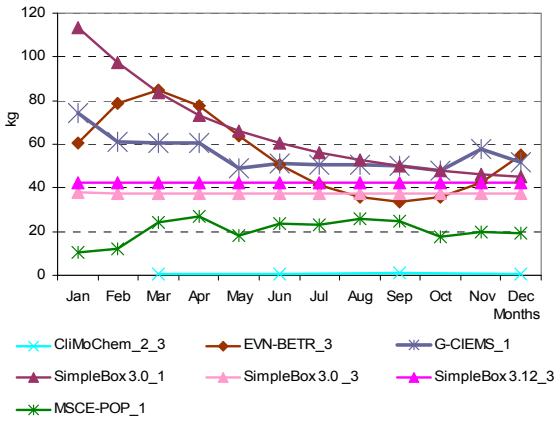


Fig. 3.1c. *PCB-153 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

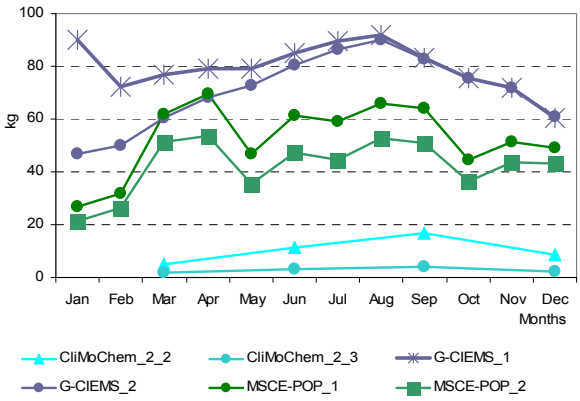


Fig. 3.2. *PCB-153 mass in the 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

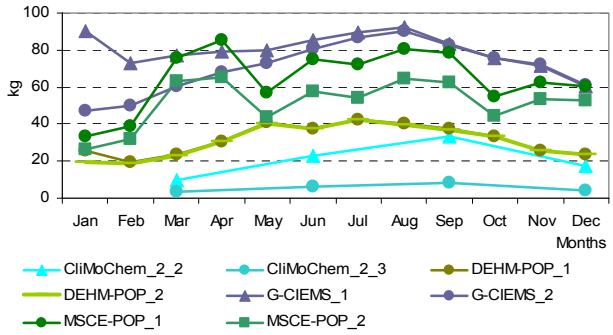


Fig. 3.3. *PCB-153 mass in the 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference data set"*

Table 3.1. *Calculation results: PCB-153 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations							*m*	σ
	EVN-BETR_1[a]	G-CIEMS_1	SimpleBox 3.0_1[b]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0_3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2	ADEPT		
Jan	3551.91	74.11	113.59	10.51	60.56		37.71	42.19	*555.80*	*1321.55*	Jan	38.66	41.27		33.73	33.73	8.32	75.90	*38.60*	*21.74*
Feb	2249.35	61.03	97.31	12.38	78.93		37.40	42.19	*368.37*	*829.90*	Feb	55.84	43.99		36.02	36.02	10.26	75.90	*43.01*	*21.99*
Mar	968.63	60.40	83.61	24.12	84.74		37.40	42.19	*185.87*	*345.93*	Mar	62.83	49.39		36.10	36.10	20.05	75.90	*46.73*	*20.27*
Seas_1	**2256.63**	**65.18**	**98.17**	**15.67**	**74.74**	**0.38**	**37.50**	**42.19**	***323.81***	***781.62***	**Seas_1**	**52.44**	**44.88**	**0.98**	**35.28**	**35.28**	**12.88**	**75.90**	***36.81***	***24.83***
Apr	356.03	60.79	73.44	27.13	77.75		37.41	42.19	*96.39*	*116.02*	Apr	59.34	53.74		36.16	36.16	20.86	52.80	*43.18*	*14.57*
May	145.43	48.83	65.98	18.14	63.99		37.41	42.19	*60.28*	*40.93*	May	50.92	45.81		36.21	36.21	13.83	52.80	*39.30*	*14.33*
Jun	76.12	50.98	60.37	23.83	50.64		37.41	42.19	*48.79*	*16.76*	Jun	42.57	49.05		36.25	36.25	18.42	52.80	*39.22*	*12.19*
Seas_2	**192.53**	**53.53**	**66.60**	**23.03**	**64.13**	**0.65**	**37.41**	**42.19**	***60.01***	***57.80***	**Seas_2**	**50.94**	**49.53**	**2.27**	**36.21**	**36.21**	**17.71**	**52.80**	***35.10***	***18.95***
Jul	50.48	50.68	56.10	23.07	41.23		37.41	42.19	*43.02*	*10.94*	Jul	36.49	49.77		36.28	36.29	17.29	52.80	*38.15*	*12.61*
Aug	40.23	50.65	52.74	25.69	35.92		37.41	42.19	*40.69*	*9.18*	Aug	32.86	50.33		36.31	36.31	20.45	52.80	*38.18*	*11.92*
Sep	36.30	50.11	50.13	25.01	33.50		37.41	42.19	*39.24*	*9.06*	Sep	31.07	50.08		36.33	36.34	19.89	52.80	*37.75*	*12.21*
Seas_3	**42.33**	**50.48**	**52.99**	**24.59**	**36.88**	**0.85**	**37.41**	**42.19**	***35.97***	***16.67***	**Seas_3**	**33.47**	**50.06**	**3.33**	**36.31**	**36.31**	**19.21**	**52.80**	***33.07***	***17.20***
Oct	38.68	47.82	48.05	17.40	35.98		37.41	42.19	*38.22*	*10.36*	Oct	33.33	48.01		36.35	36.36	14.11	75.90	*40.68*	*20.45*
Nov	45.99	57.77	46.36	19.92	42.48		37.41	42.19	*41.73*	*11.49*	Nov	38.82	58.15		36.37	36.38	16.92	75.90	*43.76*	*20.47*
Dec	60.30	51.61	44.98	19.19	55.08		37.41	42.19	*44.39*	*13.59*	Dec	49.22	52.01		36.39	36.39	16.83	75.90	*44.46*	*19.81*
Seas_4	**48.32**	**52.40**	**46.46**	**18.84**	**44.51**	**0.43**	**37.41**	**42.19**	***36.32***	***17.74***	**Seas_4**	**40.46**	**52.72**	**1.76**	**36.37**	**36.38**	**15.95**	**75.90**	***37.08***	***24.01***
Annual	**634.95**	**55.40**	**66.06**	**20.53**	**55.07**	**0.58**	**37.43**	**42.19**	***114.03***	***211.53***	**Annual**	**44.33**	**49.30**	**2.08**	**36.04**	**36.05**	**16.44**	**64.35**	***35.51***	***20.74***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.
[b] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table 3.2. *Calculation results: PCB-153 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	MSCE-POP_1	CliMoChem_2_3				G-CIEMS_2	CliMoChem_2_2	MSCE-POP_2		
Jan	89.85	26.99		*58.42*	*44.45*	Jan	46.89		21.38	*34.13*	*18.04*
Feb	72.44	31.82		*52.13*	*28.73*	Feb	49.89		26.37	*38.13*	*16.63*
Mar	76.71	61.98		*69.35*	*10.42*	Mar	60.34		51.53	*55.93*	*6.22*
Seas_1	**79.67**	**40.26**	**1.91**	***40.61***	***38.88***	**Seas_1**	**52.37**	**4.92**	**33.10**	***30.13***	***23.87***
Apr	78.95	69.71		*74.33*	*6.54*	Apr	68.06		53.61	*60.84*	*10.22*
May	79.31	46.60		*62.96*	*23.13*	May	72.64		35.55	*54.09*	*26.23*
Jun	85.05	61.22		*73.14*	*16.85*	Jun	80.54		47.33	*63.93*	*23.48*
Seas_2	**81.11**	**59.18**	**3.25**	***47.85***	***40.14***	**Seas_2**	**73.75**	**11.34**	**45.50**	***43.53***	***31.25***
Jul	89.36	59.28		*74.32*	*21.27*	Jul	86.52		44.43	*65.47*	*29.76*
Aug	91.62	66.00		*78.81*	*18.11*	Aug	90.09		52.55	*71.32*	*26.54*
Sep	83.02	64.27		*73.65*	*13.26*	Sep	82.55		51.12	*66.84*	*22.23*
Seas_3	**88.00**	**63.19**	**4.27**	***51.82***	***43.01***	**Seas_3**	**86.39**	**16.65**	**49.37**	***50.80***	***34.89***
Oct	75.55	44.72		*60.13*	*21.80*	Oct	75.64		36.25	*55.94*	*27.85*
Nov	71.64	51.19		*61.42*	*14.46*	Nov	72.03		43.47	*57.75*	*20.19*
Dec	60.58	49.30		*54.94*	*7.98*	Dec	61.00		43.24	*52.12*	*12.56*
Seas_4	**69.26**	**48.40**	**2.13**	***39.93***	***34.35***	**Seas_4**	**69.56**	**8.79**	**40.99**	***39.78***	***30.40***
Annual	**79.51**	**52.76**	**2.89**	***45.05***	***38.89***	**Annual**	**70.51**	**10.42**	**42.24**	*41.06*	*30.06*

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Calculation results on PCB-153 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table 3.3.

Monthly values of PCB-153 mass contained in 10 km layer of the atmosphere calculated by the participating models on the basis of “reference” data set are compared in Fig. 3.3.

Own/alternative data set. Calculation results on PCB-153 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data sets together with statistical parameters used for evaluation are presented in Table 3.4.

Monthly values of PCB-153 mass contained in 1 km layer of the atmosphere calculated by participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.4 a and b, respectively.

Calculation results on PCB-153 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data set together with statistical parameters used for evaluation are presented in Table 3.5.

Monthly values of PCB-153 mass contained in 5 km layer of the atmosphere calculated by the models on the basis of “own or alternative” data sets are compared in Fig. 3.5.

Calculation results on PCB-153 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data sets together with statistical parameters used for evaluation are presented in Table 3.6.

Monthly values of PCB-153 mass contained in 10 km layer of the atmosphere calculated by the participating models on the basis of “own or alternative” data sets are compared in Fig. 3.6.

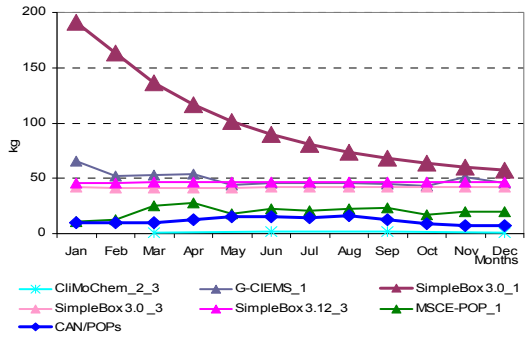


Fig. 3.4a. *PCB-153 mass contained in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions*

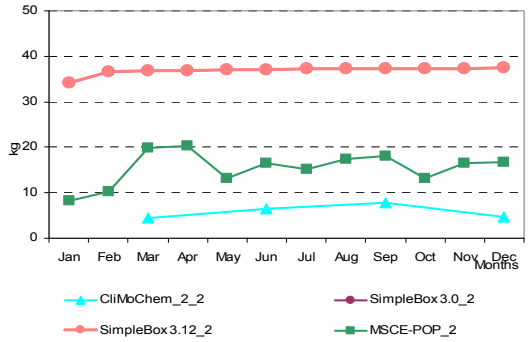


Fig.3.4b. *PCB-153 mass contained in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets and zero initial conditions*

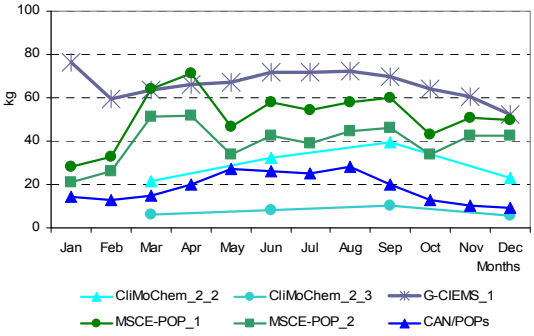


Fig. 3.5. *PCB-153 mass in the 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets*

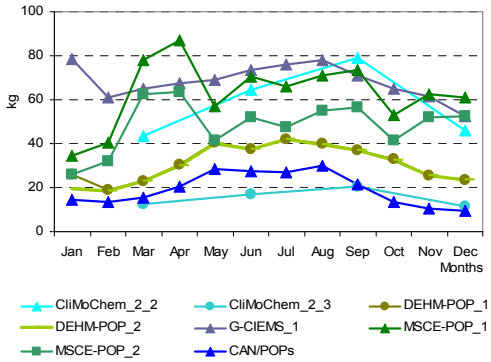


Fig. 3.6. *PCB-153 mass contained in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets*

Table 3.3. *Calculation results: PCB-153 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	G-CIEMS_1	CliMoChem_2_3				G-CIEMS_2	CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	25.99	33.01	90.27		*49.76*	*35.26*	Jan	46.90		19.59	26.15	*30.88*	*14.25*
Feb	19.35	38.91	72.80		*43.69*	*27.04*	Feb	49.94		18.79	32.25	*33.66*	*15.63*
Mar	23.46	75.80	77.24		*58.83*	*30.64*	Mar	60.50		23.15	63.02	*48.89*	*22.33*
Season_1	**22.93**	**49.24**	**80.10**	**3.81**	***39.02***	***33.12***	**Season_1**	**52.45**	**9.83**	**20.51**	**40.47**	***30.82***	***19.22***
Apr	30.53	85.25	79.40		*65.06*	*30.05*	Apr	68.29		30.26	65.56	*54.70*	*21.21*
May	40.63	56.99	79.67		*59.10*	*19.61*	May	72.88		40.35	43.47	*52.23*	*17.95*
Jun	37.75	74.87	85.29		*65.97*	*24.99*	Jun	80.72		37.50	57.89	*58.70*	*21.62*
Season_2	**36.30**	**72.37**	**81.46**	**6.50**	***49.16***	***34.48***	**Season_2**	**73.96**	**22.67**	**36.04**	**55.64**	***47.08***	***22.46***
Jul	42.37	72.50	89.72		*68.20*	*23.97*	Jul	86.83		42.11	54.33	*61.09*	*23.11*
Aug	40.17	80.72	92.05		*70.98*	*27.28*	Aug	90.49		39.93	64.27	*64.90*	*25.29*
Sep	37.28	78.60	83.15		*66.34*	*25.27*	Sep	82.68		37.12	62.51	*60.77*	*22.83*
Season_3	**39.94**	**77.27**	**88.31**	**8.55**	***53.52***	***36.43***	**Season_3**	**86.67**	**33.30**	**39.72**	**60.37**	***55.02***	***24.05***
Oct	33.13	54.69	75.62		*54.48*	*21.25*	Oct	75.71		33.05	44.33	*51.03*	*22.11*
Nov	26.02	62.61	71.69		*53.44*	*24.17*	Nov	72.07		25.98	53.16	*50.40*	*23.17*
Dec	23.72	60.29	60.62		*48.21*	*21.21*	Dec	61.05		23.69	52.88	*45.87*	*19.64*
Season_4	**27.62**	**59.19**	**69.31**	**4.27**	***40.10***	***29.76***	**Season_4**	**69.61**	**17.57**	**27.57**	**50.12**	***41.22***	***23.31***
Annual	**31.70**	**64.52**	**79.80**	**5.78**	***45.45***	***33.20***	**Annual**	**70.67**	**20.85**	**30.96**	**51.65**	***43.53***	***22.18***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
* - data of DEHM-POP are given for 15 km layer of the atmosphere.

Table 3.4. *Calculation results: PCB-153 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CAN/POPs	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	65.92	191.04	11.00	9.57		41.79	46.08	*60.90*	*67.34*	Jan		34.14	34.14	8.28	*25.52*	*14.93*
Feb	52.26	163.19	12.83	9.68		41.54	46.13	*54.27*	*56.22*	Feb		36.60	36.60	10.23	*27.81*	*15.23*
Mar	52.53	136.47	24.85	9.92		41.60	46.21	*51.93*	*44.24*	Mar		36.77	36.76	19.87	*31.13*	*9.75*
Seas_1	**56.90**	**163.57**	**16.23**	**9.72**	**1.26**	**41.64**	**46.14**	***47.92***	***54.98***	**Seas_1**	**4.36**	**35.84**	**35.84**	**12.79**	***22.21***	***16.11***
Apr	53.95	116.33	27.70	12.20		41.65	46.27	*49.68*	*35.84*	Apr		36.90	36.90	20.20	*31.33*	*9.64*
May	44.18	101.27	18.07	15.30		41.69	46.31	*44.47*	*30.94*	May		37.00	37.00	13.15	*29.05*	*13.77*
Jun	46.06	89.80	22.48	14.80		41.72	46.35	*43.54*	*26.18*	Jun		37.09	37.09	16.61	*30.27*	*11.83*
Seas_2	**48.06**	**102.47**	**22.75**	**14.10**	**1.69**	**41.69**	**46.31**	***39.58***	***32.77***	**Seas_2**	**6.44**	**37.00**	**37.00**	**16.65**	***24.27***	***15.28***
Jul	45.88	80.96	21.07	14.40		41.75	46.38	*41.74*	*23.46*	Jul		37.17	37.17	15.07	*29.80*	*12.76*
Aug	45.91	73.92	22.64	16.30		41.76	46.41	*41.16*	*20.42*	Aug		37.23	37.23	17.44	*30.64*	*11.42*
Sep	44.99	68.40	23.37	12.70		41.79	46.42	*39.61*	*19.48*	Sep		37.29	37.28	18.00	*30.86*	*11.14*
Seas_3	**45.59**	**74.43**	**22.36**	**14.47**	**2.03**	**41.77**	**46.40**	***35.29***	***24.19***	**Seas_3**	**7.92**	**37.23**	**37.23**	**16.84**	***24.80***	***14.80***
Oct	42.82	63.95	16.81	9.07		41.79	46.44	*36.81*	*20.30*	Oct		37.33	37.33	13.24	*29.30*	*13.91*
Nov	51.26	60.30	19.83	7.20		41.80	46.44	*37.81*	*20.19*	Nov		37.37	37.37	16.48	*30.41*	*12.06*
Dec	45.89	57.31	19.38	7.32		41.82	46.44	*36.36*	*18.94*	Dec		37.41	37.40	16.65	*30.49*	*11.99*
Seas_4	**46.66**	**60.52**	**18.67**	**7.86**	**1.14**	**41.80**	**46.44**	***31.87***	***22.53***	**Seas_4**	**4.61**	**37.37**	**37.37**	**15.46**	***23.70***	***16.39***
Annual	**49.30**	**100.25**	**20.00**	**11.54**	**1.53**	**41.73**	**46.32**	***38.67***	***32.75***	**Annual**	**5.83**	**36.86**	**36.86**	**15.44**	***23.75***	***15.64***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table 3.5. *Calculation results: PCB-153 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	G-CIEMS_1	MSCE-POP_1	CAN/POPs	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	76.65	28.27	14.26		*39.73*	*32.73*	Jan		21.27		
Feb	59.51	32.96	12.85		*35.11*	*23.41*	Feb		26.29		
Mar	63.51	63.86	14.97		*47.45*	*28.13*	Mar		51.07		
Season_1	**66.56**	**41.70**	**14.03**	**6.29**	***32.14***	***27.52***	**Season_1**	**21.78**	**32.88**	***27.33***	***7.85***
Apr	66.30	71.17	19.84		*52.44*	*28.34*	Apr		51.91		
May	67.43	46.42	27.00		*46.95*	*20.22*	May		33.78		
Jun	71.66	57.76	25.90		*51.77*	*23.46*	Jun		42.68		
Season_2	**68.47**	**58.45**	**24.25**	**8.43**	***39.90***	***28.26***	**Season_2**	**32.18**	**42.79**	***37.48***	***7.50***
Jul	71.80	54.13	25.00		*50.31*	*23.63*	Jul		38.73		
Aug	72.46	58.17	28.10		*52.91*	*22.64*	Aug		44.82		
Sep	69.61	60.06	19.80		*49.82*	*26.44*	Sep		46.24		
Season_3	**71.29**	**57.45**	**24.30**	**10.17**	***28.39***	***28.39***	**Season_3**	**39.62**	**43.27**	***2.58***	***2.58***
Oct	64.04	43.18	12.88		*40.03*	*25.72*	Oct		34.03		
Nov	60.76	50.96	10.10		*40.61*	*26.87*	Nov		42.34		
Dec	52.20	49.80	9.28		*37.09*	*24.12*	Dec		42.77		
Season_4	**59.00**	**47.98**	**10.75**	**5.72**	***26.59***	***26.59***	**Season_4**	**23.05**	**39.71**	***11.79***	***11.79***
Annual	**66.33**	**51.40**	**18.33**	**7.65**	***35.93***	***27.52***	**Annual**	**29.16**	**39.66**	***34.41***	***7.43***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table 3.6. *Calculation results: PCB-153 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions	*m*	*σ*	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	G-CIEMS_1	MSCE-POP_1	CAN/POPs	CliMoChem_2_3				CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	25.84	78.74	34.57	14.73		*38.47*	*28.05*	Jan		19.50	26.01	*22.76*	*4.61*
Feb	19.18	60.83	40.31	13.39		*33.43*	*21.62*	Feb		18.65	32.15	*25.40*	*9.55*
Mar	23.24	64.81	78.10	15.63		*45.44*	*30.68*	Mar		22.95	62.45	*42.70*	*27.93*
Seas_1	**22.75**	**68.13**	**50.99**	**14.58**	**12.58**	***33.81***	***24.57***	**Seas_1**	**43.56**	**20.37**	**40.21**	***34.71***	***12.54***
Apr	30.27	67.39	87.04	20.59		*51.32*	*31.21*	Apr		30.00	63.48	*46.74*	*23.67*
May	40.42	68.79	56.77	28.29		*48.57*	*17.83*	May		40.14	41.31	*40.72*	*0.83*
Jun	37.60	73.30	70.64	27.52		*52.27*	*23.15*	Jun		37.35	52.19	*44.77*	*10.50*
Seas_2	**36.10**	**69.83**	**71.48**	**25.47**	**16.86**	***43.95***	***25.32***	**Seas_2**	**64.35**	**35.83**	**52.33**	***50.84***	***14.32***
Jul	42.12	76.15	66.20	26.98		*52.86*	*22.40*	Jul		41.85	47.36	*44.61*	*3.90*
Aug	39.98	77.87	71.14	30.21		*54.80*	*23.26*	Aug		39.75	54.82	*47.28*	*10.65*
Sep	36.98	70.99	73.45	21.43		*50.71*	*25.65*	Sep		36.83	56.55	*46.69*	*13.94*
Seas_3	**39.69**	**75.00**	**70.26**	**26.21**	**20.34**	***51.33***	***25.91***	**Seas_3**	**79.24**	**39.48**	**52.91**	***57.21***	***20.22***
Oct	32.77	64.82	52.81	13.68		*41.02*	*22.52*	Oct		32.69	41.61	*37.15*	*6.31*
Nov	25.63	61.26	62.32	10.60		*39.95*	*25.95*	Nov		25.59	51.78	*38.69*	*18.52*
Dec	23.39	52.58	60.90	9.60		*36.62*	*24.15*	Dec		23.37	52.31	*37.84*	*20.46*
Seas_4	**27.26**	**59.55**	**58.67**	**11.29**	**11.44**	***39.23***	***23.85***	**Seas_4**	**46.09**	**27.22**	**48.57**	***40.63***	***11.68***
Annual	**31.45**	**68.13**	**62.85**	**19.39**	**15.30**	***39.42***	***24.59***	**Annual**	**58.31**	**30.72**	**48.50**	***45.85***	***13.98***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - data of DEHM-POP are given for 15 km layer of the atmosphere.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-153 mass contained in 1, 5 and 10 km layers of the atmosphere obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables 3.7-3.9.

Table 3.7. *The percentage difference between calculation results on PCB-153 mass contained in 1 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-11.1%	68.2%	1.2%	1.2%	10.8%	9.2%	4.7%	-0.5%
Feb			-14.4%	67.7%	1.6%	1.6%	11.1%	9.3%	3.6%	-0.3%
Mar			-13.0%	63.2%	1.8%	1.8%	11.2%	9.5%	3.0%	-0.9%
Seas_1	**343.0%**	**229.8%**	**-12.7%**	**66.6%**	**1.6%**	**1.6%**	**11.0%**	**9.4%**	**3.6%**	**-0.7%**
Apr			-11.3%	58.4%	2.0%	2.0%	11.3%	9.7%	2.1%	-3.2%
May			-9.5%	53.5%	2.2%	2.2%	11.4%	9.8%	-0.4%	-5.0%
Jun			-9.6%	48.8%	2.3%	2.3%	11.5%	9.9%	-5.7%	-9.8%
Seas_2	**183.8%**	**159.2%**	**-10.2%**	**53.9%**	**2.2%**	**2.2%**	**11.4%**	**9.8%**	**-1.2%**	**-6.0%**
Jul			-9.5%	44.3%	2.4%	2.4%	11.6%	9.9%	-8.7%	-12.8%
Aug			-9.4%	40.2%	2.5%	2.5%	11.6%	10.0%	-11.9%	-14.7%
Sep			-10.2%	36.4%	2.6%	2.6%	11.7%	10.0%	-6.5%	-9.5%
Seas_3	**137.9%**	**138.1%**	**-9.7%**	**40.5%**	**2.5%**	**2.5%**	**11.6%**	**10.0%**	**-9.1%**	**-12.4%**
Oct			-10.5%	33.1%	2.7%	2.7%	11.7%	10.1%	-3.4%	-6.1%
Nov			-11.3%	30.1%	2.8%	2.7%	11.7%	10.1%	-0.5%	-2.6%
Dec			-11.1%	27.4%	2.8%	2.8%	11.8%	10.1%	1.0%	-1.1%
Seas_4	**162.3%**	**167.9%**	**-11.0%**	**30.3%**	**2.8%**	**2.7%**	**11.7%**	**10.1%**	**-0.9%**	**-3.1%**
Annual	**179.7%**	**164.6%**	**-11.0%**	**51.8%**	**2.3%**	**2.3%**	**11.5%**	**9.8%**	**-2.6%**	**-6.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table 3.8.*The percentage difference between calculation results on PCB-153 mass contained in 5 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	MSCE-POP_1	MSCE-POP_2
Jan			-14.7%	4.7%	-0.5%
Feb			-17.9%	3.6%	-0.3%
Mar			-17.2%	3.0%	-0.9%
Seas_1	**343.0%**	**229.8%**	**-16.5%**	**3.6%**	**-0.7%**
Apr			-16.0%	2.1%	-3.2%
May			-15.0%	-0.4%	-5.0%
Jun			-15.7%	-5.7%	-9.8%
Seas_2	**183.8%**	**159.2%**	**-15.6%**	**-1.2%**	**-6.0%**
Jul			-19.7%	-8.7%	-12.8%
Aug			-20.9%	-11.9%	-14.7%
Sep			-16.2%	-6.5%	-9.5%
Seas_3	**137.9%**	**138.1%**	**-19.0%**	**-9.1%**	**-12.4%**
Oct			-15.2%	-3.4%	-6.1%
Nov			-15.2%	-0.5%	-2.6%
Dec			-13.8%	1.0%	-1.1%
Seas_4	**162.3%**	**167.9%**	**-14.8%**	**-0.9%**	**-3.1%**
Annual	**179.7%**	**164.6%**	**-16.6%**	**-2.6%**	**-6.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table 3.9. *The percentage difference between calculation results on PCB-153 mass contained in 10 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	DEHM-POP_1	DEHM-POP_2	G-CIEMS_1	MSCE-POP_1	MSCE-POP_2
Jan			-0.6%	-0.5%	-12.8%	4.7%	-0.5%
Feb			-0.9%	-0.7%	-16.4%	3.6%	-0.3%
Mar			-0.9%	-0.9%	-16.1%	3.0%	-0.9%
Seas_1	**343.0%**	**229.8%**	**-0.8%**	**-0.7%**	**-14.9%**	**3.6%**	**-0.7%**
Apr			-0.9%	-0.9%	-15.1%	2.1%	-3.2%
May			-0.5%	-0.5%	-13.7%	-0.4%	-5.0%
Jun			-0.4%	-0.4%	-14.1%	-5.7%	-9.8%
Seas_2	**183.8%**	**159.2%**	**-0.6%**	**-0.6%**	**-14.3%**	**-1.2%**	**-6.0%**
Jul			-0.6%	-0.6%	-15.1%	-8.7%	-12.8%
Aug			-0.5%	-0.5%	-15.4%	-11.9%	-14.7%
Sep			-0.8%	-0.8%	-14.6%	-6.5%	-9.5%
Seas_3	**137.9%**	**138.1%**	**-0.6%**	**-0.6%**	**-15.1%**	**-9.1%**	**-12.4%**
Oct			-1.1%	-1.1%	-14.3%	-3.4%	-6.1%
Nov			-1.5%	-1.5%	-14.5%	-0.5%	-2.6%
Dec			-1.4%	-1.4%	-13.3%	1.0%	-1.1%
Seas_4	**162.3%**	**167.9%**	**-1.3%**	**-1.3%**	**-14.1%**	**-0.9%**	**-3.1%**
Annual	**179.7%**	**164.6%**	**-0.8%**	**-0.8%**	**-14.6%**	**-2.6%**	**-6.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

3.1.2. Comparison of calculated values of PCB-153 mass in soil

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-153 contained in soil within 5 cm and 10 cm depth.

Reference data set. Calculation results on PCB-153 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.10.

Monthly values of PCB-153 mass contained in 5cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.7a and b, respectively.

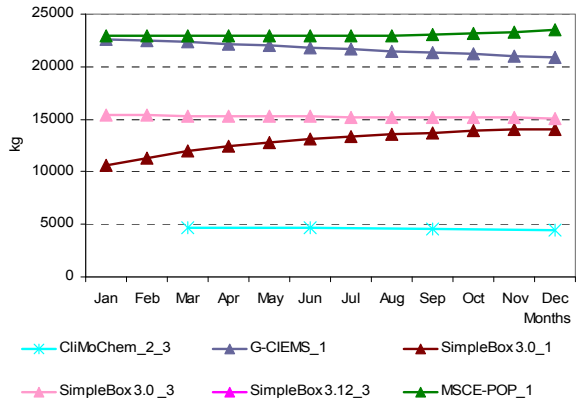


Fig.3.7a. *PCB-153 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

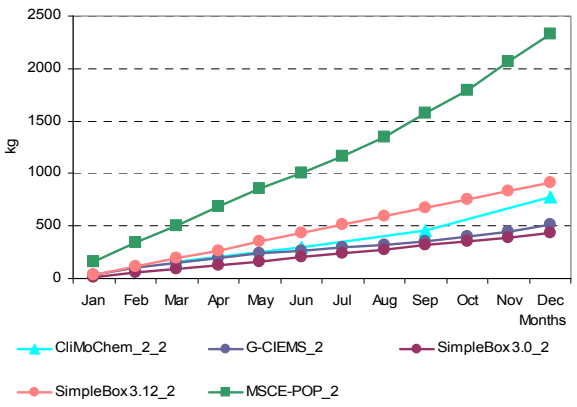


Fig.3.7b. *PCB-153 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Calculation results on PCB-153 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.11.

Monthly values of PCB-153 mass contained in 10 cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.8a and b, respectively.

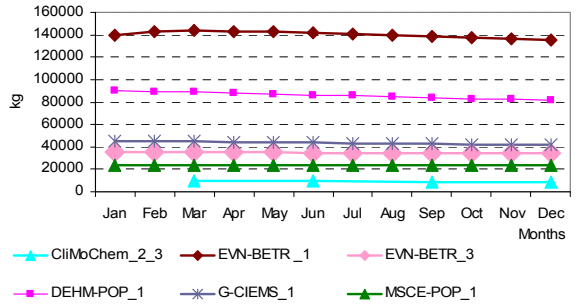


Fig.3.8a. *PCB-153 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

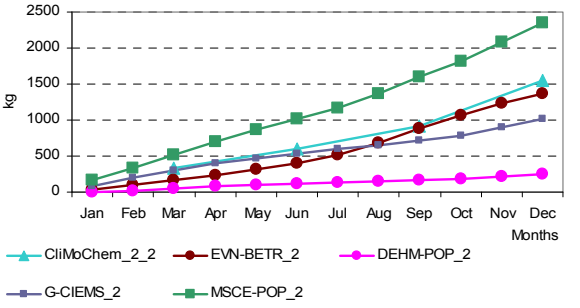


Fig.3.8b. *PCB-153 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Table 3.10. *Calculation results: PCB-153 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem _2_2	Simple Box 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	22599.4	10616.1	22907.6		15407.7	253179.2	*64942.0*	*105354.2*	Jan	39.7		16.4	34.8	158.0	*62.2*	*64.6*
Feb	22496.3	11357.6	22934.1		15379.3	253179.2	*65069.3*	*105270.1*	Feb	100.7		52.3	111.1	337.2	*150.3*	*127.2*
Mar	22353.6	11940.2	22943.3		15351.3	253179.2	*65153.5*	*105213.0*	Mar	152.2		88.8	188.8	506.4	*234.0*	*186.2*
Seas_1	**22483.1**	**11304.7**	**22928.3**	**4723.9**	**15379.4**	**253179.2**	***54999.8***	***97332.1***	**Seas_1**	**97.6**	**165.4**	**52.5**	**111.6**	**333.8**	***152.2***	***109.3***
Apr	22199.4	12413.2	22965.2		15323.1	253179.2	*65216.0*	*105170.3*	Apr	199.5		126.3	264.6	685.7	*319.0*	*250.9*
May	22030.0	12793.0	22972.4		15295.3	253179.2	*65254.0*	*105142.7*	May	234.6		164.0	348.6	855.7	*400.7*	*312.7*
Jun	21856.1	13101.9	22945.9		15267.2	253179.2	*65270.1*	*105128.2*	Jun	264.8		202.0	429.0	1003.6	*474.9*	*365.3*
Seas_2	**22028.5**	**12769.4**	**22961.2**	**4628.7**	**15295.2**	**253179.2**	***55143.7***	***97247.8***	**Seas_2**	**233.0**	**301.3**	**164.1**	**347.4**	**848.4**	***378.8***	***271.5***
Jul	21684.6	13354.5	22926.5		15239.7	253179.2	*65276.9*	*105119.9*	Jul	296.1		240.1	509.6	1162.1	*552.0*	*423.0*
Aug	21511.1	13565.5	22952.5		15212.0	251211.9	*64890.6*	*104233.5*	Aug	323.9		278.8	591.6	1345.8	*635.0*	*493.5*
Sep	21342.6	13737.1	23057.4		15184.7	253179.2	*65300.2*	*105101.8*	Sep	355.3		317.0	672.0	1574.6	*729.7*	*585.3*
Seas_3	**21512.8**	**13552.4**	**22978.8**	**4539.7**	**15212.2**	**252523.5**	***55053.2***	***96963.4***	**Seas_3**	**325.1**	**460.3**	**278.6**	**591.1**	**1360.8**	***603.2***	***440.8***
Oct	21182.8	13878.6	23154.1		15157.6	253179.2	*65310.4*	*105094.8*	Oct	394.4		355.2	752.5	1795.3	*824.3*	*671.6*
Nov	21039.6	13995.4	23324.8		15130.9	253179.2	*65334.0*	*105081.6*	Nov	449.3		393.4	832.8	2063.4	*934.7*	*777.4*
Dec	20904.4	14090.9	23492.9		15104.8	253179.2	*65354.4*	*105070.6*	Dec	511.4		430.9	907.8	2327.1	*1044.3*	*880.3*
Seas_4	**21042.2**	**13988.3**	**23323.9**	**4489.3**	**15131.1**	**253179.2**	***55192.3***	***97215.3***	**Seas_4**	**451.7**	**776.8**	**393.2**	**831.0**	**2061.9**	***902.9***	***676.0***
Annual	**21766.7**	**12903.7**	**23048.1**	**4595.4**	**15254.5**	**253015.3**	***55097.3***	***97188.3***	**Annual**	**276.8**	**426.0**	**222.1**	**470.3**	**1151.2**	***509.3***	***373.2***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-153 mass contained in 5cm layer of soil (kg) calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.12.

Monthly values of PCB-153 mass contained in 5cm layer of soil calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.9a and b, respectively.

Calculation results on PCB-153 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.13.

Monthly values of PCB-153 mass contained in 10 cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.10a and b, respectively.

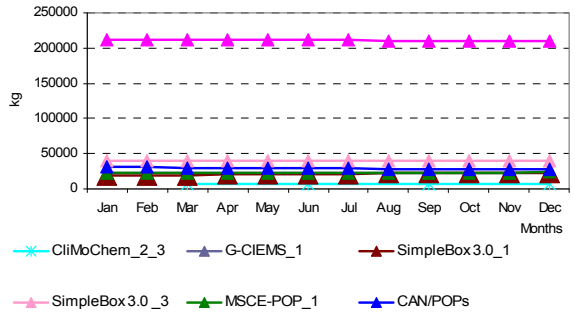


Fig. 3.9a. *PCB-153 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

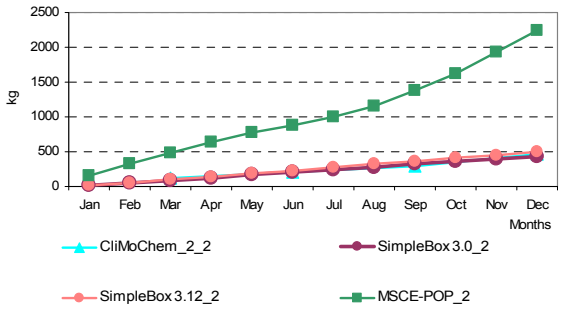


Fig. 3.9b. *PCB-153 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

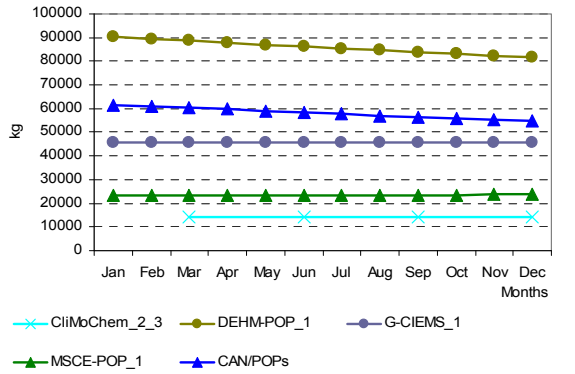


Fig.3.10a. *PCB-153 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

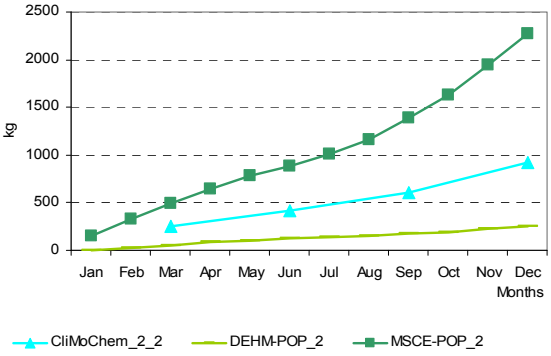


Fig.3.10b. *PCB-153 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table 3.11. *Calculation results: PCB-153 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	EVN-BETR_1[b]	G-CIEMS_1	EVN-BETR_3[b]	CliMoChem_2_3				EVN-BETR_2[b]	G-CIEMS_2	CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	90190.0	23157.9	139064.3	45198.8	35870.0		*66696.2*	*47689.3*	Jan	39.3	79.5		6.1	159.7	*71.1*	*66.2*
Feb	89380.0	23184.8	142960.5	44992.5	35630.6		*67229.7*	*49139.4*	Feb	101.0	201.5		22.7	340.9	*166.5*	*137.4*
Mar	88600.0	23194.1	143816.5	44707.3	35390.9		*67141.8*	*49452.7*	Mar	168.1	304.4		44.9	511.9	*257.3*	*200.1*
Seas_1	**89390.0**	**23179.0**	**141947.1**	**44966.2**	**35630.5**	**9447.8**	***57426.8***	***49539.0***	**Seas_1**	**102.8**	**195.1**	**330.8**	**24.5**	**337.5**	***198.1***	***138.1***
Apr	87820.0	23216.3	143341.7	44398.8	35153.0		*66786.0*	*49252.8*	Apr	237.3	399.0		81.7	693.2	*352.8*	*261.3*
May	87020.0	23223.5	142408.2	44059.9	34924.5		*66327.2*	*48878.4*	May	313.7	469.2		101.3	865.1	*437.3*	*322.6*
Jun	86240.0	23196.7	141329.3	43712.3	34710.9		*65837.8*	*48455.9*	Jun	403.4	529.6		117.7	1014.6	*516.3*	*374.2*
Seas_2	**87026.7**	**23212.1**	**142359.7**	**44057.0**	**34929.5**	**9257.4**	***56807.1***	***49524.3***	**Seas_2**	**318.1**	**466.0**	**602.7**	**100.2**	**857.6**	***468.9***	***286.2***
Jul	85450.0	23177.1	140226.6	43369.2	34526.8		*65349.9*	*48016.4*	Jul	520.3	592.1		136.7	1174.8	*606.0*	*428.7*
Aug	84680.0	23203.4	139155.6	43022.2	34391.3		*64890.5*	*47574.1*	Aug	683.3	647.8		154.2	1360.5	*711.5*	*495.5*
Sep	83910.0	23309.4	138105.2	42685.2	34285.9		*64459.1*	*47116.6*	Sep	876.2	710.6		168.9	1591.8	*836.9*	*587.0*
Seas_3	**84680.0**	**23230.0**	**139162.5**	**43025.6**	**34401.3**	**9079.4**	***55596.4***	***48265.5***	**Seas_3**	**693.3**	**650.2**	**920.6**	**153.3**	**1375.7**	***758.6***	***444.3***
Oct	83170.0	23407.2	137052.9	42365.6	34181.2		*64035.4*	*46661.5*	Oct	1069.1	788.7		189.6	1815.0	*965.6*	*674.7*
Nov	82420.0	23579.8	135978.3	42079.2	34053.1		*63622.1*	*46180.6*	Nov	1236.9	898.6		220.2	2085.9	*1110.4*	*775.7*
Dec	81690.0	23749.7	134866.5	41808.7	33886.8		*63200.3*	*45692.3*	Dec	1365.5	1022.8		245.0	2352.6	*1246.4*	*873.8*
Seas_4	**82426.7**	**23578.9**	**135965.9**	**42084.5**	**34040.3**	**8978.6**	***54512.5***	***46941.8***	**Seas_4**	**1223.8**	**903.4**	**1553.7**	**218.3**	**2084.5**	***1196.7***	***699.9***
Annual	**85880.8**	**23300.0**	**139858.8**	**43533.3**	**34750.4**	**9190.8**	***56085.7***	***48564.3***	**Annual**	**584.5**	**553.7**	**851.9**	**124.1**	**1163.8**	***655.6***	***385.6***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - data of DEHM-POP are given for 15 cm layer of soil;
[b] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.

Table 3.12. *Calculation results: PCB-153 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	CAN/POPs	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	22762.5	18372.1	30747.6	22930.8		39429.6	212172.7	*57735.9*	*76024.0*	Jan		16.1	18.4	153.2	*62.6*	*78.5*
Feb	22815.1	19223.8	30521.3	22974.7		39430.4	211972.3	*57822.9*	*75862.4*	Feb		51.7	58.9	324.9	*145.2*	*155.7*
Mar	22830.6	19909.8	30242.0	22996.4		39427.4	211773.2	*57863.2*	*75729.2*	Mar		88.2	100.6	481.8	*223.5*	*223.8*
Seas_1	**22802.7**	**19168.6**	**30503.6**	**22967.3**	**7145.5**	**39429.2**	**211972.7**	***50569.9***	***71859.0***	**Seas_1**	**123.3**	**52.0**	**59.3**	**319.9**	***138.6***	***125.0***
Apr	22834.0	20481.5	29958.2	23010.7		39427.7	211629.1	*57890.2*	*75632.9*	Apr		125.9	141.4	636.5	*301.3*	*290.4*
May	22820.5	20954.7	29604.1	22994.7		39425.4	211368.3	*57861.3*	*75509.5*	May		164.0	187.0	771.4	*374.2*	*344.2*
Jun	22801.8	21351.4	29231.3	22928.2		39425.8	211167.5	*57817.7*	*75425.2*	Jun		202.6	230.9	876.8	*436.8*	*381.3*
Seas_2	**22818.8**	**20929.2**	**29597.9**	**22977.9**	**7129.5**	**39426.3**	**211388.3**	***50609.7***	***71558.4***	**Seas_2**	**209.8**	**164.2**	**186.5**	**761.6**	***330.5***	***288.0***
Jul	22783.9	21686.5	28869.3	22874.0		39424.3	210967.2	*57767.5*	*75345.8*	Jul		241.5	275.2	995.7	*504.1*	*426.1*
Aug	22762.6	21977.8	28557.7	22884.2		39424.0	210075.1	*57613.6*	*74980.3*	Aug		281.4	320.4	1151.1	*584.3*	*491.2*
Sep	22744.6	22223.7	28298.8	23021.2		39425.7	210564.5	*57713.1*	*75165.1*	Sep		320.8	365.0	1379.3	*688.4*	*598.7*
Seas_3	**22763.7**	**21962.7**	**28575.3**	**22926.5**	**7103.7**	**39424.7**	**210535.6**	***50470.3***	***71229.6***	**Seas_3**	**300.9**	**281.2**	**320.2**	**1175.4**	***519.4***	***437.6***
Oct	22733.6	22437.0	28090.8	23171.5		39425.3	210365.2	*57703.9*	*75067.5*	Oct		360.4	409.9	1614.1	*794.8*	*709.9*
Nov	22738.1	22623.5	27919.3	23436.8		39425.4	210165.7	*57718.1*	*74957.7*	Nov		400.3	454.8	1923.8	*926.3*	*864.3*
Dec	22749.2	22784.4	27762.1	23716.5		39426.6	209971.7	*57735.1*	*74849.7*	Dec		439.5	496.5	2243.6	*1059.9*	*1025.5*
Seas_4	**22740.3**	**22615.0**	**27924.1**	**23441.6**	**7113.4**	**39425.8**	**210167.5**	***50489.7***	***71050.2***	**Seas_4**	**462.3**	**400.1**	**453.8**	**1927.2**	***810.8***	***744.7***
Annual	**22781.4**	**21168.9**	**29150.2**	**23078.3**	**7123.0**	**39426.5**	**211016.0**	***50534.9***	***71421.3***	**Annual**	**274.1**	**224.4**	**254.9**	**1046.0**	***449.9***	***398.0***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table 3.13. *Calculation results: PCB-153 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	G-CIEMS_1	MSCE-POP_1	CAN/POPs[b]	CliMoChem_2_3				CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	90190.0	45524.9	23181.4	61403.5		*55075.0*	*28175.1*	Jan		6.3	154.9	*80.6*	*105.0*
Feb	89380.0	45630.1	23225.8	60853.6		*54772.4*	*27769.5*	Feb		23.3	328.4	*175.9*	*215.7*
Mar	88600.0	45661.1	23247.7	60260.8		*54442.4*	*27391.1*	Mar		46.0	487.0	*266.5*	*311.9*
Season_1	**89390.0**	**45605.4**	**23218.3**	**60839.3**	**14290.9**	***46668.8***	***30105.2***	**Season_1**	**246.6**	**25.2**	**323.4**	***198.4***	***154.8***
Apr	87820.0	45668.0	23262.2	59663.5		*54103.4*	*27018.9*	Apr		83.4	643.5	*363.4*	*396.0*
May	87020.0	45641.0	23246.0	58999.0		*53726.5*	*26650.1*	May		103.4	779.9	*441.6*	*478.3*
Jun	86240.0	45603.7	23178.8	58317.9		*53335.1*	*26310.6*	Jun		120.3	886.3	*503.3*	*541.7*
Season_2	**87026.7**	**45637.5**	**23229.0**	**58993.5**	**14259.0**	***45829.2***	***29060.3***	**Season_2**	**419.7**	**102.4**	**769.9**	***430.7***	***333.9***
Jul	85450.0	45567.7	23124.1	57649.9		*52947.9*	*25964.2*	Jul		139.7	1006.6	*573.2*	*613.0*
Aug	84680.0	45525.2	23134.3	57029.2		*52592.2*	*25606.1*	Aug		157.6	1163.7	*660.6*	*711.4*
Sep	83910.0	45489.3	23272.8	56468.0		*52285.0*	*25202.7*	Sep		172.6	1394.3	*783.5*	*863.9*
Season_3	**84680.0**	**45527.4**	**23177.1**	**57049.0**	**14207.4**	***44928.2***	***28037.3***	**Season_3**	**601.8**	**156.6**	**1188.2**	***648.9***	***517.4***
Oct	83170.0	45467.2	23424.8	55961.1		*52005.8*	*24809.1*	Oct		193.7	1631.7	*912.7*	*1016.8*
Nov	82420.0	45476.2	23693.0	55493.2		*51770.6*	*24366.7*	Nov		224.9	1944.8	*1084.8*	*1216.1*
Dec	81690.0	45498.4	23975.8	55043.8		*51552.0*	*23927.6*	Dec		250.0	2268.2	*1259.1*	*1427.0*
Season_4	**82426.7**	**45480.6**	**23697.9**	**55499.4**	**14226.8**	***44266.3***	***26969.0***	**Season_4**	**924.7**	**222.9**	**1948.2**	***1031.9***	***867.7***
Annual	**85880.8**	**45562.7**	**23330.6**	**58095.3**	**14246.0**	***45423.1***	***28537.3***	**Annual**	**548.2**	**126.8**	**1057.4**	***577.5***	***466.0***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] – data of DEHM-POP are given for 15 cm layer of soil;
[b] - in CAN/POPs results the second layer of soil is applied as 5cm.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-153 masses contained in soil within 5 and 10 cm layers obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables 3.14-3.15.

Table 3.14. *The percentage difference between calculation results on PCB-153 masses contained within 5 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			0.7%	73.1%	-1.5%	-47.2%	155.9%	-16.2%	0.1%	-3.0%
Feb			1.4%	69.3%	-1.1%	-46.9%	156.4%	-16.3%	0.2%	-3.7%
Mar			2.1%	66.7%	-0.7%	-46.7%	156.8%	-16.4%	0.2%	-4.9%
Seas_1	**-25.5%**	**51.3%**	**1.4%**	**69.6%**	**-0.9%**	**-46.8%**	**156.4%**	**-16.3%**	**0.2%**	**-4.2%**
Apr			2.9%	65.0%	-0.3%	-46.5%	157.3%	-16.4%	0.2%	-7.2%
May			3.6%	63.8%	0.0%	-46.3%	157.8%	-16.5%	0.1%	-9.8%
Jun			4.3%	63.0%	0.3%	-46.2%	158.2%	-16.6%	-0.1%	-12.6%
Seas_2	**-30.4%**	**54.0%**	**3.6%**	**63.9%**	**0.0%**	**-46.3%**	**157.8%**	**-16.5%**	**0.1%**	**-10.2%**
Jul			5.1%	62.4%	0.6%	-46.0%	158.7%	-16.7%	-0.2%	-14.3%
Aug			5.8%	62.0%	0.9%	-45.8%	159.2%	-16.4%	-0.3%	-14.5%
Sep			6.6%	61.8%	1.2%	-45.7%	159.6%	-16.8%	-0.2%	-12.4%
Seas_3	**-34.6%**	**56.5%**	**5.8%**	**62.1%**	**0.9%**	**-45.8%**	**159.2%**	**-16.6%**	**-0.2%**	**-13.6%**
Oct			7.3%	61.7%	1.5%	-45.5%	160.1%	-16.9%	0.1%	-10.1%
Nov			8.1%	61.6%	1.7%	-45.4%	160.6%	-17.0%	0.5%	-6.8%
Dec			8.8%	61.7%	2.0%	-45.3%	161.0%	-17.1%	1.0%	-3.6%
Seas_4	**-40.5%**	**58.5%**	**8.1%**	**61.7%**	**1.8%**	**-45.4%**	**160.6%**	**-17.0%**	**0.5%**	**-6.5%**
Annual	**-35.7%**	**55.0%**	**4.7%**	**64.1%**	**1.0%**	**-45.8%**	**158.5%**	**-16.6%**	**0.1%**	**-9.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table 3.15. *The percentage difference between calculation results on PCB-153 mass contained within 10 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	DEHM-POP_1	DEHM-POP_2	G-CIEMS_1	MSCE-POP_1	MSCE-POP_2
Jan			0.0%	3.7%	0.7%	0.1%	-3.0%
Feb			0.0%	2.8%	1.4%	0.2%	-3.7%
Mar			0.0%	2.4%	2.1%	0.2%	-4.9%
Season_1	**-25.5%**	**51.3%**	**0.0%**	**2.6%**	**1.4%**	**0.2%**	**-4.2%**
Apr			0.0%	2.1%	2.9%	0.2%	-7.2%
May			0.0%	2.1%	3.6%	0.1%	-9.8%
Jun			0.0%	2.2%	4.3%	-0.1%	-12.6%
Season_2	**-30.4%**	**54.0%**	**0.0%**	**2.1%**	**3.6%**	**0.1%**	**-10.2%**
Jul			0.0%	2.2%	5.1%	-0.2%	-14.3%
Aug			0.0%	2.2%	5.8%	-0.3%	-14.5%
Sep			0.0%	2.2%	6.6%	-0.2%	-12.4%
Season_3	**-34.6%**	**56.5%**	**0.0%**	**2.2%**	**5.8%**	**-0.2%**	**-13.6%**
Oct			0.0%	2.2%	7.3%	0.1%	-10.1%
Nov			0.0%	2.1%	8.1%	0.5%	-6.8%
Dec			0.0%	2.0%	8.8%	1.0%	-3.6%
Season_4	**-40.5%**	**58.5%**	**0.0%**	**2.1%**	**8.1%**	**0.5%**	**-6.5%**
Annual	**-35.7%**	**55.0%**	**0.0%**	**2.2%**	**4.7%**	**0.1%**	**-9.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.

3.1.3. Comparison of calculated values of PCB-153 mass in water

According to the programme of Stage II model results of computational experiments on mass balance include masses of PCB-153 contained in sea within a layer of 200 m depth.

Reference data set. Calculation results on PCB-153 mass contained in 200 m layer of seawater (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.16.

Monthly values of PCB-153 mass contained in 200 m layer of seawater calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.11a and b, respectively.

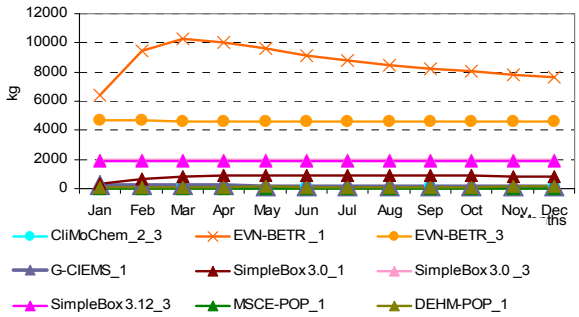


Fig. 3.11a. *PCB-153 mass contained in 200 m layer of seawater (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

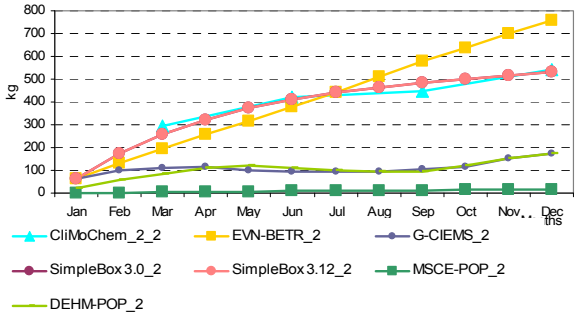


Fig. 3.11b. *PCB-153 mass contained in 200 m layer of seawater (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass contained in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.17.

Monthly values of PCB-153 mass contained in 200 m layer of water calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.12a and b, respectively.

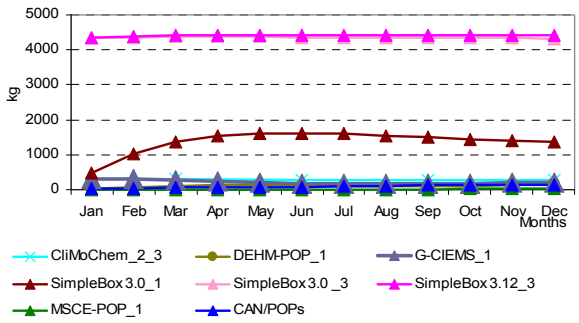


Fig. 3.12a. *PCB-153 mass contained in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

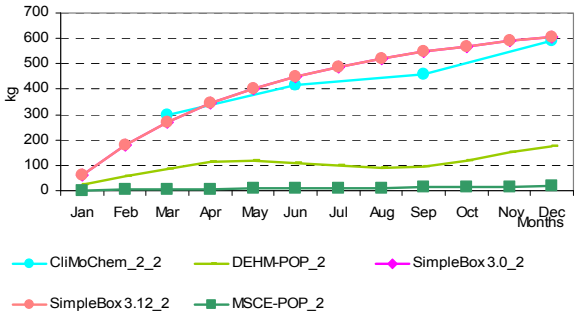


Fig. 3.12b. *PCB-153 mass contained in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table 3.16. *Calculation results: PCB-153 mass contained in 200 m layer of seawater (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data					Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations							*m*	σ
	DEHM-POP_1	MSCE-POP_1	EVN-BETR_1[a]	G-CIEMS_1	SimpleBox 3.0_1[b]	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	DEHM-POP_2	MSCE-POP_2		
Jan	48.39	2.04	6380.63	279.64	315.69	4681.94		1933.49	1923.70	*1945.69*	*2389.46*	Jan	62.40	64.26		60.97	60.96	22.06	1.68	*45.39*	*26.78*
Feb	77.42	2.80	9461.64	261.10	625.51	4662.43		1946.93	1923.70	*2370.19*	*3257.41*	Feb	130.12	101.53		173.23	173.21	56.15	2.34	*106.10*	*67.63*
Mar	99.07	4.05	10254.78	232.15	797.39	4634.48		1956.11	1923.70	*2487.72*	*3491.94*	Mar	195.53	111.33		257.56	257.55	82.86	3.46	*151.38*	*102.64*
Seas_1	**74.96**	**2.96**	**8699.02**	**257.63**	**579.53**	**4659.62**	**166.46**	**1945.51**	**1923.70**	***2034.38***	***2916.72***	**Seas_1**	**129.35**	**92.37**	**293.96**	**163.92**	**163.91**	**53.69**	**2.49**	***128.53***	***93.69***
Apr	122.60	6.45	10043.12	209.73	886.41	4604.02		1962.46	1923.70	*2469.81*	*3415.47*	Apr	256.57	115.08		322.30	322.30	110.50	5.48	*188.71*	*130.70*
May	127.10	9.23	9582.66	172.14	923.14	4580.43		1966.61	1923.70	*2410.62*	*3268.57*	May	316.50	98.83		371.59	371.57	118.60	7.78	*214.14*	*158.15*
Jun	116.00	9.99	9136.24	151.02	930.29	4568.00		1969.21	1923.70	*2350.56*	*3130.88*	Jun	378.06	94.26		409.81	409.81	110.50	8.35	*235.13*	*183.45*
Seas_2	**121.90**	**8.56**	**9587.34**	**177.63**	**913.28**	**4584.15**	**160.85**	**1966.09**	**1923.70**	***2160.39***	***3150.37***	**Seas_2**	**317.04**	**102.72**	**419.64**	**367.90**	**367.89**	**113.20**	**7.20**	***242.23***	***163.30***
Jul	104.40	10.56	8764.05	139.01	921.37	4566.54		1970.67	1923.70	*2300.04*	*3019.08*	Jul	442.38	95.74		439.99	440.00	100.70	8.80	*254.60*	*206.56*
Aug	97.76	11.54	8467.39	126.95	904.50	4575.36		1971.38	1923.70	*2259.82*	*2932.75*	Aug	510.87	95.04		464.80	464.80	95.18	9.50	*273.36*	*229.29*
Sep	99.29	15.42	8223.26	124.05	885.16	4584.58		1971.46	1923.70	*2228.36*	*2861.36*	Sep	576.52	103.34		484.98	485.00	97.36	12.66	*293.31*	*247.77*
Seas_3	**100.48**	**12.50**	**8484.90**	**130.00**	**903.67**	**4575.49**	**147.04**	**1971.17**	**1923.70**	***2027.66***	***2836.76***	**Seas_3**	**509.92**	**98.04**	**446.96**	**463.26**	**463.27**	**97.75**	**10.32**	***298.50***	***217.78***
Oct	120.70	17.26	8018.23	128.62	865.88	4592.69		1971.10	1923.70	*2204.77*	*2799.58*	Oct	639.40	117.64		502.15	502.18	119.20	14.08	*315.78*	*261.97*
Nov	152.20	19.68	7840.79	156.10	848.14	4599.04		1970.45	1923.70	*2188.76*	*2742.63*	Nov	700.71	153.57		517.15	517.20	150.90	16.09	*342.60*	*271.40*
Dec	173.90	20.87	7673.69	171.34	832.89	4596.40		1969.59	1923.70	*2170.30*	*2690.31*	Dec	755.98	175.76		530.32	530.41	172.80	17.27	*363.76*	*283.27*
Seas_4	**148.93**	**19.27**	**7844.24**	**152.02**	**848.97**	**4596.05**	**150.30**	**1970.38**	**1923.70**	*1961.54*	*2655.16*	**Seas_4**	**698.70**	**148.99**	**543.81**	**516.54**	**516.60**	**147.63**	**15.82**	***369.73***	***259.79***
Annual	**111.57**	**10.82**	**8653.87**	**179.32**	**811.36**	**4603.83**	**156.16**	**1963.29**	**1923.70**	***2045.99***	***2887.31***	**Annual**	**413.75**	**110.53**	**426.09**	**377.90**	**377.92**	**103.07**	**8.96**	***259.75***	***177.49***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
[b] - SimpleBox data presented here are masses calculated for continental level.

Table 3.17. *Calculation results: PCB-153 mass contained in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data					Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	DEHM-POP_1	G-CIEMS_1	SimpleBox 3.0_1[a]	CAN/ POPs	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	DEHM-POP_2	MSCE-POP_2		
Jan	48.75	306.41	468.13	44.41	2.24		4358.64	4366.41	*1370.71*	*2050.56*	Jan		61.33	61.32	22.21	1.78	*36.66*	*29.68*
Feb	78.40	291.15	1032.01	50.95	3.03		4366.08	4389.25	*1458.70*	*2024.52*	Feb		178.11	178.09	56.75	2.45	*103.85*	*88.56*
Mar	100.60	265.09	1356.30	56.90	4.33		4369.75	4404.60	*1508.22*	*2020.53*	Mar		270.14	270.11	83.95	3.58	*156.94*	*134.74*
Seas_1	**75.92**	**287.55**	**952.15**	**50.75**	**3.20**	**296.98**	**4364.82**	**4386.75**	***1302.26***	***1920.34***	**Seas_1**	**298.74**	**169.86**	**169.84**	**54.30**	**2.60**	***139.07***	***115.33***
Apr	124.40	246.13	1529.43	63.82	6.81		4369.75	4414.91	*1536.46*	*2019.92*	Apr		343.97	343.96	111.80	5.61	*201.33*	*170.31*
May	127.20	208.82	1602.51	72.45	9.54		4369.48	4421.31	*1544.47*	*2023.85*	May		402.51	402.47	118.40	7.78	*232.79*	*201.09*
Jun	113.80	186.47	1615.65	83.82	10.29		4366.11	4424.15	*1542.90*	*2026.39*	Jun		449.56	449.53	108.10	8.32	*253.88*	*229.58*
Seas_2	**121.80**	**213.81**	**1582.53**	**73.36**	**8.88**	**286.08**	**4368.44**	**4420.12**	***1384.38***	***1925.06***	**Seas_2**	**417.08**	**398.68**	**398.66**	**112.77**	**7.24**	***266.88***	***192.65***
Jul	100.80	173.90	1593.80	97.91	10.77		4362.07	4425.73	*1537.85*	*2026.91*	Jul		487.85	487.81	97.08	8.69	*270.36*	*253.70*
Aug	93.46	160.36	1552.71	114.86	11.65		4356.65	4423.02	*1530.39*	*2025.16*	Aug		520.00	519.96	90.84	9.27	*285.02*	*273.35*
Sep	95.26	156.82	1503.92	130.04	15.47		4350.62	4420.88	*1524.72*	*2021.19*	Sep		546.58	546.56	93.30	12.29	*299.68*	*286.99*
Seas_3	**96.51**	**163.70**	**1550.14**	**114.27**	**12.63**	**265.69**	**4356.45**	**4423.21**	***1372.82***	***1926.85***	**Seas_3**	**457.23**	**518.14**	**518.11**	**93.74**	**10.08**	***319.46***	***247.28***
Oct	118.00	162.17	1452.94	140.37	17.39		4344.19	4416.97	*1521.72*	*2014.26*	Oct		569.36	569.32	116.50	13.72	*317.22*	*294.12*
Nov	151.80	191.44	1403.42	145.83	20.03		4336.99	4412.76	*1523.18*	*2003.84*	Nov		589.26	589.20	150.50	15.87	*336.21*	*297.29*
Dec	175.90	208.01	1358.15	150.67	21.32		4330.00	4407.63	*1521.67*	*1996.23*	Dec		606.58	606.57	174.70	17.13	*351.24*	*301.76*
Seas_4	**148.57**	**187.21**	**1404.84**	**145.62**	**19.58**	**267.38**	**4337.06**	**4412.46**	***1365.34***	***1908.27***	**Seas_4**	**590.94**	**588.40**	**588.36**	**147.23**	**15.57**	***386.10***	***282.02***
Annual	**110.70**	**213.06**	**1372.42**	**96.00**	**11.07**	**279.03**	**4356.69**	**4410.64**	***1356.20***	***1917.91***	**Annual**	**441.00**	**418.77**	**418.74**	**102.01**	**8.87**	***277.88***	***205.91***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.18.

Table 3.18. *The percentage difference between calculation results on PCB-153 mass in water (kg) obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	DEHM-POP_1	DEHM-POP_2	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			0.7%	0.7%	-2.9%	48.3%	0.6%	0.6%	125.4%	127.0%	9.8%	5.6%
Feb			1.3%	1.1%	-53.5%	65.0%	2.8%	2.8%	124.3%	128.2%	8.4%	4.7%
Mar			1.5%	1.3%	-66.8%	70.1%	4.9%	4.9%	123.4%	129.0%	6.7%	3.5%
Seas_1	**1.6%**	**78.4%**	**1.3%**	**1.1%**	**-50.4%**	**64.3%**	**3.6%**	**3.6%**	**124.4%**	**128.0%**	**7.9%**	**4.3%**
Apr			1.5%	1.2%	-72.2%	72.5%	6.7%	6.7%	122.7%	129.5%	5.6%	2.3%
May			0.1%	-0.2%	-77.4%	73.6%	8.3%	8.3%	122.2%	129.8%	3.4%	0.0%
Jun			-1.9%	-2.2%	-80.0%	73.7%	9.7%	9.7%	121.7%	130.0%	3.0%	-0.4%
Seas_2	**-0.6%**	**77.9%**	**-0.1%**	**-0.4%**	**-76.6%**	**73.3%**	**8.4%**	**8.4%**	**122.2%**	**129.8%**	**3.8%**	**0.5%**
Jul			-3.4%	-3.6%	-81.1%	73.0%	10.9%	10.9%	121.3%	130.1%	2.0%	-1.3%
Aug			-4.4%	-4.6%	-82.3%	71.7%	11.9%	11.9%	121.0%	129.9%	1.0%	-2.4%
Sep			-4.1%	-4.2%	-82.3%	69.9%	12.7%	12.7%	120.7%	129.8%	0.4%	-2.9%
Seas_3	**2.3%**	**80.7%**	**-4.0%**	**-4.1%**	**-81.9%**	**71.5%**	**11.8%**	**11.8%**	**121.0%**	**129.9%**	**1.0%**	**-2.3%**
Oct			-2.2%	-2.3%	-81.3%	67.8%	13.4%	13.4%	120.4%	129.6%	0.8%	-2.5%
Nov			-0.3%	-0.3%	-77.4%	65.5%	13.9%	13.9%	120.1%	129.4%	1.8%	-1.4%
Dec			1.2%	1.1%	-75.0%	63.1%	14.4%	14.4%	119.8%	129.1%	2.2%	-0.8%
Seas_4	**8.7%**	**77.9%**	**-0.2%**	**-0.3%**	**-77.9%**	**65.5%**	**13.9%**	**13.9%**	**120.1%**	**129.4%**	**1.6%**	**-1.5%**
Annual	**3.5%**	**78.7%**	**-0.8%**	**-1.0%**	**-73.7%**	**69.1%**	**10.8%**	**10.8%**	**121.9%**	**129.3%**	**2.3%**	**-0.9%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

3.1.4. Comparison of calculated values of PCB-153 mass in vegetation

Reference data set. Calculation results on PCB-153 mass in vegetation (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.19.

Monthly values of PCB-153 mass in vegetation calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.13a and b, respectively.

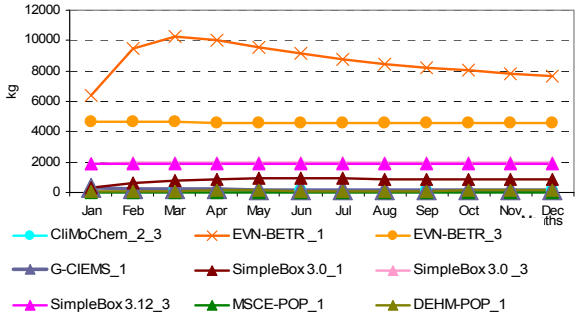


Fig. 3.13a. *PCB-153 mass contained in vegetation (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

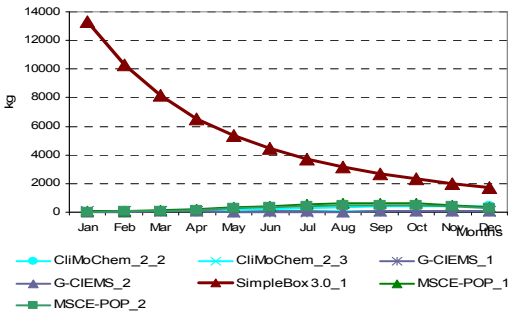


Fig. 3.13b. *PCB-153 mass contained in vegetation (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass in vegetation (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.20.

Monthly values of PCB-153 mass in vegetation calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.14a and b, respectively.

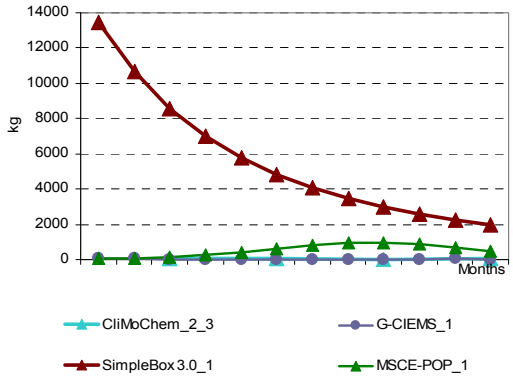


Fig. 3.14a. *PCB-153 mass contained in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

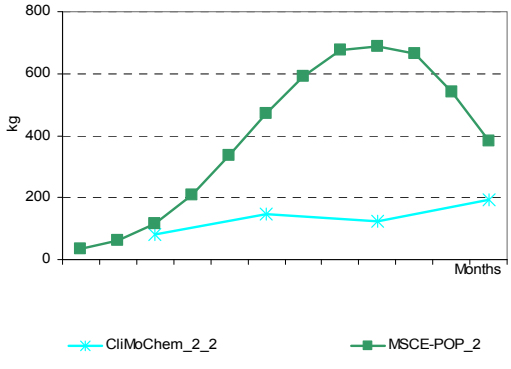


Fig. 3.14b. *PCB-153 mass contained in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table 3.19. *Calculation results: PCB-153 mass in vegetation (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3				G-CIEMS_2	CliMoChem_2_2	MSCE-POP_2		
Jan	88.00	13308.03	34.8		*4476.9*	*7648.0*	Jan	27.5		29.4	*28.4*	*1.4*
Feb	48.75	10307.84	61.9		*3472.8*	*5919.3*	Feb	33.4		52.0	*42.7*	*13.2*
Mar	43.54	8156.51	110.2		*2770.1*	*4664.9*	Mar	38.1		91.5	*64.8*	*37.7*
Season_1	**60.10**	**10590.79**	**69.0**	**96.2**	***2704.0***	***5257.9***	**Season_1**	**33.0**	**73.2**	**57.6**	***54.6***	***20.3***
Apr	43.44	6548.31	195.1		*2262.3*	*3712.6*	Apr	42.0		159.1	*100.5*	*82.9*
May	31.68	5348.60	312.9		*1897.7*	*2991.9*	May	32.5		251.4	*142.0*	*154.8*
Jun	33.48	4431.05	436.0		*1633.5*	*2431.1*	Jun	35.0		341.7	*188.4*	*216.9*
Season_2	**36.20**	**5442.65**	**314.7**	**81.1**	***1468.6***	***2652.1***	**Season_2**	**36.5**	**233.2**	**250.8**	***173.5***	***118.9***
Jul	32.92	3716.25	555.6		*1434.9*	*1992.9*	Jul	35.0		426.3	*230.7*	*276.7*
Aug	29.45	3138.80	636.5		*1268.2*	*1648.1*	Aug	31.6		482.6	*257.1*	*318.9*
Sep	34.74	2679.47	644.9		*1119.7*	*1384.8*	Sep	38.0		493.3	*265.7*	*322.0*
Season_3	**32.37**	**3178.17**	**612.3**	**95.0**	***979.5***	***1488.7***	**Season_3**	**34.9**	**381.1**	**467.4**	***294.5***	***228.9***
Oct	37.75	2302.33	615.8		*985.3*	*1176.6*	Oct	42.1		477.4	*259.7*	*307.8*
Nov	45.41	1988.08	491.0		*841.5*	*1017.6*	Nov	51.4		388.8	*220.1*	*238.6*
Dec	41.52	1728.00	344.5		*704.7*	*899.1*	Dec	48.1		279.8	*163.9*	*163.8*
Season_4	**41.56**	**2006.13**	**483.8**	**102.8**	***658.6***	***919.4***	**Season_4**	**47.2**	**437.1**	**382.0**	***288.8***	***211.0***
Annual	**42.56**	**5304.44**	**369.9**	**93.8**	***1452.7***	***2571.9***	**Annual**	**42.6**	**281.1**	**289.4**	***204.4***	***140.2***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table 3.20. *Calculation results: PCB-153 mass in vegetation (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis o zero initial concentrations		*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	68.9	13470.8	42.1		*4527.3*	*7745.3*	Jan		34.3		
Feb	36.9	10656.3	78.2		*3590.5*	*6119.2*	Feb		63.4		
Mar	33.6	8573.6	143.5		*2916.9*	*4899.2*	Mar		114.9		
Season_1	**46.5**	**10900.2**	**88.0**	**35.8**	***2767.6***	***5421.8***	**Season_1**	**81.1**	**70.9**	***76.0***	***7.2***
Apr	33.1	6975.8	267.2		*2425.4*	*3942.5*	Apr		208.7		
May	23.2	5756.8	441.2		*2073.7*	*3196.4*	May		338.0		
Jun	24.2	4808.4	630.8		*1821.2*	*2604.8*	Jun		469.9		
Season_2	**26.9**	**5847.0**	**446.4**	**34.7**	***1588.7***	***2845.6***	**Season_2**	**147.9**	**338.9**	***243.4***	***135.0***
Jul	23.9	4060.0	814.1		*1632.7*	*2138.9*	Jul		593.1		
Aug	21.2	3449.6	937.2		*1469.4*	*1775.0*	Aug		674.7		
Sep	24.8	2960.6	945.8		*1310.4*	*1501.5*	Sep		688.8		
Season_3	**23.3**	**3490.1**	**899.1**	**27.7**	***1110.0***	***1639.3***	**Season_3**	**121.9**	**652.2**	***387.1***	***374.9***
Oct	27.5	2557.2	899.0		*1161.2*	*1285.1*	Oct		665.7		
Nov	34.6	2219.8	712.6		*989.0*	*1118.5*	Nov		541.1		
Dec	32.5	1939.5	491.0		*821.0*	*995.4*	Dec		384.1		
Season_4	**31.5**	**2238.8**	**700.8**	**42.1**	***753.3***	***1038.6***	**Season_4**	**193.7**	**530.3**	***362.0***	***238.0***
Annual	**32.0**	**5619.0**	**533.6**	**35.1**	***1554.9***	***2719.6***	**Annual**	**136.1**	**398.0**	***267.1***	***185.2***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.21.

Table 3.21. *The percentage difference between calculation results on PCB-153 mass in vegetation (kg) obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	SimpleBox 3.0_1	MSCE-POP_1	MSCE-POP_2
Jan			-21.7%	1.2%	21.1%	16.7%
Feb			-24.3%	3.4%	26.3%	21.9%
Mar			-22.9%	5.1%	30.3%	25.6%
Seas_1	**10.8%**	**-62.8%**	**-22.7%**	**2.9%**	**27.6%**	**23.0%**
Apr			-23.7%	6.5%	36.9%	31.1%
May			-26.7%	7.6%	41.0%	34.4%
Jun			-27.7%	8.5%	44.7%	37.5%
Seas_2	**-36.6%**	**-57.2%**	**-25.8%**	**7.4%**	**41.9%**	**35.1%**
Jul			-27.5%	9.2%	46.5%	39.1%
Aug			-27.9%	9.9%	47.3%	39.8%
Sep			-28.5%	10.5%	46.7%	39.6%
Seas_3	**-68.0%**	**-70.9%**	**-28.0%**	**9.8%**	**46.8%**	**39.5%**
Oct			-27.2%	11.1%	46.0%	39.5%
Nov			-23.8%	11.7%	45.1%	39.2%
Dec			-21.7%	12.2%	42.5%	37.3%
Seas_4	**-55.7%**	**-59.0%**	**-24.1%**	**11.6%**	44.9%	38.8%
Annual	**-51.6%**	**-62.6%**	**-24.7%**	**5.9%**	**44.2%**	**37.5%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

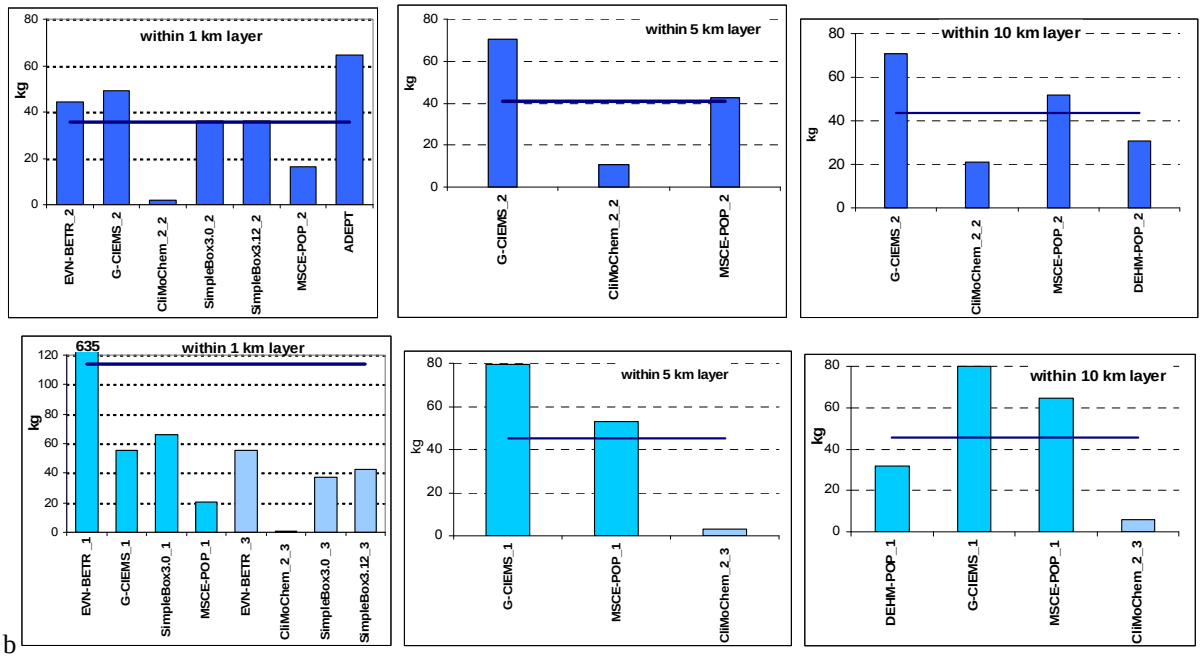
3.1.5. Comparison of distribution of PCB-153 mass between environmental media

Mass balance estimates presented in Sections 3.1.1-3.1.4 comprise masses of PCB-153 contained in different environmental compartments calculated by the participating models. The considered estimates of mass distribution in 2000 include results of one-year calculation with zero initial concentrations obtained by ADEPT, CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, MSCE-POP, SimpleBox models and with initial concentrations in media given as input data calculated by CAN/POPs, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, MSCE-POP, and SimpleBox models; as well as results of long-term calculations for 20-year period with zero initial data with historical carried out by CliMoChem, EVN-BETR and UK-MODEL and SimpleBox models. Results of CliMoChem, DEHM-POP, G-CIEMS, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of these models' calculations to the variations in the input data.

A preliminary analysis of the comparison of absolute values and relative fractions of PCB-153 mass contained in the main environmental compartments is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions (non-zero initial conditions) and for results based on zero initial conditions.

Atmosphere. According to the calculation results on PCB-153 mass contained in 1km layer of the atmosphere obtained on the basis of "***reference"*** data set and non-zero initial conditions (Table 3.1, Section 3.1.1), square deviation σ exceeds the mean value of this parameter averaged between the participating models. In the case with calculations made with zero initial conditions for 1 km layer (Table 3.1, Section 3.1.1) and with both zero and non-zero initial conditions for 5 and 10 km atmospheric layers (Tables 3.2 and 3.3, Section 3.1.1) using "reference*"* data set the participating

models give close enough results in terms of annual and monthly (seasonal) absolute values of PCB-153 atmospheric content. Comparison of annual values of PCB-153 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "reference" data set is presented in Fig.3.15a. Fig. 3.15b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



b

Fig.3.15. *Comparison of annual values of PCB-153 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The highest values of PCB-153 atmospheric content within 1 km layer are obtained by ADEPT model with zero initial concentrations (see Fig. 3.15a) and by EVN-BETR and UK-MODEL on the basis of initial conditions given as input data (see Fig. 3.15b). For 5 and 10 km layers, the maximum values calculated on the basis of zero and non-zero initial concentrations are characteristics of G-CIEMS results. The lowest values of PCB-153 mass contained in the different layers of the atmosphere are obtained by CliMoChem model. Comparison of air content profiles of annual values of PCB-153 mass calculated by three models (G-CIEMS, MSCE-POP and CliMoChem) for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set is presented in Fig.3.16.

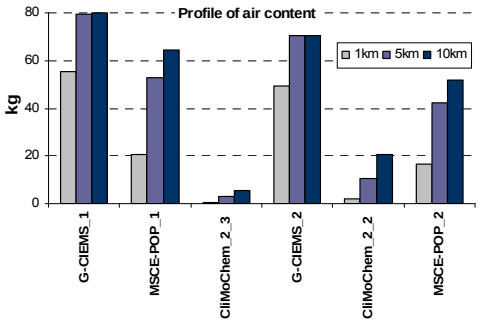


Fig. 3.16. *Comparison of air content profiles of annual values of PCB-153 mass calculated by four models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set*

Seasonal and monthly variations of PCB-153 mass contained in the considered layers of the atmosphere are observed in results of ADEPT, CliMoChem, DEHM-POP, G-CIEMS and MSCE-POP models (see Figs. 3.1a,b,c, 3.2 and 3.3 given in Section 3.1.1). Decreasing trend of this parameter values is presented in results of EVN-BETR and UK-MODEL and SimpleBox 3.0 models made with initial

concentrations given as input data (Fig. 3.1a and c). Negligible seasonal variations of the considered parameter values are characteristic of all other results of SimpleBox model (versions 3.0 and 3.12) (Fig. 3.1a, b, c).

Results on PCB-153 mass content in 1, 5 and 10 km layers of the atmosphere obtained on the basis of "***own or alternative"*** data set (Tables 3.4, 3.5 and 3.6, respectively, given in Section 3.1.1) to some extent differ from those obtained on "reference" data set due to changes in the number of models performed calculations. However, the participating models also provided rather close results in terms of absolute values of PCB-153 air content. For annual and monthly (seasonal) values of PCB-153 mass in each of these layers obtained on the basis of both zero and non-zero initial conditions, square deviation between different model results is less than the averaged value. Comparison of annual values of PCB-153 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig.3.17a. Fig. 3.17b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

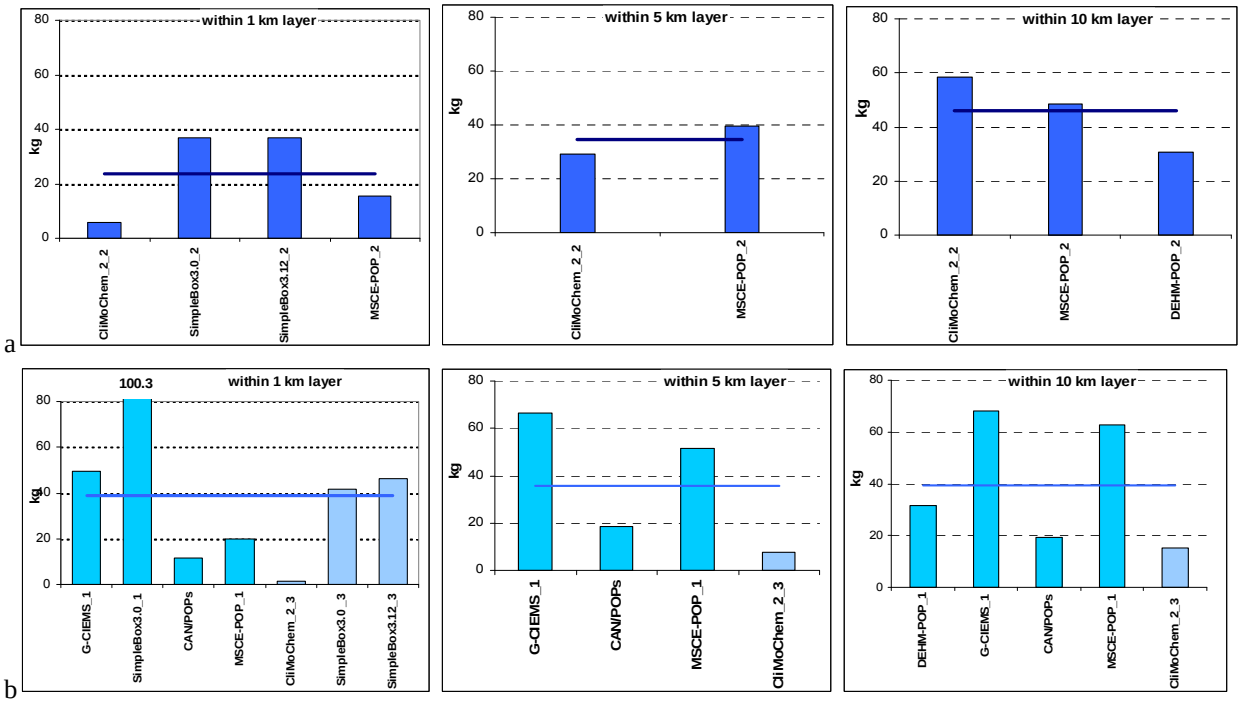


Fig. 3.17. *Comparison of annual values of PCB-153 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Values of PCB-153 atmospheric content within 1 km layer obtained by SimpleBox model with both zero and non-zero initial conditions are higher than those calculated by other models. Calculations of MSCE-POP and CliMoChem models performed on the basis of zero initial conditions are characterized by the maximum absolute values of PCB-153 mass within 5 km and 10 km layers, respectively (see Fig. 3.17a). The maximum values for 5 and 10 km layers of the atmosphere calculated on the basis of non-zero initial conditions are obtained by G-CIEMS models (see Fig. 3.17b). Results of CliMoChem model obtained on the basis of non-zero initial conditions for the

considered atmospheric layers are lower than those calculated by other models (Fig. 3.17b). Comparison of air content profiles of annual values of PCB-153 mass calculated by four models (G-CIEMS, CAN/POPs, MSCE-POP and CliMoChem) for 1, 5 and 10 km layers on the basis of "own or alternative" data sets is presented in Fig.3.18.

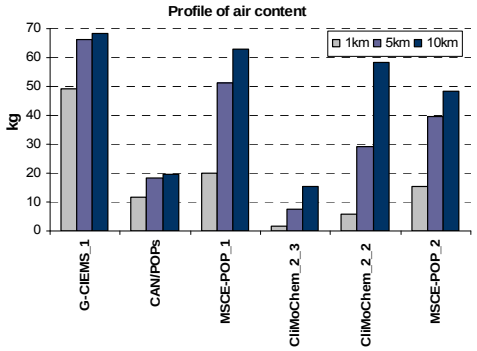


Fig. 3.18. *Comparison of air content profiles of annual values of PCB-153 mass calculated by five models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative data sets"*

For models performed calculations with the use of both physical-chemical data sets, characteristics of seasonal variations of PCB-153 mass contained in the considered layers of the atmosphere obtained with "own/alternative" data sets (see Figs. 3.4a,b, 3.5 and 3.6 given in Section 3.1.1) are similar to those for "reference" results. Monthly values of PCB-153 mass contained in the atmospheric layers presented by CAN/POPs demonstrate considerable changes depending on months.

Comparison of annual values of PCB-153 mass contained in 1, 5 and 10 km layers of the atmosphere obtained by the participating models with the use of "reference" and "own/alternative" data sets is presented in Fig. 3.19.

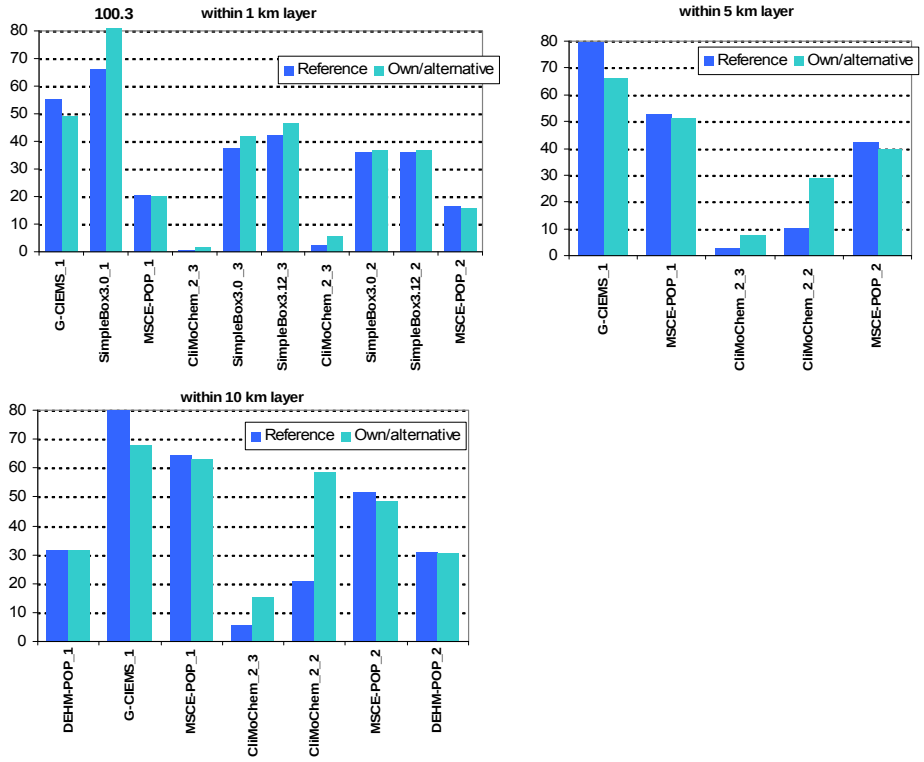


Fig.3.19. *Comparison of PCB-153 mass contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of two data set*

According to these results and data on percentage difference between PCB-153 mass values obtained with two data sets of physical-chemical properties (Tables 3.7- 3.9), for DEHM-POP, G-CIEMS and MSCE-POP models, the annual values of calculation results calculated with the use of

“own or alternative” data sets are smaller than those obtained with “reference” data set; and vice versa for CliMoChem and SimpleBox models. The most considerable differences in the results obtained with two data sets are characteristic of CliMoChem and SimpleBox 3.0_1 results. Minor differences are observed for DEHM-POP results. The results of other models show rather weak sensitivity of air content values with respect to variations of pollutant-related parameters.

Soil. Differences in calculation results of the participating models on PCB-153 mass contained in soil are more considerable than those in results on air content. It can be explained that in the case of PCBs soil is more inert media than atmosphere. Therefore, in contrast to the one-year calculations made on the basis of zero initial conditions, the usage of initial concentrations obtained within long-term calculations or historical emissions affect calculated mass accumulated in soil much more drastically than that contained in the atmosphere.

Scattering of calculated values of PCB-153 mass contained in 5 cm layers of soil obtained with the use of “***reference”*** data set and non-zero initial conditions is much higher than that calculated on the basis of zero initial conditions (Table 3.10, Section 3.1.2). In the first case, the square deviation presented for annual values exceeds considerably the mean value averaged between all models. The square deviations between results of participating models on soil content within 10 cm layer (Table 3.11, Section 3.1.2) calculated on the basis of “reference” data set and both zero and non-zero initial conditions is lower than the corresponding mean values. Comparison of annual values of PCB-153 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of “reference” data set is presented in Fig.3.20a. Fig. 3.20b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

All models’ results can be divided into two close groups: results of models performed calculations on the basis of zero initial concentrations and characterizing by low values of soil content and results of models used initial concentrations and/or historical emissions with considerably higher values. The results of MSCE-POP model on PCB-153 mass contained in soil within 5 and 10 cm layers calculated on the basis of zero initial concentrations are the highest among results of other models (see Fig 3.20a). The lowest value of soil content obtained with the use of zero initial conditions is characteristic of SimpleBox 3.0 model for 5 cm layer and of DEHM-POP model for 10 cm layer. The reason for the high scattering of soil content values for 5 cm layer based on non-zero initial conditions is more than an order of magnitude difference in simulation results of SimpleBox 3.12 model (historical emissions) and results of other models (see Fig 3.20b). This discrepancy leads to significant bias of averaged value (black line) to the maximum calculated value. The highest values of PCB-153 masses contained in soil within 10 cm layers calculated by different models on the basis of non-zero initial conditions are obtained by EVN-BETR and UK-MODEL with the use of initial concentrations given as input data; and the lowest values – by CliMoChem model.

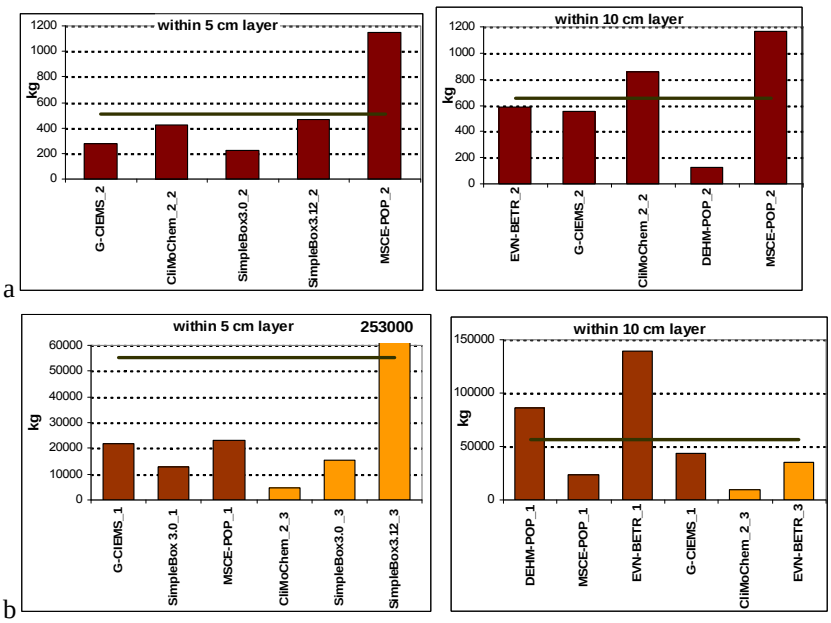


Fig. 3.20. *Comparison of annual values of PCB-153 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of soil content profiles of annual values of PCB-153 mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set is presented in Fig.3.21.

According to the MSCE-POP modeling approach, the most part of overall PCB-153 mass accumulated in soil is contained within 5 cm layer. According to the results of CliMoChem and G-CIEMS models soil content within 10 cm layer is two times higher than that within 5 cm layer.

Seasonal and monthly variations of PCB-153 mass contained in soil within 5 and 10 cm layers (see Figs. 3.7a,b and 3.8a,b, Section 3.1.2) are not essential for all participating models' results.

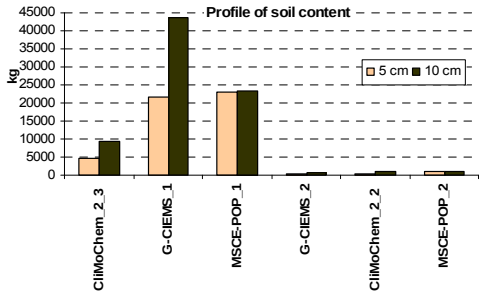


Fig. 3.21. *Comparison of soil content profiles of annual values of PCB-153 mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set*

Like in the case of calculations performed on the basis of "reference" data set, there is also rather large difference between values on PCB-153 mass contained in 5cm layer of soil obtained with the use of "***own or alternative"*** data sets and non-zero initial conditions (Table 3.12, Section 3.1.2). The scattering of results on soil content within 5 cm layer calculated on the basis of zero initial conditions is considerably lower. For the results on soil content within 10 cm layer obtained by the participating models with the use of both zero and non-zero initial conditions, square deviation of annual values does not exceed the mean values averaged between all models (Table 3.13, Section 3.1.2). Comparison of annual values of PCB-153 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig.3.22a. Fig. 3.22b shows the same results but obtained on the basis of initial concentrations or historical emissions. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem

calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

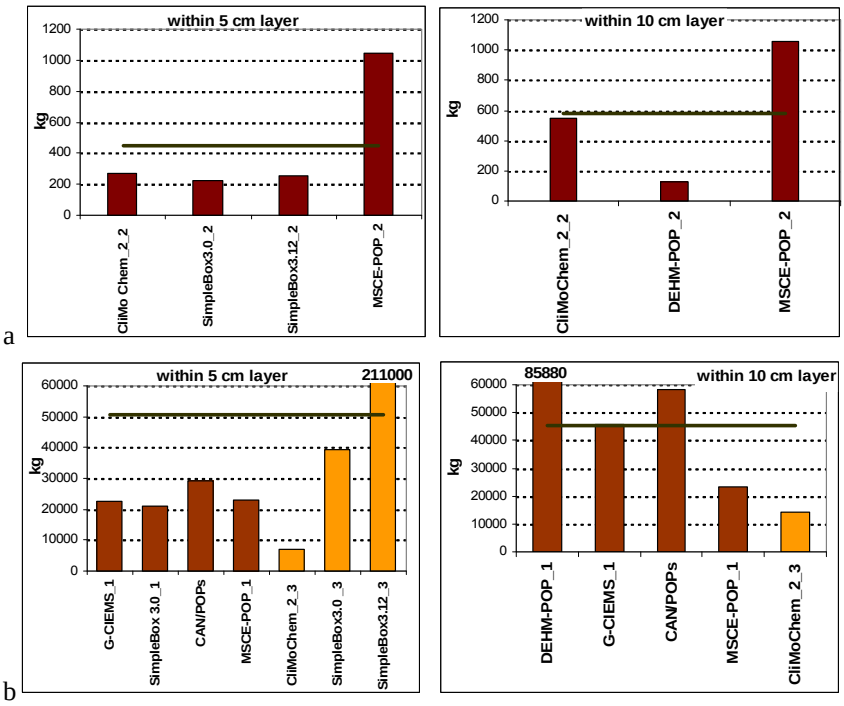


Fig. 3.22. *Comparison of annual values of PCB-153 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non- zero initial conditions)*

The difference in calculated absolute values obtained with the use of zero and non-zero initial conditions is again considerable. The highest values of PCB-153 mass contained in soil within 5 and 10 cm layers calculated on the basis of zero initial concentrations are observed for MSCE-POP model (see Fig 3.22a). The lowest values of soil content obtained with zero initial conditions for 5 and 10 cm layers are characteristic of SimpleBox 3.0 and DEHM-POP model, respectively. According to the data based on non-zero initial conditions (see Fig 3.22b), the highest and lowest values of PCB-153 mass contained in 5 cm soil layer are characteristic of SimpleBox 3.12 and CliMoChem models calculated on the basis of historical emissions. The minimum and maximum values for 10 cm soil layer are obtained by CliMoChem and DEHM-POP models, respectively.

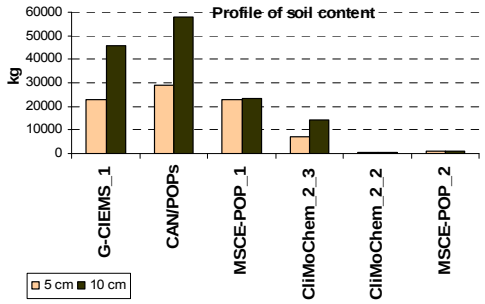


Fig. 3.23. *Comparison of soil content profiles of annual values of PCB-153 mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets*

Comparison of soil content profiles of annual values of PCB-153 mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets is presented in Fig.3.23.

In all models' results obtained on the basis of "own/alternative" data set calculated masses of PCB-153 in the considered soil layers (see Figs. 3.9 and 3.10, Section 3.1.2) are not subjected to the considerable seasonal and/or monthly variations.

Comparison of annual values of PCB-153 mass contained in the considered different layers of soil obtained with "reference" and "own/alternative" data sets is presented in Fig. 3.24.

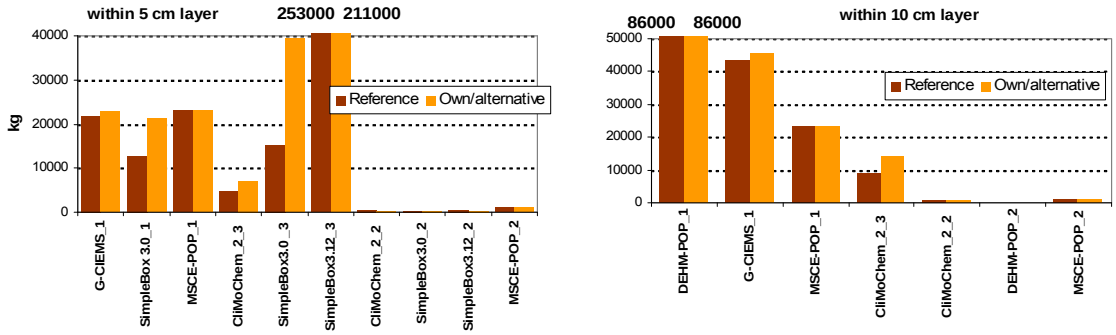


Fig.3.24. *Comparison of PCB-153 mass contained within 5 and 10 cm soil layers calculated by different models on the basis of two data set*

Contrary to the results of most models, values of PCB-153 soil content obtained by CliMoChem 2_2, SimpleBox 3.12_2, SimpleBox 3.12_3 and MSCE-POP_2 models with the use of "own or alternative" data sets are less than those obtained with "reference" data set. The largest difference in the results calculated with two data sets is characteristic of SimpleBox 3.0 results based on historical emissions. According to the data presented in Table 3.14 (Section 3.1.2), the difference in results of this model totals approximately to 160%. For other models percentage difference between calculation results on PCB-153 mass contained in soil is not high varying from 0.1 to 64%. There is no difference for results of DEHM-POP obtained with the use of initial conditions on the basis of two data sets: "reference" and "alternative" data sets.

Water. The difference between annual and monthly values of PCB-153 mass contained in water layer of 200 m calculated by the participating models with the use of "***reference***" data set and non-zero initial conditions is more essential than that between values obtained on the basis of zero initial concentrations (Table 3.16, Section 3.1.3). Square deviation of these values in the second group of results is lower than mean values averaged between all models results. Comparison of annual values of PCB-153 water content calculated by different models on the basis of zero initial concentrations and with the use of "reference*"* data set is presented in Fig.3.25a. Fig. 3.25b shows the same results but obtained on the basis of initial concentrations or historical emissions. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plot shows the value of the corresponding parameter averaged between models.

For results obtained on the basis of zero initial conditions (see Fig. 3.25a), the highest and the lowest values are characteristic of CliMoChem and MSCE-POP models, respectively. According to the data presented in Fig 3.25b, absolute value of PCB-153 water content obtained by EVN-BETR and UK-MODEL on the basis of initial concentrations given as input data exceeds essentially results of other models. Then come values of EVN-BETR and UK-MODEL, SimpleBox 3.0 and 3.12 models calculated using historical emissions. In comparison with them, results of CliMoChem, DEHM-POP, G-CIEMS and SimpleBox 3.0 (initial concentrations) are considerably lower. The minimum value of PCB-153 water content is obtained by MSCE-POP model.

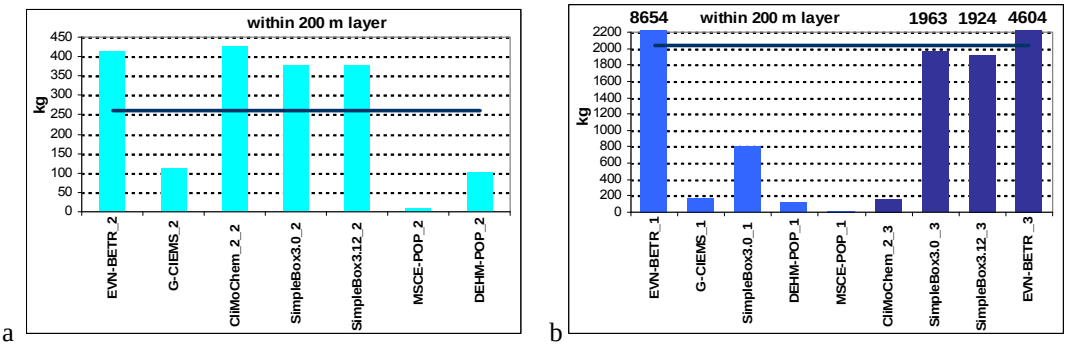


Fig. 3.25. *Comparison of annual values of PCB-153 masses contained in water within 200 m layer calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

In results on water content within 200 m layer calculated with the use of "***own/alternative***" data set, square deviation of values obtained by the participating models on the basis of zero initial conditions does not exceed the mean value averaged between all models; and vice versa for results based on non-zero initial conditions (Table 3.17, Section 3.1.3). Figs.3.26a and 3.26b show the annual values of PCB-153 masses contained in water layer of 200 m and calculated by different models on the basis of "own or alternative" data set and zero and non-zero initial conditions, respectively (blue line corresponds to the averaged value). Different colour of columns corresponds to the different types of calculations (a - one-year calculations on the basis of zero initial conditions; b - one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

The dispersion of absolute values of PCB water content calculated on the basis of zero initial conditions with the use of "own or alternative" data set (see Fig. 3.26a) is similar to that in the results obtained with the use of "reference" data set. The highest and the lowest values are also characteristic of CliMoChem and MSCE-POP models, respectively. In the results obtained on the basis of non-zero initial conditions (see Fig. 3.26b) the difference in absolute values of different models is also considerable. The maximum value obtained by SimpleBox 3.0 and 3.12 model with the use of historical emissions differs more than two orders of magnitude from the minimum value calculated by MSCE-POP model.

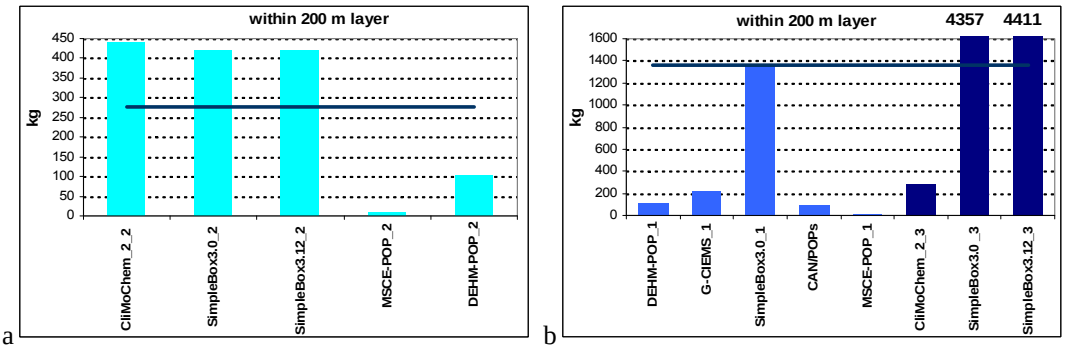


Fig. 3.26. *Comparison of annual values of PCB-153 masses contained in water within 200 m layer calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

According to the data presented (see Figs. 3.11a,b and 3.12a,b, Section 3.1.3), seasonal variations of PCB-153 mass contained in water layer of 200 m are minor in both sets of SimpleBox 3.0 and 3.12

results calculated on the basis of historical emissions. Increasing trends of water content are characteristic of all models' results based on zero initial conditions.

Comparison of annual values of PCB-153 mass contained in the 200m layer of water obtained by the participating models on the basis of "reference" and "own/alternative" data sets is presented in Fig. 3.27.

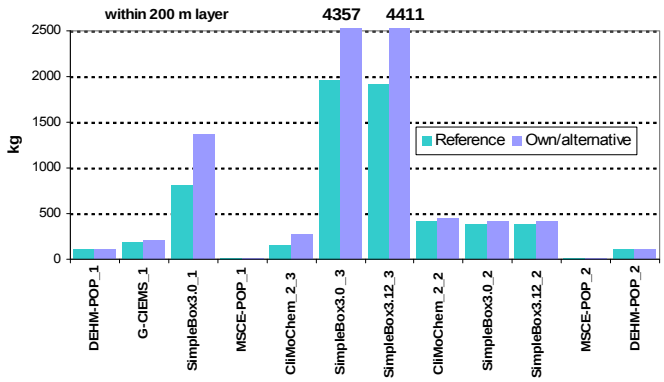


Fig.3.27. *Comparison of PCB-153 mass contained within 200 m water layer calculated by different models on the basis of two data sets*

For the results of most models, values of PCB-153 water content calculated on the basis of "own or alternative" data sets exceed those obtained with the use of "reference" data set (Table 3.18, Section 3.1.3). The largest difference in the results obtained with two data sets equal to 130% is characteristic of SimpleBox 3.12 (calculations with historical emissions). For results of DEHM-POP_1 and *2,* G-CIEMS_1 and MSCE-POP_2, the values of PCB-153 masses contained in water obtained with the use of "own or alternative" data sets are smaller than those obtained with "reference" data set.

Vegetation. The scattering in values of PCB-153 mass contained in vegetation obtained by the participating models on the basis of non-zero initial conditions is rather large for both results based on two different data sets of physical-chemical properties (Tables 3.19 and 3.20, Section 3.1.4). The difference between the maximum values obtained by SimpleBox model and the minimum values calculated by G-CIEMS on the basis of initial concentrations given as input data reaches several orders of magnitude. Square deviation σ between different model results obtained on the basis of zero initial conditions does not exceed the mean value of this parameter.

Annual values of PCB-153 mass contained in vegetation obtained on the basis of zero initial conditions and with the use of "reference" and "own/alternative" data sets are presented in Fig. 3.28a. Fig. 3.28b shows the results obtained with the use of non-zero initial conditions.

According to the calculation results of CliMoChem and G-CIEMS models, the values of PCB-153 mass in vegetation obtained with the use of "own or alternative" data sets are smaller than those obtained with "reference" data set; and vice versa for MSCE-POP and SimpleBox results. The largest difference in the results obtained with two data sets equal to 63% is characteristic of CliMoChem results (Table 3.21, Section 3.1.4). Percentage difference between results of other models calculated with the use of both data sets varies from 6 to 52 %.

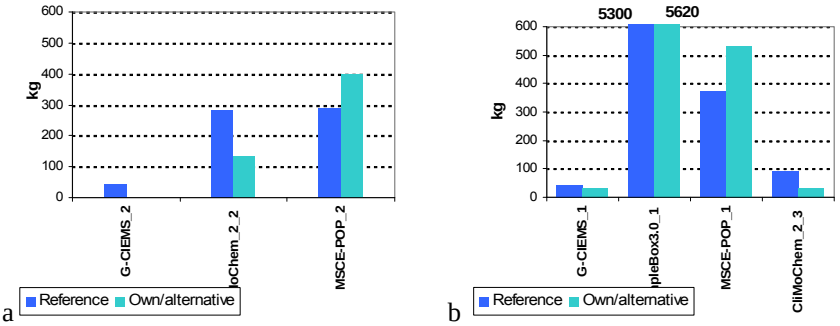


Fig.3.28. *Comparison of PCB-153 mass contained in vegetation calculated by different models on the basis of "reference" and "own/alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Relative distribution of PCB mass. According to the results on relative distribution of PCB-153 mass between different environmental compartments, all models show that bulk fraction of overall environmental PCB content is accumulated in soil. The average distribution of PCB-153 mass between main environmental compartments is presented for the results of participating models obtained on the basis of zero and non-zero initial conditions in Fig. 3.29a and b, respectively. In these figures results calculated with the use of "reference" and "own/alternative" data sets are given. Of note, values of average fraction of PCB-153 mass in each medium calculated with two different data sets of physical-chemical properties could not be directly compared between each other since calculation results of different number of participating models are enclosed in them.

The distribution of PCB-153 mass between main environmental compartments obtained by the participating models on the basis of zero initial conditions (see Fig. 3.29a) shows that soil compartment contains the largest fraction of overall environmental mass (more than 50%). Then come seawater compartment with 27 and 32% in "reference" and "own/alternative" results, respectively and vegetation compartment with 9 and 12% in "reference" and "own/alternative" results, respectively. The atmospheric content of PCB-153 is equal to approximately 5 %. According to the calculations performed on the basis of non-zero initial conditions (see Fig. 3.29b), PCB-153 is mainly accumulated in soil (96%) and only about 4% of its overall mass in the environment is distributed between other compartments. The difference between relative values calculated with "reference" and "own/alternative" data sets is not high.

To show redistribution of the pollutant between main environmental compartments for each participating model in more detail, plots of PCB-153 fractions in different environmental compartments calculated by the models on the basis of zero and non-zero initial conditions are presented below. Fractions of PCB-153 mass contained in soil calculated by the different models with the use of "reference" and "own/alternative" data sets are compared in Figs. 3.30a and b. The red line in the plots shows the value of the corresponding fraction averaged between models.

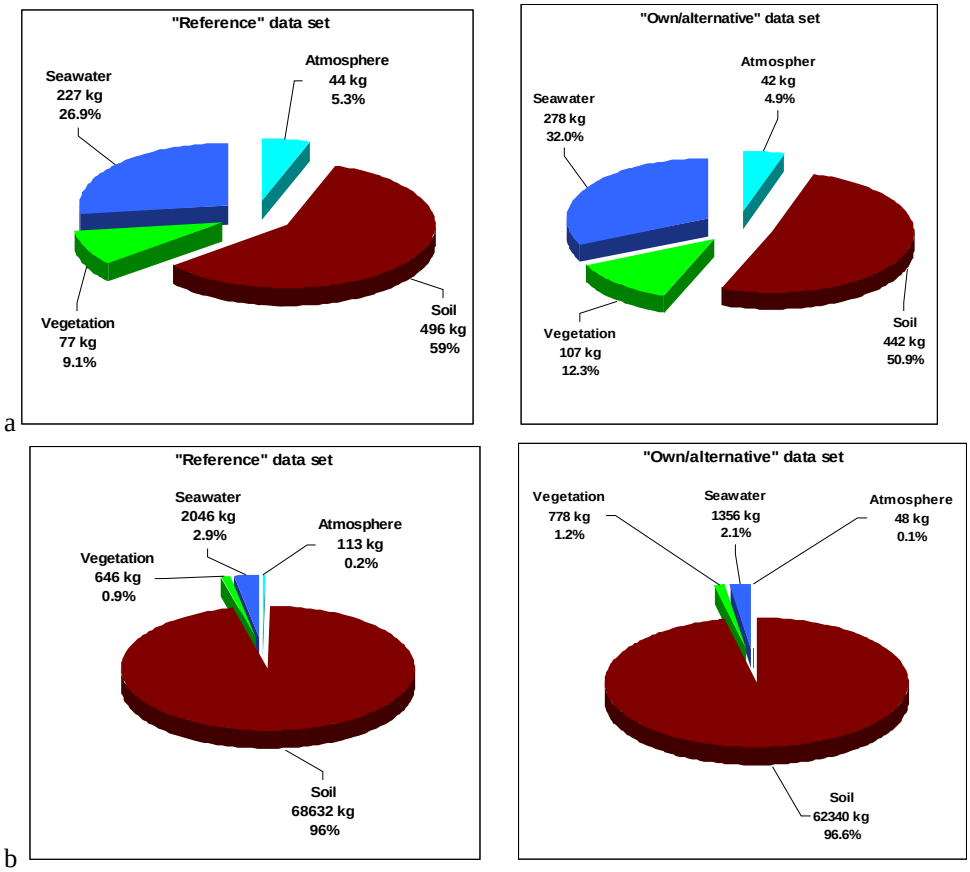


Fig. 3.29. *Distribution of PCB-153 mass between environmental compartments (kg) averaged for all participating models and calculated on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

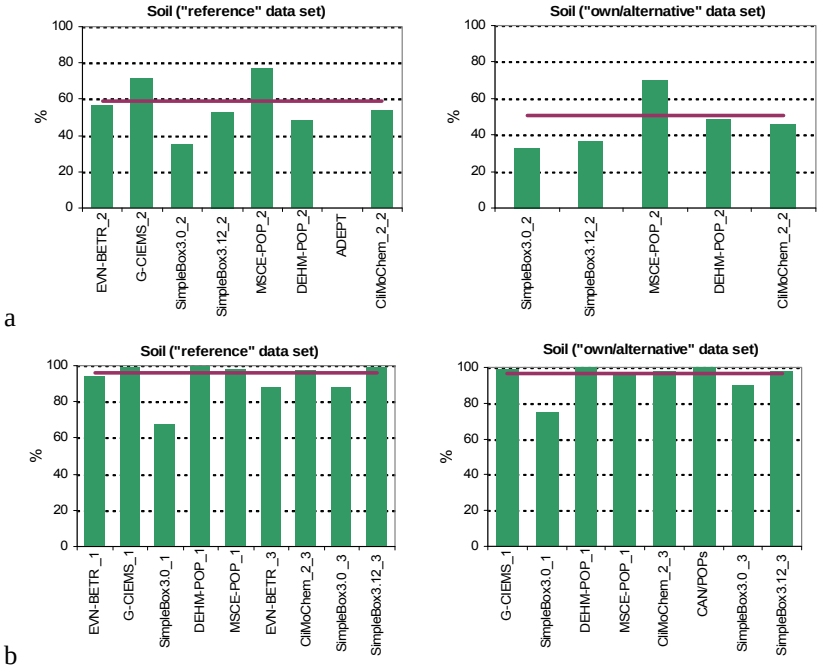


Fig. 3.30. *Fractions of PCB-153 mass in soil calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The values of PCB fraction in soil obtained by the participants on the basis of zero initial concentrations (Fig. 3.30a) vary from 35 to 77% in the case of use of “reference” and from 33 to 70% in the case of use of “own or alternative” data sets. ADEPT model does not include soil compartment like any other compartments except the atmospheric one. For MSCE-POP and SimpleBox 3.12 results (zero initial conditions), the fraction of overall environmental mass of PCB-153 accumulated in soil calculated on the basis of “reference” data set is noticeably higher than that obtained with the use of “own or alternative” data set. For most models the fraction of overall environmental content in soil calculated using initial conditions in media or historical emissions (see Fig. 3.30b) is higher than 90% for results of both physical-chemical data sets (“reference” and “own/alternative”). The value of SimpleBox 3.0 model calculated with initial concentrations of the pollutant in media with the use of “own/alternative” data set is higher than that based on “reference” data set.

PCB fractions in all other compartments are lower than those in soil. Fractions of PCB-153 mass in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. 3.31a and b, respectively. In these figures fractions of PCB-153 mass in the atmosphere calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.

Since ADEPT model is a purely atmospheric one, all environmental content of PCB-153 calculated by this model is concentrated in this medium making up respectively 100%. The results of other models calculated on the basis of zero initial concentrations (see Fig.3.31a) are characterised by higher values of relative fractions of total environmental mass of PCB-153 contained in the atmosphere (1.3-12%) than the results obtained with initial conditions or historical emissions (0.02-0.43%) (Fig.3.31b). The considerable difference between calculations made on two different data sets of physical-chemical properties is observed in results of G-CIEMS_1, SimpleBox 3.0_3 and 3.12_2 and CliMoChem_2-3 models.

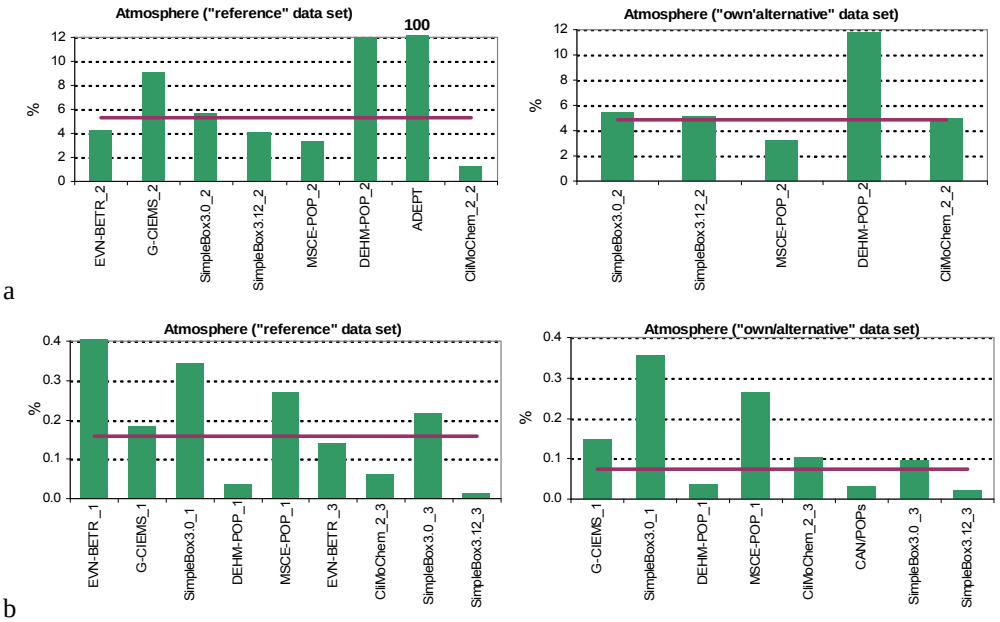


Fig. 3.31. *Fractions of PCB-153 mass in the atmosphere calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of PCB-153 mass in seawater calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. 3.32a and b, respectively. In these figures fractions of PCB-153 mass in seawater calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.

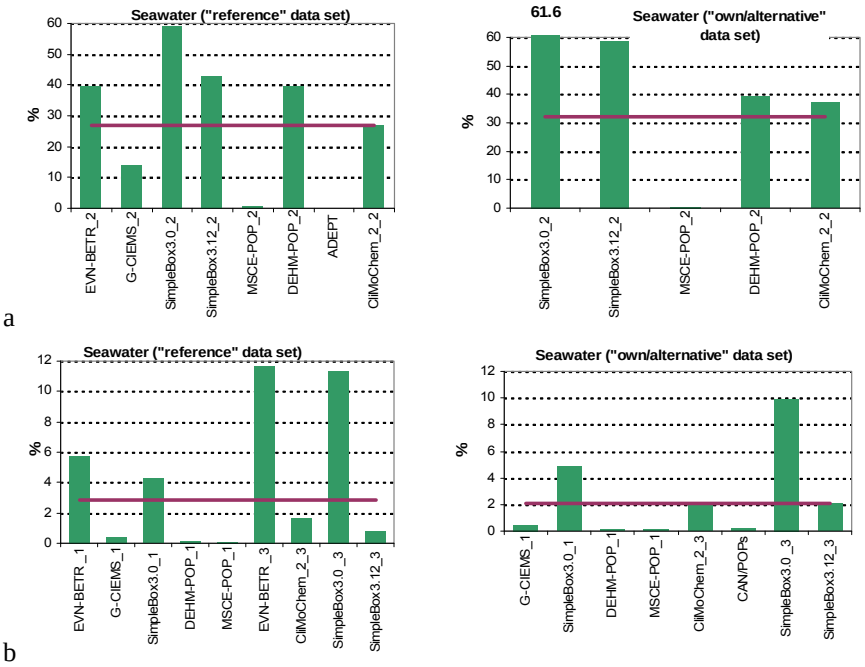


Fig. 3.32. *Fractions of PCB-153 mass in seawater calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

As in the case of atmospheric content, relative fractions of PCB-153 water content obtained by most models on the basis of zero initial concentrations and both physical-chemical data sets vary from 14 to 62% and considerably exceed values calculated with initial conditions (See Fig. 3.32 a). MSCE-POP model provided the minimum seawater fractions equal to 0.6 % in both cases. The results of participating models obtained on the basis of initial concentrations of the pollutant in media or historical emissions (See Fig. 3.32b) strongly differ between each other. The highest values among these results are obtained by EVN-BETR and UK-MODEL and SimpleBox 3.0 model using historical emissions. The lowest values are characteristic of results of MSCE-POP, DEHM-POP, CAN/POPs and G-CIEMS models calculated using initial conditions. Considerable difference between fractions of PCB-153 water content calculated with the use of two different physical-chemical data sets can be seen for SimpleBox results.

Fractions of total environmental mass of PCB-153 contained in vegetation calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. 3.33a and b, respectively. In these figures fractions of PCB-153 mass in vegetation calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models. Of note, the models, for which vegetation compartment was not included into calculations of mass balance, are also shown in the plots.

Fig. 3.33a shows that fractions of total environmental mass of PCB-153 contained in vegetation calculated by MSCE-POP model on the basis of zero initial conditions are the highest among other models for both data sets of physical-chemical properties. At that the value obtained on the basis of "reference" data set is lower than that based on "own/alternative" data set. The results obtained by the participating models on the basis of non-zero initial conditions differ considerably between each other (see Fig. 3.33b). The scattering of calculated lowest and highest fractions of vegetation content between models reaches two orders of magnitude. The highest and the lowest fractions of vegetation content are obtained by SimpleBox 3.0 and by G-CIEMS models, respectively. In all models' results except those of G-CIEMS there is noticeable difference between calculated values based on two different data sets of physical-chemical properties.

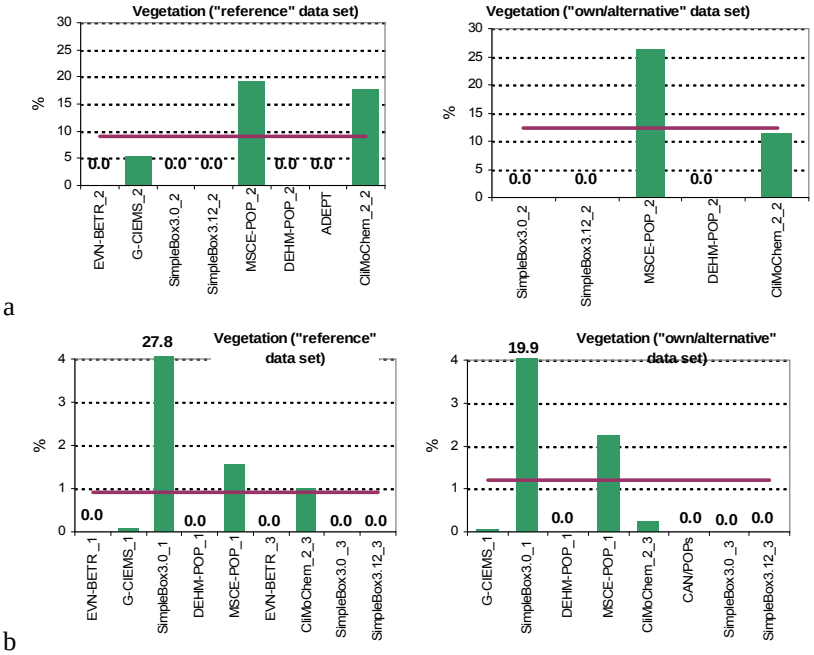


Fig. 3.33. *Fractions of PCB-153 mass in vegetation calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Thus, according to the results of most participating models' based of both physical-chemical data sets ("reference" and "own/alternative"), the absolute values of PCB-153 mass contained in the considered layers of the atmosphere are rather close. Differences in calculated values of PCB-153 mass accumulated in other media than atmosphere are more considerable.

According to the results presented by most models, PCB-153 is mainly accumulated in soil. PCB fractions in all other compartments are essentially lower and depend on type of calculations performed. The variability between PCB fractions in other environmental compartments is higher.
For most participating models the comparison of absolute and relative values of PCB-153 mass in the environmental media calculated with two different data sets ("reference" and "own/alternative") show relatively weak sensitivity of mass balance values with respect to variations of pollutant-related parameters. Only in some cases the differences are essential.

3.2. Masses degraded in the environmental compartments

3.2.1. Comparison of calculated values of PCB-153 mass degraded in the atmosphere

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-153 degraded in the atmosphere within layers of 1 km, 5 km and 10 km height.

Reference data set. Calculation results on PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.22.

Monthly values of PCB-153 mass degraded in 1 km layer of the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.34 a and b, respectively. Seasonal variations of low values of mass contained in 1 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. 3.34c in more detail.

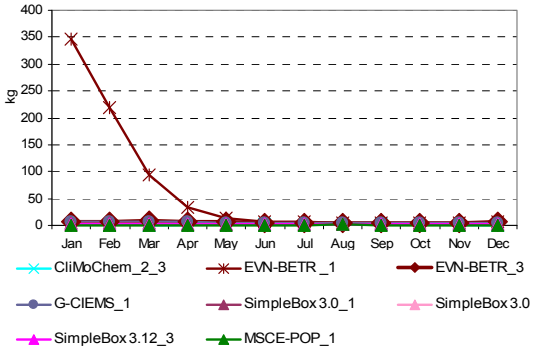


Fig. 3.34a. *PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

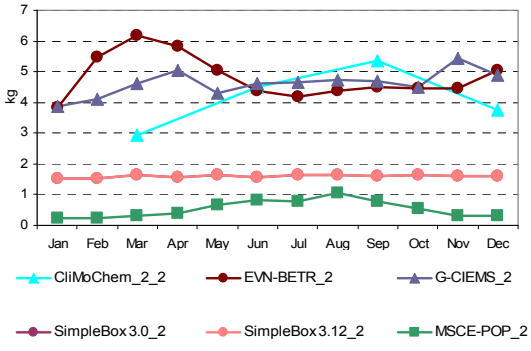


Fig. 3.34b. *PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

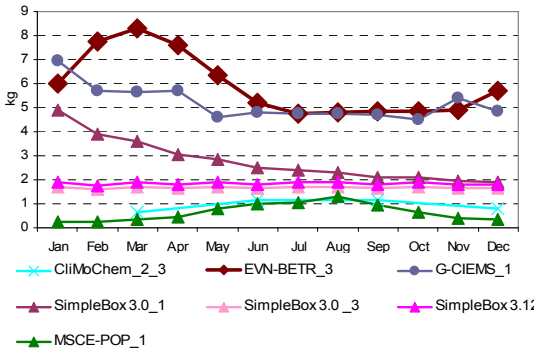


Fig. 3.34c. *PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Calculation results on PCB-153 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table 3.23.

Monthly values of PCB-153 mass degraded in 5 km layer of the atmosphere calculated by the models on the basis of “reference” data set are compared in Fig. 3.35.

Calculation results on PCB-153 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table 3.24.

Monthly values of PCB-153 mass degraded in 10 km layer of the atmosphere calculated by the participating models on the basis of “reference” data set are compared in Fig. 3.36.

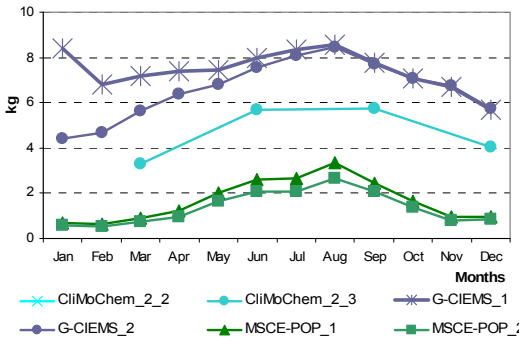


Fig. 3.35. *PCB-153 mass degraded in 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of “reference” data set*

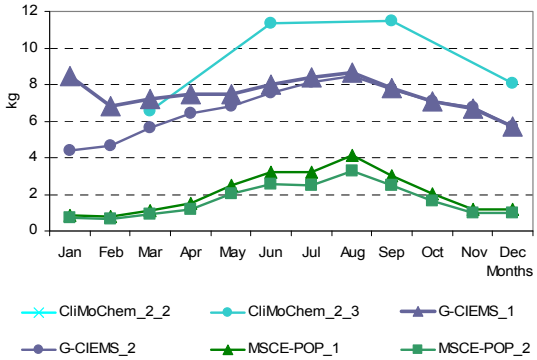


Fig.3.36. *PCB-153 mass degraded in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of “reference” data set*

Table 3.22. *Calculation results: PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	MSCE-POP_1	EVN-BETR _1[a]	G-CIEMS_1	SimpleBox 3.0_1[b]	EVN-BETR _3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	0.26	347.37	6.95	4.88	6.00		1.70	1.88	*52.72*	*129.95*	Jan	3.84	3.87		1.53	1.53	0.23	*2.20*	*1.60*
Feb	0.25	218.72	5.72	3.90	7.74		1.58	1.76	*34.24*	*81.39*	Feb	5.49	4.12		1.52	1.52	0.22	*2.57*	*2.16*
Mar	0.35	93.93	5.66	3.58	8.29		1.68	1.88	*16.48*	*34.26*	Mar	6.16	4.63		1.63	1.63	0.30	*2.87*	*2.43*
Seas_1	**0.86**	**660.02**	**18.33**	**12.35**	**22.04**	**0.66**	**4.96**	**5.52**	***90.59***	***230.22***	**Seas_1**	**15.49**	**12.62**	2.93	**4.68**	**4.68**	**0.74**	***6.86***	***5.83***
Apr	0.47	34.46	5.70	3.04	7.62		1.63	1.82	*7.82*	*12.01*	Apr	5.82	5.04		1.58	1.58	0.38	*2.88*	*2.40*
May	0.80	14.15	4.58	2.83	6.33		1.68	1.88	*4.61*	*4.61*	May	5.04	4.29		1.63	1.63	0.65	*2.65*	*1.90*
Jun	1.02	7.68	4.78	2.51	5.22		1.63	1.82	*3.52*	*2.43*	Jun	4.38	4.60		1.58	1.58	0.81	*2.59*	*1.76*
Seas_2	**2.29**	**56.29**	**15.05**	**8.38**	**19.17**	**1.14**	**4.94**	**5.52**	***14.10***	***18.15***	**Seas_2**	**15.25**	**13.93**	4.51	**4.79**	**4.80**	**1.84**	***7.52***	***5.60***
Jul	1.03	5.69	4.75	2.42	4.75		1.68	1.88	*3.17*	*1.84*	Jul	4.18	4.67		1.64	1.64	0.80	*2.58*	*1.72*
Aug	1.30	5.29	4.75	2.28	4.82		1.68	1.88	*3.15*	*1.73*	Aug	4.38	4.72		1.64	1.64	1.04	*2.68*	*1.72*
Sep	0.95	5.18	4.70	2.10	4.87		1.63	1.82	*3.04*	*1.80*	Sep	4.48	4.69		1.59	1.59	0.80	*2.63*	*1.82*
Seas_3	**3.29**	**16.16**	**14.20**	**6.80**	**14.44**	**1.15**	**5.00**	**5.58**	***8.33***	***5.74***	**Seas_3**	**13.04**	**14.08**	5.34	**4.86**	**4.86**	**2.65**	***7.47***	***4.82***
Oct	0.64	5.13	4.48	2.09	4.85		1.68	1.88	*2.97*	*1.80*	Oct	4.47	4.50		1.64	1.64	0.53	*2.56*	*1.82*
Nov	0.38	5.24	5.42	1.96	4.91		1.63	1.82	*3.05*	*2.07*	Nov	4.47	5.45		1.59	1.59	0.32	*2.68*	*2.17*
Dec	0.37	6.16	4.84	1.91	5.68		1.63	1.82	*3.20*	*2.30*	Dec	5.06	4.88		1.59	1.59	0.32	*2.69*	*2.15*
Seas_4	**1.39**	**16.53**	**14.74**	**5.96**	**15.44**	**0.80**	**4.94**	**5.52**	***8.17***	***6.42***	**Seas_4**	**13.99**	**14.83**	3.75	**4.81**	**4.81**	**1.17**	***7.23***	***5.73***
Annual	**7.83**	**749.01**	**62.32**	**33.49**	**71.09**	**3.75**	**19.84**	**22.15**	***121.19***	***254.83***	**Annual**	**57.78**	**55.46**	**16.53**	**19.15**	**19.15**	**6.40**	***29.08***	***21.86***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
[b] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table 3.23. *Calculation results: PCB-153 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	MSCE-POP_1	CliMoChem_2_3				G-CIEMS_2	CliMoChem_2_2	MSCE-POP_2		
Jan	8.42	0.68		*4.55*	*5.48*	Jan	4.40		0.59	*2.49*	*2.69*
Feb	6.79	0.65		*3.72*	*4.35*	Feb	4.68		0.55	*2.62*	*2.91*
Mar	7.19	0.90		*4.04*	*4.45*	Mar	5.66		0.76	*3.21*	*3.46*
Seas_1	**22.4**	**2.22**	**3.28**	***9.30***	***11.36***	**Seas_1**	**14.7**	**14.63**	**1.91**	***10.42***	***7.37***
Apr	7.40	1.22		*4.31*	*4.37*	Apr	6.38		0.98	*3.68*	*3.82*
May	7.43	2.05		*4.74*	*3.81*	May	6.81		1.67	*4.24*	*3.63*
Jun	7.97	2.61		*5.29*	*3.79*	Jun	7.55		2.08	*4.81*	*3.87*
Seas_2	**22.8**	**5.88**	**5.68**	***11.46***	***9.83***	**Seas_2**	**20.7**	**22.53**	**4.72**	***16.00***	***9.81***
Jul	8.38	2.65		*5.52*	*4.05*	Jul	8.11		2.06	*5.08*	*4.28*
Aug	8.59	3.35		*5.97*	*3.70*	Aug	8.45		2.68	*5.56*	*4.07*
Sep	7.78	2.45		*5.12*	*3.77*	Sep	7.74		2.05	*4.90*	*4.02*
Seas_3	**24.7**	**8.45**	**5.74**	***12.98***	***10.28***	**Seas_3**	**24.3**	**26.71**	**6.80**	***19.27***	***10.87***
Oct	7.08	1.65		*4.37*	*3.84*	Oct	7.09		1.36	*4.23*	*4.05*
Nov	6.72	0.97		*3.84*	*4.07*	Nov	6.75		0.82	*3.78*	*4.20*
Dec	5.68	0.94		*3.31*	*3.35*	Dec	5.72		0.83	*3.27*	*3.46*
Seas_4	**19.5**	**3.56**	**4.02**	***9.02***	***9.06***	**Seas_4**	**19.6**	**18.76**	**3.01**	***13.78***	***9.33***
Annual	**89.44**	**20.11**	**18.73**	***42.76***	***40.43***	**Annual**	**79.32**	**82.64**	**16.44**	***59.47***	***37.30***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

Table 3.24. *Calculation results: PCB-153 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	MSCE-POP_1	CliMoChem_2_3				G-CIEMS_2	CliMoChem_2_2	MSCE-POP_2		
Jan	8.46	0.83		*4.64*	*5.40*	Jan	4.40		0.73	*2.56*	*2.60*
Feb	6.82	0.79		*3.81*	*4.27*	Feb	4.68		0.68	*2.68*	*2.83*
Mar	7.24	1.10		*4.17*	*4.34*	Mar	5.67		0.93	*3.30*	*3.35*
Seas_1	**22.53**	**2.71**	**6.57**	***10.60***	***10.50***	**Seas_1**	**14.8**	**29.26**	**2.33**	***15.45***	***13.48***
Apr	7.44	1.49		*4.47*	*4.21*	Apr	6.40		1.20	*3.80*	*3.68*
May	7.47	2.50		*4.99*	*3.51*	May	6.83		2.04	*4.44*	*3.39*
Jun	8.00	3.20		*5.60*	*3.39*	Jun	7.57		2.54	*5.05*	*3.56*
Seas_2	**22.91**	**7.19**	**11.36**	***13.82***	***8.14***	**Seas_2**	**20.8**	**45.07**	**5.78**	***23.88***	***19.83***
Jul	8.41	3.24		*5.83*	*3.65*	Jul	**8.14**		2.52	*5.33*	*3.97*
Aug	8.63	4.10		*6.36*	*3.20*	Aug	**8.48**		3.28	*5.88*	*3.68*
Sep	7.80	3.00		*5.40*	*3.39*	Sep	**7.75**		2.51	*5.13*	*3.70*
Seas_3	**24.84**	**10.34**	**11.48**	***15.55***	***8.06***	**Seas_3**	**24.4**	**53.42**	**8.31**	***28.70***	***22.87***
Oct	7.09	2.02		*4.55*	*3.59*	Oct	**7.10**		1.67	*4.38*	*3.84*
Nov	6.72	1.18		*3.95*	*3.92*	Nov	**6.76**		1.00	*3.88*	*4.07*
Dec	5.68	1.15		*3.42*	*3.20*	Dec	**5.72**		1.01	*3.37*	*3.33*
Seas_4	**19.49**	**4.35**	**8.04**	***10.63***	***7.89***	**Seas_4**	**19.6**	**37.52**	**3.68**	***20.26***	***16.93***
Annual	**89.76**	**24.60**	**37.45**	***50.60***	***34.52***	**Annual**	**79.50**	**165.27**	**20.10**	***88.29***	***72.98***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Own/alternative data set. Calculation results on PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.25.

Monthly values of PCB-153 mass degraded in 1 km layer of the atmosphere calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.37 a and b, respectively.

Calculation results on PCB-153 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data set together with statistical parameters used for evaluation are presented in Table 3.26.

Monthly values of PCB-153 mass degraded in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. 3.38.

Calculation results on PCB-153 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative data sets" together with statistical parameters used for evaluation are presented in Table 3.27.

Monthly values of PCB-153 mass degraded in 10 km layer of the atmosphere calculated by the participating models on the basis of "own or alternative" data sets are compared in Fig. 3.39.

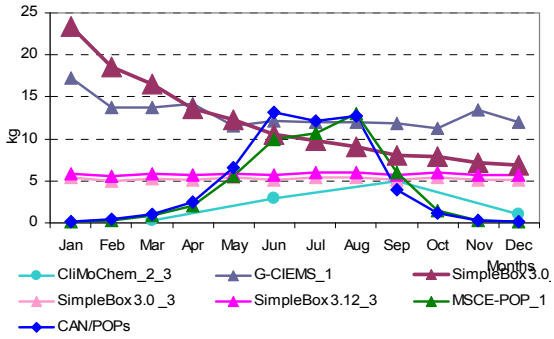


Fig. 3.37a. *PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

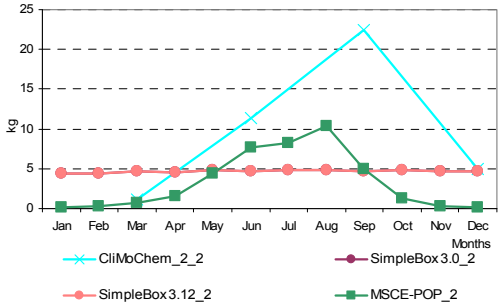


Fig. 3.37b. *PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

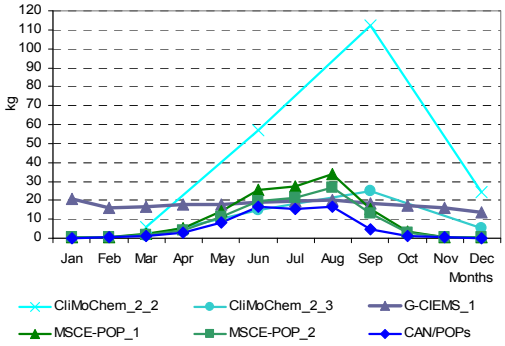


Fig. 3.38. *PCB-153 mass in 5 km layer of the atmosphere (kg) degraded by the participating models on the basis of "own or alternative" data sets*

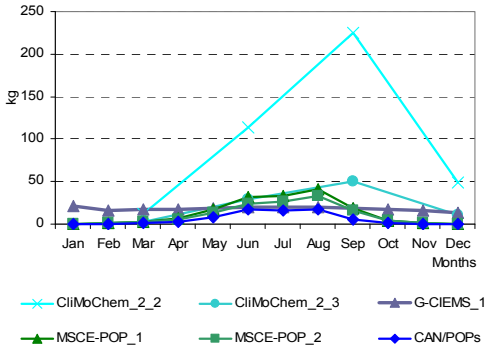


Fig. 3.39. *PCB-153 mass degraded in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own or alternative" data sets*

Table 3.25. *Calculation results: PCB-153 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	G-CIEMS_1	SimpleBox 3.0_1[a]	CAN/ POPs	CliMo Chem_ 2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.18	17.27	23.34	0.19		5.36	5.89	*8.70*	*9.51*	Jan		4.42	4.42	0.15	*3.00*	*2.46*
Feb	0.32	13.69	18.57	0.39		4.98	5.52	*7.24*	*7.39*	Feb		4.41	4.41	0.27	*3.03*	*2.39*
Mar	0.84	13.76	16.56	1.06		5.33	5.90	*7.24*	*6.54*	Mar		4.73	4.73	0.70	*3.39*	*2.33*
Seas_1	**1.33**	**44.71**	**58.47**	**1.64**	**0.28**	**15.67**	**17.31**	***19.92***	***23.06***	**Seas_1**	**1.20**	**13.56**	**13.56**	**1.12**	***7.36***	***7.16***
Apr	2.02	14.13	13.64	2.47		5.17	5.72	*7.19*	*5.39*	Apr		4.59	4.59	1.56	*3.58*	*1.75*
May	5.56	11.57	12.27	6.56		5.34	5.92	*7.87*	*3.17*	May		4.76	4.76	4.37	*4.63*	*0.23*
Jun	9.96	12.07	10.54	13.13		5.18	5.73	*9.43*	*3.29*	Jun		4.62	4.62	7.61	*5.62*	*1.73*
Seas_2	**17.55**	**37.77**	**36.45**	**22.16**	**2.94**	**15.69**	**17.37**	***21.42***	***12.24***	**Seas_2**	**11.36**	**13.97**	**13.97**	**13.55**	***13.21***	***1.25***
Jul	10.73	12.02	9.84	12.08		5.35	5.92	*9.32*	*2.98*	Jul		4.78	4.78	8.22	*5.93*	*1.98*
Aug	13.07	12.03	9.00	12.67		5.35	5.93	*9.67*	*3.44*	Aug		4.79	4.79	10.33	*6.63*	*3.20*
Sep	5.94	11.78	8.08	3.94		5.18	5.74	*6.78*	*2.80*	Sep		4.64	4.64	5.01	*4.76*	*0.21*
Seas_3	**29.75**	**35.83**	**26.92**	**28.69**	**4.98**	**15.88**	**17.58**	***22.81***	***10.51***	**Seas_3**	**22.48**	**14.20**	**14.20**	**23.55**	***18.61***	***5.11***
Oct	1.46	11.22	7.83	1.14		5.35	5.93	*5.49*	*3.84*	Oct		4.80	4.80	1.22	*3.60*	*2.07*
Nov	0.29	13.43	7.17	0.27		5.18	5.74	*5.35*	*4.90*	Nov		4.65	4.65	0.25	*3.18*	*2.54*
Dec	0.15	12.02	6.84	0.11		5.19	5.74	*5.01*	*4.49*	Dec		4.65	4.65	0.13	*3.15*	*2.61*
Seas_4	**1.90**	**36.66**	**21.84**	**1.52**	**1.08**	**15.72**	**17.40**	***13.73***	***13.28***	**Seas_4**	**4.90**	**14.10**	**14.10**	**1.60**	***8.67***	***6.41***
Annual	**50.53**	**154.98**	**143.68**	**54.02**	**9.28**	**62.97**	**69.66**	***77.87***	***52.58***	**Annual**	**39.94**	**55.83**	**55.83**	**39.82**	***47.86***	***9.21***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table 3.26. *Calculation results: PCB-153 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	CAN/POPs	G-CIEMS_1	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	0.24	20.52	0.46		*7.07*	*11.65*	Jan		0.40		
Feb	0.43	15.86	0.81		*5.70*	*8.80*	Feb		0.69		
Mar	1.23	16.89	2.16		*6.76*	*8.78*	Mar		1.80		
Seas_1	**1.90**	**53.27**	**3.43**	**1.38**	***15.00***	***25.53***	**Seas_1**	**6.02**	**2.88**	***4.45***	***2.21***
Apr	2.93	17.58	5.20		*8.57*	*7.89*	Apr		4.02		
May	8.06	17.96	14.29		*13.44*	*5.00*	May		11.23		
Jun	16.89	19.16	25.59		*20.55*	*4.51*	Jun		19.56		
Seas_2	**27.89**	**54.70**	**45.09**	**14.71**	***35.60***	***17.80***	**Seas_2**	**56.78**	**34.81**	***45.79***	***15.53***
Jul	15.60	19.88	27.58		*21.02*	*6.07*	Jul		21.11		
Aug	16.59	20.31	33.59		*23.50*	*8.94*	Aug		26.54		
Sep	5.01	18.57	15.27		*12.95*	*7.07*	Sep		12.86		
Seas_3	**37.20**	**58.76**	**76.44**	**24.88**	***49.32***	***22.87***	**Seas_3**	**112.38**	**60.52**	***86.45***	***36.67***
Oct	1.38	16.96	3.75		*7.36*	*8.40*	Oct		3.13		
Nov	0.31	16.04	0.75		*5.70*	*8.96*	Nov		0.64		
Dec	0.13	13.76	0.39		*4.76*	*7.80*	Dec		0.34		
Seas_4	**1.81**	**46.77**	**4.88**	**5.41**	***14.72***	***21.43***	**Seas_4**	**24.51**	**4.11**	***14.31***	***14.43***
Annual	**68.80**	**213.50**	**129.84**	**46.38**	***114.63***	***74.75***	**Annual**	**199.68**	**102.32**	***151.00***	***68.84***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table 3.27. *Calculation results: PCB-153 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	G-CIEMS_1	MSCE-POP_1	CAN/POPs	CliMoChem_2_3				CliMo Chem_2_2	MSCE-POP_2		
Jan	20.63	0.56	0.24		*7.14*	*11.68*	Jan		0.48		
Feb	15.93	0.99	0.43		*5.79*	*8.79*	Feb		0.84		
Mar	16.98	2.64	1.23		*6.95*	*8.71*	Mar		2.20		
Seas_1	**53.54**	**4.19**	**1.90**	**2.76**	***15.60***	***25.31***	**Seas_1**	**12.03**	**3.53**	***7.78***	***6.01***
Apr	17.65	6.36	2.93		*8.98*	*7.70*	Apr		4.92		
May	18.02	17.48	8.07		*14.52*	*5.60*	May		13.73		
Jun	19.20	31.30	16.89		*22.47*	*7.74*	Jun		23.92		
Seas_2	**54.87**	**55.14**	**27.89**	**29.42**	***41.83***	***15.23***	**Seas_2**	**113.55**	**42.57**	***78.06***	***50.19***
Jul	19.95	33.73	15.61		*23.09*	*9.46*	Jul		25.82		
Aug	20.40	41.08	16.59		*26.02*	*13.18*	Aug		32.46		
Sep	18.60	18.67	5.01		*14.09*	*7.86*	Sep		15.73		
Seas_3	**58.94**	**93.48**	**37.21**	**49.77**	***59.85***	***24.13***	**Seas_3**	**224.76**	**74.01**	***149.38***	***106.59***
Oct	16.98	4.58	1.38		*7.65*	*8.24*	Oct		3.83		
Nov	16.05	0.91	0.31		*5.76*	*8.92*	Nov		0.78		
Dec	13.77	0.47	0.13		*4.79*	*7.78*	Dec		0.42		
Seas_4	**46.80**	**5.97**	**1.81**	**10.82**	***16.35***	***20.63***	**Seas_4**	**49.02**	**5.03**	***27.02***	***31.11***
Annual	**214.15**	**158.79**	**68.81**	**92.77**	***133.63***	***65.80***	**Annual**	**399.37**	**125.14**	***262.25***	***193.91***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-153 mass degraded in 1, 5 and 10 km layers of obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables 3.28 – 3.30.

Table 3.28. *The percentage difference between calculation results on PCB-153 mass degraded in 1 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			149%	378%	189%	189%	216%	213%	-32%	-33%
Feb			139%	376%	190%	190%	216%	213%	26%	24%
Mar			143%	363%	190%	190%	217%	214%	141%	137%
Seas_1	-59%	-58%	144%	373%	190%	190%	216%	213%	55%	51%
Apr			148%	349%	191%	191%	217%	214%	327%	311%
May			153%	334%	191%	191%	217%	214%	598%	572%
Jun			152%	320%	192%	192%	218%	215%	879%	843%
Seas_2	152%	159%	151%	335%	191%	191%	217%	214%	667%	637%
Jul			153%	307%	192%	192%	218%	215%	940%	925%
Aug			153%	295%	192%	192%	218%	215%	902%	889%
Sep			151%	284%	193%	192%	218%	215%	523%	526%
Seas_3	321%	333%	152%	296%	192%	192%	218%	215%	804%	790%
Oct			150%	274%	193%	193%	218%	215%	127%	129%
Nov			148%	266%	193%	193%	218%	215%	-23%	-22%
Dec			148%	259%	193%	193%	218%	215%	-59%	-59%
Seas_4	31%	35%	149%	267%	193%	193%	218%	215%	37%	37%
Annual	142%	148%	149%	329%	192%	192%	217%	214%	545%	522%

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Table 3.29. *The percentage difference between calculation results on PCB-153 mass degraded in 5 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	MSCE-POP_1	MSCE-POP_2
Jan			144%	-32%	-33%
Feb			134%	26%	24%
Mar			135%	141%	137%
Seas_1	-59%	-58%	138%	55%	51%
Apr			138%	327%	311%
May			142%	598%	572%
Jun			140%	879%	843%
Seas_2	152%	159%	140%	667%	637%
Jul			137%	940%	925%
Aug			137%	902%	889%
Sep			139%	523%	526%
Seas_3	321%	333%	137%	804%	790%
Oct			140%	127%	129%
Nov			139%	-23%	-22%
Dec			142%	-59%	-59%
Seas_4	31%	35%	140%	37%	37%
Annual	142%	148%	139%	545%	522%

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table 3.30. *The percentage difference between calculation results on PCB-153 mass degraded in 10 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	MSCE-POP_1	MSCE-POP_2
Jan			144%	-32%	-33%
Feb			134%	26%	24%
Mar			134%	141%	137%
Seas_1	-59%	-58%	138%	55%	51%
Apr			137%	327%	311%
May			141%	598%	572%
Jun			140%	879%	843%
Seas_2	152%	159%	140%	667%	637%
Jul			137%	940%	925%
Aug			136%	902%	889%
Sep			139%	523%	526%
Seas_3	321%	333%	137%	804%	790%
Oct			139%	127%	129%
Nov			139%	-23%	-22%
Dec			142%	-59%	-59%
Seas_4	31%	35%	140%	37%	37%
Annual	142%	148%	139%	545%	522%

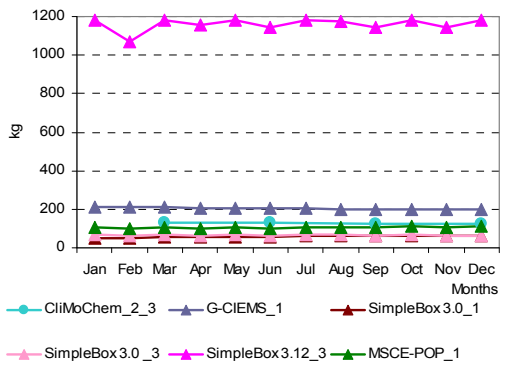
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

3.2.2. Comparison of calculated values of PCB-153 mass degraded in soil

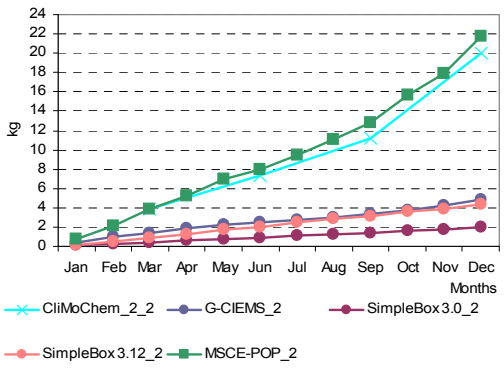
According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-153 degraded in soil within 5 cm and 10 cm depth.

Reference data set. Calculation results on PCB-153 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.31.

Monthly values of PCB-153 mass degraded in 5 cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.40a and b, respectively.



a



b

Fig. 3.40a. *PCB-153 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. 3.40b. *PCB-153 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Calculation results on PCB-153 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table 3.32.

Monthly values of PCB-153 mass degraded in 10 cm layer of soil calculated by all participating models on the basis of “reference” data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.41a and b, respectively. Seasonal variations of low values of mass degraded in 10 cm layer of soil calculated by the participating models on the basis of “reference” data set and non-zero initial conditions are also shown in Fig. 3.41c in more detail.

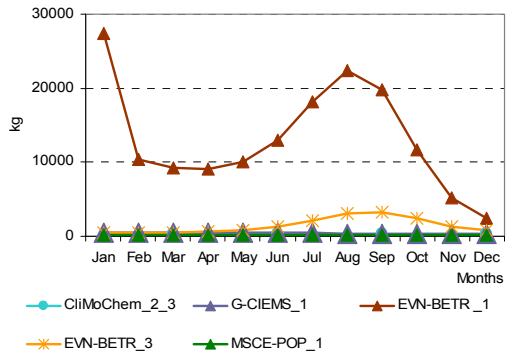


Fig.3.41a. *PCB-153 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and non-zero initial conditions (all models)*

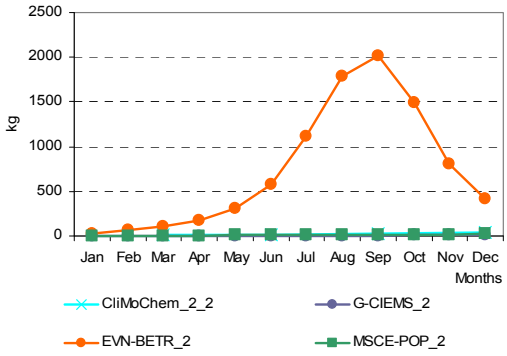


Fig.3.41b. *PCB-153 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and zero-initial conditions*

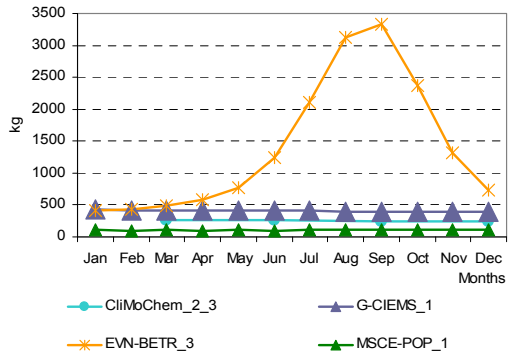


Fig.3.41c. *PCB-153 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and non-zero initial conditions (models with low values)*

Table 3.31. *Calculation results: PCB-153 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	MSCE-POP_1	G-CIEMS_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	103.9	211.9	48.1		67.8	1183.0	*322.9*	*485.0*	Jan	0.4		0.1	0.2	0.7	*0.3*	*0.3*
Feb	97.5	210.9	48.1		63.2	1068.5	*297.6*	*435.6*	Feb	0.9		0.2	0.5	2.1	*1.0*	*0.8*
Mar	104.6	209.6	53.9		67.4	1183.0	*323.7*	*484.2*	Mar	1.4		0.4	0.9	3.9	*1.7*	*1.5*
Seas_1	**305.9**	**632.3**	**150.1**	**131.9**	**198.4**	**3434.6**	***808.9***	***1299.5***	**Seas_1**	**2.7**	**3.9**	**0.7**	**1.6**	**6.7**	***3.1***	***2.3***
Apr	101.6	208.1	54.2		65.1	1156.8	*317.1*	*473.3*	Apr	1.9		0.6	1.2	5.3	*2.2*	*2.1*
May	105.2	206.5	57.6		67.1	1183.0	*323.9*	*483.9*	May	2.2		0.8	1.7	6.9	*2.9*	*2.7*
Jun	101.8	204.9	56.9		64.8	1144.9	*314.7*	*467.8*	Jun	2.5		0.9	2.0	8.0	*3.3*	*3.1*
Seas_2	**308.6**	**619.5**	**168.7**	**129.2**	**197.0**	**3484.6**	***817.9***	***1318.4***	**Seas_2**	**6.6**	**7.4**	**2.2**	**5.0**	**20.1**	***8.3***	***6.9***
Jul	105.2	203.3	59.9		66.8	1183.0	*323.6*	*483.8*	Jul	2.8		1.1	2.5	9.5	*4.0*	*3.8*
Aug	105.6	201.7	60.7		66.6	1175.5	*322.0*	*480.4*	Aug	3.0		1.3	2.9	11.0	*4.6*	*4.4*
Sep	103.5	200.1	59.4		64.3	1144.9	*314.4*	*467.6*	Sep	3.3		1.4	3.2	12.8	*5.2*	*5.1*
Seas_3	**314.2**	**605.0**	**180.0**	**126.6**	**197.8**	**3503.4**	***821.2***	***1325.2***	**Seas_3**	**9.1**	**11.1**	**3.8**	**8.5**	**33.3**	***13.2***	***11.5***
Oct	108.9	198.6	61.9		66.3	1183.0	*323.8*	*483.5*	Oct	3.7		1.7	3.7	15.7	*6.2*	*6.4*
Nov	107.9	197.2	60.3		64.1	1144.9	*314.9*	*467.2*	Nov	4.2		1.8	3.9	17.9	*7.0*	*7.4*
Dec	114.6	196.0	61.4		64.3	1183.0	*323.9*	*483.4*	Dec	4.8		2.0	4.4	21.8	*8.2*	*9.1*
Seas_4	**331.4**	**591.8**	**183.7**	**125.2**	**194.7**	**3510.9**	***823.0***	***1327.4***	**Seas_4**	**12.7**	**20.0**	**5.4**	**12.0**	**55.4**	***21.1***	***19.9***
Annual	**1260.2**	**2448.6**	**682.5**	**513.0**	**787.9**	**13933.5**	***3270.9***	***5270.3***	**Annual**	**31.1**	**42.4**	**12.2**	**27.0**	**115.6**	***45.7***	***40.5***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

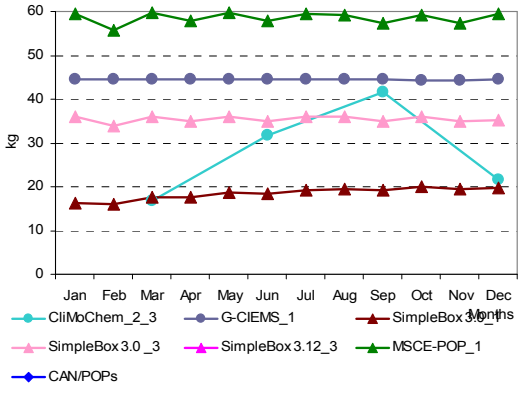
Table 3.32. *Calculation results: PCB-153 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	EVN-BETR_1[a]	G-CIEMS_1	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3				EVN-BETR_2[a]	G-CIEMS_2	CliMo Chem_2_2	MSCE-POP_2		
Jan	27437.1	423.7	105.0	420.5		*7096.6*	*13561.2*	Jan	31.3	0.7		0.7	*10.9*	*17.6*
Feb	10358.2	421.8	98.5	427.6		*2826.5*	*5023.5*	Feb	69.1	1.9		2.2	*24.4*	*38.7*
Mar	9260.7	419.1	105.7	482.2		*2566.9*	*4465.5*	Mar	113.3	2.9		3.9	*40.0*	*63.5*
Seas_1	**47056.0**	**1264.6**	**309.3**	**1330.2**	**263.8**	***10044.8***	***20696.1***	**Seas_1**	**213.6**	**5.5**	**7.7**	**6.8**	***58.4***	***103.5***
Apr	9079.4	416.2	102.7	577.6		*2544.0*	*4361.4*	Apr	181.0	3.7		5.3	*63.4*	*101.9*
May	10002.6	413.0	106.4	778.8		*2825.2*	*4792.8*	May	308.5	4.4		7.0	*106.6*	*174.9*
Jun	12957.7	409.8	102.9	1233.1		*3675.9*	*6206.3*	Jun	579.6	5.0		8.0	*197.5*	*330.9*
Seas_2	**32039.7**	**1239.0**	**312.0**	**2589.5**	**258.4**	***7287.7***	***13869.0***	**Seas_2**	**1069.1**	**13.1**	**14.7**	**20.4**	***279.3***	***526.6***
Jul	18155.0	406.6	106.3	2100.3		*5192.1*	*8686.4*	Jul	1110.3	5.6		9.6	*375.1*	*636.6*
Aug	22413.5	403.3	106.7	3122.7		*6511.5*	*10687.8*	Aug	1791.0	6.1		11.1	*602.7*	*1029.1*
Sep	19809.1	400.1	104.6	3323.1		*5909.2*	*9379.7*	Sep	2018.1	6.7		12.9	*679.2*	*1159.5*
Seas_3	**60377.5**	**1210.0**	**317.7**	**8546.0**	**253.2**	*14140.9*	*26078.2*	**Seas_3**	**4919.4**	**18.3**	**22.3**	**33.6**	*1248.4*	*2447.3*
Oct	11641.1	397.2	110.1	2376.8		*3631.3*	*5434.1*	Oct	1486.5	7.4		15.8	*503.2*	*851.5*
Nov	5211.2	394.5	109.1	1311.9		*1756.6*	*2359.5*	Nov	807.7	8.4		18.1	*278.1*	*458.7*
Dec	2417.7	391.9	115.9	735.2		*915.2*	*1033.2*	Dec	416.7	9.6		22.0	*149.4*	*231.5*
Seas_4	**19270.0**	**1183.6**	**335.1**	**4424.0**	**250.5**	***5092.6***	***8105.6***	**Seas_4**	**2710.8**	**25.4**	**40.1**	**56.0**	***708.1***	***1335.2***
Annual	**158743.2**	**4897.2**	**1274.0**	**16889.8**	**1026.0**	***36566.0***	***68603.8***	**Annual**	**8912.9**	**62.3**	**84.8**	**116.8**	***2294.2***	***4412.5***

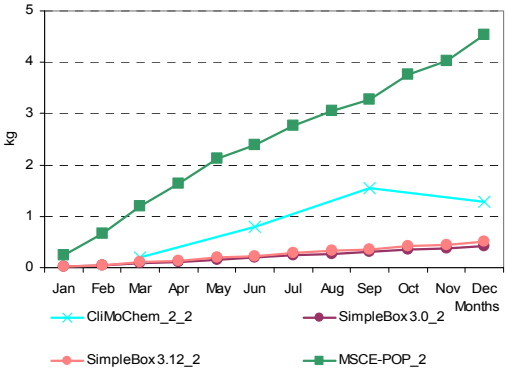
EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
a - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.

Own/alternative data set. Calculation results on PCB-153 mass degraded in 5cm layer of soil (kg) calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.33.

Monthly values of PCB-153 mass degraded in 5cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.42a and b, respectively.



a



b

Fig. 3.42a. *PCB-153 mass degraded in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

Fig. 3.42b. *PCB-153 mass degraded in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table 3.33. *Calculation results: PCB-153 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	MSCE-POP_1	G-CIEMS_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	281.5	59.6	44.4	16.2		36.1	230.8	*111.4*	*114.1*	Jan		0.0	0.0	0.2	*0.1*	*0.1*
Feb	261.3	55.8	44.5	15.9		33.8	208.2	*103.2*	*104.1*	Feb		0.0	0.1	0.7	*0.3*	*0.4*
Mar	276.7	59.7	44.6	17.6		36.1	230.2	*110.8*	*112.3*	Mar		0.1	0.1	1.2	*0.5*	*0.6*
Seas_1	**819.4**	**175.1**	**133.6**	**49.7**	**16.7**	**106.0**	**669.2**	***281.4***	***323.4***	**Seas_1**	0.2	**0.1**	**0.2**	**2.1**	***0.7***	***1.0***
Apr	265.2	57.9	44.6	17.6		34.9	226.0	*107.7*	*108.3*	Apr		0.1	0.1	1.6	*0.6*	*0.9*
May	270.7	59.8	44.6	18.6		36.1	229.7	*109.9*	*110.2*	May		0.2	0.2	2.1	*0.8*	*1.1*
Jun	258.6	57.8	44.5	18.3		34.9	222.0	*106.0*	*105.4*	Jun		0.2	0.2	2.4	*0.9*	*1.3*
Seas_2	**794.5**	**175.5**	**133.7**	**54.5**	**31.6**	**105.9**	**677.7**	***281.9***	***315.7***	**Seas_2**	0.8	**0.5**	**0.6**	**6.2**	***2.0***	***2.8***
Jul	263.8	59.5	44.5	19.2		36.1	229.1	*108.7*	*108.1*	Jul		0.2	0.3	2.8	*1.1*	*1.4*
Aug	260.9	59.3	44.4	19.5		36.1	228.3	*108.1*	*107.0*	Aug		0.3	0.3	3.0	*1.2*	*1.6*
Sep	250.1	57.3	44.4	19.1		34.9	221.2	*104.5*	*102.8*	Sep		0.3	0.4	3.3	*1.3*	*1.7*
Seas_3	**774.7**	**176.0**	**133.3**	**57.8**	**41.6**	**107.0**	**678.6**	***281.3***	***308.8***	**Seas_3**	1.6	**0.8**	**1.0**	**9.1**	***3.1***	***4.0***
Oct	256.5	59.2	44.4	19.9		36.1	228.3	*107.4*	*105.7*	Oct		0.3	0.4	3.8	*1.5*	*1.9*
Nov	246.6	57.4	44.4	19.4		34.9	220.7	*103.9*	*101.6*	Nov		0.4	0.4	4.0	*1.6*	*2.1*
Dec	253.4	59.4	44.4	19.7		35.1	227.8	*106.6*	*104.9*	Dec		0.4	0.5	4.5	*1.8*	*2.4*
Seas_4	**756.5**	**175.9**	**133.2**	**59.1**	**21.7**	**106.0**	**676.8**	***275.6***	***306.2***	**Seas_4**	1.3	**1.1**	**1.4**	**12.3**	***4.0***	***5.5***
Annual	**3145.1**	**702.5**	**533.8**	**221.1**	**111.5**	**424.9**	**2702.3**	***1120.2***	***1253.7***	**Annual**	**3.8**	**2.6**	**3.1**	**29.7**	***9.8***	***13.3***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Calculation results on PCB-153 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.34.

Table 3.34. *Calculation results: PCB-153 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on he basis of historica emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	CAN/POPs	G-CIEMS_1	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	MSCE-POP_2		
Jan	562.0	88.9	60.2		*237.0*	*281.8*	Jan		0.2		
Feb	520.9	89.1	56.4		*222.1*	*259.3*	Feb		0.7		
Mar	551.3	89.2	60.4		*233.6*	*275.5*	Mar		1.2		
Seas_1	**1634.3**	**267.1**	**177.0**	**33.3**	***527.9***	***743.8***	**Seas_1**	**0.4**	**2.1**	***1.3***	***1.2***
Apr	528.1	89.2	58.5		*225.3*	*262.7*	Apr		1.7		
May	539.4	89.1	60.5		*229.7*	*268.6*	May		2.1		
Jun	515.8	89.0	58.4		*221.1*	*255.7*	Jun		2.4		
Seas_2	**1583.3**	**267.3**	**177.4**	**63.2**	***522.8***	***711.9***	**Seas_2**	**1.6**	**6.2**	***3.9***	***3.3***
Jul	526.7	89.0	60.1		*225.3*	*261.5*	Jul		2.8		
Aug	520.9	88.9	59.9		*223.2*	*258.2*	Aug		3.1		
Sep	499.0	88.8	57.9		*215.2*	*246.2*	Sep		3.3		
Seas_3	**1546.6**	**266.7**	**178.0**	**83.1**	***518.6***	***689.5***	**Seas_3**	**3.1**	**9.2**	***6.1***	***4.3***
Oct	510.9	88.8	59.9		*219.8*	*252.4*	Oct		3.8		
Nov	490.1	88.8	58.0		*212.3*	*241.1*	Nov		4.1		
Dec	502.2	88.8	60.0		*217.0*	*247.4*	Dec		4.6		
Seas_4	**1503.2**	**266.4**	**177.9**	**43.4**	***497.7***	***676.6***	**Seas_4**	**2.5**	**12.5**	***7.5***	***7.0***
Annual	**6267.5**	**1067.6**	**710.2**	**223.1**	***2067.1***	***2821.6***	**Annual**	**7.7**	**30.0**	***18.8***	***15.8***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
a - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model on the basis of initial concentrations given as input data;
[b]– in CAN/POPs results the second layer of soil is applied as 5cm;

Monthly values of PCB-153 mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.43a and b, respectively.

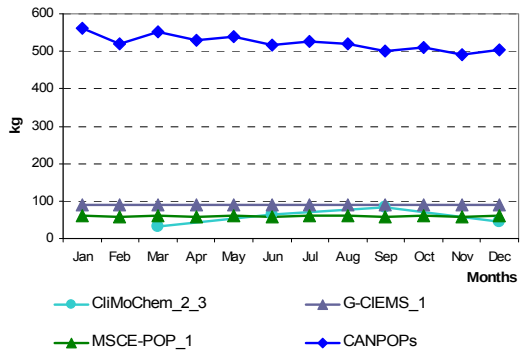


Fig.3.43a. *PCB-153 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

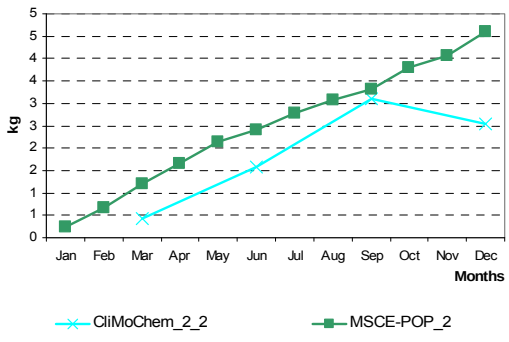


Fig.3.43b. *PCB-153 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-153 mass degraded in soil within 5 and 10 cm layers obtained with two different data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables 3.35-3.36.

Table 3.35. *The percentage difference between calculation results on PCB-153 mass degraded within 5 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-79%	-66%	-79%	-89%	-47%	-80%	-43%	-67%
Feb			-79%	-67%	-79%	-89%	-47%	-81%	-43%	-69%
Mar			-79%	-67%	-79%	-89%	-46%	-81%	-43%	-69%
Seas_1	**-95%**	**-87%**	**-79%**	**-67%**	**-79%**	**-89%**	**-47%**	**-81%**	**-43%**	**-69%**
Apr			-79%	-68%	-79%	-89%	-46%	-80%	-43%	-69%
May			-78%	-68%	-79%	-89%	-46%	-81%	-43%	-69%
Jun			-78%	-68%	-79%	-89%	-46%	-81%	-43%	-70%
Seas_2	**-89%**	**-76%**	**-78%**	**-68%**	**-79%**	**-89%**	**-46%**	**-81%**	**-43%**	**-69%**
Jul			-78%	-68%	-79%	-89%	-46%	-81%	-43%	-71%
Aug			-78%	-68%	-79%	-89%	-46%	-81%	-44%	-72%
Sep			-78%	-68%	-79%	-89%	-46%	-81%	-45%	-74%
Seas_3	**-86%**	**-67%**	**-78%**	**-68%**	**-79%**	**-89%**	**-46%**	**-81%**	**-44%**	**-73%**
Oct			-78%	-68%	-79%	-89%	-46%	-81%	-46%	-76%
Nov			-77%	-68%	-79%	-89%	-46%	-81%	-47%	-78%
Dec			-77%	-68%	-79%	-89%	-45%	-81%	-48%	-79%
Seas_4	**-94%**	**-83%**	**-77%**	**-68%**	**-79%**	**-89%**	**-46%**	**-81%**	**-47%**	**-78%**
Annual	**-91%**	**-78%**	**-78%**	**-68%**	**-79%**	**-89%**	**-46%**	**-81%**	**-44%**	**-74%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Table 3.36. *The percentage difference between calculation results on PCB-153 mass degraded within 10 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	MSCE-POP_1	MSCE-POP_2
Jan			-79%	-43%	-67%
Feb			-79%	-43%	-69%
Mar			-79%	-43%	-69%
Seas_1	-95%	-87%	-79%	-43%	-69%
Apr			-79%	-43%	-69%
May			-78%	-43%	-69%
Jun			-78%	-43%	-70%
Seas_2	-89%	-76%	-78%	-43%	-69%
Jul			-78%	-43%	-71%
Aug			-78%	-44%	-72%
Sep			-78%	-45%	-74%
Seas_3	-86%	-67%	-78%	-44%	-73%
Oct			-78%	-46%	-76%
Nov			-77%	-47%	-78%
Dec			-77%	-48%	-79%
Seas_4	-94%	-83%	-77%	-47%	-78%
Annual	-91%	-78%	-78%	-44%	-74%

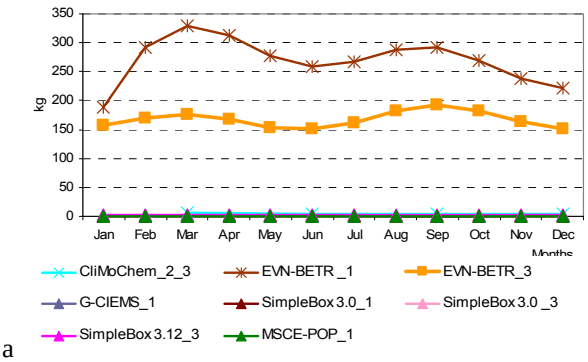
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

3.2.3. Comparison of calculated values of PCB-153 mass degraded in water

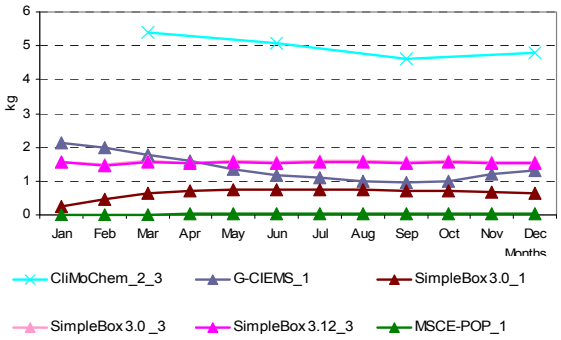
According to the programme of Stage II model results of computational experiments on mass balance include masses of PCB-153 degraded in sea within a layer of 200 m depth.

Reference data set. Calculation results on PCB-153 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.37.

Monthly values of PCB-153 mass degraded in 200 m layer of water calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.44a and b, respectively. Seasonal variations of low values of mass degraded in 200 m layer of water calculated by the participating models on the basis of "reference" data set and zero initial conditions are also shown in Fig. 3.44c in more detail.



a



b

Fig. 3.44a. *PCB-153 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. 3.44b. *PCB-153 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

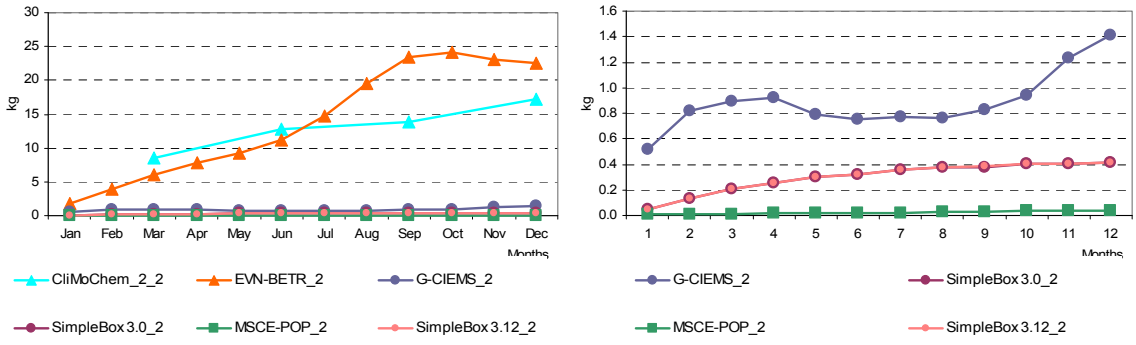


Fig. 3.44c. *PCB-153 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions (models with low values)*

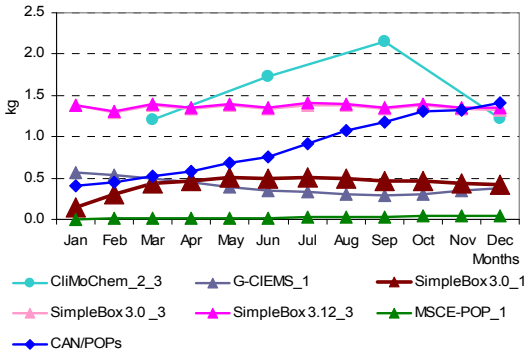
Table 3.37. *Calculation results: PCB-153 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	EVN-BETR_1[a]	G-CIEMS_1	SimpleBox 3.0_1[b]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	187.50	2.12	0.26	0.01	157.79		1.57	1.56	*50.12*	*84.15*	Jan	1.82	0.52		0.05	0.05	0.01	*0.49*	*0.77*
Feb	291.36	1.98	0.48	0.01	169.45		1.48	1.46	*66.60*	*117.30*	Feb	3.92	0.82		0.13	0.13	0.01	*1.00*	*1.66*
Mar	328.72	1.77	0.65	0.01	175.30		1.59	1.56	*72.80*	*130.19*	Mar	6.07	0.89		0.21	0.21	0.01	*1.48*	*2.59*
Seas_1	**807.58**	**5.87**	**1.38**	**0.03**	**502.55**	**5.39**	**4.64**	**4.59**	***166.50***	***312.38***	**Seas_1**	**11.80**	**2.23**	**8.53**	**0.39**	**0.39**	**0.03**	***3.89***	***5.03***
Apr	311.71	1.61	0.70	0.02	166.92		1.54	1.51	*69.14*	*123.54*	Apr	7.74	0.92		0.25	0.25	0.02	*1.84*	*3.32*
May	277.49	1.34	0.75	0.02	153.72		1.60	1.56	*62.35*	*110.62*	May	9.15	0.79		0.30	0.30	0.02	*2.11*	*3.94*
Jun	259.90	1.18	0.73	0.03	150.40		1.55	1.51	*59.33*	*104.51*	Jun	11.21	0.76		0.32	0.32	0.02	*2.53*	*4.86*
Seas_2	**849.09**	**4.13**	**2.18**	**0.07**	**471.03**	**5.07**	**4.69**	**4.59**	***167.60***	***320.31***	**Seas_2**	**28.10**	**2.47**	**12.72**	**0.88**	**0.88**	**0.06**	***7.52***	***11.14***
Jul	267.85	1.09	0.75	0.03	162.20		1.60	1.56	*62.15*	*108.80*	Jul	14.77	0.77		0.36	0.36	0.02	*3.26*	*6.44*
Aug	287.40	1.00	0.73	0.03	181.77		1.60	1.56	*67.73*	*117.99*	Aug	19.55	0.76		0.38	0.38	0.02	*4.22*	*8.58*
Sep	292.12	0.97	0.70	0.03	191.98		1.55	1.51	*69.84*	*121.15*	Sep	23.38	0.83		0.38	0.38	0.03	*5.00*	*10.28*
Seas_3	**847.37**	**3.06**	**2.18**	**0.09**	**535.96**	**4.62**	**4.75**	**4.64**	***175.33***	***329.38***	**Seas_3**	**57.70**	**2.36**	**13.86**	**1.12**	**1.12**	**0.08**	***12.71***	***22.63***
Oct	269.82	1.00	0.70	0.04	182.31		1.60	1.56	*65.29*	*112.70*	Oct	24.23	0.94		0.41	0.41	0.04	*5.20*	*10.64*
Nov	238.21	1.20	0.67	0.05	162.85		1.55	1.51	*58.01*	*99.77*	Nov	23.08	1.23		0.41	0.41	0.04	*5.03*	*10.10*
Dec	220.90	1.31	0.65	0.05	150.50		1.55	1.51	*53.78*	*92.38*	Dec	22.48	1.41		0.42	0.42	0.04	*4.95*	*9.81*
Seas_4	**728.93**	**3.50**	**2.02**	**0.14**	**495.67**	**4.81**	**4.70**	**4.59**	***155.55***	***288.73***	**Seas_4**	**69.78**	**3.59**	**17.26**	**1.23**	**1.23**	**0.12**	***15.53***	***27.33***
Annual	**3232.97**	**16.56**	**7.76**	**0.33**	**2005.20**	**19.88**	**18.77**	**18.40**	***664.98***	***1249.96***	**Annual**	**167.39**	**10.65**	**52.36**	**3.61**	**3.61**	**0.28**	***39.65***	***65.52***

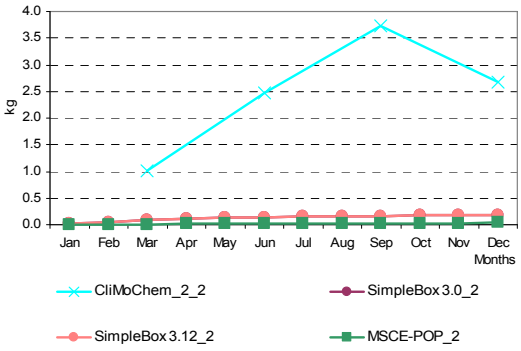
EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
b - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-153 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.38.

Monthly values of PCB-153 mass degraded in 200 m layer of water calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.45a and b, respectively.



a



b

Fig. 3.45a. *PCB-153 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

Fig. 3.45b. *PCB-153 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table 3.38. *Calculation results: PCB-153 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	0.41	0.56	0.15	0.004		1.38	1.38	*0.65*	*0.60*	Jan		0.02	0.02	0.003	*0.01*	*0.01*
Feb	0.44	0.53	0.31	0.007		1.30	1.30	*0.65*	*0.53*	Feb		0.05	0.05	0.006	*0.04*	*0.03*
Mar	0.53	0.49	0.43	0.009		1.39	1.40	*0.71*	*0.56*	Mar		0.09	0.09	0.008	*0.06*	*0.04*
Seas_1	**1.39**	**1.58**	**0.88**	**0.021**	**1.21**	**4.06**	**4.08**	***1.89***	***1.57***	**Seas_1**	**1.00**	**0.16**	**0.16**	**0.017**	***0.33***	***0.45***
Apr	0.58	0.46	0.47	0.014		1.34	1.35	*0.70*	*0.54*	Apr		0.11	0.11	0.012	*0.07*	*0.05*
May	0.68	0.39	0.51	0.019		1.39	1.40	*0.73*	*0.56*	May		0.13	0.13	0.016	*0.09*	*0.06*
Jun	0.76	0.35	0.50	0.021		1.34	1.36	*0.72*	*0.54*	Jun		0.14	0.14	0.017	*0.10*	*0.07*
Seas_2	**2.01**	**1.20**	**1.47**	**0.054**	**1.73**	**4.07**	**4.11**	***2.09***	***1.50***	**Seas_2**	**2.47**	**0.37**	**0.37**	**0.044**	***0.82***	***1.12***
Jul	0.92	0.33	0.51	0.024		1.38	1.40	*0.76*	*0.57*	Jul		0.15	0.15	0.019	*0.11*	*0.08*
Aug	1.07	0.30	0.49	0.026		1.38	1.40	*0.78*	*0.59*	Aug		0.16	0.16	0.020	*0.12*	*0.08*
Sep	1.18	0.29	0.46	0.028		1.33	1.36	*0.78*	*0.58*	Sep		0.17	0.17	0.023	*0.12*	*0.08*
Seas_3	**3.17**	**0.92**	**1.46**	**0.078**	**2.16**	**4.10**	**4.16**	***2.29***	***1.58***	**Seas_3**	**3.73**	**0.49**	**0.49**	**0.062**	***1.19***	***1.70***
Oct	1.31	0.30	0.46	0.038		1.38	1.40	*0.82*	*0.62*	Oct		0.18	0.18	0.030	*0.13*	*0.09*
Nov	1.32	0.35	0.43	0.041		1.33	1.35	*0.81*	*0.60*	Nov		0.18	0.18	0.032	*0.13*	*0.09*
Dec	1.41	0.38	0.42	0.046		1.33	1.35	*0.82*	*0.61*	Dec		0.19	0.19	0.037	*0.14*	*0.09*
Seas_4	**4.05**	**1.04**	**1.31**	**0.125**	**1.22**	**4.04**	**4.11**	***2.27***	***1.72***	**Seas_4**	**2.68**	**0.55**	**0.55**	**0.099**	***0.97***	***1.16***
Annual	**10.61**	**4.74**	**5.12**	**0.278**	**6.31**	**16.26**	**16.47**	***8.54***	***6.14***	**Annual**	**9.89**	**1.56**	**1.56**	**0.223**	***3.31***	***4.43***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.39.

Table 3.39. *The percentage difference between calculation results on PCB-153 mass degraded in 200 m layer of water obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	Simple Box 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-74%	-42%	-61%	-61%	-12%	-11%	-41%	-44%
Feb			-73%	-36%	-60%	-60%	-12%	-11%	-35%	-37%
Mar			-72%	-34%	-59%	-59%	-13%	-11%	-29%	-32%
Seas_1	-88%	-78%	-73%	-36%	-60%	-60%	-12%	-11%	-34%	-37%
Apr			-72%	-33%	-58%	-58%	-13%	-10%	-26%	-28%
May			-71%	-32%	-58%	-58%	-13%	-10%	-18%	-21%
Jun			-70%	-32%	-57%	-57%	-13%	-10%	-16%	-19%
Seas_2	-81%	-66%	-71%	-32%	-58%	-58%	-13%	-10%	-19%	-22%
Jul			-70%	-32%	-57%	-57%	-14%	-10%	-15%	-18%
Aug			-70%	-33%	-56%	-56%	-14%	-10%	-14%	-18%
Sep			-70%	-34%	-56%	-56%	-14%	-10%	-14%	-18%
Seas_3	-73%	-53%	-70%	-33%	-56%	-56%	-14%	-10%	-14%	-18%
Oct			-70%	-34%	-56%	-56%	-14%	-10%	-13%	-16%
Nov			-70%	-35%	-56%	-56%	-14%	-10%	-12%	-16%
Dec			-71%	-36%	-55%	-55%	-14%	-11%	-9%	-12%
Seas_4	-84%	-75%	-70%	-35%	-56%	-56%	-14%	-10%	-11%	-15%
Annual	-81%	-68%	-71%	-34%	-57%	-57%	-13%	-10%	-16%	-19%

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.2.4. Comparison of calculated values of PCB-153 mass degraded in vegetation

Reference data set. Calculation results on PCB-153 mass degraded in vegetation (kg) calculated by models on the basis of "reference" data set are presented in Table 3.40.

Monthly values of PCB-153 mass degraded in vegetation calculated by the participating models on the basis of "reference" data set are compared in Fig. 3.46.

Table 3.40. *Calculation results: PCB-153 mass degraded in vegetation (kg) calculated by models on the basis of "reference" data set*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	Results obtained on the basis of zero initial concentrations	
	G-CIEMS_1	CliMoChem_2_3	G-CIEMS_2	CliMoChem_2_2
Jan	27.8		0.3	
Feb	15.4		0.3	
Mar	13.8		0.4	
Seas_1	**57.0**	**0.0**	**0.9**	**0.0**
Apr	13.7		0.4	
May	10.0		0.3	
Jun	10.6		0.3	
Seas_2	**34.3**	**0.0**	**1.0**	**0.0**
Jul	10.4		0.3	
Aug	9.3		0.3	
Sep	11.0		0.4	
Seas_3	**30.7**	**0.0**	**1.0**	**0.0**
Oct	11.9		0.4	
Nov	14.4		0.5	
Dec	13.1		0.5	
Seas_4	**39.4**	**0.0**	**1.3**	**0.0**
Annual	**161.4**	0.0	**4.3**	0.0

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
* - In MSCE-POP model degradation in vegetation is not taken into account.

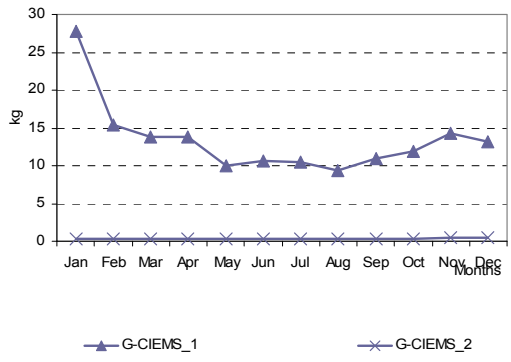


Fig. 3.46. *PCB-153 mass degraded in vegetation (kg) calculated by the participating models on the basis of "reference" data set)*

Own/alternative data set. Calculation results on PCB-153 mass degraded in vegetation (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.41.

Table 3.41. *Calculation results: PCB-153 mass degraded in vegetation (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations
	G-CIEMS_1	CliMoChem_2_3				CliMoChem_2_2
Jan	21.8				Jan	
Feb	11.7				Feb	
Mar	10.6				Mar	
Seas_1	**44.1**	17.1	***30.6***	***13.5***	**Seas_1**	32.4
Apr	10.5				Apr	
May	7.3				May	
Jun	7.7				Jun	
Seas_2	**25.5**	42.6	***34.1***	***8.6***	**Seas_2**	179.1
Jul	7.5				Jul	
Aug	6.7				Aug	
Sep	7.9				Sep	
Seas_3	**22.1**	70.1	***46.1***	***24.0***	**Seas_3**	322.6
Oct	8.7				Oct	
Nov	10.9				Nov	
Dec	10.3				Dec	
Seas_4	**29.9**	40.4	***35.2***	***5.3***	**Seas_4**	186.4
Annual	**121.5**	170.3	***145.9***	***24.4***	**Annual**	720.5

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
* - In MSCE-POP model degradation in vegetation is not taken into account.

Monthly values of PCB-153 mass degraded in vegetation calculated by the participating models on the basis of "own or alternative" data sets are compared in Fig. 3.47.

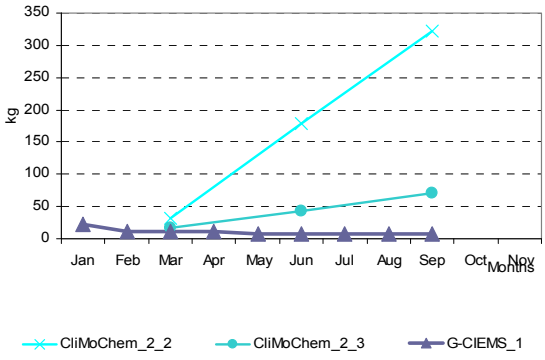


Fig. 3.47. *PCB-153 mass degraded in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained by G-CIEMS model with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.42.

Table 3.42. *The percentage difference between calculation results on PCB-153 mass degraded in vegetation obtained by G-CIEMS models on the basis of two data sets: "own or alternative" and "reference"*

Month	G-CIEMS_1
Jan	-21.7%
Feb	-24.3%
Mar	-22.9%
Seas_1	-22.7%
Apr	-23.7%
May	-26.7%
Jun	-27.7%
Seas_2	-25.8%
Jul	-27.5%
Aug	-27.9%
Sep	-28.5%
Seas_3	-28.0%
Oct	-27.2%
Nov	-23.8%
Dec	-21.7%
Seas_4	-24.1%
Annual	-24.7%

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;

3.2.5. Comparison of distribution of PCB-153 mass degraded in the environment

Sections from 3.2.1 to 3.2.4 above are devoted to the comparison between the results of participating models on PCB-153 mass degraded in the main environmental compartments (atmosphere, soil, water and vegetation). The comparison includes results of one-year calculations made on the basis of initial conditions (CAN/POPs, EVN-BETR and UK-MODEL, G-CIEMS, MSCE-POP, SimpleBox) and zero initial concentrations (CliMoChem, EVN-BETR and UK-MODEL, G-CIEMS, MSCE-POP and SimpleBox) along with results of long-term calculations performed with historical emissions (CliMoChem, EVN-BETR and UK-MODEL and SimpleBox). Calculation results obtained with the use of two different physical-chemical data sets are submitted by CliMoChem, G-CIEMS, MSCE-POP and SimpleBox models.

A preliminary analysis of the main results on comparison of absolute and relative values of PCB-153 mass degraded in the main environmental compartments is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions and for results based on zero-initial conditions.

Atmosphere. In the results obtained by the participating models on the basis of "***reference"*** data set and non-zero initial conditions the scattering of absolute values on PCB-153 mass degraded in 1 km layer of the atmosphere is higher than that in results based on zero initial conditions as well as than difference in the results for 5 and 10 km atmospheric layers (Tables 3.22 – 3.24 given in Section 3.2.1). Square deviation σ of annual values of degraded mass presented by different participating models for 5 and 10 km layers do not exceed the averaged value.

Comparison of annual values of PCB-153 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "reference" data set is presented in Fig.3.48a. Fig. 3.48b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

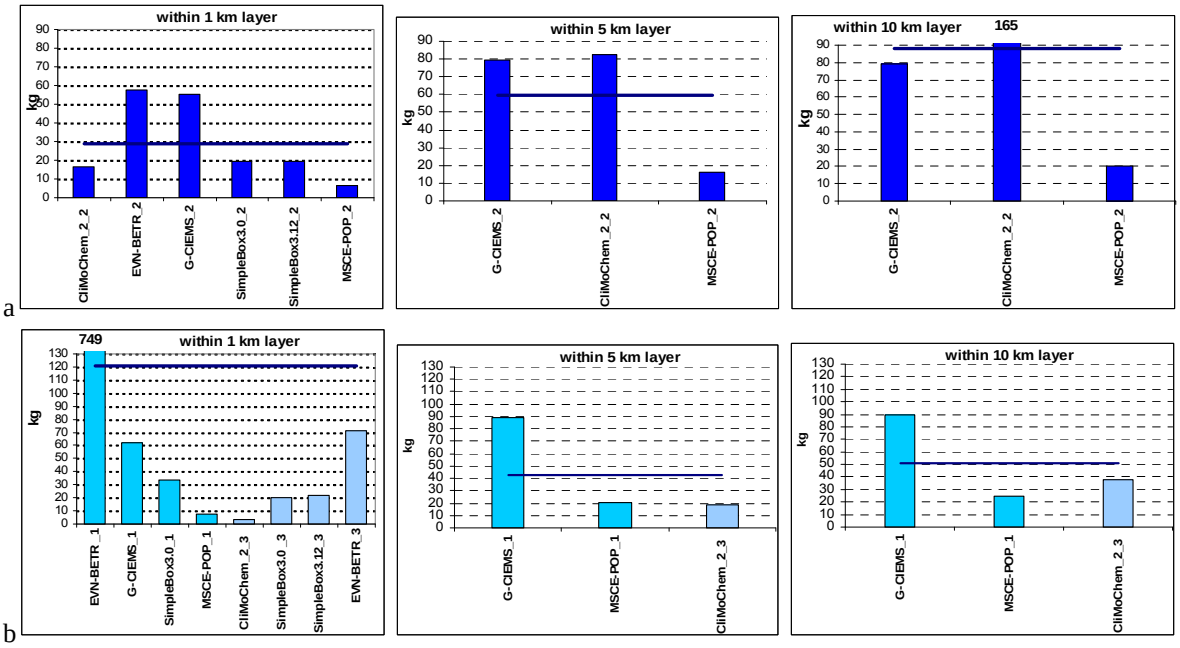


Fig.3.48. *Comparison of annual values of PCB-153 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The difference in absolute values on PCB-153 mass degraded in the atmosphere obtained by the models on the basis of "reference" data set and zero initial conditions is within a factor of nine for 1 km layer, - within a factor of five for 5 km layer, and – within a factor of eight for 10 km layer (see Fig. 3.48a). The difference between the maximum and minimum annual values of PCB-153 mass degraded within 1 km atmospheric layer, which are obtained on the basis of non-zero initial conditions, reaches more than two orders of magnitude (see Fig. 3.48b). For 5 and 10 km layers, the maximum annual values exceed the minimum ones 5 and 4 times, respectively. Comparison of profiles of annual values of PCB-153 degraded mass calculated by three models (G-CIEMS, CliMoChem and MSCE-POP) for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set is presented in Fig.3.49.

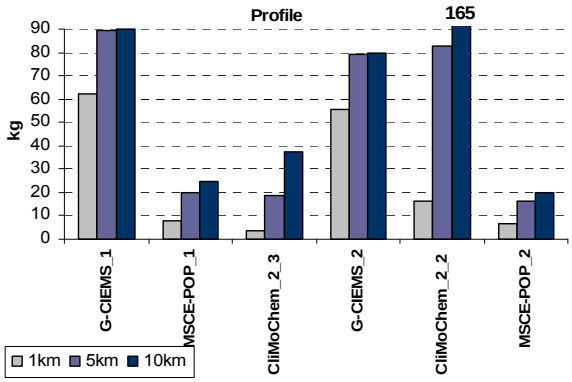


Fig. 3.49. *Comparison of profiles of annual values of PCB-153 degraded mass calculated by four models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference data set»*

Results on PCB-153 mass degraded in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions and with the use of "***own or alternative"*** data set (Tables 3.25 – 3.27 given in Section 3.2.1) demonstrate reasonable agreement between all model calculations for each considered layer. For annual and most monthly values of PCB-153 mass degraded in each of these layers, square deviation do not exceed the averaged value.

Comparison of annual values of PCB-153 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig.3.50a. Fig. 3.50b shows the same results but obtained on

the basis of given initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

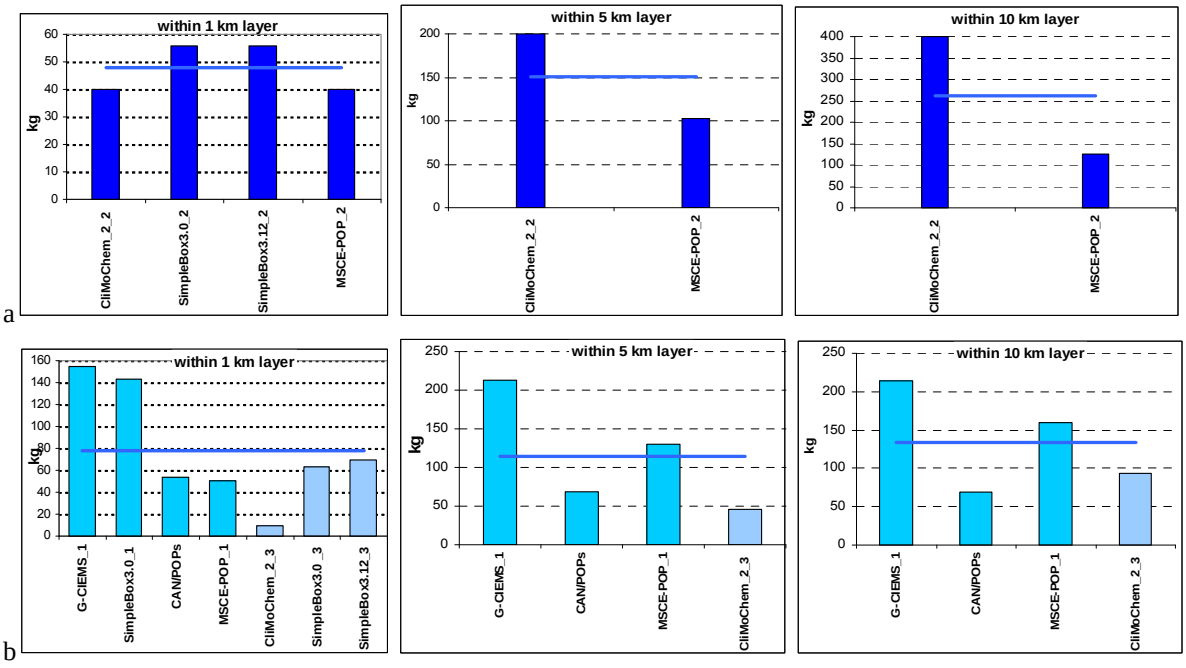


Fig. 3.50. *Comparison of annual values of PCB-153 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

According to the results obtained on the basis of zero initial conditions (see Fig. 3.50a), the maximum and minimum absolute values of PCB-153 masses degraded in the atmosphere differ between each other 1.4 times for 1 km layer, 2 times for 5 km layer, and 3 times for 10 km layer. The highest absolute value of PCB mass degraded in 1 km atmospheric layer obtained on the basis of non-zero initial conditions exceed the lowest value approximately 17 times (see Fig. 3.50b). The scattering of values obtained for 5 and 10 km layers is within a factor of 5 and 3, respectively. Comparison of profiles of annual values of PCB-153 degraded mass calculated by four models (G-CIEMS, CAN/POPs, CliMoChem and MSCE-POP) for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative" data sets is presented in Fig.3.51.

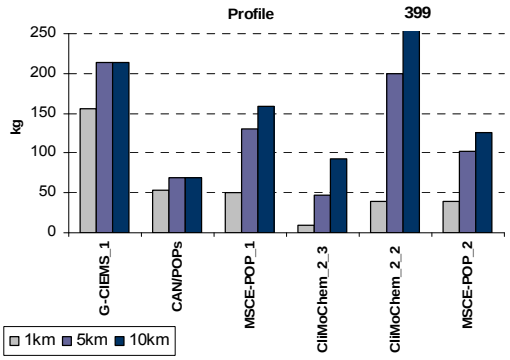


Fig. 3.51. *Comparison of profiles of annual values of PCB-153 degraded mass calculated by five models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative data sets"*

For the results obtained on the basis of both physical-chemical data sets, it is obvious that absolute values of PCB-153 mass degraded in the considered layers of the atmosphere presented by CAN/POPs, CliMoChem and MSCE-POP models show seasonal variations with some increase in summer time (see Figs. 3.34 – 3.36 and 3.37-3.39 given in Section 3.2.1). This increase is especially noticeable in results obtained on the basis of "own" data sets. It can be explained that in these models degradation processes in the atmosphere as gas-phase reaction of the pollutant with hydroxyl radicals

is described using temperature dependent second order rate constant [*Shatalov et al*., 2004]. Decrease in PCB degraded mass within the year is observed in results obtained by EVN-BETR and UK-MODEL and SimpleBox 3.0 models on the basis of initial concentrations given as input data (Fig. 3.34a,c and 3.37a).

Comparison of annual values of PCB-153 mass degraded in the considered different layers of the atmosphere obtained with “reference” and “own/alternative” data sets is presented in Fig. 3.52.

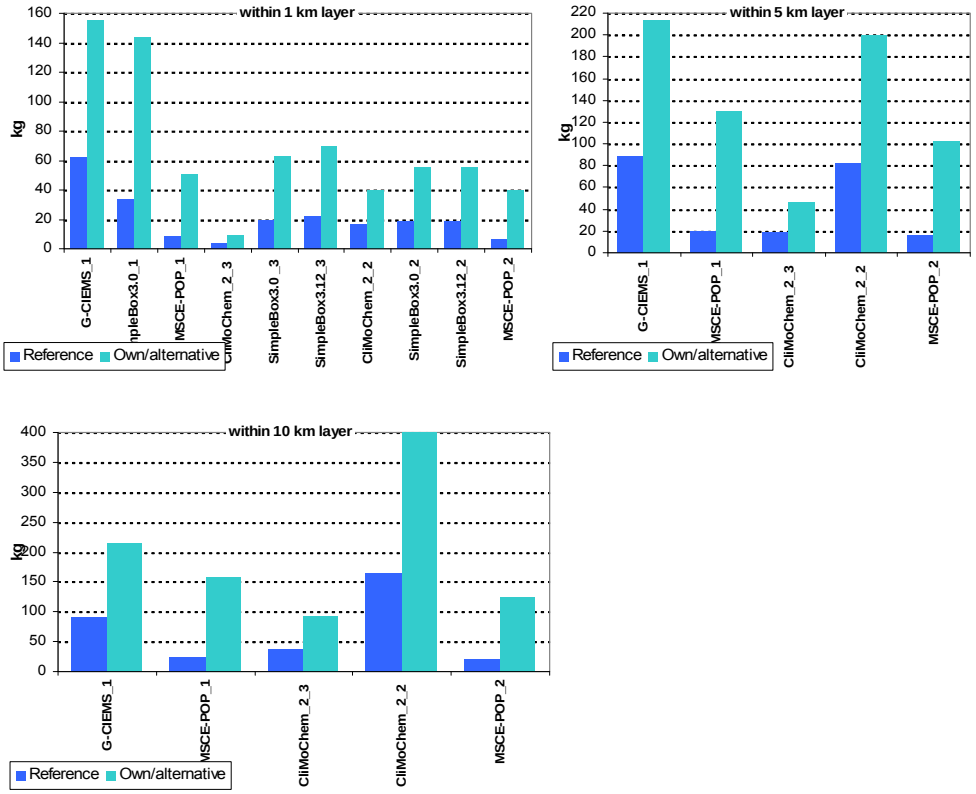


Fig.3.52. *Comparison of PCB-153 mass degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of two data set*

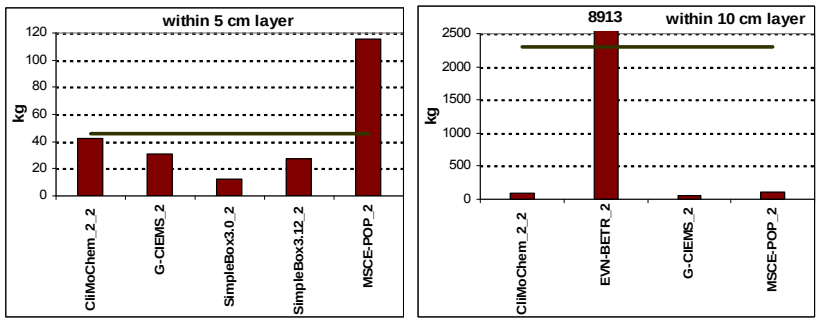
For the participating models, the annual values of calculation results on PCB-153 masses degraded in the atmosphere obtained with the use of “own or alternative” data sets noticeably exceed those obtained with “reference” data set. According to the data presented in Tables 3.28-3.30 (see Section 3.2.1), percentage difference between results obtained with two data sets of physical-chemical properties varies from 142 to 545%. The largest difference in the results obtained with two data sets is characteristic of MSCE-POP results calculated on the basis of initial concentrations given as input data.

Soil. There is a considerable difference in calculated values of PCB-153 mass degraded in 5 and 10 cm soil layers obtained on the basis of “***reference”*** data set (Tables 3.31 and 3.32, Section 3.2.2). Only in the results based on zero initial conditions for 5 cm layer, the square deviation presented for annual value does not exceed the mean value averaged between the different models.

Comparison of annual values of PCB-153 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of “reference” data set is presented in Fig.3.53a. Fig. 3.53b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the

different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

a



b

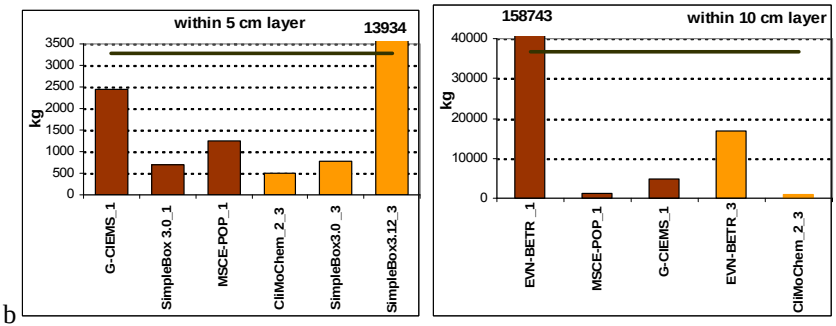


Fig. 3.53. *Comparison of annual values of PCB-153 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Results of most models performed calculations on the basis of zero initial concentrations are characterized by relatively low values of mass degraded in soil (see Fig. 3.53a). Results with higher values of PCB-153 mass degraded in soil are obtained by the models, which used initial concentrations and/or historical emissions (see Fig. 3.53b). For both types of calculations the maximum values of PCB-153 mass degraded in 5 cm soil layer are characteristic of MSCE-POP (zero initial conditions) and of SimpleBox 3.12 (historical emissions) models. For 10 cm layer EVN-BETR and UK-MODEL provided the maximum annual values of PCB-153 degraded mass.

A comparison of profiles of annual values of PCB-153 degraded mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set is presented in Fig.3.54.

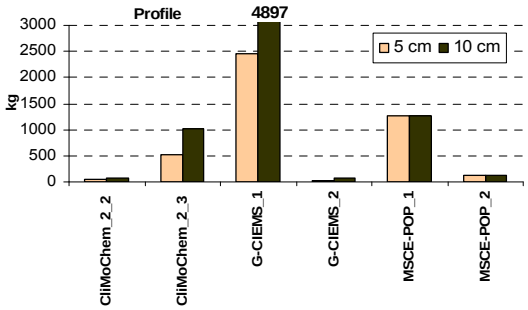


Fig. 3.54. *Comparison of profiles of annual values of PCB-153 degraded mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "reference data set"*

In compliance with the results of CliMoChem and G-CIEMS on soil content profile, values of PCB-153 mass degraded within 10 cm layer is approximately two times higher than that degraded within 5 cm layer. For MSCE-POP model results, values of mass degraded in both layers are equal to each other.

According to the calculation results on PCB-153 mass degraded in 5 cm layers of soil calculated by models on the basis of zero and non-zero initial conditions and with the use of "***own or alternative"***

data sets (Table 3.33 given in Section 3.1.2), square deviation σ between different model results for each of these layers exceed the averaged value. The same can be noted for the results obtained by the models for 10 cm layer with the use of non-zero initial conditions. At that, square deviation of the absolute values of PCB-153 mass degraded in 10 cm layers of soil calculated on the basis of zero initial conditions is less than the averaged value (see Table 3.34 given in Section 3.1.2). Comparison of annual values of PCB-153 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig.3.55a. Fig. 3.55b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

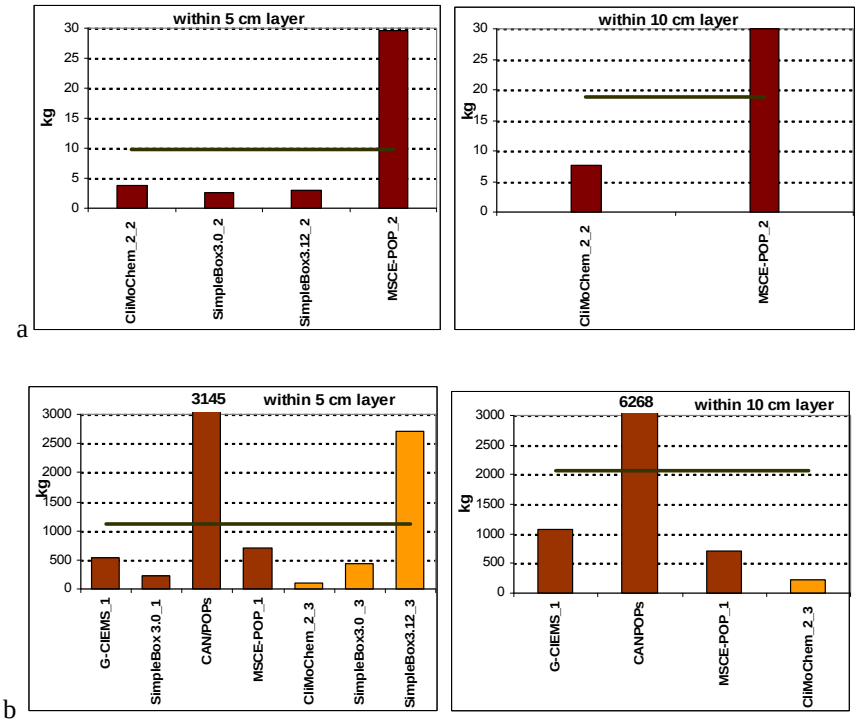


Fig. 3.55. *Comparison of annual values of PCB-153 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The highest results for 5 and 10 cm soil layers obtained using zero initial conditions (see Fig. 3.55a) are characteristic of MSCE-POP model. According to the results presented in Fig. 3.55b, the maximum values of PCB-153 mass degraded in 5 and 10 cm soil layers are characteristic of CAN/POPs results calculated on the basis of initial concentrations given as input data.

Comparison of profiles of annual values of PCB-153 degraded mass calculated by the participating models for

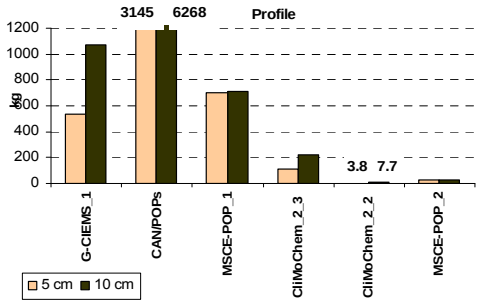


Fig. 3.56. *Comparison of profiles of annual values of PCB-153 degraded mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative data sets"*

the considered soil layers (5 and 10 cm) on the basis of “own or alternative” data sets is presented in Fig.3.56.

According to the results of CAN/POPs, CliMoChem and G-CIEMS obtained on the basis of “own or alternative” data set, values of PCB-153 mass degraded within 10 cm layer exceed those for 5 cm layer about two times. MSCE-POP model presented approximately equal values of mass degraded in both layers.

Seasonal variations in absolute values of PCB-153 mass degraded in soil within 5 and 10 cm layers (see Figs. 3.40 – 3.43 given in Section 3.2.2) are observed in results of CliMoChem model obtained on the basis of their own physical-chemical data set and EVN-BETR and UK-MODEL results based on “reference” data set.

Comparison of annual values of PCB-153 mass degraded in the considered different layers of soil obtained with “reference” and “own/alternative” data sets is presented in Fig. 3.57.

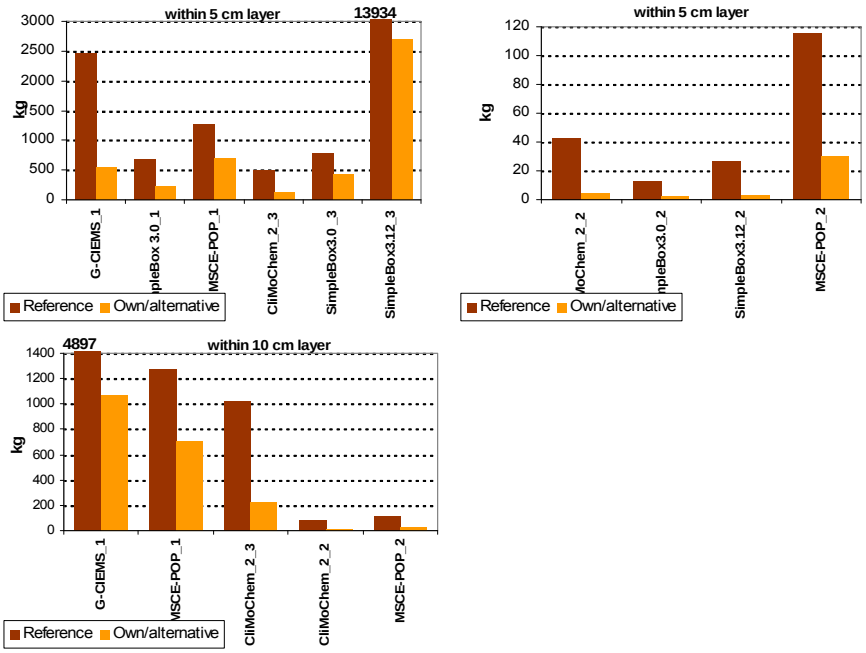


Fig.3.57. *Comparison of PCB-153 mass degraded within 5 and 10 cm soil layers calculated by different models on the basis of two data set*

For all models’ results, the values of PCB-153 masses degraded in soil obtained with the use of “own or alternative” data sets are less than those obtained with “reference” data set. The largest difference in the results obtained with two data sets exceeding 90% is characteristic of CliMoChem results calculated using zero initial conditions. According to the data on percentage difference between calculation results on PCB-153 mass degraded in soil (Tables 3.35 and 3.36 Section 3.2.2), the difference in other models’ results varies from 44 to 89%.

Water. Most models provide relatively close annual and monthly values of PCB-153 masses degraded in water layer of 200 m calculated on the basis of non-zero initial conditions and “own/alternative” physical-chemical data sets (see Tables 3.37 and 3.38 given in Section 3.2.3). In all other cases, square deviation of annual values between different model results considerably exceeds the mean values.

Comparison of annual values of PCB-153 masses degraded in water layer of 200 m calculated by different models on the basis of zero initial concentrations and with the use of "***reference"*** data set is presented in Fig.3.58a. Fig. 3.58b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plot shows the value of the corresponding parameter averaged between models.

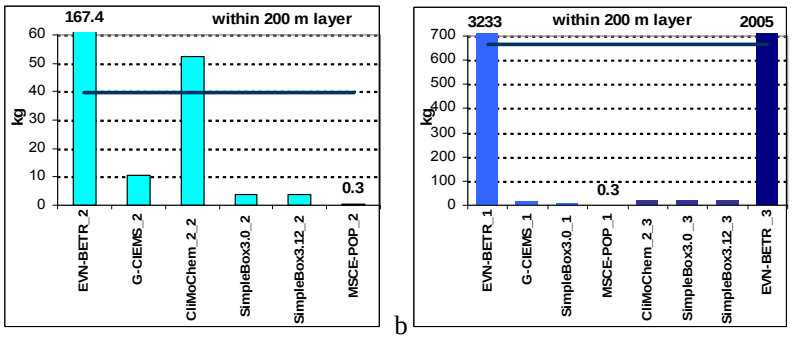


Fig. 3.58. *Comparison of annual values of PCB-153 masses degraded in water within 200 m layer calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

According to the results based on zero initial conditions (see Fig. 3.58a), the maximum absolute value of PCB-153 mass degraded in water layer of 200 m calculated by EVN-BETR and UK-MODEL considerably exceed the minimum one obtained by MSCE-POP model (more than 600 times). In the results calculated on the basis of initial conditions or historical emissions (see Fig. 3.58b), the maximum calculated value is characteristic of EVN-BETR and UK-MODEL results based on given initial concentrations. At that the minimum value of PCB-153 mass degraded in water is also obtained by MSCE-POP model.

Comparison of annual values of PCB-153 mass degraded in water layer of 200 m calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative"*** data sets is presented in Fig.3.59a (blue line corresponds to the averaged value). Fig. 3.59b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

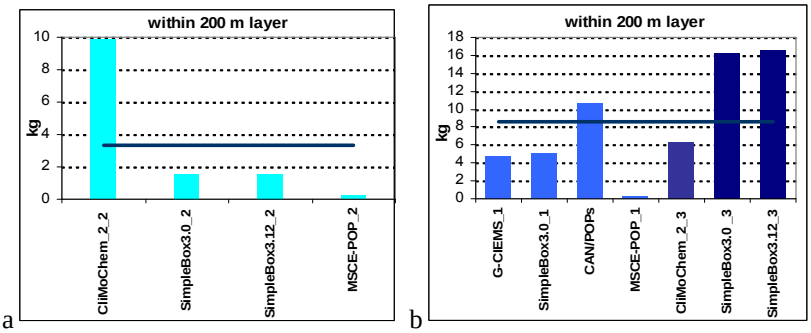


Fig. 3.59. *Comparison of annual values of PCB-153 masses degraded in water within 200 m layer calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

For all models performed calculations on both zero and non-zero initial conditions, the results obtained on the basis of initial conditions or historical emissions exceed those calculated with zero initial concentrations (except for CliMoChem). In MSCE-POP results both calculated values are equally small in comparison with other models' results. The maximum values in results obtained on the basis of zero and non-zero initial conditions are characteristic of CliMOChem and SimpleBox 3.12 models, respectively.

According to the data presented (see Figs. 3.44a,b and 3.45a,b Section 3.2.3), some seasonal variations of PCB-153 mass degraded in water layer of 200 m are observed in and CliMoChem, EVN-BETR and UK-MODEL and G-CIEMS results. Increasing trend of water content is characteristic of CAN/POPs results. There are no any considerable seasonal variations in results of SimpleBox 3.0 and 3.12 calculated with historical emissions.

Annual values of PCB-153 mass degraded in the 200m layer of water obtained by the participating models on the basis of "reference" and "own/alternative" data sets are compared in Fig. 3.60.

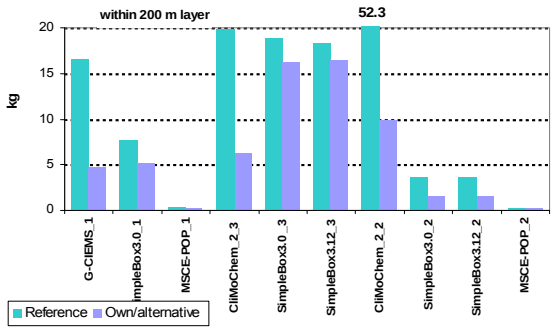


Fig. 3.60. *Comparison of PCB-153 mass degraded within 200 m water layer calculated by different models on the basis of two data sets*

For all models' results, the values of PCB-153 masses degraded in water obtained with the use of "own or alternative" data sets are less than those obtained with "reference" data set (see also Table 3.39 given in Section 3.2.3). The percentage difference between results of both calculations varies from 10 to 81%.

Vegetation. The difference between results on PCB-153 masses degraded in vegetation obtained on the basis of "reference" and "own or alternative" data set is considerable (see Tables 3.40 and 3.41, Section 3.2.4). Annual values of PCB-153 mass degraded in vegetation obtained by the participating models on the basis of "reference" and "own/alternative" data sets are shown in Fig. 3.61.

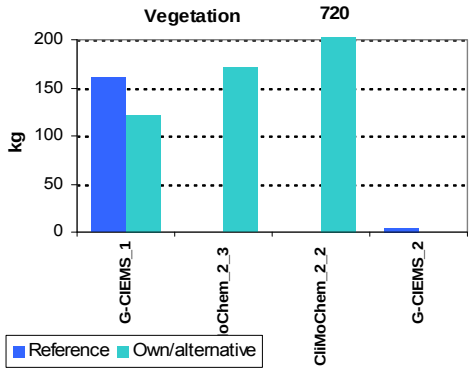


Fig.3.61. *Comparison of PCB-153 mass degraded in vegetation calculated by different models on the basis of two data sets*

The values of PCB-153 mass degraded in vegetation obtained by G-CIEMS model with the use of "own or alternative" data sets on the basis of initial concentrations given as input data are smaller than those obtained by this model with "reference" data set. The difference in the results obtained with two data sets is equal to 25% (see Table 3.42, Section 3.2.4).

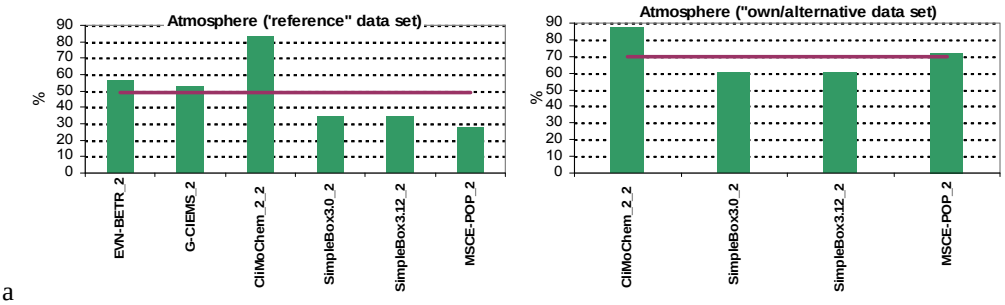
Relative distribution of PCB mass degraded in the environmental compartments

The presented estimates of PCB-153 masses degraded in the main environmental compartments allow one to reveal the relative contributions of degradation process occurs in this or that media to the overall mass of PCB-153 in the whole environment. Below, the comparison of relative fractions of PCB-153

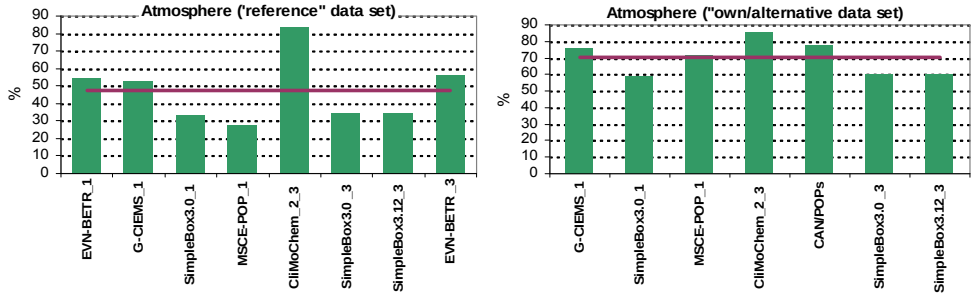
mass degraded in the main environmental media in relation to the mass balance estimates is presented. Of note, here and hereinafter fractions of mass degraded in different media are the ratios of the degraded mass and the mass contained in the considered compartment (taking into account also degraded mass).

Fractions of PCB-153 mass degraded in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Figs. 3.62a and b, respectively. In these figures fractions of PCB-153 mass degraded in the atmosphere calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.

According to the results obtained on the basis of zero and non-zero initial conditions and with the use of both physical-chemical data sets, most models provide rather close values of the fraction of PCB-153 mass degraded in the atmosphere. For most models the fraction of PCB-153 mass degraded in the atmosphere calculated on the basis of "own or alternative" data set exceed essentially that obtained with the use of "reference" data set. The results based on zero initial conditions vary from 28 to 89% ("reference" data set) and from 60 to 87% ("own/alternative" data set) of the overall mass contained originally in this compartment (See Fig. 3.62a). According to the results obtained with the use of non-zero initial conditions (see Fig. 3.62b) mass of PCB-153 degraded in the atmosphere makes up from 28 to 87% ("reference" data set) and from 59 to 86% ("own/alternative" data set) of the overall mass in this compartment.



a



b

Fig. 3.62. *Fractions of PCB-153 mass degraded in the atmosphere calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

In Fig. 3.63 a and b fractions of PCB-153 mass degraded in soil calculated by the different models on the basis of zero and non-zero initial conditions are presented, respectively. In these figures fractions of PCB-153 mass degraded in soil calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.

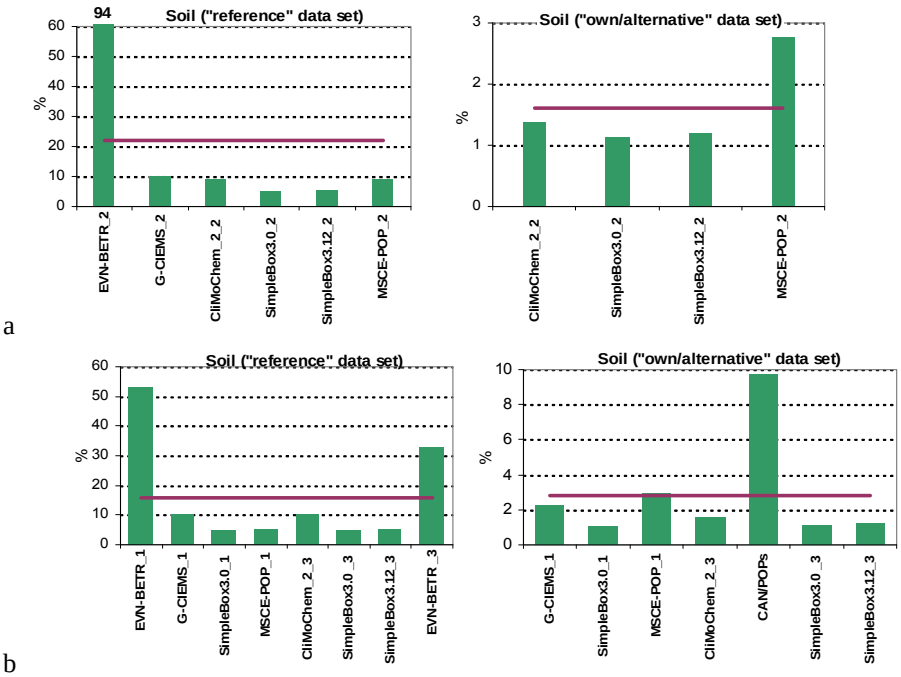


Fig. 3.63. *Fractions of PCB-153 mass degraded in soil calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The results obtained by most models on the basis of both zero and non-zero initial conditions are in reasonable agreement between each other. The fraction of PCB-153 mass degraded in soil calculated by all models on the basis of "reference» data set is considerably higher than that obtained with the use of "own or alternative" data set. The values of fraction of PCB-153 mass degraded in soil obtained on the basis of zero initial conditions and "reference" data set (see Fig. 3.63a) vary from 5 to 94% and are higher than those calculated using "own or alternative" data set (1.1 – 2.8%). The fractions of PCB-153 mass degraded in soil obtained on the basis of non-zero initial conditions and "reference" data set (see Fig. 3.63b) are observed in the range from 5 to 53%; the results calculated using "own or alternative" data set vary from 1.0 to 9.7%.

Fractions of PCB-153 mass degraded in seawater calculated by the participating on the basis of zero and non-zero initial conditions are presented in Figs. 3.64a and b, respectively. In these figures fractions of PCB-153 mass degraded in the atmosphere calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.

Results of SimpleBox model based on both zero and non-zero initial conditions as well as on "reference" and "own or alternative" data sets are lower than results of others models. The maximum values in results obtained on the basis of zero initial conditions are characteristic of EVN-BETR and UK-MODEL ("reference") and MSCE-POP model ("own/alternative') (See Fig. 3.64a). The maximum fractions of PCB-153 mass degraded in water based on non-zero initial conditions are obtained by EVN-BETR and UK-MODEL with "reference" data set and by CAN/POPs model with "own or alternative" data set (See Fig. 3.64b). As in the case of results on fractions of mass degraded in soil, for all models the values of fraction of PCB-153 mass degraded in water obtained on the basis of "reference» data set exceed those obtained with the use of "own or alternative" data set.

For the participating models provided results on PCB-153 degradation in vegetation, fractions of PCB-153 mass degraded in vegetation calculated on the basis of zero and non-zero initial conditions are

presented in Figs. 3.65a and b, respectively. In this figure fractions of PCB-153 mass degraded in the atmosphere calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. Results obtained by CliMoChem and G-CIEMS models using non-zero initial conditions and “own/alternative” data set are rather close to each other.

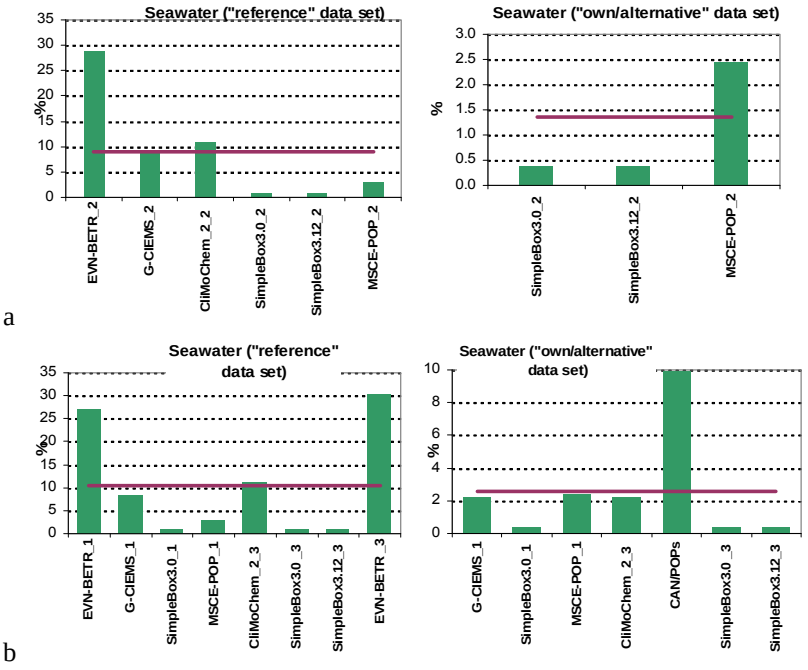


Fig. 3.64. *Fractions of PCB-153 mass degraded in seawater calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

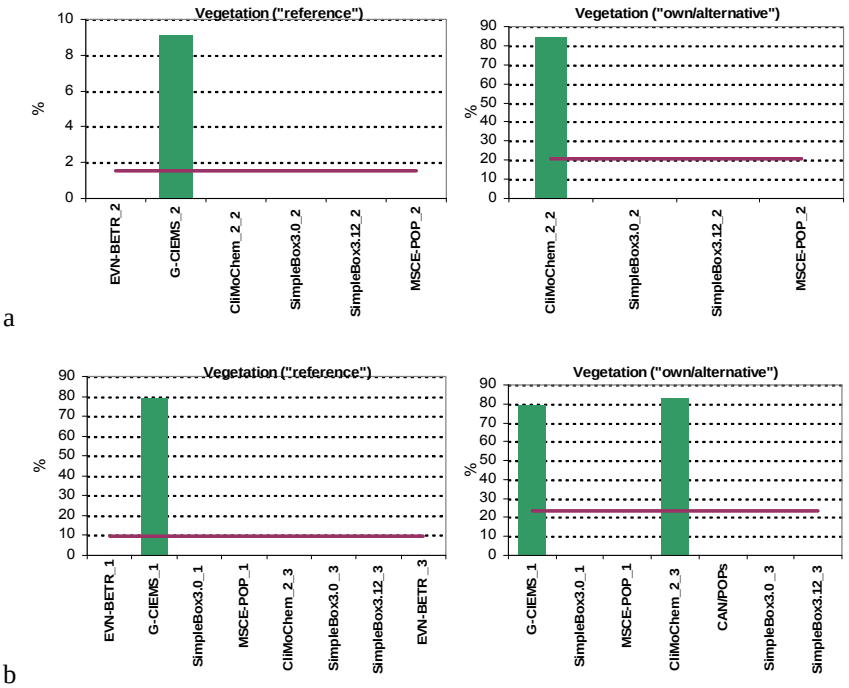


Fig. 3.65. *Fractions of PCB-153 mass degraded in vegetation calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Thus, in calculations based on both physical-chemical data sets ('reference" and "own/alternative") most participating models provide rather close absolute values of PCB-153 mass degraded in the atmosphere, soil and water. Noticeable seasonal variations in absolute values obtained are mostly characteristic of models that use temperature dependent degradation rates.

The comparison of masses degraded in main environmental media calculated with "reference" and "own/alternative" data sets shows that almost all models use higher degradation rates in the atmosphere in their "own or alternative" set of parameters compared with that in "reference" data set. That is why the annual values of calculation results on PCB-153 masses degraded in the atmosphere obtained with the use of "own or alternative" data sets noticeably exceed those obtained with "reference" data set. On the opposite, degradation rates in soil and water used by models are lower than that given in "reference" data set. Therefore, for all models' results, the values of PCB-153 masses degraded in these media obtained with the use of "own or alternative" data sets are less than those obtained with "reference" data set.

A preliminary analysis of relative fractions of PCB-153 mass degraded in the main environmental media that are ratios of the degraded mass and the mass contained in the considered compartment (taking into account also degraded mass) shows that most models closely describe degradation in the atmosphere, soil and water.

3.2.6. Comparison of calculated values of PCB-153 mass deposited into deep sea

In this section a comparison of results calculated by CliMoChem model with historical emission scenario on the basis of their own Land Cover Data [*DeFries and Townshend*, 1994] and Land Cover Data given as input data for this intercomparison study [*Guo and Chen*, 1994] is presented. Of note, contrary to the calculations discussed in the previous and subsequent sections in this simulation, PCB-153 is emitted as pulse emission into air each year at the beginning of season one.

Reference data set. Two sets of calculated values of PCB-153 mass deposited into deep sea (kg) obtained by CliMoChem model on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.43.

Table 3.43. *Calculation results: PCB-153 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "reference" data set and statistical parameters used for evaluation*

Month	CliMoChem_1_3	CliMoChem_2_3	*m*	σ
Season_1	135.308	155.224	145.27	14.08
Season_2	87.353	99.588	93.47	8.65
Season_3	54.413	61.803	58.11	5.22
Season_4	44.870	51.616	48.24	4.77
Annual	**321.944**	**368.230**	**345.09**	**32.73**

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

Seasonal values of PCB-153 mass deposited into deep sea calculated by CliMoChem model on the basis of "reference" data set are compared in Fig. 3.66.

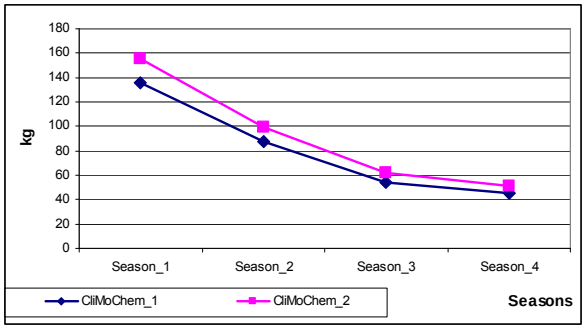


Fig. 3.66. *PCB-153 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "reference" data set*

Own/alternative data set. Two versions of calculation results on PCB-153 mass deposited into deep sea (kg) obtained by CliMoChem model on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.44.

Table 3.44. *Calculation results: PCB-153 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	CliMoChem_1_3	CliMoChem_2_3	*m*	σ
Season_1	92.538	114.090	103.31	15.24
Season_2	68.027	83.628	75.83	11.03
Season_3	49.630	61.286	55.46	8.24
Season_4	50.966	64.479	57.72	9.56
Annual	261.162	323.484	292.32	44.07

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

Seasonal values of PCB-153 mass deposited into deep sea calculated by CliMoChem model on the basis of "own or alternative" data sets are compared in Fig. 3.67.

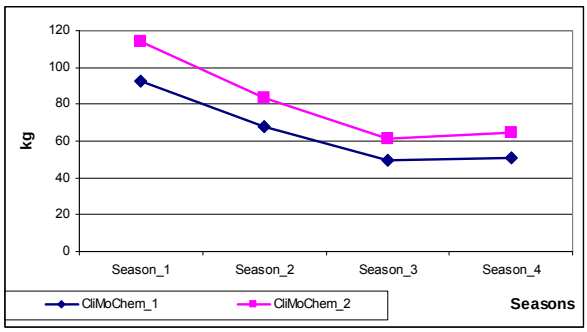


Fig. 3.67. *PCB-153 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "own or alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.45.

Table 3.45. *The percentage difference between calculation results on PCB-153 mass deposited into deep sea obtained by CliMoChem model on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_1_3	CliMoChem_2_3
Season_1	-31.6%	-26.5%
Season_2	-22.1%	-16.0%
Season_3	-8.8%	-0.8%
Season_4	13.6%	24.9%
Annual	-18.9%	-12.2%

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

For both variants of CliMoChem results, the annual values and practically all seasonal values of PCB-153 masses deposited into deep sea obtained with the use of "own or alternative" data sets (except those obtained for season 4) are less than those obtained with "reference" data set.

3.3. Mass flows transported in/out the specified domain: inflow and outflow

Mass flows of PCB-153 transported in/out the specified domain (inflow and outflow) are calculated by the participating models on the basis of atmospheric emission estimates presented by [*Breivik et al*. 2002a] (see also www.nilu.no/projects/globalpcb/). The higher (or worst-case) emission estimates for 1981-2000 are applied.

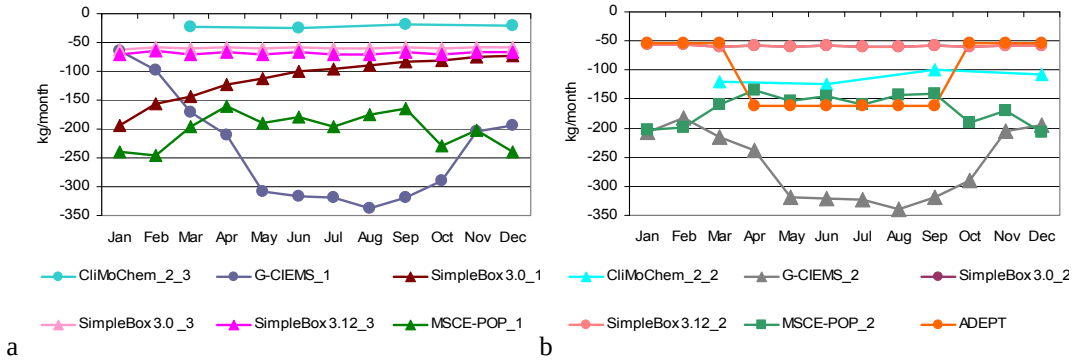
All amount of emissions is released into the atmosphere and is uniformly distributed throughout a year. In calculations of ADEPT, CAN/POPs, G-CIEMS, SimpleBox and MSCE-POP models, a value of PCB-153 total annual emissions in 2000 totals on average 5600 kg. In CliMoChem model the global emission data were summarized to zone-specific emissions (10 zones) and for the specified domain emission data for the model zones 2 and 3 (of 10) are used. At that emission value in 2000 used by CliMoChem for PCB-153 totals to 8953 kg.

It should be noted that transport into the calculation domain is supposed to be positive.

3.3.1. Comparison of calculated values of PCB-153 mass flows transported in/out the calculation domain through the atmosphere.

Reference data set. Calculation results on PCB-153 mass flows transported in/out the calculation domain through the atmosphere calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.46.

Monthly values of PCB-153 mass flows transported in/out the calculation domain through the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.68 a and b, respectively.



a b

Fig. 3.68a. *PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. 3.68b. *PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported in/out the calculation domain through the atmosphere calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.47.

Monthly values of PCB-153 mass flows transported in/out of the calculation domain through atmosphere calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.69 a and b, respectively.

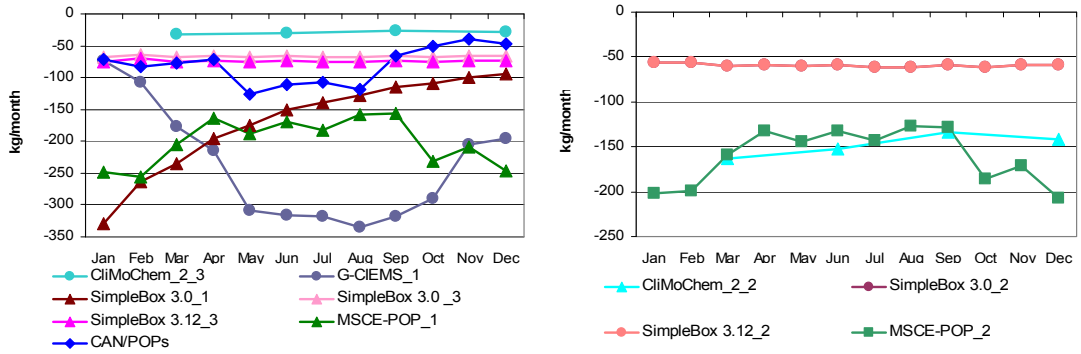


Fig. 3.69a. *PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

Fig. 3.69b. *PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.48.

Table 3.46. *Calculation results: PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	-65.1	-194.7	-239.7		-61.9	-69.9	*-126.2*	*84.6*	Jan	-206.5		-55.1	-55.1	-203.3	-53.0	*-114.6*	*82.4*
Feb	-97.9	-156.1	-245.0		-57.3	-65.4	*-124.4*	*77.8*	Feb	-182.4		-55.2	-55.2	-199.8	-53.0	*-109.1*	*75.1*
Mar	-171.4	-143.6	-196.0		-61.3	-69.9	*-128.4*	*60.4*	Mar	-216.1		-59.1	-59.1	-159.6	-53.0	*-109.4*	*74.4*
Seas_1	**-334.4**	**-494.3**	**-680.7**	**-67.0**	**-180.5**	**-205.2**	***-327.0***	***226.7***	**Seas_1**	**-605.0**	**-361.9**	**-169.4**	**-169.4**	**-562.7**	**-159.0**	***-337.9***	***205.5***
Apr	-210.9	-122.0	-160.6		-59.3	-67.7	*-124.1*	*63.8*	Apr	-238.3		-57.3	-57.3	-134.2	-162.5	*-129.9*	*76.4*
May	-309.0	-113.1	-190.2		-61.3	-69.9	*-148.7*	*103.1*	May	-318.6		-59.3	-59.3	-153.7	-162.5	*-150.7*	*106.1*
Jun	-317.1	-100.0	-179.8		-59.3	-67.7	*-144.8*	*107.4*	Jun	-321.6		-57.5	-57.5	-145.1	-162.5	*-148.8*	*108.1*
Seas_2	**-837.1**	**-335.1**	**-530.7**	**-72.3**	**-180.0**	**-205.2**	***-360.0***	***281.6***	**Seas_2**	**-878.5**	**-373.3**	**-174.2**	**-174.2**	**-433.0**	**-487.5**	***-420.1***	***260.0***
Jul	-318.4	-95.7	-196.8		-61.3	-69.9	*-148.4*	*109.3*	Jul	-323.1		-59.5	-59.5	-159.0	-162.5	*-152.7*	*107.9*
Aug	-336.5	-89.7	-174.4		-61.3	-69.9	*-146.4*	*115.4*	Aug	-339.9		-59.5	-59.5	-143.6	-162.5	*-153.0*	*114.7*
Sep	-319.3	-82.3	-164.9		-59.3	-67.7	*-138.7*	*109.3*	Sep	-319.7		-57.6	-57.6	-139.9	-162.5	*-147.5*	*107.3*
Seas_3	**-974.2**	**-267.8**	**-536.0**	**-58.2**	**-182.0**	**-207.5**	***-370.9***	***335.3***	**Seas_3**	**-982.7**	**-297.1**	**-176.6**	**-176.6**	**-442.5**	**-487.5**	***-427.2***	***301.7***
Oct	-289.6	-81.3	-229.5		-61.3	-69.9	*-146.3*	*105.8*	Oct	-290.7		-59.6	-59.6	-189.7	-53.0	*-130.5*	*106.4*
Nov	-203.2	-75.7	-201.6		-59.3	-67.7	*-121.5*	*74.1*	Nov	-204.9		-57.7	-57.7	-169.6	-53.0	*-108.6*	*72.9*
Dec	-193.4	-73.2	-240.0		-59.3	-67.7	*-126.7*	*83.9*	Dec	-194.2		-57.7	-57.7	-206.4	-53.0	*-113.8*	*79.1*
Seas_4	**-686.2**	**-230.2**	**-671.1**	**-64.4**	**-180.0**	**-205.2**	***-339.5***	***268.8***	**Seas_4**	**-689.9**	**-324.7**	**-175.0**	**-175.0**	**-565.7**	**-159.0**	***-348.2***	***228.2***
Annual	**-2831.9**	**-1327.4**	**-2418.5**	**-261.9**	**-722.4**	**-823.1**	***-1397.5***	***1017.8***	**Annual**	**-3156.1**	**-1357.0**	**-695.2**	**-695.3**	**-2003.9**	**-1293.0**	***-1533.4***	***932.6***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data are presented for moderate scale.

Table 3.47. *Calculation results: PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-72.1	-74.1	-329.3	-248.1		-68.1	-75.1	*-144.5*	*114.7*	Jan		-55.8	-55.8	-202.1	*-104.6*	*84.5*
Feb	-82.1	-107.3	-263.6	-255.6		-63.3	-70.3	*-140.4*	*93.6*	Feb		-56.1	-56.1	-199.6	*-104.0*	*82.8*
Mar	-76.6	-177.2	-236.1	-204.4		-67.8	-75.3	*-139.6*	*75.1*	Mar		-60.3	-60.3	-159.4	*-93.3*	*57.2*
Seas_1	**-230.7**	**-358.6**	**-829.0**	**-708.1**	**-97.2**	**-199.2**	**-220.6**	***-377.6***	***279.9***	**Seas_1**	**-490.3**	**-172.3**	**-172.3**	**-561.1**	***-349.0***	***206.1***
Apr	-71.3	-214.3	-195.0	-164.2		-65.7	-73.0	*-130.6*	*68.3*	Apr		-58.6	-58.6	-132.2	*-83.1*	*42.5*
May	-126.7	-308.1	-175.4	-187.5		-67.9	-75.5	*-156.9*	*89.0*	May		-60.7	-60.7	-144.6	*-88.7*	*48.4*
Jun	-111.9	-316.2	-150.4	-170.2		-65.8	-73.1	*-147.9*	*92.2*	Jun		-58.9	-58.9	-132.5	*-83.4*	*42.5*
Seas_2	**-309.9**	**-838.6**	**-520.9**	**-521.9**	**-92.4**	**-199.4**	**-221.5**	***-386.4***	***256.7***	**Seasl_2**	**-459.0**	**-178.2**	**-178.2**	**-409.4**	***-306.2***	***149.2***
Jul	-106.3	-317.6	-139.9	-182.5		-68.0	-75.6	*-148.3*	*93.2*	Jul		-61.0	-61.0	-143.5	*-88.5*	*47.6*
Aug	-118.2	-335.3	-127.5	-158.8		-68.1	-75.6	*-147.2*	*98.1*	Aug		-61.1	-61.1	-127.4	*-83.2*	*38.3*
Sep	-66.1	-318.0	-113.9	-155.6		-65.9	-73.2	*-132.1*	*97.6*	Sep		-59.2	-59.2	-128.9	*-82.5*	*40.2*
Seas_3	**-290.6**	**-970.9**	**-381.3**	**-496.9**	**-80.9**	**-202.0**	**-224.4**	***-378.2***	***293.3***	**Seas_3**	**-402.8**	**-181.4**	**-181.4**	**-399.8**	***-291.3***	***127.0***
Oct	-50.6	-288.9	-109.7	-230.7		-68.1	-75.7	*-137.3*	*98.6*	Oct		-61.3	-61.3	-185.2	*-102.6*	*71.5*
Nov	-38.8	-205.0	-99.8	-208.4		-65.9	-73.3	*-115.2*	*73.5*	Nov		-59.4	-59.4	-170.5	*-96.4*	*64.2*
Dec	-46.6	-194.8	-94.6	-247.0		-66.0	-73.3	*-120.4*	*81.1*	Dec		-59.5	-59.5	-207.4	*-108.8*	*85.4*
Seas_4	**-136.0**	**-688.8**	**-304.2**	**-686.1**	**-84.4**	**-200.0**	**-222.2**	***-331.7***	***252.5***	**Seas_4**	**-424.2**	**-180.1**	**-180.1**	**-563.1**	***-336.9***	***189.7***
Annual	**-967.2**	**-2856.8**	**-2035.4**	**-2413.1**	**-354.9**	**-800.6**	**-888.8**	***-1473.8***	***950.0***	**Annual**	**-1776.3**	**-712.0**	**-712.0**	**-1933.3**	***-1283.4***	***662.9***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table 3.48. *Comparison of the calculation results on PCB-153 mass flows transported in/out the calculation domain through the atmosphere (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative"*

Month	CliMoChem_2_3		G-CIEMS_1		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	own	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-65.1	-74.1	-194.7	-329.3	-55.1	-55.8	-55.1	-55.8	-61.9	-68.1	-69.9	-75.1	-239.7	-248.1	-203.3	-202.1		
Feb			-97.9	-107.3	-156.1	-263.6	-55.2	-56.1	-55.2	-56.1	-57.3	-63.3	-65.4	-70.3	-245.0	-255.6	-199.8	-199.6		
Mar			-171.4	-177.2	-143.6	-236.1	-59.1	-60.3	-59.1	-60.3	-61.3	-67.8	-69.9	-75.3	-196.0	-204.4	-159.6	-159.4		
Seas_1	**-67.0**	**-97.2**	**-334.4**	**-358.6**	**-494.3**	**-829.0**	**-169.4**	**-172.3**	**-169.4**	**-172.3**	**-180.5**	**-199.2**	**-205.2**	**-220.6**	**-680.7**	**-708.1**	**-562.7**	**-561.1**	**-361.9**	**-490.3**
Apr			-210.9	-214.3	-122.0	-195.0	-57.3	-58.6	-57.3	-58.6	-59.3	-65.7	-67.7	-73.0	-160.6	-164.2	-134.2	-132.2		
May			-309.0	-308.1	-113.1	-175.4	-59.3	-60.7	-59.3	-60.7	-61.3	-67.9	-69.9	-75.5	-190.2	-187.5	-153.7	-144.6		
Jun			-317.1	-316.2	-100.0	-150.4	-57.5	-58.9	-57.5	-58.9	-59.3	-65.8	-67.7	-73.1	-179.8	-170.2	-145.1	-132.5		
Seas_2	**-72.3**	**-92.4**	**-837.1**	**-838.6**	**-335.1**	**-520.9**	**-174.2**	**-178.2**	**-174.2**	**-178.2**	**-180.0**	**-199.4**	**-205.2**	**-221.5**	**-530.7**	**-521.9**	**-433.0**	**-409.4**	**-373.3**	**-459.0**
Jul			-318.4	-317.6	-95.7	-139.9	-59.5	-61.0	-59.5	-61.0	-61.3	-68.0	-69.9	-75.6	-196.8	-182.5	-159.0	-143.5		
Aug			-336.5	-335.3	-89.7	-127.5	-59.5	-61.1	-59.5	-61.1	-61.3	-68.1	-69.9	-75.6	-174.4	-158.8	-143.6	-127.4		
Sep			-319.3	-318.0	-82.3	-113.9	-57.6	-59.2	-57.6	-59.2	-59.3	-65.9	-67.7	-73.2	-164.9	-155.6	-139.9	-128.9		
Seas_3	**-58.2**	**-80.9**	**-974.2**	**-970.9**	**-267.8**	**-381.3**	**-176.6**	**-181.4**	**-176.6**	**-181.4**	**-182.0**	**-202.0**	**-207.5**	**-224.4**	**-536.0**	**-496.9**	**-442.5**	**-399.8**	**-297.1**	**-402.8**
Oct			-289.6	-288.9	-81.3	-109.7	-59.6	-61.3	-59.6	-61.3	-61.3	-68.1	-69.9	-75.7	-229.5	-230.7	-189.7	-185.2		
Nov			-203.2	-205.0	-75.7	-99.8	-57.7	-59.4	-57.7	-59.4	-59.3	-65.9	-67.7	-73.3	-201.6	-208.4	-169.6	-170.5		
Dec			-193.4	-194.8	-73.2	-94.6	-57.7	-59.5	-57.7	-59.5	-59.3	-66.0	-67.7	-73.3	-240.0	-247.0	-206.4	-207.4		
Seas_4	**-64.4**	**-84.4**	**-686.2**	**-688.8**	**-230.2**	**-304.2**	**-175.0**	**-180.1**	**-175.0**	**-180.1**	**-180.0**	**-200.0**	**-205.2**	**-222.2**	**-671.1**	**-686.1**	**-565.7**	**-563.1**	**-324.7**	**-424.2**
Annual	**-261.9**	**-354.9**	**-2831.9**	**-2856.8**	**-1327.4**	**-2035.4**	**-695.2**	**-712.0**	**-695.3**	**-712.0**	**-722.4**	**-800.6**	**-823.1**	**-888.8**	**-2418.5**	**-2413.1**	**-2003.9**	**-1933.3**	**-1357.0**	**-1776.3**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;

CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.3.2. Comparison of calculated values of PCB-153 mass flows transported in/out the calculation domain through ocean

Reference data set. Calculation results on PCB-153 mass flows transported in/out the calculation domain through ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.49.

Monthly values of PCB-153 mass flows transported in/out the calculation domain through ocean calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.70 a and b, respectively.

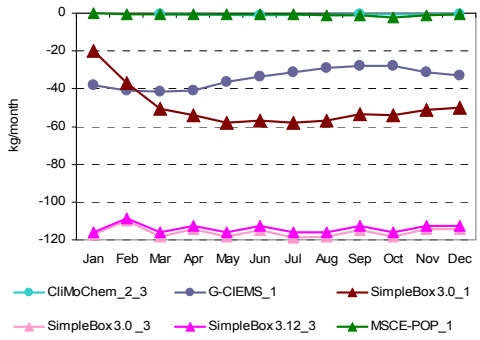


Fig. 3.70a. *PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

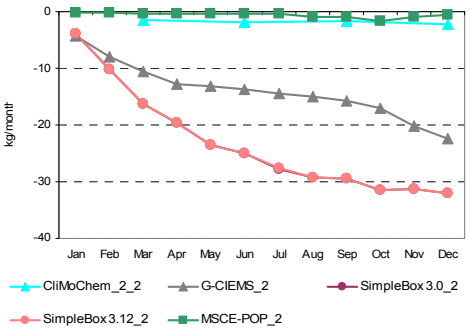


Fig. 3.70b. *PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported in/out the calculation domain through ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.50.

Monthly values of PCB-153 mass flows transported in/out the calculation domain through ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.71 a and b, respectively.

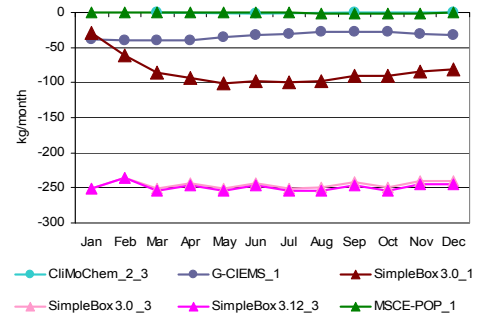


Fig. 3.71a. *PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

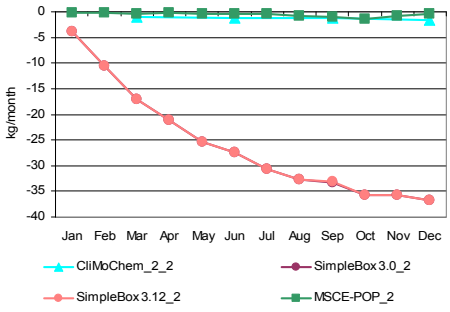


Fig. 3.71b. *PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.51.

Table 3.49. *Calculation results: PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	MSCE-POP_1	G-CIEMS_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-0.2	-38.3	-20.1		-116.9	-116.2	*-58.3*	*54.8*	Jan	-4.3		-3.9	-3.9	-0.1	*-3.0*	*2.0*
Feb	-0.3	-41.1	-37.1		-110.0	-108.7	*-59.5*	*48.3*	Feb	-8.0		-10.3	-10.3	-0.3	*-7.2*	*4.8*
Mar	-0.4	-41.6	-50.5		-118.1	-116.2	*-65.4*	*50.9*	Mar	-10.6		-16.3	-16.3	-0.3	*-10.9*	*7.5*
Seas_1	**-0.8**	**-121.1**	**-107.7**	**-2.4**	**-345.0**	**-341.2**	***-153.0***	***155.7***	**Seas_1**	**-22.9**	**-4.3**	**-30.5**	**-30.4**	**-0.7**	***-17.8***	***14.3***
Apr	-0.3	-41.0	-54.2		-114.6	-112.5	*-64.5*	*49.0*	Apr	-12.7		-19.7	-19.7	-0.3	*-13.1*	*9.2*
May	-0.4	-36.6	-58.2		-118.5	-116.2	*-66.0*	*51.3*	May	-13.1		-23.5	-23.4	-0.3	*-15.1*	*11.0*
Jun	-0.5	-33.5	-56.6		-114.8	-112.5	*-63.6*	*49.9*	Jun	-13.8		-25.0	-25.0	-0.4	*-16.0*	*11.7*
Seas_2	**-1.2**	**-111.1**	**-169.0**	**-2.6**	**-347.9**	**-341.2**	***-162.2***	***155.3***	**Seas_2**	**-39.6**	**-5.4**	**-68.2**	**-68.1**	**-1.0**	***-36.5***	***32.5***
Jul	-0.5	-31.4	-57.9		-118.6	-116.2	*-64.9*	*52.1*	Jul	-14.5		-27.7	-27.7	-0.4	*-17.6*	*13.0*
Aug	-1.0	-28.9	-56.7		-118.5	-116.2	*-64.3*	*52.3*	Aug	-14.9		-29.2	-29.2	-0.8	*-18.5*	*13.6*
Sep	-1.3	-27.7	-53.6		-114.6	-112.5	*-61.9*	*50.6*	Sep	-15.8		-29.5	-29.4	-1.0	*-18.9*	*13.6*
Seas_3	**-2.9**	**-88.0**	**-168.1**	**-2.4**	**-351.8**	**-345.0**	***-159.7***	***158.6***	**Seas_3**	**-45.2**	**-5.1**	**-86.4**	**-86.3**	**-2.3**	***-45.0***	***41.3***
Oct	-2.0	-27.7	-54.0		-118.4	-116.2	*-63.7*	*52.3*	Oct	-17.1		-31.5	-31.5	-1.6	*-20.4*	*14.3*
Nov	-1.2	-31.3	-51.1		-114.4	-112.5	*-62.1*	*50.2*	Nov	-20.1		-31.3	-31.3	-0.9	*-20.9*	*14.3*
Dec	-0.7	-33.0	-50.1		-114.3	-112.5	*-62.1*	*50.1*	Dec	-22.5		-32.1	-32.1	-0.5	*-21.8*	*14.9*
Seas_4	**-3.9**	**-91.9**	**-155.3**	**-2.2**	**-347.1**	**-341.2**	***-156.9***	***156.0***	**Seas_4**	**-59.7**	**-6.5**	**-94.9**	**-94.8**	**-3.0**	***-51.8***	***45.3***
Annual	**-8.7**	**-412.0**	**-600.1**	**-9.7**	**-1391.7**	**-1368.7**	***-631.8***	***623.7***	**Annual**	**-167.5**	**-21.2**	**-279.9**	**-279.7**	**-7.1**	***-151.1***	***133.2***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data are presented for moderate scale.

Table 3.50. *Calculation results: PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-37.8	-29.8	-0.2		-251.1	-251.5	*-114.1*	*126.1*	Jan		-3.9	-3.9	-0.1	*-2.6*	*2.2*
Feb	-40.3	-61.2	-0.3		-235.3	-236.5	*-114.7*	*112.8*	Feb		-10.6	-10.6	-0.3	*-7.1*	*5.9*
Mar	-40.5	-85.9	-0.4		-251.6	-253.6	*-126.4*	*119.1*	Mar		-17.1	-17.1	-0.4	*-11.5*	*9.7*
Seas_1	**-118.6**	**-176.8**	**-0.9**	**-2.1**	**-738.0**	**-741.6**	***-296.3***	***350.2***	**Seas_1**	**-2.9**	**-31.6**	**-31.5**	**-0.8**	***-16.7***	***17.2***
Apr	-39.9	-93.5	-0.3		-243.4	-245.9	*-124.6*	*114.5*	Apr		-21.1	-21.0	-0.3	*-14.1*	*12.0*
May	-35.6	-101.1	-0.4		-251.4	-254.4	*-128.6*	*119.1*	May		-25.4	-25.4	-0.3	*-17.0*	*14.5*
Jun	-32.6	-98.4	-0.5		-242.9	-246.3	*-124.2*	*115.5*	Jun		-27.4	-27.4	-0.4	*-18.4*	*15.6*
Seas_2	**-108.1**	**-293.0**	**-1.2**	**-2.4**	**-737.7**	**-746.6**	***-314.9***	***347.7***	**Seas_2**	**-3.9**	**-73.9**	**-73.9**	**-1.0**	***-38.2***	***41.3***
Jul	-30.6	-100.1	-0.5		-250.7	-254.5	*-127.3*	*120.0*	Jul		-30.7	-30.7	-0.4	*-20.6*	*17.5*
Aug	-28.2	-97.3	-1.0		-250.2	-254.2	*-126.2*	*120.3*	Aug		-32.7	-32.7	-0.8	*-22.1*	*18.4*
Sep	-27.0	-91.0	-1.3		-241.7	-245.7	*-121.3*	*116.4*	Sep		-33.2	-33.2	-0.9	*-22.5*	*18.6*
Seas_3	**-85.7**	**-288.4**	**-2.8**	**-2.2**	**-742.6**	**-754.3**	***-312.7***	***353.4***	**Seas_3**	**-3.7**	**-96.6**	**-96.6**	**-2.1**	***-49.8***	***54.1***
Oct	-27.0	-90.7	-2.0		-249.2	-253.5	*-124.5*	*120.3*	Oct		-35.7	-35.7	-1.5	*-24.3*	*19.7*
Nov	-30.5	-84.6	-1.1		-240.7	-245.0	*-120.4*	*115.7*	Nov		-35.7	-35.7	-0.8	*-24.1*	*20.1*
Dec	-32.2	-81.7	-0.6		-240.1	-244.6	*-119.9*	*115.5*	Dec		-36.7	-36.7	-0.5	*-24.6*	*20.9*
Seas_4	**-89.7**	**-256.9**	**-3.7**	**-2.0**	**-730.0**	**-743.1**	***-304.2***	***347.5***	**Seas_4**	**-4.6**	**-108.1**	**-108.1**	**-2.8**	***-55.9***	***60.3***
Annual	**-402.2**	**-1015.2**	**-8.6**	**-8.7**	**-2948.3**	**-2985.7**	***-1228.1***	***1396.4***	**Annual**	**-15.1**	**-310.3**	**-310.1**	**-6.7**	***-160.5***	***172.8***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

a - SimpleBox data are presented for moderate scale.

Table 3.51. *Comparison of the calculation results on PCB-153 mass flows transported in/out the calculation domain through ocean (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		G-CIEMS_1		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-38.3	-37.8	-20.1	-29.8	-3.9	-3.9	-3.9	-3.9	-116.9	-251.1	-116.2	-251.5	-0.2	-0.2	-0.1	-0.1		
Feb			-41.1	-40.3	-37.1	-61.2	-10.3	-10.6	-10.3	-10.6	-110.0	-235.3	-108.7	-236.5	-0.3	-0.3	-0.3	-0.3		
Mar			-41.6	-40.5	-50.5	-85.9	-16.3	-17.1	-16.3	-17.1	-118.1	-251.6	-116.2	-253.6	-0.4	-0.4	-0.3	-0.4		
Seas_1	**-2.4**	**-2.1**	**-121.1**	**-118.6**	**-107.7**	**-176.8**	**-30.5**	**-31.6**	**-30.4**	**-31.5**	**-345.0**	**-738.0**	**-341.2**	**-741.6**	**-0.8**	**-0.9**	**-0.7**	**-0.8**	**-4.3**	**-2.9**
Apr			-41.0	-39.9	-54.2	-93.5	-19.7	-21.1	-19.7	-21.0	-114.6	-243.4	-112.5	-245.9	-0.3	-0.3	-0.3	-0.3		
May			-36.6	-35.6	-58.2	-101.1	-23.5	-25.4	-23.4	-25.4	-118.5	-251.4	-116.2	-254.4	-0.4	-0.4	-0.3	-0.3		
Jun			-33.5	-32.6	-56.6	-98.4	-25.0	-27.4	-25.0	-27.4	-114.8	-242.9	-112.5	-246.3	-0.5	-0.5	-0.4	-0.4		
Seas_2	**-2.6**	**-2.4**	**-111.1**	**-108.1**	**-169.0**	**-293.0**	**-68.2**	**-73.9**	**-68.1**	**-73.9**	**-347.9**	**-737.7**	**-341.2**	**-746.6**	**-1.2**	**-1.2**	**-1.0**	**-1.0**	**-5.4**	**-3.9**
Jul			-31.4	-30.6	-57.9	-100.1	-27.7	-30.7	-27.7	-30.7	-118.6	-250.7	-116.2	-254.5	-0.5	-0.5	-0.4	-0.4		
Aug			-28.9	-28.2	-56.7	-97.3	-29.2	-32.7	-29.2	-32.7	-118.5	-250.2	-116.2	-254.2	-1.0	-1.0	-0.8	-0.8		
Sep			-27.7	-27.0	-53.6	-91.0	-29.5	-33.2	-29.4	-33.2	-114.6	-241.7	-112.5	-245.7	-1.3	-1.3	-1.0	-0.9		
Seas_3	**-2.4**	**-2.2**	**-88.0**	**-85.7**	**-168.1**	**-288.4**	**-86.4**	**-96.6**	**-86.3**	**-96.6**	**-351.8**	**-742.6**	**-345.0**	**-754.3**	**-2.9**	**-2.8**	**-2.3**	**-2.1**	**-5.1**	**-3.7**
Oct			-27.7	-27.0	-54.0	-90.7	-31.5	-35.7	-31.5	-35.7	-118.4	-249.2	-116.2	-253.5	-2.0	-2.0	-1.6	-1.5		
Nov			-31.3	-30.5	-51.1	-84.6	-31.3	-35.7	-31.3	-35.7	-114.4	-240.7	-112.5	-245.0	-1.2	-1.1	-0.9	-0.8		
Dec			-33.0	-32.2	-50.1	-81.7	-32.1	-36.7	-32.1	-36.7	-114.3	-240.1	-112.5	-244.6	-0.7	-0.6	-0.5	-0.5		
Seas_4	**-2.2**	**-2.0**	**-91.9**	**-89.7**	**-155.3**	**-256.9**	**-94.9**	**-108.1**	**-94.8**	**-108.1**	**-347.1**	**-730.0**	**-341.2**	**-743.1**	**-3.9**	**-3.7**	**-3.0**	**-2.8**	**-6.5**	**-4.6**
Annual	**-9.7**	**-8.7**	**-412.0**	**-402.2**	**-600.1**	**-1015.2**	**-279.9**	**-310.3**	**-279.7**	**-310.1**	**-1391.7**	**-2948.3**	**-1368.7**	**-2985.7**	**-8.7**	**-8.6**	**-7.1**	**-6.7**	**-21.2**	**-15.1**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.3.3. Calculated values of PCB-153 mass flows transported in/out the calculation domain through other compartments

Reference data set. Calculation results on PCB-153 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.52.

Monthly values of PCB-153 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "reference" data set are presented in Fig. 3.72.

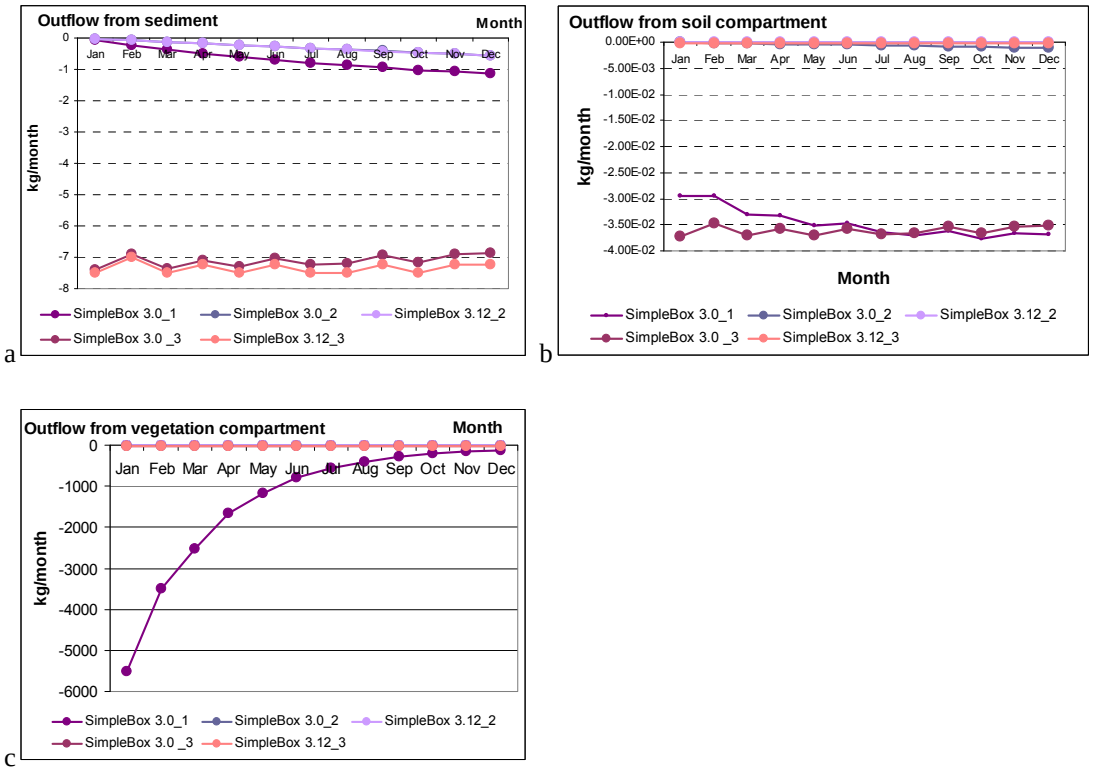


Fig. 3.72. *PCB-153 mass flows transported in/out the calculation domain through sediment (a), soil (b) and vegetation(c) calculated by SimpleBox on the basis of "reference" data set*

Own/alternative data set. Calculation results on PCB-153 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.53.

Monthly values of PCB-153 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "alternative" data set are compared in Fig. 3.73.

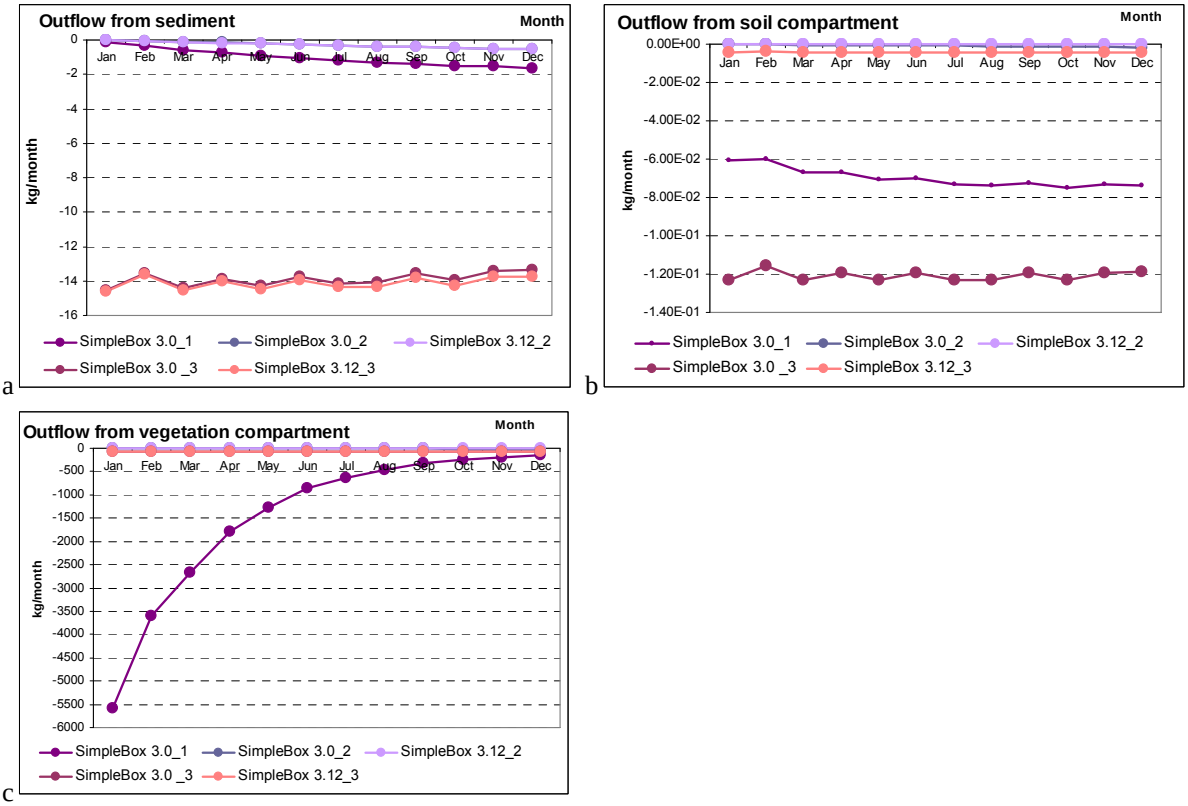


Fig. 3.73. *PCB-153 mass flows transported in/out the calculation domain through sediment (a), soil (b) and vegetation(c) calculated by SimpleBox on the basis of "alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two different data sets of physical-chemical properties (for SimpleBox model) is shown in Table 3.54.

In results on mass flows of PCB-153 transported in/out the calculation domain through sediments, soil and vegetation obtained on the basis of "alternative" and "reference" data sets, there is the largest difference between values of mass flows transported out soil observed for SimpleBox 3.12_2 and SimpleBox 3.12_3 output.

Table 3.52. *Calculation results: PCB-153 mass flows transported in/out the calculation domain through sediments, soil and vegetation (kg/month) calculated by SimpleBox on the basis of "reference" data set*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	-0.08	-0.02	-0.02	-7.41	-7.49	-2.95E-02	-4.31E-05	-1.18E-08	-3.73E-02	-1.37E-04	-5522.1	-1.8	-1.8	-34.9	-34.9
Feb	-0.23	-0.07	-0.07	-6.90	-7.00	-2.95E-02	-1.28E-04	-3.42E-08	-3.48E-02	-1.28E-04	-3493.3	-4.5	-4.4	-32.6	-32.7
Mar	-0.38	-0.12	-0.12	-7.35	-7.49	-3.31E-02	-2.33E-04	-6.12E-08	-3.71E-02	-1.37E-04	-2538.2	-6.9	-6.7	-34.8	-34.9
Apr	-0.48	-0.17	-0.17	-7.09	-7.24	-3.32E-02	-3.20E-04	-8.33E-08	-3.58E-02	-1.32E-04	-1664.4	-8.1	-7.9	-33.6	-33.8
May	-0.61	-0.22	-0.23	-7.29	-7.49	-3.52E-02	-4.29E-04	-1.11E-07	-3.70E-02	-1.37E-04	-1174.1	-9.4	-9.1	-34.7	-34.9
Jun	-0.68	-0.27	-0.27	-7.03	-7.24	-3.48E-02	-5.11E-04	-1.31E-07	-3.57E-02	-1.32E-04	-782.0	-9.7	-9.4	-33.5	-33.8
Jul	-0.80	-0.33	-0.33	-7.24	-7.49	-3.65E-02	-6.27E-04	-1.60E-07	-3.68E-02	-1.37E-04	-563.6	-10.6	-10.1	-34.6	-34.9
Aug	-0.88	-0.38	-0.38	-7.21	-7.49	-3.70E-02	-7.28E-04	-1.84E-07	-3.67E-02	-1.37E-04	-397.4	-10.9	-10.4	-34.6	-34.9
Sep	-0.93	-0.41	-0.42	-6.95	-7.24	-3.61E-02	-8.01E-04	-2.01E-07	-3.55E-02	-1.32E-04	-278.6	-10.9	-10.3	-33.4	-33.8
Oct	-1.03	-0.47	-0.48	-7.15	-7.49	-3.76E-02	-9.27E-04	-2.32E-07	-3.66E-02	-1.37E-04	-214.6	-11.4	-10.8	-34.5	-34.9
Nov	-1.06	-0.51	-0.51	-6.90	-7.24	-3.66E-02	-9.93E-04	-2.47E-07	-3.53E-02	-1.32E-04	-159.8	-11.2	-10.5	-33.3	-33.8
Dec	-1.13	-0.55	-0.56	-6.87	-7.24	-3.68E-02	-1.09E-03	-2.69E-07	-3.53E-02	-1.32E-04	-128.1	-11.4	-10.6	-33.3	-33.8
Annual	**-8.29**	**-3.51**	**-3.56**	**-85.38**	**-88.13**	**-4.16E-01**	**-6.83E-03**	**-1.72E-06**	**-4.34E-01**	**-1.61E-03**	**-16916.1**	**-106.9**	**-101.9**	**-408.0**	**-411.4**

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

* - SimpleBox data are presented for moderate scale

Table 3.53. *Calculation results: PCB-153 mass flows transported in/out the calculation domain through sediment, soil and vegetation (kg/month) calculated by SimpleBox on the basis of "alternative data sets"*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox x 3.12_3
Jan	-0.13	-0.02	-0.02	-14.52	-14.63	-6.09E-02	-6.13E-05	-3.17E-07	-1.23E-01	-4.27E-03	-5576.0	-1.9	-1.8	-69.3	-69.5
Feb	-0.36	-0.07	-0.07	-13.52	-13.65	-6.02E-02	-1.83E-04	-9.48E-07	-1.15E-01	-3.99E-03	-3596.6	-4.8	-4.7	-66.0	-66.6
Mar	-0.60	-0.12	-0.12	-14.39	-14.55	-6.71E-02	-3.33E-04	-1.73E-06	-1.23E-01	-4.26E-03	-2663.1	-7.4	-7.2	-71.5	-72.3
Apr	-0.76	-0.17	-0.17	-13.86	-14.03	-6.69E-02	-4.59E-04	-2.38E-06	-1.19E-01	-4.12E-03	-1779.6	-8.7	-8.4	-69.8	-70.7
May	-0.94	-0.22	-0.23	-14.26	-14.46	-7.08E-02	-6.18E-04	-3.21E-06	-1.23E-01	-4.25E-03	-1278.4	-10.1	-9.8	-72.5	-73.6
Jun	-1.04	-0.26	-0.27	-13.74	-13.95	-6.98E-02	-7.38E-04	-3.83E-06	-1.19E-01	-4.11E-03	-866.5	-10.6	-10.2	-70.5	-71.5
Jul	-1.20	-0.32	-0.33	-14.13	-14.38	-7.31E-02	-9.09E-04	-4.71E-06	-1.23E-01	-4.24E-03	-634.7	-11.5	-11.0	-73.0	-74.1
Aug	-1.32	-0.37	-0.38	-14.07	-14.34	-7.40E-02	-1.06E-03	-5.48E-06	-1.23E-01	-4.24E-03	-454.2	-11.9	-11.4	-73.1	-74.2
Sep	-1.37	-0.41	-0.42	-13.56	-13.83	-7.23E-02	-1.17E-03	-6.04E-06	-1.19E-01	-4.10E-03	-322.4	-11.9	-11.3	-70.9	-71.9
Oct	-1.51	-0.47	-0.48	-13.95	-14.26	-7.53E-02	-1.35E-03	-7.01E-06	-1.23E-01	-4.23E-03	-250.6	-12.5	-11.9	-73.3	-74.3
Nov	-1.55	-0.50	-0.51	-13.44	-13.76	-7.34E-02	-1.45E-03	-7.53E-06	-1.19E-01	-4.09E-03	-187.7	-12.3	-11.6	-70.9	-71.9
Dec	-1.62	-0.55	-0.56	-13.38	-13.72	-7.38E-02	-1.59E-03	-8.26E-06	-1.19E-01	-4.08E-03	-150.7	-12.5	-11.7	-70.9	-71.9
Annual	**-12.39**	**-3.49**	**-3.55**	**-166.83**	**-169.55**	**-8.38E-01**	**-9.92E-03**	**-5.14E-05**	**-1.45E+00**	**-5.00E-02**	**-17760.5**	**-115.9**	**-111.1**	**-851.8**	**-862.6**

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

* - SimpleBox data are presented for moderate scale.

Table 3.54. *The percentage difference between calculation results on PCB-153 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of two data sets: "reference" and "alternative"*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	53.6%	-3.3%	-3.2%	96.0%	95.5%	106%	42%	2583%	231%	3026%	1%	4%	5%	98%	99%
Feb	57.7%	-2.4%	-2.3%	95.9%	94.9%	104%	43%	2674%	231%	3023%	3%	5%	6%	102%	104%
Mar	57.2%	-2.0%	-1.9%	95.8%	94.3%	103%	43%	2723%	232%	3019%	5%	6%	7%	105%	107%
Apr	55.8%	-1.7%	-1.6%	95.7%	93.7%	102%	44%	2762%	233%	3016%	7%	7%	7%	108%	109%
May	54.3%	-1.4%	-1.3%	95.6%	93.2%	101%	44%	2796%	233%	3012%	9%	8%	8%	109%	111%
Jun	52.7%	-1.2%	-1.1%	95.4%	92.6%	101%	44%	2826%	234%	3008%	11%	8%	9%	110%	111%
Jul	51.1%	-1.0%	-0.8%	95.3%	92.1%	100%	45%	2853%	235%	3005%	13%	9%	9%	111%	112%
Aug	49.5%	-0.7%	-0.6%	95.2%	91.5%	100%	45%	2879%	235%	3001%	14%	9%	10%	112%	112%
Sep	48.1%	-0.5%	-0.4%	95.1%	91.0%	100%	46%	2903%	236%	2997%	16%	9%	10%	112%	113%
Oct	46.7%	-0.3%	-0.2%	95.0%	90.4%	100%	46%	2925%	236%	2994%	17%	9%	10%	112%	113%
Nov	45.3%	-0.1%	0.1%	94.9%	89.9%	100%	46%	2947%	237%	2990%	17%	10%	10%	113%	113%
Dec	44.1%	0.1%	0.3%	94.8%	89.4%	101%	47%	2967%	238%	2987%	18%	10%	10%	113%	113%
Annual	**49.5%**	**-0.7%**	**-0.5%**	**95.4%**	**92.4%**	**101%**	**45%**	**2882%**	**234%**	**3007%**	**5%**	**8%**	**9%**	**109%**	**110%**

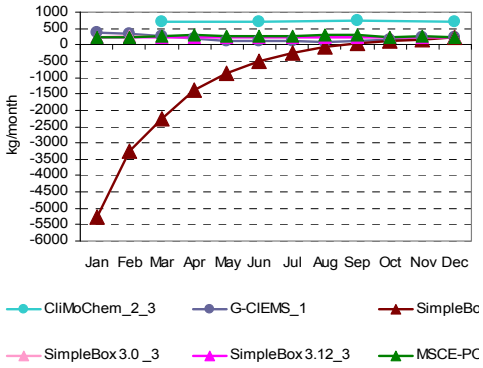
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

3.3.4. Comparison of calculated values of PCB-153 total mass flows transported in/out the specified domain

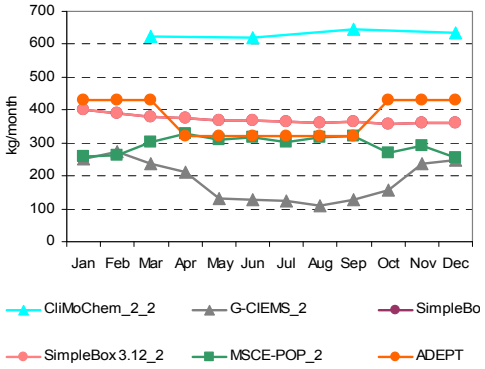
Values of total mass flow transported in/out the calculation domain are calculated as sum of inflow (emissions) and all outflows through the main transport media.

Reference data set. Calculation results on PCB-153 total mass flows transported in/out the specified domain calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.55.

Monthly values of total PCB-153 total mass flows transported in/out the specified domain calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.74 a and b, respectively. Seasonal variations of positive values of total PCB-153 total mass flows transported in/out the specified domain calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. 3.74c in more detail.



a



b

Fig. 3.74a. *PCB-153 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. 3.74b. *PCB-153 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

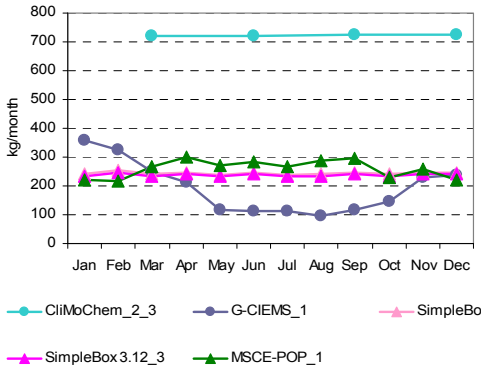
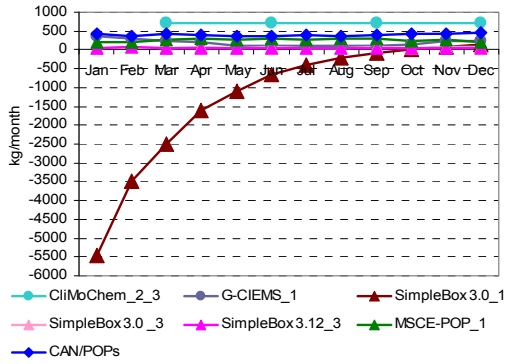


Fig. 3.74c. *PCB-153 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (positive values)*

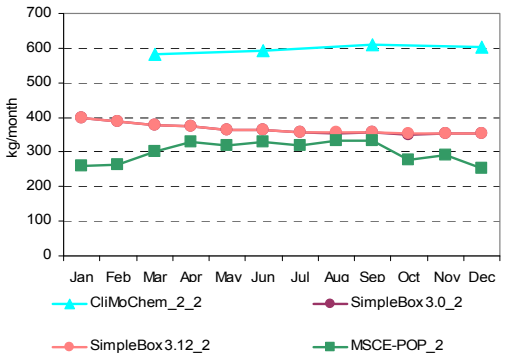
Own/alternative data set. Calculation results on PCB-153 total mass flows transported in/out the specified domain calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.56.

Monthly values of total PCB-153 mass flows transported in/out the specified domain calculated by the participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.75 a and b, respectively. Seasonal variations of positive values of total PCB-153 total mass flows transported in/out the specified domain calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions are also shown in Fig. 3.74c in more detail.



a

Fig. 3.75a. *PCB-153 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of “own or alternative” data set and non-zero initial conditions*



b

Fig. 3.75b. *PCB-153 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of “own or alternative” data set and zero initial conditions*

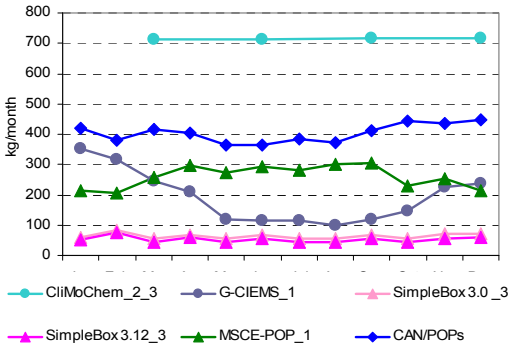


Fig. 3.75c. *PCB-153 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (positive values)*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.57.

Table 3.55. *Calculation results: PCB-153 total mass flows transported in/out the specified domain (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	359.6	-5266.8	222.4		240.2	232.7	*-842.4*	*2473.9*	Jan	252.2		400.5	400.5	258.8	430.3	*348.5*	*85.7*
Feb	324.0	-3262.2	216.9		254.4	247.4	*-443.9*	*1576.0*	Feb	272.7		391.2	391.3	262.1	430.3	*349.5*	*76.7*
Mar	250.1	-2262.5	265.9		239.7	232.7	*-254.8*	*1122.4*	Mar	236.3		378.8	379.0	302.3	430.3	*345.3*	*76.2*
Seas_1	**933.6**	**-10791.5**	**705.2**	**2168.7**	**734.2**	**712.8**	***-922.8***	***4867.6***	**Seas_1**	**761.2**	**1871.9**	**1170.5**	**1170.8**	**823.2**	**1290.9**	***1181.4***	***398.5***
Apr	211.2	-1386.2	301.3		246.6	240.1	*-77.4*	*732.4*	Apr	212.0		376.0	376.2	327.7	320.8	*322.5*	*67.1*
May	117.4	-875.9	271.6		239.4	232.7	*-3.0*	*491.5*	May	131.3		368.9	369.2	308.2	320.8	*299.7*	*98.1*
Jun	112.4	-484.4	281.9		246.6	240.1	*79.3*	*321.6*	Jun	127.7		368.8	369.1	316.7	320.8	*300.6*	*99.9*
Seas_2	**441.0**	**-2746.5**	**854.8**	**2163.3**	**732.6**	**712.8**	***359.7***	***1638.1***	**Seas_2**	**471.0**	**1859.4**	**1113.6**	**1114.5**	**952.6**	**962.4**	***1078.9***	***449.6***
Jul	113.3	-247.9	264.9		239.5	232.7	*120.5*	*214.1*	Jul	125.4		363.2	363.7	302.8	320.8	*295.2*	*98.5*
Aug	97.6	-74.6	286.8		239.6	232.7	*156.4*	*147.1*	Aug	108.2		361.2	361.8	317.8	320.8	*294.0*	*106.0*
Sep	116.1	39.5	296.0		246.9	240.1	*187.7*	*106.2*	Sep	127.5		362.9	363.5	321.3	320.8	*299.2*	*98.3*
Seas_3	**327.0**	**-283.0**	**847.8**	**2177.5**	**726.0**	**705.4**	***750.1***	***811.9***	**Seas_3**	**361.2**	**1936.0**	**1087.3**	**1088.9**	**941.9**	**962.4**	***1063.0***	***506.1***
Oct	145.7	119.2	230.7		239.9	232.7	*193.6*	*56.7*	Oct	155.2		358.3	359.0	270.9	430.3	*314.7*	*105.6*
Nov	228.6	167.3	259.5		247.2	240.1	*228.5*	*36.1*	Nov	238.0		360.5	361.2	291.8	430.3	*336.4*	*73.6*
Dec	236.7	217.6	221.5		247.4	240.1	*232.6*	*12.7*	Dec	246.4		359.5	360.3	255.2	430.3	*330.4*	*78.2*
Seas_4	**611.0**	**504.0**	**711.7**	**2171.5**	**734.6**	**712.8**	***907.6***	***625.2***	**Seas_4**	**639.6**	**1906.9**	**1078.3**	**1080.5**	**817.9**	**1290.9**	***1135.7***	***441.0***
Annual	**2312.6**	**-13317.0**	**3119.5**	**8680.9**	**2927.4**	**2843.9**	***1094.5***	***7446.5***	**Annual**	**2232.9**	**7574.3**	**4449.8**	**4454.8**	**3535.7**	**4507.0**	***4459.1***	***1761.6***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table 3.56. *Calculation results: PCB-153 total mass flows transported in/out the specified domain (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	420.2	351.2	-5465.1	214.0		58.1	50.6	*-728.5*	*2325.3*	Jan		399.7	399.7	260.0	*353.1*	*80.7*
Feb	378.4	315.4	-3497.2	206.3		83.0	74.3	*-406.6*	*1519.0*	Feb		389.7	389.8	262.3	*347.3*	*73.6*
Mar	415.7	245.4	-2515.6	257.4		55.9	45.5	*-249.3*	*1118.9*	Mar		376.4	376.6	302.5	*351.8*	*42.7*
Seas_1	**1214.2**	**912.0**	**-11478.0**	**677.6**	**2138.8**	**197.0**	**170.4**	***-881.1***	***4720.8***	**Seas_1**	**1744.9**	**1165.8**	**1166.1**	**824.8**	***1225.4***	***381.9***
Apr	405.1	208.9	-1614.0	297.7		68.5	57.6	*-96.1*	*755.5*	Apr		372.8	373.0	329.7	*358.5*	*24.9*
May	365.5	119.3	-1085.8	274.3		55.1	43.4	*-38.0*	*528.8*	May		364.8	365.1	317.3	*349.1*	*27.5*
Jun	364.4	114.2	-661.5	291.5		68.2	56.4	*38.9*	*365.3*	Jun		364.1	364.5	329.3	*352.6*	*20.2*
Seas_2	**1135.0**	**442.4**	**-3361.4**	**863.5**	**2143.3**	**191.7**	**157.4**	***224.6***	***1723.9***	**Seas_2**	**1775.3**	**1101.7**	**1102.6**	**976.3**	***1239.0***	***362.4***
Jul	385.9	114.9	-405.9	279.2		55.3	42.7	*78.7*	*273.0*	Jul		357.7	358.2	318.3	*344.7*	*22.9*
Aug	374.1	99.6	-210.2	302.4		55.7	42.9	*110.7*	*208.3*	Aug		355.1	355.7	334.0	*348.3*	*12.4*
Sep	410.3	118.1	-73.8	305.3		69.2	56.6	*147.6*	*177.9*	Sep		356.5	357.1	332.4	*348.7*	*14.1*
Seas_3	**1170.2**	**332.5**	**-689.9**	**887.0**	**2155.0**	**180.1**	**142.2**	***596.7***	***908.0***	**Seas_3**	**1831.6**	**1069.4**	**1071.0**	**984.8**	***1239.2***	***397.0***
Oct	441.7	147.1	17.6	229.6		56.6	43.4	*156.0*	*160.5*	Oct		351.3	352.0	275.6	*326.3*	*43.9*
Nov	437.5	227.5	81.2	252.7		70.2	57.3	*187.7*	*148.6*	Nov		353.3	354.1	290.9	*332.8*	*36.3*
Dec	445.6	236.0	141.4	214.6		70.7	57.8	*194.3*	*142.8*	Dec		352.1	352.9	254.4	*319.8*	*56.6*
Seas_4	**1324.8**	**610.6**	**240.2**	**696.8**	**2151.8**	**197.5**	**158.5**	***768.6***	***733.7***	**Seas_4**	**1809.3**	**1056.7**	**1058.9**	**820.8**	***1186.4***	***430.0***
Annual	**4844.3**	**2297.5**	**-15289.1**	**3124.9**	**8588.8**	**766.4**	**628.6**	***708.8***	***7566.4***	**Annual**	**7161.1**	**4393.6**	**4398.6**	**3606.6**	***4890.0***	***1559.2***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table 3.57. *Comparison of the calculation results on PCB-153 mass flows transported in/out the specified domain (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative"*

Month	CliMoChem_2_3		G-CIEMS_1		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0_3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			359.6	351.2	-5266.8	-5465.1	400.5	399.7	400.5	399.7	240.2	58.1	232.7	50.6	222.4	214.0	258.8	260.0		
Feb			324.0	315.4	-3262.2	-3497.2	391.2	389.7	391.3	389.8	254.4	83.0	247.4	74.3	216.9	206.3	262.1	262.3		
Mar			250.1	245.4	-2262.5	-2515.6	378.8	376.4	379.0	376.6	239.7	55.9	232.7	45.5	265.9	257.4	302.3	302.5		
Seas_1	**2168.7**	**2138.8**	**933.6**	**912.0**	**-10791.5**	**-11478.0**	**1170.5**	**1165.8**	**1170.8**	**1166.1**	**734.2**	**197.0**	**712.8**	**170.4**	**705.2**	**677.6**	**823.2**	**824.8**	**1871.9**	**1744.9**
Apr			211.2	208.9	-1386.2	-1614.0	376.0	372.8	376.2	373.0	246.6	68.5	240.1	57.6	301.3	297.7	327.7	329.7		
May			117.4	119.3	-875.9	-1085.8	368.9	364.8	369.2	365.1	239.4	55.1	232.7	43.4	271.6	274.3	308.2	317.3		
Jun			112.4	114.2	-484.4	-661.5	368.8	364.1	369.1	364.5	246.6	68.2	240.1	56.4	281.9	291.5	316.7	329.3		
Seas_2	**2163.3**	**2143.3**	**441.0**	**442.4**	**-2746.5**	**-3361.4**	**1113.6**	**1101.7**	**1114.5**	**1102.6**	**732.6**	**191.7**	**712.8**	**157.4**	**854.8**	**863.5**	**952.6**	**976.3**	**1859.4**	**1775.3**
Jul			113.3	114.9	-247.9	-405.9	363.2	357.7	363.7	358.2	239.5	55.3	232.7	42.7	264.9	279.2	302.8	318.3		
Aug			97.6	99.6	-74.6	-210.2	361.2	355.1	361.8	355.7	239.6	55.7	232.7	42.9	286.8	302.4	317.8	334.0		
Sep			116.1	118.1	39.5	-73.8	362.9	356.5	363.5	357.1	246.9	69.2	240.1	56.6	296.0	305.3	321.3	332.4		
Seas_3	**2177.5**	**2155.0**	**327.0**	**332.5**	**-283.0**	**-689.9**	**1087.3**	**1069.4**	**1088.9**	**1071.0**	**726.0**	**180.1**	**705.4**	**142.2**	**847.8**	**887.0**	**941.9**	**984.8**	**1936.0**	**1831.6**
Oct			145.7	147.1	119.2	17.6	358.3	351.3	359.0	352.0	239.9	56.6	232.7	43.4	230.7	229.6	270.9	275.6		
Nov			228.6	227.5	167.3	81.2	360.5	353.3	361.2	354.1	247.2	70.2	240.1	57.3	259.5	252.7	291.8	290.9		
Dec			236.7	236.0	217.6	141.4	359.5	352.1	360.3	352.9	247.4	70.7	240.1	57.8	221.5	214.6	255.2	254.4		
Seas_4	**2171.5**	**2151.8**	**611.0**	**610.6**	**504.0**	**240.2**	**1078.3**	**1056.7**	**1080.5**	**1058.9**	**734.6**	**197.5**	**712.8**	**158.5**	**711.7**	**696.8**	**817.9**	**820.8**	**1906.9**	**1809.3**
Annual	**8680.9**	**8588.8**	**2312.6**	**2297.5**	**-13317.0**	**-15289.1**	**4449.8**	**4393.6**	**4454.8**	**4398.6**	**2927.4**	**766.4**	**2843.9**	**628.6**	**3119.5**	**3124.9**	**3535.7**	**3606.6**	**7574.3**	**7161.1**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

3.3.5. Comparison of PCB-153 mass flows transported in/out the specified domain

The calculation results on PCB-153 transport inside and outside the calculation domain through main transport media such as atmosphere and seawater are discussed in this subsection. Transport of this pollutant from sediment, soil and vegetation compartments due to such processes as burial, leaching and harvest of agricultural vegetation, respectively, is considered in SimpleBox model.

The results considered in Sections 3.3.1-3.3.4 above are obtained with one-year calculations with zero initial concentrations (ADEPT, CliMoChem, G-CIEMS, MSCE-POP, SimpleBox) and with initial concentrations in media (CAN/POPs, G-CIEMS, MSCE-POP, SimpleBox); and with long-term calculations with historical emissions (CliMoChem, SimpleBox). CliMoChem, G-CIEMS, MSCE-POP, and SimpleBox models presented results obtained on the basis of two different physical-chemical data sets. Of note, the calculated values compared below are negative in the case if a model predicted PCB-153 transport out the calculation domain through the considered media.

A preliminary analysis of the comparison of absolute values PCB-153 transport mass flows inside and outside the calculation domain through main transport media is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions and for results based on zero initial conditions.

Transport through the atmosphere. According to the results on PCB-153 mass flows transported out the calculation domain through the atmosphere calculated on the basis of "reference" and 'own/alternative" data sets (see Tables 3.46 and 3.47 in Section 3.3.1), all models in two groups performed calculations on the basis of non-zero and zero initial conditions give rather close values in terms of annual and monthly absolute values. Square deviation σ does not exceed the mean value of this parameter averaged between the participating models.

Comparison of annual values of PCB-153 mass flows transported out the calculation domain through the atmosphere calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig.3.76a together with the averaged value given as the blue line. Fig. 3.76b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

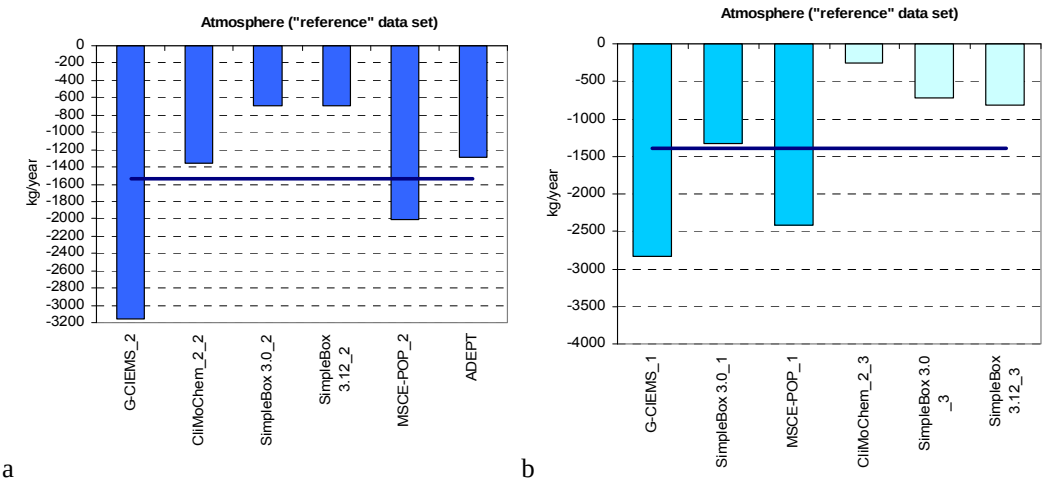
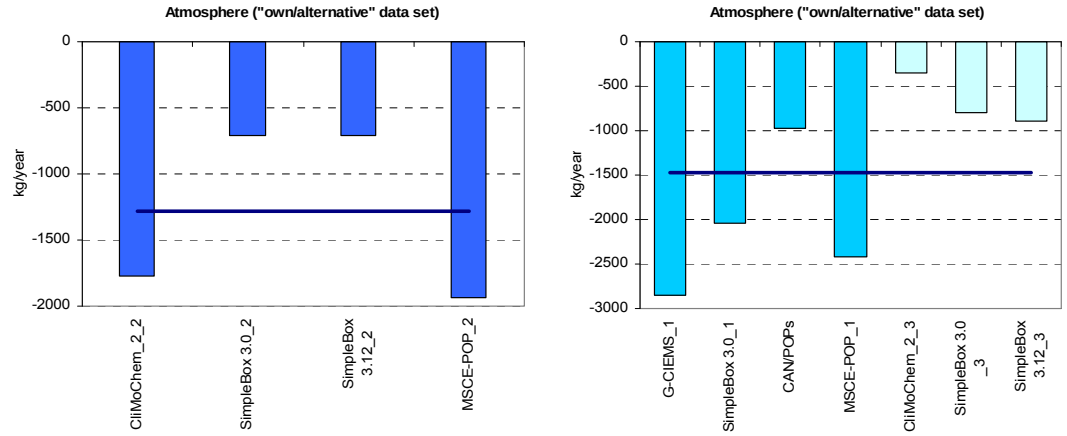


Fig.3.76. *Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

According to the results based on zero initial conditions (see Fig. 3.76a), the difference in absolute values of PCB-153 mass flows transported out the calculation domain through the atmosphere is within a factor of 4.5. At that G-CIEMS and MSCE-POP results calculated on the basis of zero initial conditions exceed the same results of CliMOChem, SimpleBox and ADEPT models and the mean value averaged for all models' results. The calculated absolute values obtained by G-CIEMS, MSCE-POP and SimpleBox 3.0 on the basis of initial conditions are higher than those obtained by CliMoChem and SimpleBox 3.0 and 3.12 with the use of historical emissions (see Fig. 3.76b). The maximum value of PCB-153 mass flows transported out the calculation domain through the atmosphere was obtained by G-CIEMS; the minimum – by CliMoChem model.

Fig.3.77a demonstrates the comparison of the annual values of PCB-153 mass flows transported out the calculation domain through the atmosphere calculated on the basis of zero initial concentrations and with the use of "**own or alternative"** data sets. Fig. 3.77b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig.3.77. *Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

As in the case of results obtained with the use of "reference" data set, absolute values of PCB-153 mass flows transported out the calculation domain through the atmosphere results calculated by MSCE-POP and CliMoChem models on the basis of zero initial conditions are higher than those of SimpleBox model and the mean averaged value (see Fig. 3.77a). The scattering between different results based on non-zero initial conditions is less considerable than that in the case of calculations made with the use of "reference" data set (see Fig. 3.77b). The maximum and the minimum absolute values obtained on the basis of non-zero initial conditions are characteristic of G-CIEMS and CliMoChem models' results.

Comparison of annual values of PCB-153 mass flows transported out the calculation domain through the atmosphere obtained with "reference" and "own/alternative" data sets is presented in Fig. 3.78 (see also Table 3.48 given in Section 3.3.1).

According to the data presented, for MSCE-POP results based on initial concentrations of the pollutant in the environmental media there is practically no difference between the annual values calculated with the use of both physical-chemical data sets. In calculations made by this model with zero initial conditions, the usage of "reference" data set slightly increases the absolute value of the considered parameter in comparison with the use of "own or alternative" data. All other models provided higher results obtained on the basis of "own or alternative" data set than those based on "reference" data set.

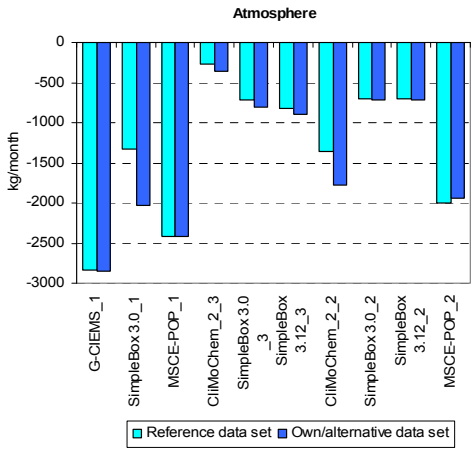


Fig.3.78. *Comparison of PCB-153 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of two physical-chemical data sets*

Transport through ocean. The difference between participating models in terms of description of PCB transport through seawater compartment is more considerable than that in the case of atmospheric transport. This is observed for results obtained with the use of "own/alternative" data sets both on the basis of zero initial conditions and historical emissions and initial concentrations of the pollutant in the media (see Tables 3.49 and 3.50 given in Section 3.3.2). In the results based on "reference" data set, the square deviation presented for annual and monthly values mainly does not exceed the averaged values.

Comparison of annual values of PCB-153 mass flows transported out the calculation domain through ocean calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig.3.79a. Fig. 3.79b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

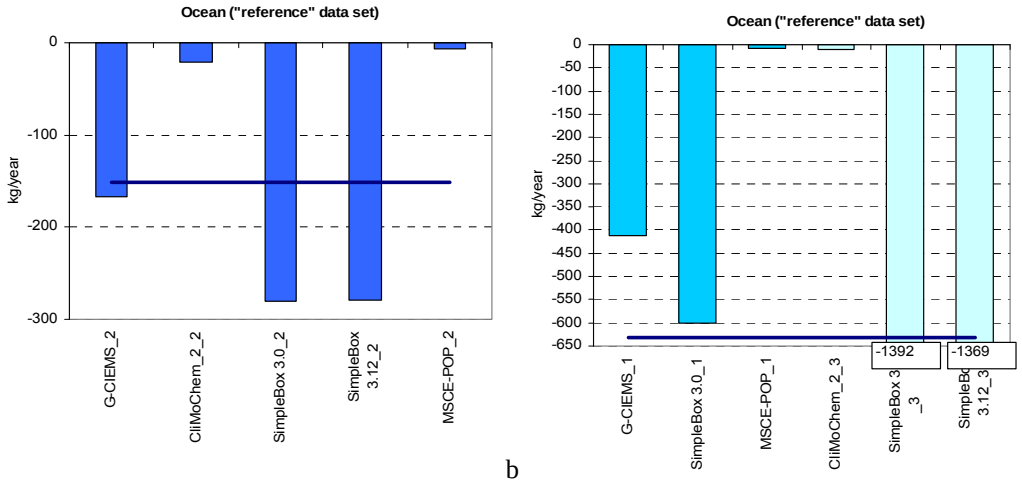


Fig.3.79. *Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The absolute value of PCB-153 mass flows transported out the calculation domain through ocean calculated by MSCE-POP and CliMoChem models on the basis of zero initial conditions is lower than the same values of G-CIEMS and SimpleBox 3.0 and 3.12 (see Fig. 3.79a). The difference in annual values of PCB-153 mass flows transported out the calculation domain through ocean based on the initial conditions reaches several orders of magnitude due to the minimum and maximum values corresponding to the results of MSCE-POP and SimpleBox 3.0 models, respectively (see Fig. 3.79 b). Three groups of the models' results can be conditionally divided in this experiment: results with the high absolute values (SimpleBox 3.0 and 3.12 used historical emissions); with the medium values (G-CIEMS, and SimpleBox 3.0 based on initial concentrations) and with the low values (MSCE-POP and CliMoChem).

Comparison of annual values of PCB-153 mass flows transported out the calculation domain through ocean calculated by different models on the basis of zero initial concentrations and with the use of "**own or alternative"** data sets is presented in Fig.3.80a. Fig. 3.80b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

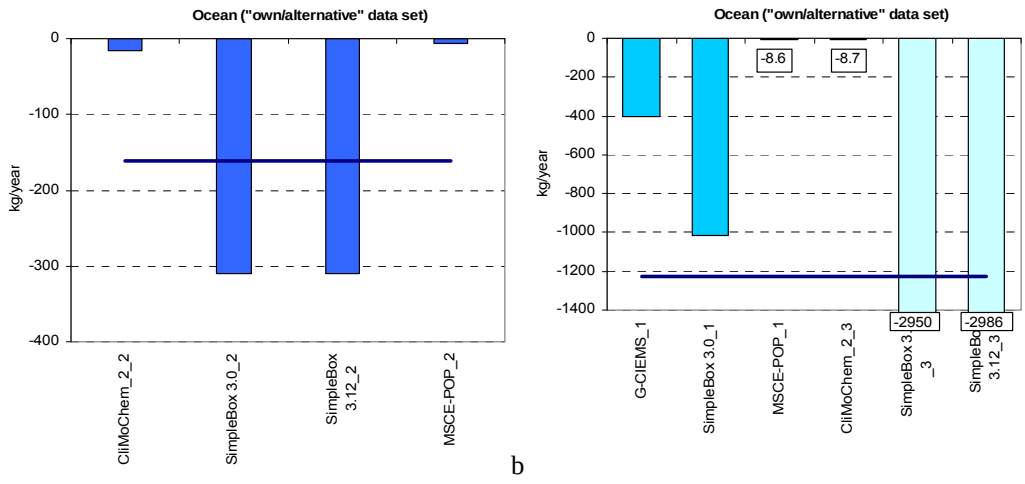


Fig.3.80. *Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The absolute values of PCB-153 mass flows transported out the calculation domain through ocean calculated by SimpleBox 3.0 and 3.12 on the basis of zero initial conditions exceed that obtained by MSCE-POP and CliMoChem models (see Fig. 3.80a). The highest values of PCB-153 mass flows transported out the calculation domain through ocean based on non-zero initial conditions are calculated by SimpleBox model on the basis of historical emissions; and the lowest values are characteristic of results of MSCE-POP and CliMOChem calculations (see Fig. 3.80b).

Comparison of annual values of PCB-153 mass flows transported out the calculation domain through ocean obtained with “reference” and “own/alternative” data sets is presented in Table 3.51 given in Section 3.3.2 and in Fig. 3.81a below. The same data for models with low values of mass flows transported out the calculation domain through ocean are also shown in Fig. 3.81b in more detail.

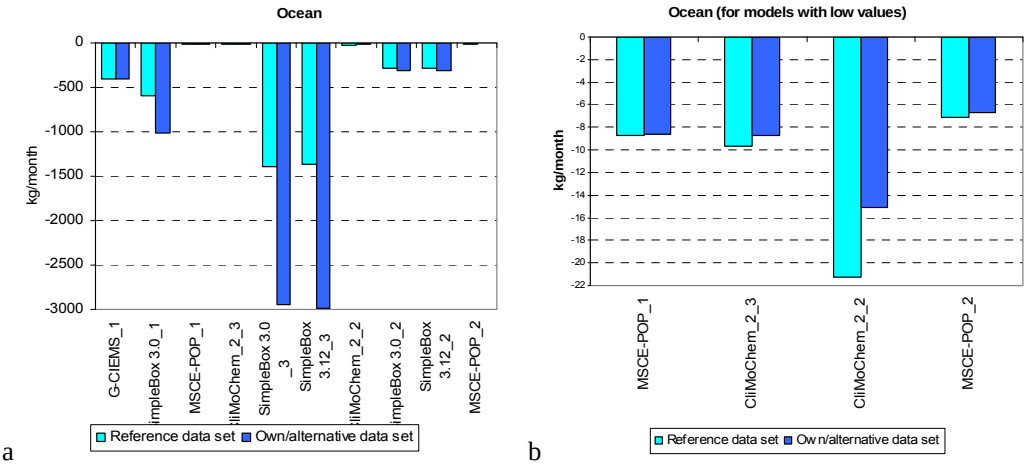


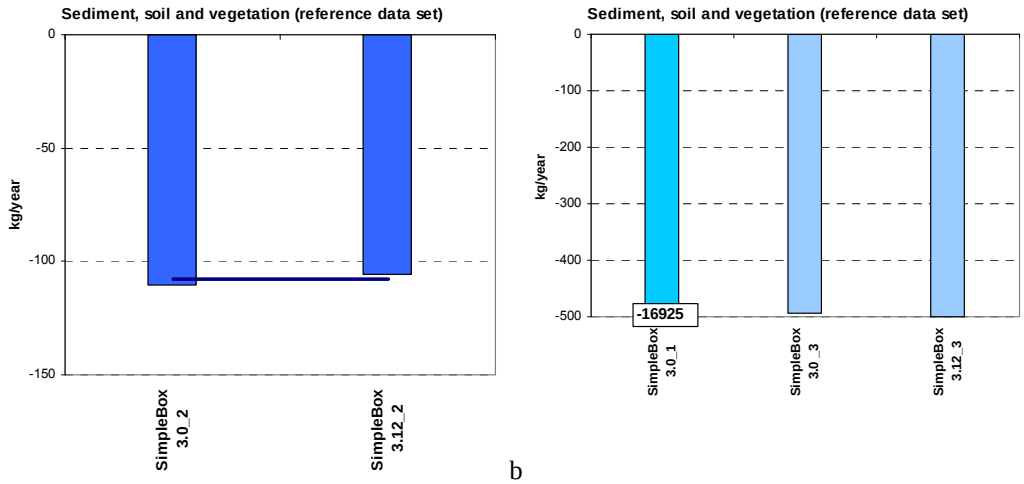
Fig.3.81. *Comparison of PCB-153 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of two data sets (a - all models; b – models with low values of PCB-153 mass flows transported in/out of ocean).*

For G-CIEMS, MSCE-POP and CliMoChem models, absolute values of PCB-153 mass flows transported out the calculation domain through ocean obtained with “reference” data set are somewhat higher than those obtained with “own/alternative” data set. The most considerable difference between two sets of results is characteristic of SimpleBox 3.0 and 3.12 calculations carried out on the basis of historical emissions.

Transport through other media. In addition to the results on mass flows of PCB-153 transported out the calculation domain via the atmosphere and ocean, SimpleBox model presented calculated values of outflows from sediments, soil and vegetation. Transport of this pollutant from these compartments is considered to be due to such processes as burial, leaching and harvest of agricultural vegetation, respectively.

According to the data presented in Tables 3.52 and 3.53 (see Section 3.3.3), the scattering between absolute values of PCB-153 mass flows transported out the calculation domain obtained on the basis of both data sets with different type of SimpleBox 3.0 and 3.12 calculations exceed an order of magnitude for sediment compartment; two orders of magnitude for vegetation compartments and four orders of magnitude for soil compartments. The highest absolute values are characteristic of PCB-153 outflow through vegetation compartment; then come transport via sediments and then – outflow from soil compartment.

Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of zero initial concentrations and with the use of “**reference”** data set is presented in Fig.3.82a. Fig. 3.82b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between calculations of different types.

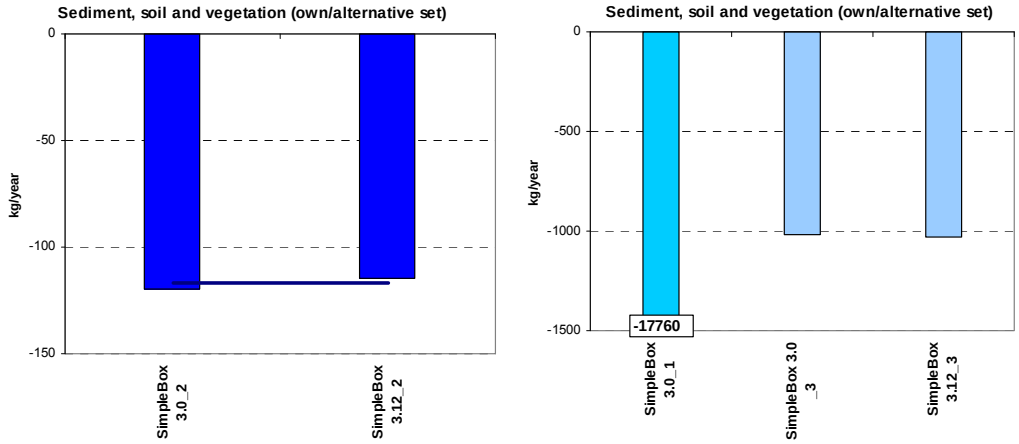


a b

Fig.3.82. *Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions).*

The maximum annual value of PCB-153 mass flows transported out the calculation domain through three considered media as a whole is obtained by SimpleBox model (version 3.0) on the basis of initial concentrations given as input data (see Fig. 3.82b). The smaller are values calculated by SimpleBox 3.0 and 3.12 with the use of historical emissions. Then come results based on zero initial conditions (see Fig. 3.82a).

The annual values of PCB-153 mass flows transported out the calculation domain through three considered media calculated by SimpleBox model on the basis of zero initial concentrations and "**alternative**" data set are compared in Fig.3.83a. Fig. 3.83b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between different versions of this model.



a b

Fig.3.83. *Comparison of annual values of PCB-153 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Annual values of PCB-153 mass flows transported out the calculation domain through such media as sediment, soil and vegetation obtained with “reference” and “own/alternative” data sets are compared in Fig. 3.84.

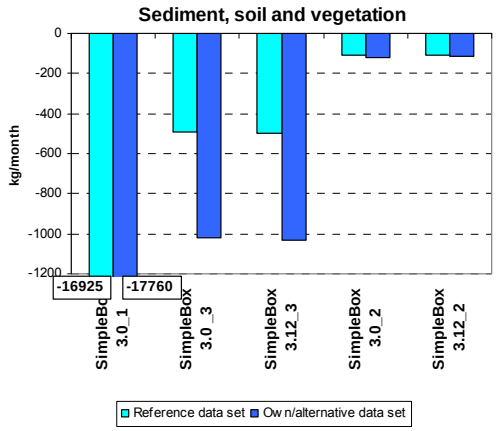


Fig.3.84. *Comparison of PCB-153 mass flows transported in/out the calculation domain through the atmosphere (a), other media (sediment, soil and vegetation)(b) and seawater(c, d) calculated by different models on the basis of two data sets*

This comparison demonstrates that the considered values of PCB-153 mass flows transported out the calculation domain through all three considered media as a whole obtained on the basis of “alternative” data set are higher than those based on “reference” data set. At that, for sediment (see Table 3.54 Section 3.3.3), results of calculations of SimpleBox model (versions 3.0 and 3.12) based on zero initial conditions and “reference” data set exceed slightly those obtained on the basis of “alternative” data set. According to the data on percentage difference between calculation results presented in Table 3.54, the major difference between two sets of results is found in results of SimpleBox 3.12 on PCB-153 mass flows transported out the calculation domain through soil making up approximately 3000%.

Total mass flow. The scattering of total mass flow values calculated on the basis of historical emissions and initial concentrations is rather high both in results based on “reference” and ‘own/alternative” data sets (Tables 3.55 and 3.56 in Section 3.3.4). However, the difference between results obtained with the use of zero initial conditions is considerably lower. According to the results of most models obtained on the basis of two different data sets, total mass flow calculated as sum of emissions and outflows through the considered media is transported into the calculation domain. Exceptions are results of SimpleBox 3.0 model obtained on the basis of initial concentrations given as input data.

Comparison of annual values of PCB-153 total mass flows transported in/out the calculation domain calculated by different models on the basis of zero initial concentrations and with the use of “***reference*”** data set is presented in Fig.3.85a. Fig. 3.85b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

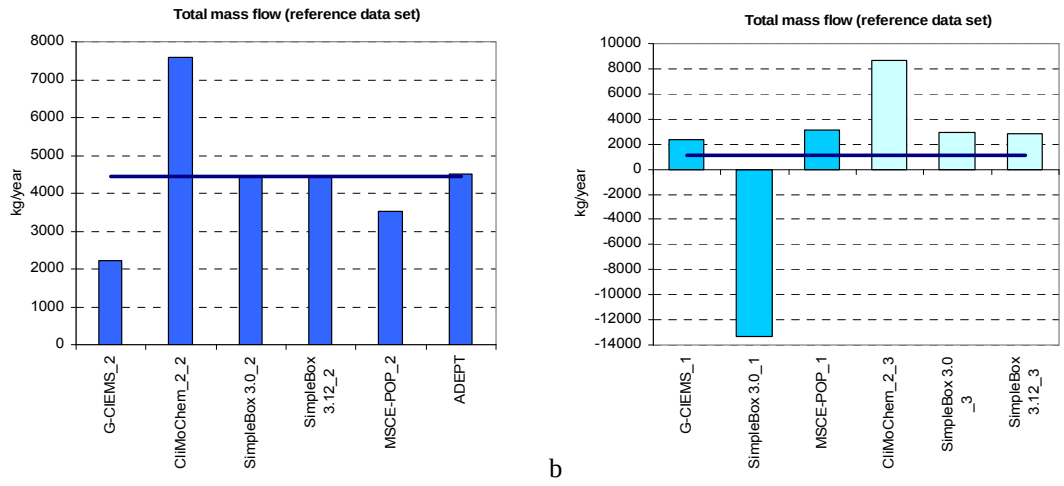


Fig.3.85. *Comparison of annual values of PCB-153 total mass flows transported in/out the calculation domain calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

The most part of participating models performed calculations on the basis of zero initial conditions provide rather close estimates of total mass flow (see Fig. 3.85a). According to the results of SimpleBox 3.0 models obtained on the basis of initial concentrations given as input data, PCB-153 emissions value in the considered year do not exceed the value of total mass flow of this pollutant transported outside calculation domain (see Fig. 3.85b). The only negative absolute value is characteristic of SimpleBox 3.0 result obtained on the basis of initial conditions. The highest value among flows directed to the calculation domain is obtained by CliMoChem model.

Comparison of annual values of PCB-153 total mass flows transported in/out the calculation domain calculated by different models on the basis of zero initial concentrations and "***own or alternative***" data sets is presented in Fig.3.86a. Fig. 3.86b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

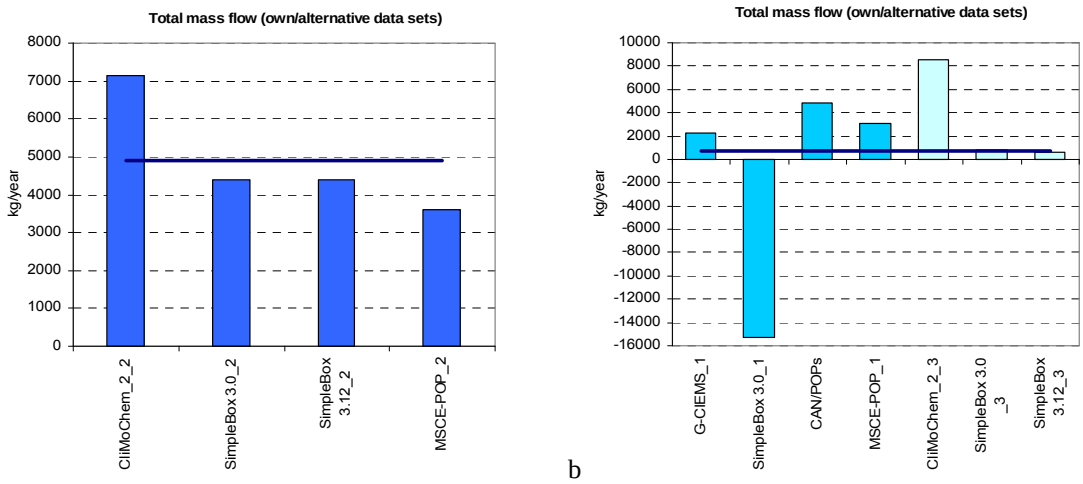


Fig.3.86. *Comparison of annual values of PCB-153 total mass flows transported in/out the calculation domain calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

As in the case of results obtained on the basis of “reference” data set, the results on total mass flow obtained on the basis of zero initial conditions are close for most participating models (see Fig. 3.86a). The main difference in total mass flow obtained on the basis of non-zero initial conditions reaching several orders of magnitude is observed between results of SimpleBox 3.0 models obtained on the basis of initial concentrations given as input data and CliMoChem results based on historical emissions (see Fig. 3.86b).

For models performed calculations on two data sets, the annual values of PCB-153 mass flow transported inside and outside the calculation domain (taking into account emissions) obtained with “reference” and “own/alternative” data sets are compared in Fig. 3.87a. Fig. 3.87b presents also the comparison of absolute values of overall mass flow transported outside the calculation domain (not taking into account emission value).

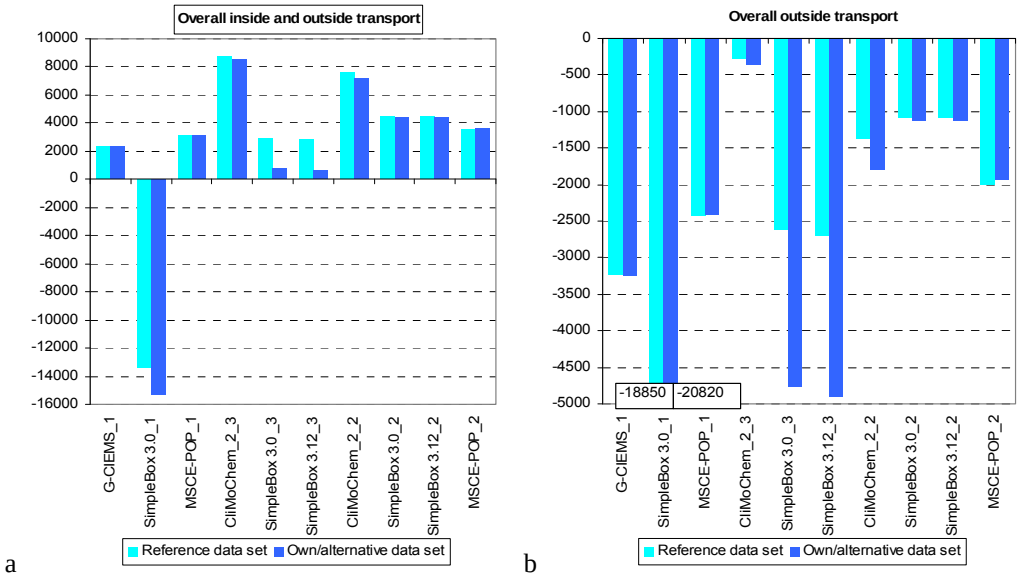
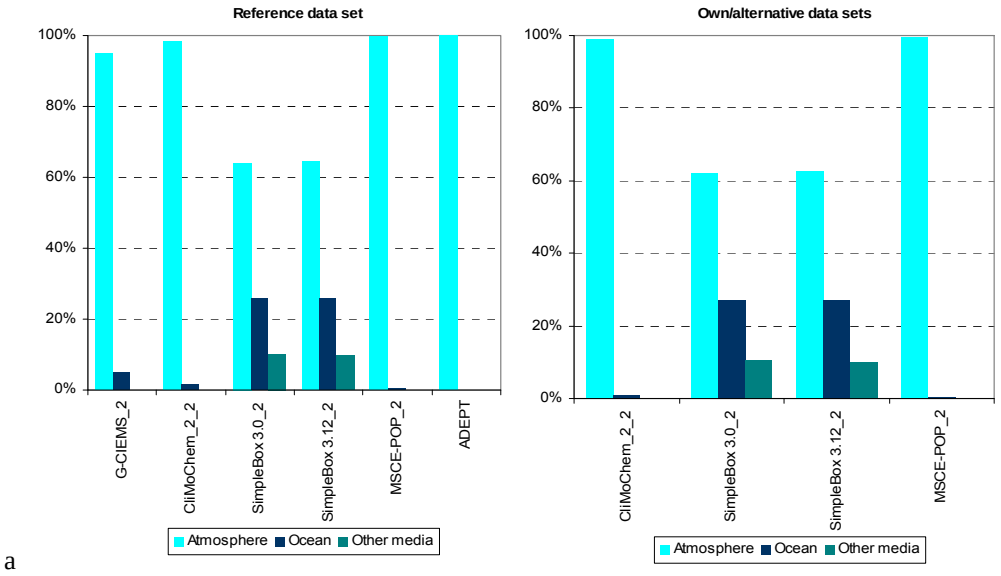


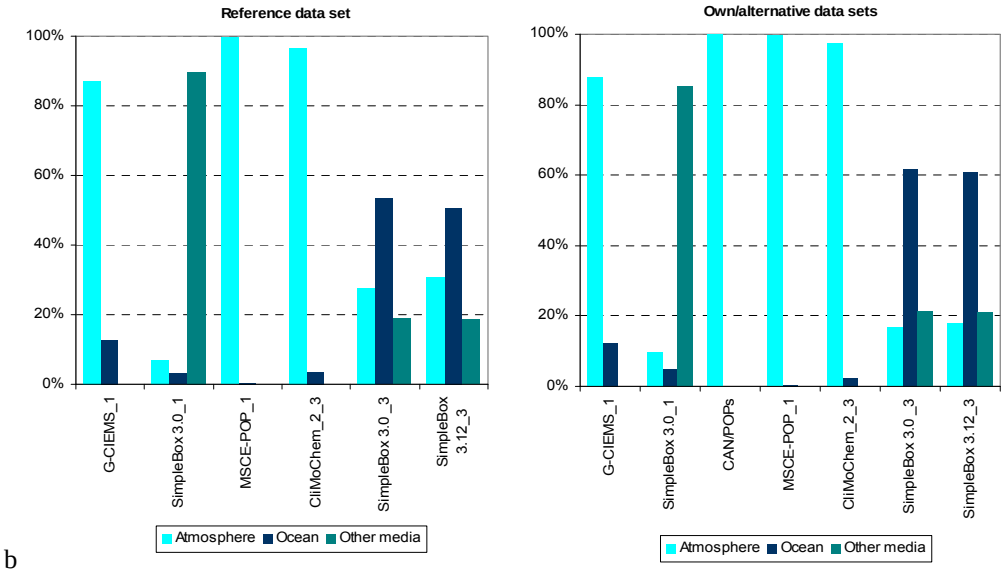
Fig.3.87. *Comparison of PCB-153 overall transport inside and outside the calculation domain (taking into account emissions) (a) and overall transport outside the calculation domain (b) calculated by different models on the basis of two data sets*

According to the data presented in Figs. 3.87 a and b, it can be concluded that the largest difference in the results obtained with two data sets (‘reference” and ‘own/alternative”) is characteristic of SimpleBox 3.0 and 3.12 calculations performed on the basis of initial concentrations and historical emissions. At that results of these model on overall outside transport flow obtained with the use of “own or alternative” data sets are higher than those obtained with “reference” data set (see Fig. 3.87 b). For other models difference in two sets of results is not essential. The latter figure also testifies that the highest and lowest absolute values of overall mass flow transported outside the calculation domain and calculated not taking into account emission value are obtained by SimpleBox 3.0 and CliMoChem models on the basis of initial conditions and historical emissions, respectively.

Fractions of overall outside transport through atmosphere, ocean and other media (sediment, soil and vegetation) calculated on the basis of zero and non-zero initial conditions are presented in Figs. 3.88a and b, respectively. In these figures fractions of PCB-153 mass in soil calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared.



a



b

Fig.3.88. *Comparison of PCB-153 fractions of overall outside transport through atmosphere, ocean and other media (sediment, soil and vegetation) calculated by different models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

According to the data presented for both "reference" and "own/alternative" data sets, in ADEPT, CAN/POPS and MSCE-POP model results the atmosphere is the main media of PCB-153 outside transport. Calculated fractions of overall outside transport through atmosphere considerably exceed those for other media in results of G-CIEMS, CliMoChem and SimpleBox 3.0 and 3.12 (zero initial conditions) models. It is worth noting that results of SimpleBoxs 3.0 and 3.12 based on historical emissions are characterised by higher annual transport in the marine environment than in the atmosphere. The most considerable contribution to the outside transport of PCB-153 due to the other considered media (sediment, soil and vegetation) than ocean and atmosphere is observed in the results of SimpleBox 3.0 model made on the basis of initial conditions.

3.4. Mass flows transported from one compartment to another in both directions

3.4.1. Comparison of calculated values of PCB-153 mass flows transported from the atmosphere to soil

Dry deposition

Reference data set. Calculation results on PCB-153 mass flows transported from the atmosphere to soil: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.58.

Monthly values of PCB-153 mass flows transported from the atmosphere to soil: dry deposition calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.89 a and b, respectively.

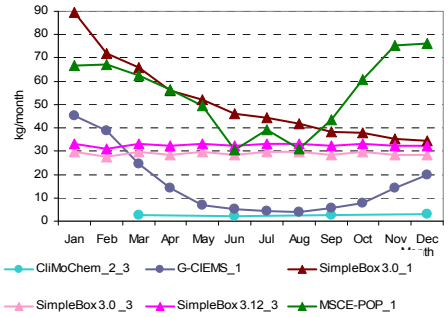


Fig. 3.89a. *PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

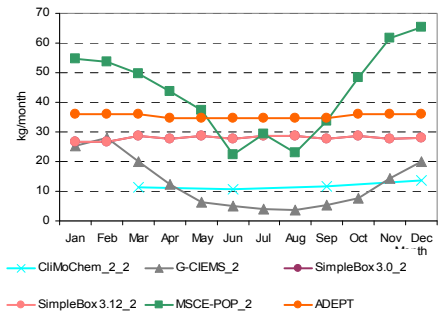


Fig. 3.89b. *PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported from the atmosphere to soil: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.59.

Monthly values of PCB-153 mass flows transported from the atmosphere to soil: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.90 a and b, respectively.

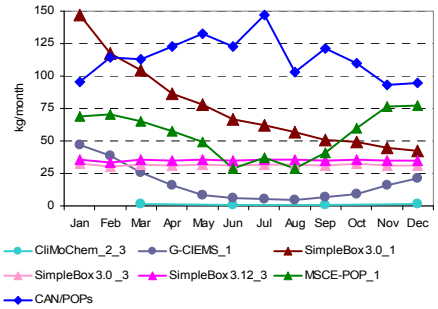


Fig. 3.89a. *PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

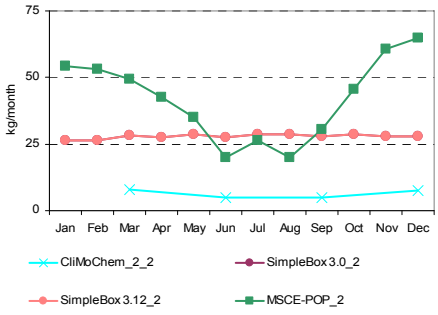


Fig. 3.89b. *PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.58. *Calculation results: PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	45.21	89.58	66.70		29.81	33.33	*52.93*	*25.06*	Jan	25.17		26.67	26.67	54.80	36.10	*33.88*	*12.47*
Feb	38.96	71.78	67.20		27.65	31.18	*47.35*	*20.68*	Feb	28.08		26.64	26.64	53.60	36.10	*34.21*	*11.53*
Mar	24.35	65.92	62.60		29.56	33.33	*43.15*	*19.57*	Mar	19.91		28.54	28.54	49.60	36.10	*32.54*	*11.13*
Seas_1	**108.52**	**227.28**	**196.50**	**7.41**	**87.02**	**97.85**	***120.76***	***79.68***	**Seas_1**	**73.16**	**34.460**	**81.85**	**81.85**	**158.00**	**108.30**	***89.60***	***41.13***
Apr	14.06	56.04	56.20		28.61	32.26	*37.43*	*18.37*	Apr	12.43		27.67	27.67	43.70	34.60	*29.21*	*11.46*
May	6.83	52.02	49.60		29.57	33.33	*34.27*	*18.21*	May	6.41		28.63	28.63	37.30	34.60	*27.11*	*12.18*
Jun	5.12	46.07	30.40		28.62	32.26	*28.49*	*14.77*	Jun	4.93		27.73	27.73	22.20	34.60	*23.44*	*11.24*
Seas_2	**26.01**	**154.14**	**136.20**	**6.63**	**86.80**	**97.85**	***84.61***	***58.63***	**Seas_2**	**23.76**	**31.524**	**84.02**	**84.03**	**103.20**	**103.80**	***71.72***	***35.32***
Jul	4.15	44.25	39.30		29.57	33.33	*30.12*	*15.56*	Jul	4.08		28.68	28.69	29.20	34.60	*25.05*	*11.99*
Aug	3.74	41.61	30.90		29.57	33.33	*27.83*	*14.25*	Aug	3.72		28.70	28.71	22.90	34.60	*23.73*	*11.93*
Sep	5.47	38.28	43.40		28.62	32.26	*29.60*	*14.63*	Sep	5.46		27.80	27.80	33.60	34.60	*25.85*	*11.83*
Seas_3	**13.36**	**124.13**	**113.60**	**7.27**	**87.77**	**98.93**	***74.18***	***51.04***	**Seas_3**	**13.26**	**34.582**	**85.18**	**85.19**	**85.70**	**103.80**	***67.95***	***35.49***
Oct	7.63	37.92	60.70		29.57	33.33	*33.83*	*19.00*	Oct	7.66		28.74	28.74	48.30	36.10	*29.91*	*14.78*
Nov	14.08	35.41	75.30		28.62	32.26	*37.13*	*22.84*	Nov	14.17		27.82	27.83	61.80	36.10	*33.55*	*17.65*
Dec	19.84	34.36	76.30		28.62	32.26	*38.28*	*21.97*	Dec	19.99		27.84	27.84	65.30	36.10	*35.41*	*17.65*
Seas_4	**41.55**	**107.69**	**212.30**	**8.47**	**86.81**	**97.85**	***92.45***	***69.71***	**Seas_4**	**41.83**	**41.063**	**84.40**	**84.41**	**175.40**	**108.30**	***89.23***	***49.80***
Annual	**189.44**	**613.24**	**658.60**	**29.78**	**348.40**	**392.48**	***371.99***	***241.56***	**Annual**	**152.01**	**141.630**	**335.46**	**335.49**	**522.30**	**424.20**	***318.51***	***149.86***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.59. *Calculation results: PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			***m***	**σ**	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	95.60	46.99	146.88	69.20		32.21	35.51	*71.07*	*44.06*	Jan		26.33	26.33	54.20	*35.62*	*16.09*
Feb	114.46	38.98	117.35	70.10		29.95	33.26	*67.35*	*40.23*	Feb		26.40	26.40	53.30	*35.37*	*15.53*
Mar	113.02	25.54	104.89	65.20		32.06	35.61	*62.72*	*38.40*	Mar		28.34	28.34	49.30	*35.33*	*12.10*
Seas_1	**323.08**	**111.51**	**369.11**	**204.50**	**5.18**	**94.22**	**104.38**	***173.1***	***132.2***	**Seas_1**	**23.50**	**81.07**	**81.07**	**156.80**	***85.6***	***54.7***
Apr	122.48	15.71	86.52	57.50		31.07	34.51	*57.96*	*40.09*	Apr		27.53	27.53	42.50	*32.52*	*8.65*
May	132.30	8.14	77.82	49.40		32.13	35.69	*55.91*	*43.85*	May		28.53	28.53	35.10	*30.72*	*3.80*
Jun	122.51	6.26	66.79	28.90		31.12	34.57	*48.36*	*41.17*	Jun		27.67	27.67	20.00	*25.11*	*4.43*
Seas_2	**377.29**	**30.12**	**231.13**	**135.80**	**3.12**	**94.32**	**104.76**	***139.5***	***128.3***	**Seas_2**	**14.65**	**83.73**	**83.72**	**97.60**	***69.9***	***37.4***
Jul	146.94	5.17	62.23	37.30		32.18	35.74	*53.26*	*49.34*	Jul		28.65	28.65	26.50	*27.93*	*1.24*
Aug	103.21	4.69	56.82	28.50		32.19	35.76	*43.53*	*33.65*	Aug		28.70	28.70	20.10	*25.83*	*4.97*
Sep	121.57	6.60	50.89	41.20		31.17	34.61	*47.67*	*39.10*	Sep		27.82	27.81	30.50	*28.71*	*1.55*
Seas_3	**371.72**	**16.46**	**169.95**	**107.00**	**3.23**	**95.53**	**106.12**	***124.3***	***123.2***	**Seas_3**	**15.02**	**85.17**	**85.16**	**77.10**	***65.6***	***33.9***
Oct	110.11	8.90	49.17	59.50		32.21	35.79	*49.28*	*34.38*	Oct		28.78	28.78	45.60	*34.38*	*9.71*
Nov	93.15	15.66	44.88	76.20		31.18	34.63	*49.28*	*29.46*	Nov		27.88	27.88	60.70	*38.82*	*18.95*
Dec	94.46	21.27	42.66	77.50		31.19	34.63	*50.29*	*28.99*	Dec		27.91	27.90	64.70	*40.17*	*21.24*
Seas_4	**297.72**	**45.83**	**136.71**	**213.20**	**4.83**	**94.58**	**105.06**	***128.3***	***99.8***	**Seas_4**	**23.13**	**84.56**	**84.56**	**171.00**	***90.8***	***60.8***
Annual	**1369.80**	**203.92**	**906.91**	**660.50**	**16.37**	**378.66**	**420.32**	***565.21***	***458.39***	**Annual**	**76.30**	**334.53**	**334.51**	**502.50**	***311.96***	***175.93***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.60.

Table 3.60. *The percentage difference between calculation results on PCB-153 mass flows transported from the atmosphere to soil: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			3.9%	64.0%	-1.3%	-1.3%	8.1%	6.5%	3.7%	-1.1%
Feb			0.1%	63.5%	-0.9%	-0.9%	8.3%	6.7%	4.3%	-0.6%
Mar			4.9%	59.1%	-0.7%	-0.7%	8.5%	6.8%	4.2%	-0.6%
Seas_1	**-31.8%**	**-30.1%**	**2.8%**	**62.4%**	**-1.0%**	**-1.0%**	**8.3%**	**6.7%**	**4.1%**	**-0.8%**
Apr			11.8%	54.4%	-0.5%	-0.5%	8.6%	7.0%	2.3%	-2.7%
May			19.2%	49.6%	-0.3%	-0.4%	8.7%	7.1%	-0.4%	-5.9%
Jun			22.3%	45.0%	-0.2%	-0.2%	8.7%	7.2%	-4.9%	-9.9%
Seas_2	**-53.5%**	**-53.0%**	**15.8%**	**50.0%**	**-0.4%**	**-0.4%**	**8.7%**	**7.1%**	**-0.3%**	**-5.4%**
Jul			24.5%	40.6%	-0.1%	-0.1%	8.8%	7.2%	-5.1%	-9.2%
Aug			25.4%	36.6%	0.0%	0.0%	8.8%	7.3%	-7.8%	-12.2%
Sep			20.7%	33.0%	0.1%	0.0%	8.9%	7.3%	-5.1%	-9.2%
Seas_3	**-56.6%**	**-55.5%**	**23.2%**	**36.9%**	**0.0%**	**0.0%**	**8.9%**	**7.3%**	**-5.8%**	**-10.0%**
Oct			16.7%	29.7%	0.1%	0.1%	8.9%	7.4%	-2.0%	-5.6%
Nov			11.2%	26.7%	0.2%	0.2%	8.9%	7.4%	1.2%	-1.8%
Dec			7.2%	24.2%	0.2%	0.2%	9.0%	7.4%	1.6%	-0.9%
Seas_4	**-43.7%**	**-43.0%**	**10.3%**	**27.0%**	**0.2%**	**0.2%**	**8.9%**	**7.4%**	**0.4%**	**-2.5%**
Annual	**-46.1%**	**-45.0%**	**7.6%**	**47.9%**	**-0.3%**	**-0.3%**	**8.7%**	**7.1%**	**0.3%**	**-3.8%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Wet deposition

Reference data set. Calculation results on PCB-153 mass flows transported from the atmosphere to soil: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.61.

Monthly values of PCB-153 mass flows transported from the atmosphere to soil: wet deposition calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.91 a and b, respectively.

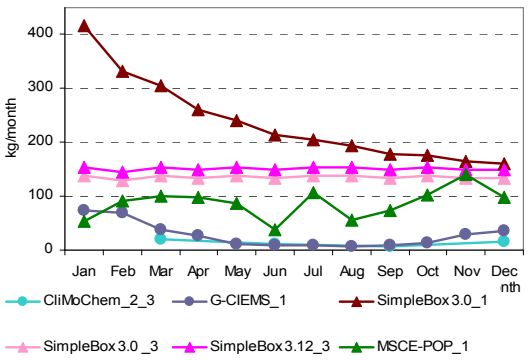


Fig. 3.91a. *PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

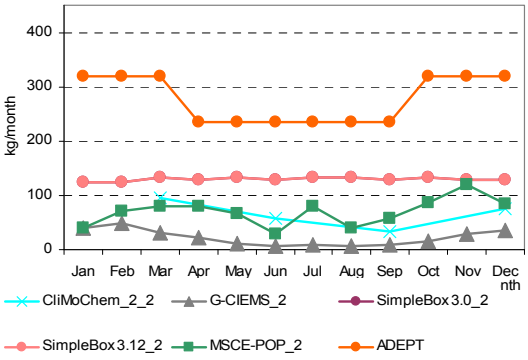


Fig. 3.91b. *PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported from the atmosphere to soil: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.62.

Monthly values of PCB-153 mass flows transported from the atmosphere to soil: wet deposition calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.92 a and b, respectively.

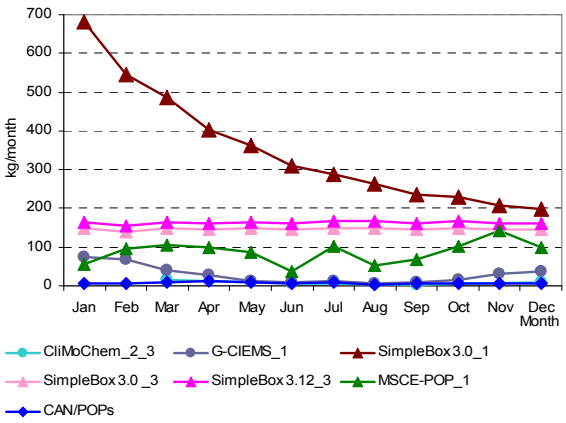


Fig. 3.92a. *PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

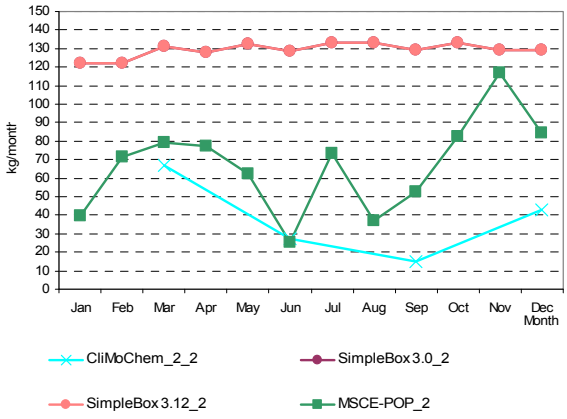


Fig. 3.92b. *PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.61. *Calculation results: PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by models on the basis of "reference" data set" and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	MSCE-POP_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	ADEPT		
Jan	72.54	415.63	52.70		138.27	154.63	*166.75*	*145.59*	Jan	40.39		39.60	123.71	123.71	318.20	*129.12*	*113.68*
Feb	68.85	333.02	91.00		128.27	144.65	*153.16*	*104.90*	Feb	49.62		71.10	123.57	123.58	318.20	*137.21*	*106.27*
Mar	38.00	305.85	101.00		137.13	154.63	*147.32*	*99.23*	Mar	31.08		79.60	132.38	132.38	318.20	*138.73*	*108.83*
Seas_1	**179.39**	**1054.50**	**244.70**	**62.01**	**403.66**	**453.91**	***399.70***	***351.66***	**Seas_1**	**121.09**	**288.58**	**190.30**	**379.66**	**379.66**	**954.60**	***385.65***	***297.10***
Apr	25.96	260.01	97.50		132.73	149.64	*133.17*	*85.33*	Apr	22.95		79.20	128.32	128.33	234.80	*118.72*	*78.09*
May	10.71	241.37	86.80		137.16	154.63	*126.13*	*85.27*	May	10.06		66.50	132.78	132.79	234.80	*115.39*	*84.18*
Jun	8.06	213.76	38.20		132.74	149.64	*108.48*	*84.25*	Jun	7.74		27.90	128.64	128.65	234.80	*105.54*	*91.33*
Seas_2	**44.74**	**715.14**	**222.50**	**36.56**	**402.63**	**453.91**	***312.58***	***263.13***	**Seas_2**	**40.76**	**173.77**	**173.60**	**389.74**	**389.77**	**704.40**	***312.01***	***235.76***
Jul	8.83	205.30	107.00		137.17	154.63	*122.58*	*72.91*	Jul	8.68		80.10	133.05	133.06	234.80	*117.94*	*82.89*
Aug	5.81	193.03	54.90		137.18	154.63	*109.11*	*76.67*	Aug	5.77		40.80	133.15	133.16	234.80	*109.53*	*89.86*
Sep	8.19	177.59	72.60		132.75	149.64	*108.15*	*67.83*	Sep	8.20		57.50	128.93	128.95	234.80	*111.68*	*85.73*
Seas_3	**22.83**	**575.92**	**234.50**	**21.65**	**407.10**	**458.89**	***286.81***	***232.55***	**Seas_3**	**22.64**	**103.03**	**178.40**	**395.12**	**395.17**	**704.40**	***299.79***	***249.86***
Oct	14.39	175.91	103.00		137.17	154.63	*117.02*	*63.28*	Oct	14.45		86.40	133.30	133.32	318.20	*137.14*	*112.29*
Nov	29.11	164.27	141.00		132.75	149.64	*123.35*	*53.96*	Nov	29.34		119.00	129.06	129.08	318.20	*144.94*	*105.55*
Dec	35.61	159.42	98.60		132.75	149.64	*115.20*	*50.15*	Dec	35.96		84.80	129.12	129.14	318.20	*139.44*	*107.08*
Seas_4	**79.11**	**499.59**	**342.60**	**46.88**	**402.68**	**453.91**	***304.13***	***194.24***	**Seas_4**	**79.75**	**227.22**	**290.20**	**391.48**	**391.54**	**954.60**	***389.13***	***300.49***
Annual	**326.07**	**2845.15**	**1044.30**	**167.09**	**1616.07**	**1820.61**	***1303.21***	***1005.56***	**Annual**	**264.24**	**792.59**	**832.50**	**1556.00**	**1556.14**	**3318.00**	***1386.58***	***1068.39***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.62. *Calculation results: PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPS	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	5.08	75.19	681.20	55.90		149.35	164.65	*188.56*	*248.56*	Jan		122.06	122.06	39.40	*94.51*	*47.73*
Feb	6.38	68.70	544.25	95.90		138.87	154.21	*168.05*	*191.72*	Feb		122.40	122.40	71.40	*105.40*	*29.44*
Mar	10.68	39.73	486.48	105.00		148.67	165.11	*159.28*	*171.19*	Mar		131.41	131.41	79.50	*114.11*	*29.97*
Seas_1	**22.14**	**183.63**	**1711.93**	**256.80**	**44.16**	**436.89**	**483.97**	***448.5***	***584.5***	**Seas_1**	**200.46**	**375.88**	**375.87**	**190.30**	***285.6***	***104.3***
Apr	10.89	28.90	401.27	99.30		144.04	160.00	*140.73*	*140.95*	Apr		127.63	127.63	77.30	*110.85*	*29.06*
May	8.86	12.70	360.96	86.30		148.98	165.49	*130.55*	*130.62*	May		132.27	132.26	62.60	*109.04*	*40.22*
Jun	5.68	9.79	309.79	36.50		144.29	160.28	*111.06*	*118.27*	Jun		128.31	128.30	25.20	*93.94*	*59.53*
Seas_2	**25.43**	**51.40**	**1072.01**	**222.10**	**17.26**	**437.32**	**485.76**	***330.2***	***380.0***	**Seas_2**	**81.08**	**388.20**	**388.19**	**165.10**	***255.6***	***156.9***
Jul	10.50	10.91	288.62	103.00		149.19	165.74	*121.33*	*105.40*	Jul		132.85	132.84	73.40	*113.03*	*34.32*
Aug	4.57	7.23	263.54	51.70		149.24	165.82	*107.02*	*103.20*	Aug		133.08	133.07	36.70	*100.95*	*55.64*
Sep	5.71	9.82	236.04	68.90		144.52	160.49	*104.25*	*91.68*	Sep		128.97	128.96	52.40	*103.44*	*44.20*
Seas_3	**20.78**	**27.96**	**788.20**	**223.60**	**9.64**	**442.96**	**492.05**	***286.5***	***299.0***	**Seas_3**	**44.78**	**394.89**	**394.87**	**162.50**	***249.3***	***174.9***
Oct	7.14	16.70	228.06	101.00		149.35	165.94	*111.37*	*87.14*	Oct		133.43	133.42	82.60	*116.48*	*29.35*
Nov	7.44	32.25	208.14	143.00		144.55	160.59	*115.99*	*78.51*	Nov		129.27	129.26	117.00	*125.17*	*7.08*
Dec	5.23	38.05	197.86	100.00		144.64	160.59	*107.73*	*74.43*	Dec		129.39	129.38	84.30	*114.36*	*26.03*
Seas_4	**19.81**	**87.00**	**634.05**	**344.00**	**27.04**	**438.55**	**487.12**	***291.1***	***246.8***	**Seas_4**	**129.48**	**392.09**	**392.06**	**283.90**	***299.4***	***124.2***
Annual	**88.16**	**349.99**	**4206.19**	**1046.50**	**98.10**	**1755.72**	**1948.91**	***1356.22***	***1468.13***	**Annual**	**455.80**	**1551.06**	**1550.99**	**801.80**	***1089.91***	***550.86***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.63.

Table 3.63. *The percentage difference between calculation results on PCB-153 mass flows transported from the atmosphere to soil: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			3.7%	63.9%	-1.3%	-1.3%	8.0%	6.5%	6.1%	-0.5%
Feb			-0.2%	63.4%	-1.0%	-1.0%	8.3%	6.6%	5.4%	0.4%
Mar			4.5%	59.1%	-0.7%	-0.7%	8.4%	6.8%	4.0%	-0.1%
Seas_1	**-30.5%**	**-28.8%**	**2.4%**	**62.3%**	**-1.0%**	**-1.0%**	**8.2%**	**6.6%**	**4.9%**	**0.0%**
Apr			11.3%	54.3%	-0.5%	-0.5%	8.5%	6.9%	1.8%	-2.4%
May			18.6%	49.5%	-0.4%	-0.4%	8.6%	7.0%	-0.6%	-5.9%
Jun			21.4%	44.9%	-0.3%	-0.3%	8.7%	7.1%	-4.5%	-9.7%
Seas_2	**-53.3%**	**-52.8%**	**14.9%**	**49.9%**	**-0.4%**	**-0.4%**	**8.6%**	**7.0%**	**-0.2%**	**-4.9%**
Jul			23.5%	40.6%	-0.1%	-0.2%	8.8%	7.2%	-3.7%	-8.4%
Aug			24.5%	36.5%	-0.1%	-0.1%	8.8%	7.2%	-5.8%	-10.0%
Sep			19.9%	32.9%	0.0%	0.0%	8.9%	7.3%	-5.1%	-8.9%
Seas_3	**-56.5%**	**-55.5%**	**22.5%**	**36.9%**	**-0.1%**	**-0.1%**	**8.8%**	**7.2%**	**-4.6%**	**-8.9%**
Oct			16.1%	29.6%	0.1%	0.1%	8.9%	7.3%	-1.9%	-4.4%
Nov			10.8%	26.7%	0.2%	0.1%	8.9%	7.3%	1.4%	-1.7%
Dec			6.9%	24.1%	0.2%	0.2%	9.0%	7.3%	1.4%	-0.6%
Seas_4	**-43.0%**	**-42.3%**	**10.0%**	**26.9%**	**0.2%**	**0.1%**	**8.9%**	**7.3%**	**0.4%**	**-2.2%**
Annual	**-42.5%**	**-41.3%**	**7.3%**	**47.8%**	**-0.3%**	**-0.3%**	**8.6%**	**7.0%**	**0.2%**	**-3.7%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Gaseous exchange

Reference data set. Calculation results on PCB-153 mass flows between the atmosphere and soil: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.64.

Monthly values of PCB-153 mass flows between the atmosphere and soil: gaseous exchange calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.93 a and b, respectively.

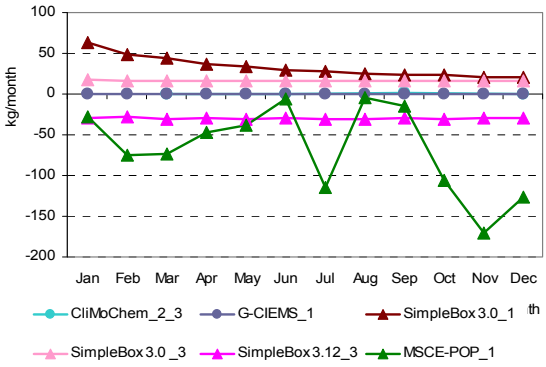


Fig. 3.93a. *PCB-153 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

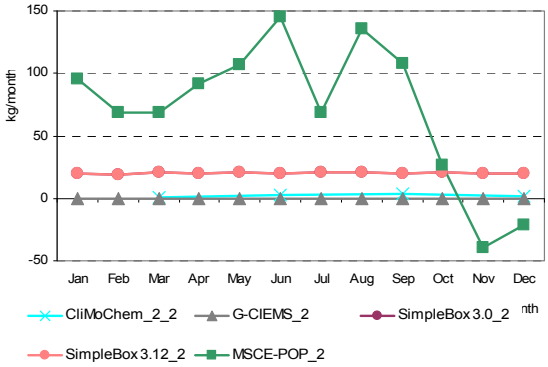


Fig. 3.93b. *PCB-153 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows between the atmosphere and soil: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.65.

Monthly values of PCB-153 mass flows between the atmosphere and soil: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.94 a and b, respectively.

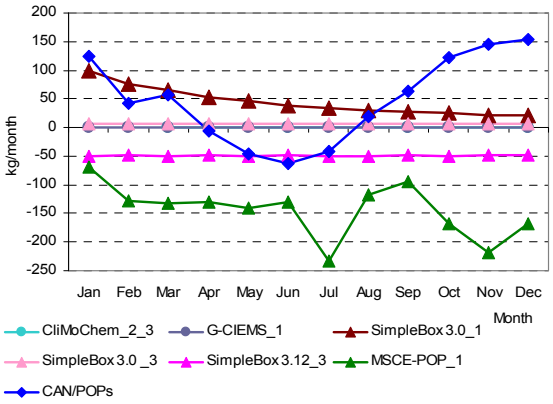


Fig. 3.94a. *PCB-153 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

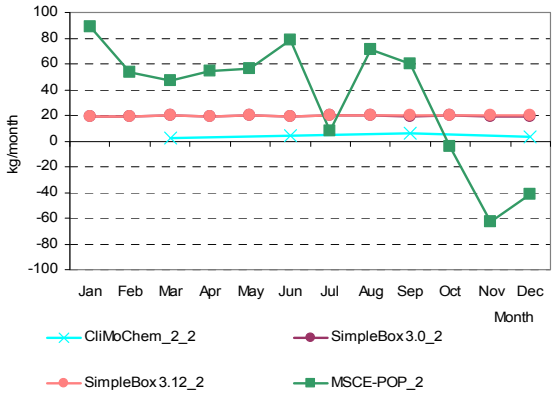


Fig. 3.94b. *PCB-153 mass between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.66.

Table 3.64. *Calculation results: PCB-153 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3a	SimpleBox 3.12_3a				G-CIEMS_2	CliMoChem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE- POP_2		
Jan	0.22	62.64	-28.10		17.22	-29.78	*4.44*	*38.08*	Jan	0.14		19.60	19.59	95.60	*33.73*	*42.25*
Feb	0.19	48.68	-74.80		15.57	-28.27	*-7.73*	*46.66*	Feb	0.15		19.24	19.23	69.10	*26.93*	*29.52*
Mar	0.15	43.96	-73.30		16.66	-30.22	*-8.55*	*45.08*	Mar	0.15		20.60	20.58	68.80	*27.53*	*29.15*
Seas_1	**0.56**	**155.28**	**-176.20**	**0.57**	**49.45**	**-88.27**	***-9.8***	***113.9***	**Seas_1**	**0.43**	**2.56**	**59.43**	**59.40**	**233.50**	***71.1***	***95.3***
Apr	0.12	36.73	-47.60		16.13	-29.24	*-4.77*	*33.97*	Apr	0.14		19.95	19.93	92.00	*33.01*	*40.42*
May	0.06	33.52	-38.90		16.68	-30.22	*-3.77*	*30.65*	May	0.12		20.64	20.61	107.00	*37.09*	*47.60*
Jun	0.04	29.21	-6.39		16.16	-29.24	*1.96*	*22.31*	Jun	0.13		19.98	19.94	145.00	*46.26*	*66.49*
Seas_2	**0.22**	**99.46**	**-92.89**	**1.39**	**48.97**	**-88.70**	***-5.3***	***75.7***	**Seas_2**	**0.39**	**6.54**	**60.57**	**60.48**	**344.00**	***94.4***	***142.4***
Jul	0.02	27.64	-115.00		16.70	-30.22	*-20.17*	*57.33*	Jul	0.13		20.65	20.61	68.80	*27.55*	*29.15*
Aug	0.01	25.63	-3.75		16.72	-30.22	*1.68*	*21.50*	Aug	0.13		20.66	20.61	136.00	*44.35*	*61.86*
Sep	0.05	23.30	-14.40		16.19	-29.24	*-0.82*	*21.59*	Sep	0.13		19.99	19.93	108.00	*37.01*	*48.24*
Seas_3	**0.07**	**76.57**	**-133.15**	**2.39**	**49.60**	**-89.67**	***-15.7***	***80.8***	**Seas_3**	**0.39**	**11.52**	**61.30**	**61.15**	**312.80**	***89.4***	***127.9***
Oct	0.07	22.82	-106.00		16.73	-30.22	*-19.32*	*52.64*	Oct	0.13		20.66	20.59	26.70	*17.02*	*11.62*
Nov	0.11	21.11	-170.00		16.20	-29.24	*-32.36*	*79.41*	Nov	0.15		19.99	19.92	-39.70	*0.09*	*28.12*
Dec	0.12	20.31	-126.00		16.21	-29.24	*-23.72*	*60.40*	Dec	0.15		19.98	19.91	-21.40	*4.66*	*19.72*
Seas_4	**0.30**	**64.24**	**-402.00**	**0.99**	**49.15**	**-88.70**	***-62.7***	***174.6***	**Seas_4**	**0.42**	**4.67**	**60.62**	**60.42**	**-34.40**	***18.3***	***41.4***
Annual	**1.16**	**395.56**	**-804.24**	**5.34**	**197.18**	**-355.33**	***-93.39***	***428.04***	**Annual**	**1.64**	**25.29**	**241.92**	**241.45**	**855.90**	***273.24***	***345.23***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.65. *Calculation results: PCB-153 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	124.03	0.15	98.37	-69.10		6.52	-50.07	*18.32*	*77.94*	Jan		18.95	18.95	88.80	*42.23*	*40.33*
Feb	42.04	0.12	75.79	-128.00		5.55	-47.19	*-8.61*	*71.70*	Feb		18.65	18.65	53.30	*30.20*	*20.01*
Mar	57.63	0.08	65.98	-133.00		5.97	-50.32	*-8.94*	*74.10*	Mar		20.00	20.01	47.30	*29.10*	*15.76*
Seas_1	**223.71**	**0.35**	**240.13**	**-330.10**	**1.44**	**18.04**	**-147.57**	***0.9***	***199.5***	**Seas_1**	**6.61**	**57.59**	**57.61**	**189.40**	***77.8***	***78.2***
Apr	-6.24	0.04	52.87	-130.00		5.81	-48.59	*-21.02*	*62.41*	Apr		19.41	19.42	54.40	*31.08*	*20.20*
May	-46.46	-0.03	46.12	-141.00		6.03	-50.10	*-30.91*	*64.78*	May		20.10	20.11	56.60	*32.27*	*21.07*
Jun	-62.11	-0.07	38.36	-131.00		5.86	-48.39	*-32.89*	*60.62*	Jun		19.48	19.49	78.20	*39.06*	*33.90*
Seas_2	**-114.81**	**-0.05**	**137.35**	**-402.00**	**2.15**	**17.70**	**-147.08**	***-72.4***	***172.7***	**Seas_2**	**11.85**	**58.98**	**59.02**	**189.20**	***79.8***	***76.3***
Jul	-42.84	-0.10	34.62	-234.00		6.07	-49.91	*-47.69*	*96.61*	Jul		20.15	20.17	7.81	*16.04*	*7.13*
Aug	18.77	-0.12	30.62	-117.00		6.08	-49.81	*-18.58*	*55.55*	Aug		20.16	20.18	70.80	*37.05*	*29.23*
Sep	63.37	-0.06	26.59	-94.90		5.91	-48.13	*-7.87*	*56.05*	Sep		19.52	19.55	60.40	*33.16*	*23.59*
Seas_3	**39.29**	**-0.28**	**91.82**	**-445.90**	**2.74**	**18.06**	**-147.85**	***-63.2***	***184.0***	**Seas_3**	**19.30**	**59.83**	**59.89**	**139.01**	***69.5***	***50.1***
Oct	121.40	-0.02	24.93	-168.00		6.11	-49.64	*-10.87*	*95.26*	Oct		20.18	20.21	-4.18	*12.07*	*14.07*
Nov	146.26	0.04	22.11	-219.00		5.92	-47.96	*-15.44*	*118.95*	Nov		19.53	19.56	-62.60	*-7.84*	*47.43*
Dec	153.70	0.06	20.45	-167.00		5.94	-47.89	*-5.79*	*103.98*	Dec		19.53	19.56	-41.60	*-0.84*	*35.30*
Seas_4	**421.37**	**0.08**	**67.49**	**-554.00**	**1.98**	**17.96**	**-145.49**	***-27.2***	***290.2***	**Seas_4**	**9.99**	**59.23**	**59.33**	**-108.38**	***5.0***	***79.1***
Annual	**569.56**	**0.11**	**536.79**	**-1732.00**	**8.32**	**71.77**	**-587.98**	***-161.92***	***793.70***	**Annual**	**47.75**	**235.64**	**235.85**	**409.23**	***232.11***	***147.63***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.66. *Comparison of the calculation results on PCB-153 mass flows between the atmosphere and soil: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets.*

Month	CliMoChem_2_3		G-CIEMS_1		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			0.22	0.15	62.64	98.37	19.60	18.95	19.59	18.95	17.22	6.52	-29.78	-50.07	-28.10	-69.10	95.60	88.80		
Feb			0.19	0.12	48.68	75.79	19.24	18.65	19.23	18.65	15.57	5.55	-28.27	-47.19	-74.80	-128.00	69.10	53.30		
Mar			0.15	0.08	43.96	65.98	20.60	20.00	20.58	20.01	16.66	5.97	-30.22	-50.32	-73.30	-133.00	68.80	47.30		
Seas_1	**0.57**	**1.44**	**0.56**	**0.35**	**155.28**	**240.13**	**59.43**	**57.59**	**59.40**	**57.61**	**49.45**	**18.04**	**-88.27**	**-147.57**	**-176.20**	**-330.10**	**233.50**	**189.40**	**2.56**	**6.61**
Apr			0.12	0.04	36.73	52.87	19.95	19.41	19.93	19.42	16.13	5.81	-29.24	-48.59	-47.60	-130.00	92.00	54.40		
May			0.06	-0.03	33.52	46.12	20.64	20.10	20.61	20.11	16.68	6.03	-30.22	-50.10	-38.90	-141.00	107.00	56.60		
Jun			0.04	-0.07	29.21	38.36	19.98	19.48	19.94	19.49	16.16	5.86	-29.24	-48.39	-6.39	-131.00	145.00	78.20		
Seas_2	**1.39**	**2.15**	**0.22**	**-0.05**	**99.46**	**137.35**	**60.57**	**58.98**	**60.48**	**59.02**	**48.97**	**17.70**	**-88.70**	**-147.08**	**-92.89**	**-402.00**	**344.00**	**189.20**	**6.54**	**11.85**
Jul			0.02	-0.10	27.64	34.62	20.65	20.15	20.61	20.17	16.70	6.07	-30.22	-49.91	-115.00	-234.00	68.80	7.81		
Aug			0.01	-0.12	25.63	30.62	20.66	20.16	20.61	20.18	16.72	6.08	-30.22	-49.81	-3.75	-117.00	136.00	70.80		
Sep			0.05	-0.06	23.30	26.59	19.99	19.52	19.93	19.55	16.19	5.91	-29.24	-48.13	-14.40	-94.90	108.00	60.40		
Seas_3	**2.39**	**2.74**	**0.07**	**-0.28**	**76.57**	**91.82**	**61.30**	**59.83**	**61.15**	**59.89**	**49.60**	**18.06**	**-89.67**	**-147.85**	**-133.15**	**-445.90**	**312.80**	**139.01**	**11.52**	**19.30**
Oct			0.07	-0.02	22.82	24.93	20.66	20.18	20.59	20.21	16.73	6.11	-30.22	-49.64	-106.00	-168.00	26.70	-4.18		
Nov			0.11	0.04	21.11	22.11	19.99	19.53	19.92	19.56	16.20	5.92	-29.24	-47.96	-170.00	-219.00	-39.70	-62.60		
Dec			0.12	0.06	20.31	20.45	19.98	19.53	19.91	19.56	16.21	5.94	-29.24	-47.89	-126.00	-167.00	-21.40	-41.60		
Seas_4	**0.99**	**1.98**	**0.30**	**0.08**	**64.24**	**67.49**	**60.62**	**59.23**	**60.42**	**59.33**	**49.15**	**17.96**	**-88.70**	**-145.49**	**-402.00**	**-554.00**	**-34.40**	**-108.38**	**4.67**	**9.99**
Annual	**5.34**	**8.32**	**1.16**	**0.11**	**395.56**	**536.79**	**241.92**	**235.64**	**241.45**	**235.85**	**197.18**	**71.77**	**-355.33**	**-587.98**	**-804.24**	**-1732.00**	**855.90**	**409.23**	**25.29**	**47.75**

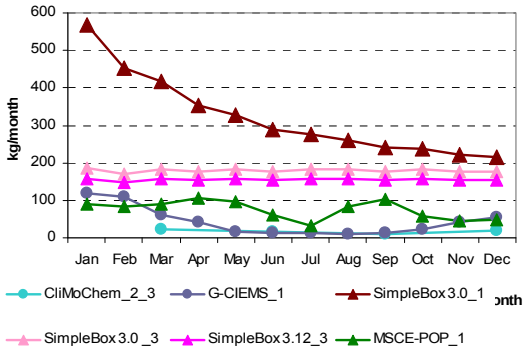
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Net mass flows between the atmosphere and soil

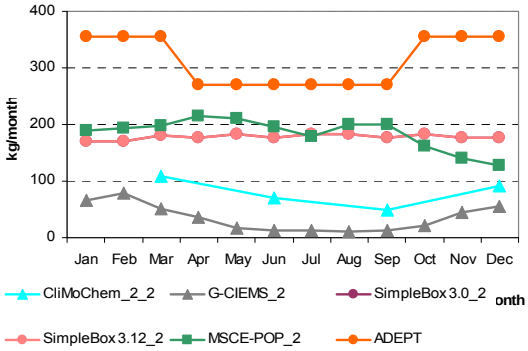
Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-153 net mass flows between the atmosphere and soil calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.67.

Monthly values of PCB-153 net mass flows between the atmosphere and soil calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.95 a and b, respectively.



a



b

Fig. 3.95a. *PCB-153 net mass flows between the atmosphere and soil (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

Fig. 3.95b. *PCB-153 net mass flows between the atmosphere and soil (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table 3.67. *Calculation results: PCB-153 net mass flows between the atmosphere and soil (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT[b]		
Jan	117.98	567.86	91.30		185.30	158.18	*224.12*	*195.53*	Jan	65.70		169.97	169.97	190.00	354.30	*189.99*	*103.98*
Feb	107.99	453.47	83.40		171.49	147.57	*192.79*	*149.68*	Feb	77.85		169.45	169.44	193.80	354.30	*192.97*	*100.48*
Mar	62.50	415.73	90.30		183.35	157.75	*181.93*	*139.56*	Mar	51.13		181.51	181.50	198.00	354.30	*193.29*	*107.74*
Seas_1	**288.47**	**1437.06**	**265.00**	**69.99**	**540.14**	**463.49**	***510.69***	***482.75***	**Seas_1**	**194.68**	**325.60**	**520.94**	**520.92**	**581.80**	**1062.90**	***534.47***	***296.96***
Apr	40.14	352.78	106.10		177.47	152.66	*165.83*	*116.86*	Apr	35.52		175.94	175.93	214.90	269.40	*174.34*	*86.54*
May	17.60	326.91	97.50		183.41	157.75	*156.63*	*114.61*	May	16.59		182.04	182.02	210.80	269.40	*172.17*	*94.00*
Jun	13.22	289.05	62.21		177.52	152.66	*138.93*	*107.12*	Jun	12.80		176.35	176.33	195.10	269.40	*165.99*	*93.84*
Seas_2	**70.97**	**968.74**	**265.81**	**44.58**	**538.40**	**463.06**	***391.93***	***346.06***	**Seas_2**	**64.91**	**211.83**	**534.33**	**534.28**	**620.80**	**808.20**	***462.39***	***274.15***
Jul	13.00	277.19	31.30		183.45	157.75	*132.54*	*110.33*	Jul	12.89		182.38	182.35	178.10	269.40	*165.02*	*93.29*
Aug	9.56	260.27	82.05		183.46	157.75	*138.62*	*96.22*	Aug	9.62		182.51	182.47	199.70	269.40	*168.74*	*95.90*
Sep	13.70	239.17	101.60		177.56	152.66	*136.94*	*84.83*	Sep	13.79		176.72	176.68	199.10	269.40	*167.14*	*93.78*
Seas_3	**36.26**	**776.62**	**214.95**	**31.30**	**544.47**	**468.15**	***345.29***	***300.63***	**Seas_3**	**36.30**	**149.12**	**541.60**	**541.51**	**576.90**	**808.20**	***442.27***	***290.69***
Oct	22.08	236.65	57.70		183.48	157.75	*131.53*	*89.25*	Oct	22.24		182.70	182.65	161.40	354.30	*180.66*	*117.93*
Nov	43.31	220.78	46.30		177.58	152.66	*128.12*	*79.88*	Nov	43.66		176.88	176.83	141.10	354.30	*178.55*	*112.35*
Dec	55.57	214.09	48.90		177.59	152.66	*129.76*	*74.10*	Dec	56.10		176.94	176.89	128.70	354.30	*178.59*	*109.97*
Seas_4	**120.96**	**671.52**	**152.90**	**56.34**	**538.64**	**463.06**	***333.90***	***256.02***	**Seas_4**	**122.00**	**272.95**	**536.51**	**536.37**	**431.20**	**1062.90**	***493.66***	***322.01***
Annual	**516.67**	**3853.95**	**898.66**	**202.20**	**2161.64**	**1857.76**	***1581.81***	***1347.55***	**Annual**	**417.89**	**959.51**	**2133.38**	**2133.07**	**2210.70**	**3742.20**	***1932.79***	***1155.31***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates;
b - ADEPT results refer to bulk depositions (sum of dry and wet deposition mass flows).

3.4.2. Comparison of calculated values of PCB-153 mass flows transported from vegetation to soil: Litterfall

Reference data set. Calculation results on PCB-153 mass flows transported from the vegetation to soil: litterfall calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.68.

Monthly values of PCB-153 mass flows transported from vegetation to soil: litterfall calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.96 a and b, respectively. Seasonal variations of low values of mass flows transported from vegetation to soil calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. 3.96c in more detail.

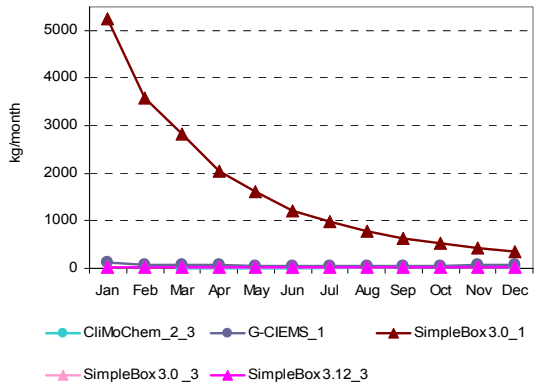
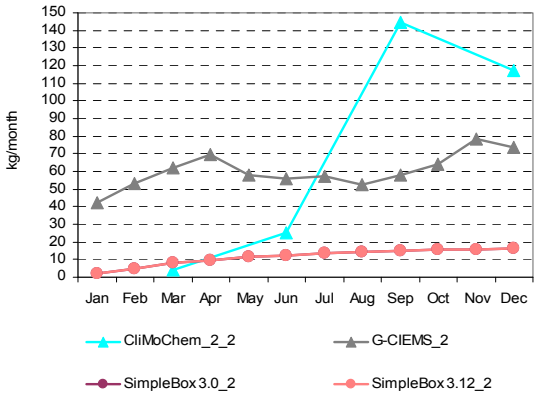


Fig. 3.96a. *PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*



b

Fig. 3.96b. *PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

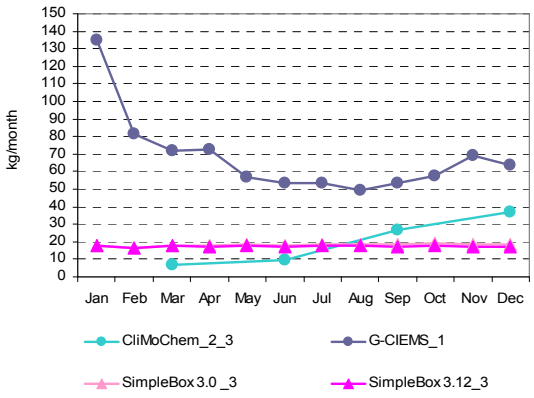
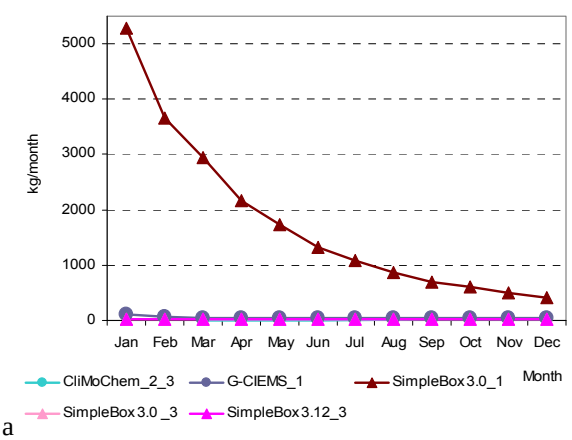


Fig. 3.96c. *PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

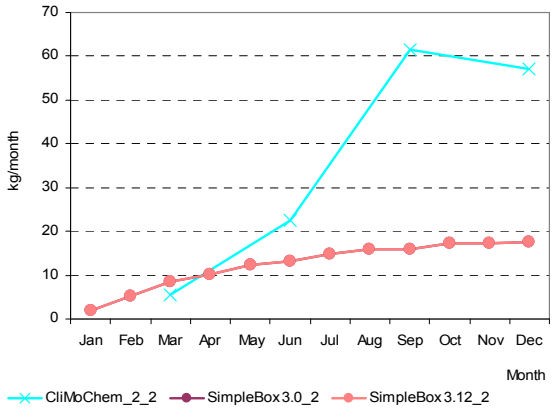
Own/alternative data set. Calculation results on PCB-153 mass flows transported from vegetation to soil: litterfall calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.69.

Monthly values of PCB-153 mass flows transported from vegetation to soil: litterfall calculated by all participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.97 a and b, respectively. Seasonal variations of low values of mass flows transported from vegetation to soil calculated by the participating models on the basis of “reference” data set and non-zero initial conditions are also shown in Fig. 3.97c in more detail.



a

Fig. 3.97a. *PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (all models)*



b

Fig. 3.97b. *PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and zero-initial conditions*

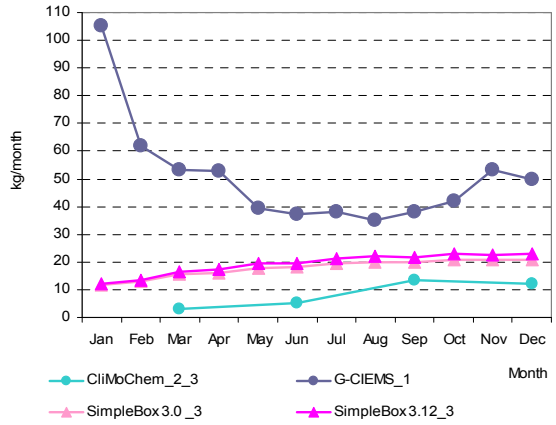


Fig. 3.97c. *PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (models with low values)*

Table 3.68. *Calculation results: PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	CliMoChem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	134.68	5246.46		17.70	17.56	*1354.10*	*2595.50*	Jan	42.06		1.90	1.90	*15.29*	*23.19*
Feb	81.26	3571.90		16.76	16.43	*921.58*	*1767.14*	Feb	53.20		4.99	4.99	*21.06*	*27.83*
Mar	71.66	2825.96		18.10	17.56	*733.32*	*1395.33*	Mar	61.78		7.93	7.93	*25.88*	*31.09*
Seas_1	**287.60**	**11644.32**	**20.06**	**52.56**	**51.54**	***2411.22***	***5162.58***	**Seas_1**	**157.04**	**13.03**	**14.82**	**14.82**	***49.93***	***71.41***
Apr	72.27	2046.61		17.69	16.99	*538.39*	*1005.81*	Apr	69.27		9.62	9.62	*29.50*	*34.44*
May	56.73	1611.97		18.43	17.56	*426.17*	*790.74*	May	57.77		11.50	11.50	*26.92*	*26.71*
Jun	53.21	1210.01		17.96	16.99	*324.54*	*590.55*	Jun	55.58		12.32	12.32	*26.74*	*24.97*
Seas_2	**182.21**	**4868.59**	**28.12**	**54.08**	**51.54**	***1036.91***	***2142.83***	**Seas_2**	**182.61**	**75.06**	**33.45**	**33.45**	***81.14***	***70.43***
Jul	53.64	987.39		18.68	17.56	*269.32*	*479.01*	Jul	56.98		13.72	13.72	*28.14*	*24.98*
Aug	49.16	789.83		18.79	17.56	*218.83*	*380.94*	Aug	52.76		14.53	14.53	*27.28*	*22.07*
Sep	53.17	622.97		18.27	16.99	*177.85*	*297.22*	Sep	58.12		14.70	14.70	*29.17*	*25.07*
Seas_3	**155.98**	**2400.18**	**80.25**	**55.74**	**52.11**	***548.85***	***1035.77***	**Seas_3**	**167.86**	**434.41**	**42.94**	**42.95**	***172.04***	***184.56***
Oct	57.77	532.00		18.96	17.56	*156.57*	*250.98*	Oct	64.38		15.73	15.73	*31.95*	*28.09*
Nov	69.50	430.46		18.41	16.99	*133.84*	*199.25*	Nov	78.64		15.67	15.67	*36.66*	*36.36*
Dec	63.54	364.67		18.47	16.99	*115.92*	*167.24*	Dec	73.64		16.04	16.04	*35.24*	*33.26*
Seas_4	**190.82**	**1327.13**	**111.71**	**55.84**	**51.54**	***347.41***	***550.56***	**Seas_4**	**216.66**	**351.31**	**47.44**	**47.44**	***165.71***	***147.22***
Annual	**816.61**	**20240.22**	**240.14**	**218.22**	**206.75**	***4344.39***	***8889.78***	**Annual**	**724.18**	**873.81**	**138.65**	**138.66**	***468.83***	***386.11***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.69. *Calculation results: PCB-153 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1a	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a		
Jan	105.43	5292.50		11.77	12.02	*1355.43*	*2625.08*	Jan		1.99	1.99	*1.99*	*0.00*
Feb	61.72	3664.20		12.91	13.56	*938.10*	*1817.54*	Feb		5.26	5.26	*5.26*	*0.00*
Mar	53.39	2943.90		15.39	16.44	*757.28*	*1457.85*	Mar		8.41	8.41	*8.41*	*0.00*
Seas_1	**220.55**	**11900.59**	**8.95**	**40.07**	**42.03**	***2442.44***	***5287.93***	**Seas_1**	**16.49**	**15.65**	**15.65**	***15.93***	***0.48***
Apr	52.93	2162.96		16.15	17.44	*562.37*	*1067.20*	Apr		10.27	10.27	*10.27*	*0.00*
May	39.53	1725.81		17.75	19.29	*450.59*	*850.20*	May		12.35	12.35	*12.35*	*0.00*
Jun	37.33	1310.69		18.01	19.67	*346.43*	*642.90*	Jun		13.30	13.30	*13.30*	*0.00*
Seas_2	**129.79**	**5199.45**	**15.99**	**51.92**	**56.40**	***1090.71***	***2297.23***	**Seas_2**	**67.33**	**35.92**	**35.92**	***46.39***	***18.13***
Jul	38.20	1080.80		19.33	21.19	*289.88*	*527.35*	Jul		14.86	14.86	*14.86*	*0.00*
Aug	35.13	872.88		19.95	21.92	*237.47*	*423.66*	Aug		15.80	15.80	*15.80*	*0.00*
Sep	38.02	694.46		19.80	21.80	*193.52*	*334.06*	Sep		16.03	16.03	*16.03*	*0.00*
Seas_3	**111.35**	**2648.15**	**40.82**	**59.08**	**64.90**	***584.86***	***1153.71***	**Seas_3**	**184.23**	**46.70**	**46.70**	***92.54***	***79.41***
Oct	42.07	597.80		20.89	23.04	*170.95*	*284.72*	Oct		17.21	17.21	*17.21*	*0.00*
Nov	53.23	487.34		20.58	22.72	*145.97*	*228.07*	Nov		17.18	17.18	*17.18*	*0.00*
Dec	49.74	415.77		20.88	23.08	*127.37*	*192.71*	Dec		17.63	17.63	*17.63*	*0.00*
Seas_4	**145.04**	**1500.91**	**36.91**	**62.35**	**68.83**	***362.81***	***637.49***	**Seas_4**	**171.09**	**52.03**	**52.02**	***91.71***	***68.74***
Annual	**606.72**	**21249.10**	**102.68**	**213.42**	**232.15**	***4480.81***	***9375.68***	**Annual**	**439.14**	**150.30**	**150.30**	***246.58***	***166.76***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.70.

Table 3.70. *The percentage difference between calculation results on PCB-153 mass flows transported from vegetation to soil: litterfall obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan			-21.7%	0.9%	4.4%	4.3%	-33.5%	-31.5%
Feb			-24.0%	2.6%	5.3%	5.3%	-23.0%	-17.4%
Mar			-25.5%	4.2%	6.1%	6.1%	-15.0%	-6.4%
Seas_1	**26.6%**	**-55.4%**	**-23.3%**	**2.2%**	**5.6%**	**5.6%**	**-23.8%**	**-18.5%**
Apr			-26.8%	5.7%	6.8%	6.8%	-8.7%	2.6%
May			-30.3%	7.1%	7.4%	7.4%	-3.7%	9.8%
Jun			-29.8%	8.3%	7.9%	7.9%	0.3%	15.8%
Seas_2	**-10.3%**	**-43.1%**	**-28.8%**	**6.8%**	**7.4%**	**7.4%**	**-4.0%**	**9.4%**
Jul			-28.8%	9.5%	8.4%	8.3%	3.5%	20.7%
Aug			-28.5%	10.5%	8.8%	8.7%	6.2%	24.8%
Sep			-28.5%	11.5%	9.1%	9.1%	8.4%	28.3%
Seas_3	**-57.6%**	**-49.1%**	**-28.6%**	**10.3%**	**8.7%**	**8.7%**	**6.0%**	**24.5%**
Oct			-27.2%	12.4%	9.4%	9.4%	10.2%	31.2%
Nov			-23.4%	13.2%	9.7%	9.7%	11.7%	33.7%
Dec			-21.7%	14.0%	9.9%	9.9%	13.1%	35.8%
Seas_4	**-51.3%**	**-67.0%**	**-24.0%**	**13.1%**	**9.7%**	**9.7%**	**11.7%**	**33.5%**
Annual	**-49.7%**	**-57.2%**	**-25.7%**	**5.0%**	**8.4%**	**8.4%**	**-2.2%**	**12.3%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.4.3. Comparison of calculated values of PCB-153 mass flows transported from the atmosphere to water

Dry deposition

Reference data set. Calculation results on PCB-153 mass flows transported from the atmosphere to water: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.71.

Monthly values of PCB-153 mass flows transported from the atmosphere to water: dry deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.98 a and b, respectively.

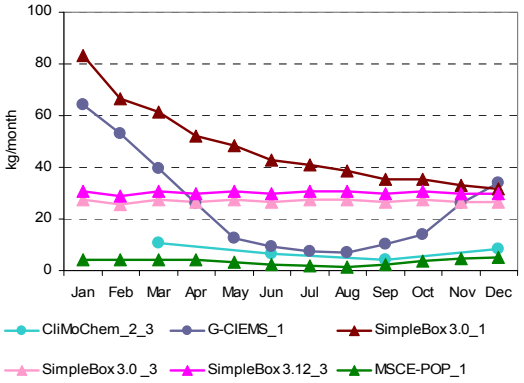


Fig. 3.98a. *PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

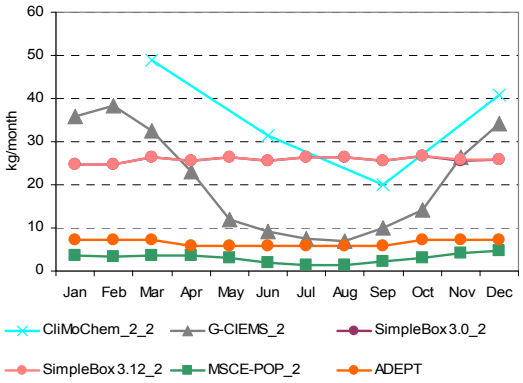


Fig. 3.98b. *PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported from the atmosphere to water: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.72.

Monthly values of PCB-153 mass flows transported from the atmosphere to water: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.99 a and b, respectively.

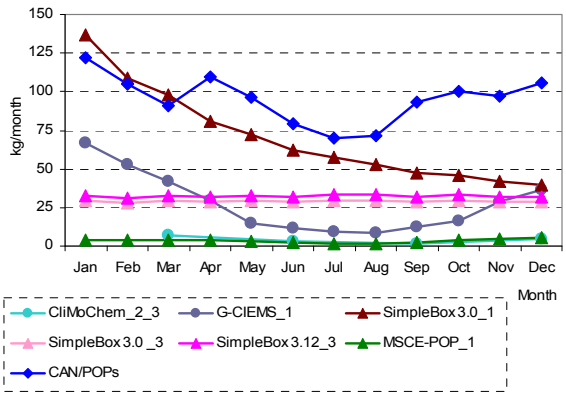


Fig. 3.99a. *PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

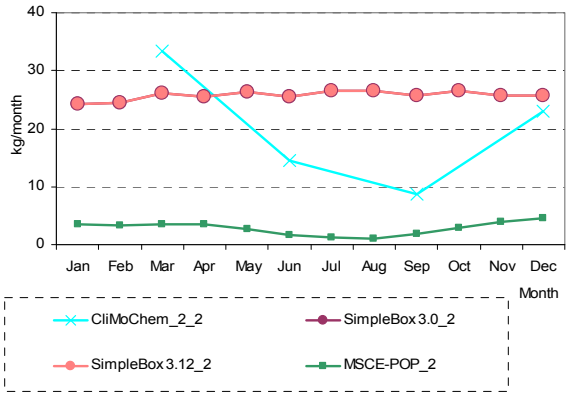


Fig. 3.99b. *PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.71. *Calculation results: PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	64.36	83.19	4.13		27.53	30.82	*42.01*	*31.48*	Jan	35.84		24.61	24.61	3.51	7.10	*19.13*	*13.49*
Feb	53.00	66.68	4.04		25.54	28.83	*35.62*	*24.56*	Feb	38.20		24.60	24.60	3.45	7.10	*19.59*	*14.26*
Mar	39.71	61.25	4.31		27.30	30.82	*32.68*	*20.63*	Mar	32.47		26.35	26.35	3.75	7.10	*19.20*	*12.88*
Seas_1	**157.07**	**211.11**	**12.48**	**31.49**	**80.37**	**90.47**	***97.17***	***75.35***	**Seas_1**	**106.51**	**146.48**	**75.55**	**75.55**	**10.71**	**21.30**	***72.68***	***51.16***
Apr	26.07	52.07	4.24		26.42	29.82	*27.72*	*16.98*	Apr	23.04		25.54	25.54	3.65	5.70	*16.70*	*11.04*
May	12.62	48.33	3.42		27.31	30.82	*24.50*	*17.33*	May	11.84		26.43	26.43	2.92	5.70	*14.66*	*11.22*
Jun	9.44	42.79	2.33		26.43	29.82	*22.16*	*16.26*	Jun	9.08		25.60	25.61	1.95	5.70	*13.59*	*11.26*
Seas_2	**48.12**	**143.18**	**9.99**	**19.83**	**80.16**	**90.47**	***65.29***	***49.68***	**Seas_2**	**43.96**	**94.24**	**77.58**	**77.58**	**8.52**	**17.10**	***53.16***	***35.38***
Jul	7.65	41.08	1.65		27.31	30.82	*21.70*	*16.50*	Jul	7.51		26.48	26.49	1.39	5.70	*13.51*	*12.05*
Aug	6.86	38.61	1.51		27.31	30.82	*21.02*	*16.02*	Aug	6.82		26.50	26.51	1.26	5.70	*13.36*	*12.18*
Sep	10.07	35.51	2.54		26.43	29.82	*20.87*	*13.95*	Sep	10.07		25.66	25.67	2.12	5.70	*13.84*	*11.15*
Seas_3	**24.58**	**115.19**	**5.70**	**12.54**	**81.05**	**91.46**	***55.09***	***46.45***	**Seas_3**	**24.40**	**59.66**	**78.65**	**78.66**	**4.77**	**17.10**	***43.87***	***32.54***
Oct	14.12	35.16	3.80		27.31	30.82	*22.24*	*12.96*	Oct	14.18		26.53	26.54	3.16	7.10	*15.50*	*10.82*
Nov	26.12	32.82	4.71		26.43	29.82	*23.98*	*11.12*	Nov	26.30		25.69	25.69	4.03	7.10	*17.76*	*11.19*
Dec	33.98	31.84	5.21		26.43	29.82	*25.46*	*11.65*	Dec	34.24		25.70	25.71	4.67	7.10	*19.48*	*12.92*
Seas_4	**74.22**	**99.81**	**13.72**	**25.33**	**80.17**	**90.47**	***63.95***	***35.70***	**Seas_4**	**74.72**	**122.76**	**77.93**	**77.94**	**11.86**	**21.30**	***64.42***	***41.22***
Annual	**304.00**	**569.30**	**41.89**	**89.18**	**321.75**	**362.87**	***281.50***	***192.86***	**Annual**	**249.58**	**423.14**	**309.71**	**309.73**	**35.86**	**76.80**	***234.14***	***149.30***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.72. *Calculation results: PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	122.03	66.91	136.51	4.19		29.76	32.82	*65.37*	*53.56*	Jan		24.30	24.30	3.42	*17.34*	*12.05*
Feb	105.30	53.04	109.12	4.05		27.67	30.74	*54.99*	*43.35*	Feb		24.38	24.38	3.35	*17.37*	*12.14*
Mar	90.97	41.67	97.56	4.27		29.62	32.91	*49.50*	*36.90*	Mar		26.17	26.17	3.61	*18.65*	*13.03*
Seas_1	**318.30**	**161.62**	**343.19**	**12.51**	**22.02**	**87.05**	**96.47**	***148.74***	***134.09***	**Seas_1**	**99.91**	**74.84**	**74.84**	**10.38**	***64.99***	***38.28***
Apr	109.67	29.17	80.49	4.15		28.70	31.89	*47.34*	*39.41*	Apr		25.42	25.42	3.46	*18.10*	*12.68*
May	96.05	15.07	72.40	3.18		29.69	32.99	*41.56*	*35.52*	May		26.34	26.34	2.62	*18.44*	*13.70*
Jun	79.47	11.57	62.13	2.11		28.75	31.95	*36.00*	*29.62*	Jun		25.56	25.55	1.71	*17.61*	*13.77*
Seas_2	**285.19**	**55.82**	**215.02**	**9.44**	**9.33**	**87.14**	**96.83**	***108.39***	***104.55***	**Seas_2**	**43.79**	**77.32**	**77.32**	**7.79**	***51.55***	***33.18***
Jul	69.61	9.55	57.87	1.46		29.73	33.04	*33.54*	*26.50*	Jul		26.46	26.46	1.20	*18.04*	*14.58*
Aug	71.51	8.65	52.83	1.31		29.74	33.06	*32.85*	*26.40*	Aug		26.51	26.51	1.07	*18.03*	*14.69*
Sep	92.91	12.19	47.30	2.31		28.80	32.00	*35.92*	*32.05*	Sep		25.69	25.69	1.86	*17.75*	*13.76*
Seas_3	**234.02**	**30.39**	**158.01**	**5.08**	**5.58**	**88.27**	**98.09**	***88.49***	***84.96***	**Seas_3**	**25.91**	**78.66**	**78.65**	**4.13**	***46.84***	***37.80***
Oct	99.94	16.50	45.69	3.58		29.76	33.08	*38.09*	*33.57*	Oct		26.58	26.58	2.89	*18.68*	*13.68*
Nov	96.99	29.08	41.68	4.64		28.81	32.02	*38.87*	*30.99*	Nov		25.75	25.75	3.88	*18.46*	*12.63*
Dec	106.06	36.45	39.61	5.13		28.82	32.01	*41.35*	*33.97*	Dec		25.77	25.77	4.52	*18.69*	*12.27*
Seas_4	**302.98**	**82.03**	**126.98**	**13.35**	**14.45**	**87.39**	**97.11**	***103.47***	***97.61***	**Seas_4**	**69.16**	**78.10**	**78.10**	**11.29**	***59.16***	***32.19***
Annual	**1140.49**	**329.86**	**843.19**	**40.38**	**51.38**	**349.85**	**388.51**	***449.09***	***405.44***	**Annual**	**238.76**	**308.92**	**308.91**	**33.59**	***222.55***	***130.24***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.73.

Table 3.73. *The percentage difference between calculation results on PCB-153 mass flows transported from the atmosphere to water: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			4.0%	64.1%	-1.3%	-1.3%	8.1%	6.5%	1.5%	-2.6%
Feb			0.1%	63.7%	-0.9%	-0.9%	8.4%	6.6%	0.2%	-2.9%
Mar			4.9%	59.3%	-0.7%	-0.7%	8.5%	6.8%	-0.9%	-3.7%
Seas_1	**-31.8%**	**-30.1%**	**2.9%**	**62.6%**	**-0.9%**	**-0.9%**	**8.3%**	**6.6%**	**0.2%**	**-3.1%**
Apr			11.9%	54.6%	-0.5%	-0.5%	8.6%	6.9%	-2.1%	-5.2%
May			19.5%	49.8%	-0.3%	-0.3%	8.7%	7.0%	-7.0%	-10.3%
Jun			22.6%	45.2%	-0.2%	-0.2%	8.8%	7.1%	-9.4%	-12.3%
Seas_2	**-53.5%**	**-53.0%**	**16.0%**	**50.2%**	**-0.3%**	**-0.3%**	**8.7%**	**7.0%**	**-5.5%**	**-8.6%**
Jul			24.9%	40.9%	-0.1%	-0.1%	8.9%	7.2%	-11.5%	-13.7%
Aug			26.0%	36.8%	0.0%	0.0%	8.9%	7.3%	-13.2%	-15.1%
Sep			21.0%	33.2%	0.1%	0.1%	9.0%	7.3%	-9.1%	-12.3%
Seas_3	**-56.6%**	**-55.5%**	**23.6%**	**37.2%**	**0.0%**	**0.0%**	**8.9%**	**7.2%**	**-10.9%**	**-13.4%**
Oct			16.9%	30.0%	0.2%	0.1%	9.0%	7.3%	-5.8%	-8.5%
Nov			11.3%	27.0%	0.2%	0.2%	9.0%	7.3%	-1.5%	-3.7%
Dec			7.3%	24.4%	0.3%	0.3%	9.1%	7.3%	-1.5%	-3.2%
Seas_4	**-43.7%**	**-43.0%**	**10.5%**	**27.2%**	**0.2%**	**0.2%**	**9.0%**	**7.3%**	**-2.7%**	**-4.8%**
Annual	**-43.6%**	**-42.4%**	**8.5%**	**48.1%**	**-0.3%**	**-0.3%**	**8.7%**	**7.1%**	**-3.6%**	**-6.3%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Wet deposition

Reference data set. Calculation results on PCB-153 mass flows transported from the atmosphere to water: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.74.

Monthly values of PCB-153 mass flows transported from the atmosphere to water: wet deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.100 a and b, respectively.

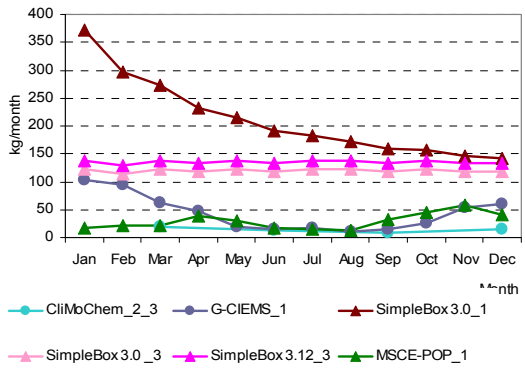


Fig. 3.100a. *PCB-153 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "reference data set" and non-zero initial conditions*

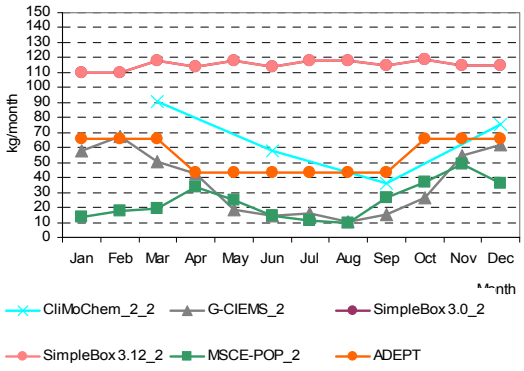


Fig. 3.100b. *PCB-153 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "reference data set" and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported from the atmosphere to water: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.75.

Monthly values of PCB-153 mass flows transported from the atmosphere to water: wet deposition calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.101 a and b, respectively.

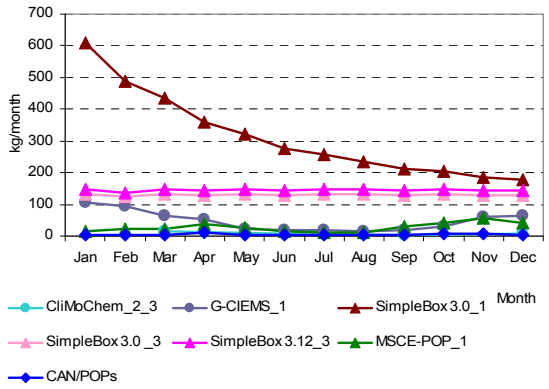


Fig. 3.101a. *PCB-153 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

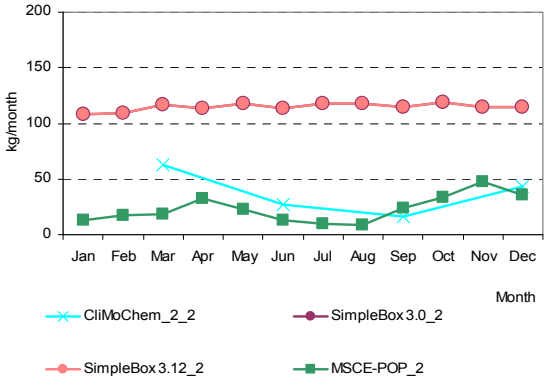


Fig. 3.101b. *PCB-153 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.76.

Gaseous exchange

Reference data set. Calculation results on PCB-153 mass flows between the atmosphere and water: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.77.

Monthly values of PCB-153 mass flows between the atmosphere and water: gaseous exchange calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.102 a and b, respectively.

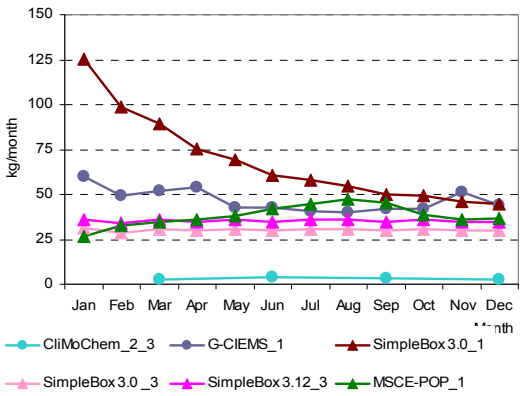


Fig. 3.102a. *PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

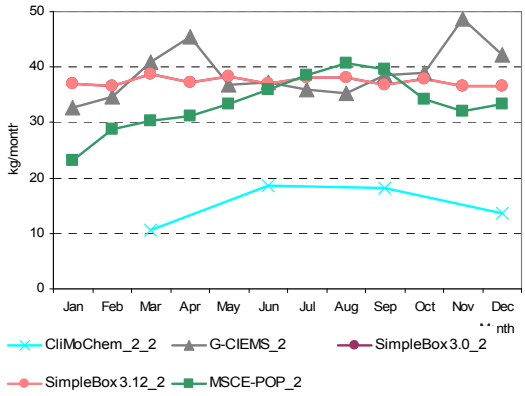


Fig. 3.102b. *PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table 3.74. *Calculation results: PCB-153 mass flows between the atmosphere and water: wet deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	103.26	371.13	16.50		122.82	137.49	*150.24*	*132.10*	Jan	57.50		109.79	109.79	13.60	65.70	*71.27*	*40.35*
Feb	93.68	297.47	21.00		113.92	128.62	*130.94*	*101.86*	Feb	67.51		109.73	109.73	17.40	65.70	*74.01*	*38.30*
Mar	61.97	273.24	22.50		121.80	137.49	*123.40*	*95.67*	Mar	50.68		117.55	117.55	19.50	65.70	*74.20*	*42.94*
Seas_1	**258.91**	**941.85**	**60.00**	**58.18**	**358.54**	**403.61**	***346.85***	***325.80***	**Seas_1**	**175.69**	**270.74**	**337.06**	**337.07**	**50.50**	**197.10**	***228.03***	***110.28***
Apr	48.15	232.28	39.10		117.89	133.06	*114.10*	*77.97*	Apr	42.56		113.95	113.96	34.00	43.50	*69.59*	*40.66*
May	19.80	215.59	29.60		121.82	137.49	*104.86*	*81.42*	May	18.59		117.91	117.92	24.90	43.50	*64.56*	*49.55*
Jun	14.85	190.88	17.50		117.90	133.06	*94.84*	*76.81*	Jun	14.26		114.23	114.24	14.20	43.50	*60.09*	*50.86*
Seas_2	**82.79**	**638.76**	**86.20**	**36.40**	**357.62**	**403.61**	***267.56***	***238.70***	**Seas_2**	**75.41**	**173.00**	**346.09**	**346.11**	**73.10**	**130.50**	***190.70***	***125.98***
Jul	16.26	183.26	14.10		121.84	137.49	*94.59*	*75.93*	Jul	15.99		118.15	118.16	11.50	43.50	*61.46*	*53.19*
Aug	10.66	172.24	12.70		121.84	137.49	*90.99*	*74.66*	Aug	10.58		118.24	118.25	9.92	43.50	*60.10*	*54.79*
Sep	15.09	158.40	32.20		117.91	133.06	*91.33*	*63.75*	Sep	15.11		114.50	114.51	26.80	43.50	*62.88*	*48.19*
Seas_3	**42.01**	**513.90**	**59.00**	**22.95**	**361.60**	**408.05**	***234.59***	***217.69***	**Seas_3**	**41.67**	**109.26**	**350.88**	**350.92**	**48.22**	**130.50**	***171.91***	***142.81***
Oct	26.63	156.84	44.10		121.84	137.49	*97.38*	*58.28*	Oct	26.75		118.38	118.40	36.90	65.70	*73.23*	*43.63*
Nov	54.02	146.41	57.70		117.92	133.06	*101.82*	*43.17*	Nov	54.43		114.62	114.63	49.30	65.70	*79.74*	*32.40*
Dec	60.99	142.04	41.20		117.92	133.06	*99.04*	*45.16*	Dec	61.59		114.66	114.68	36.40	65.70	*78.61*	*34.78*
Seas_4	**141.63**	**445.29**	**143.00**	**46.67**	**357.67**	**403.61**	***256.31***	***165.91***	**Seas_4**	**142.77**	**226.22**	**347.66**	**347.71**	**122.60**	**197.10**	***230.68***	***97.92***
Annual	**525.35**	**2539.81**	**348.20**	**164.20**	**1435.43**	**1618.88**	***1105.31***	***919.32***	**Annual**	**435.55**	**779.22**	**1381.70**	**1381.82**	**294.42**	**655.20**	***821.32***	***465.62***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.75. *Calculation results: PCB-153 mass flows between the atmosphere and water: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	3.45	107.07	608.76	16.80		132.71	146.36	*169.19*	*223.44*	Jan		108.35	108.35	13.30	*76.66*	*54.87*
Feb	3.13	93.50	486.62	21.30		123.40	137.08	*144.17*	*176.24*	Feb		108.70	108.70	17.00	*78.14*	*52.95*
Mar	2.82	64.82	435.09	22.30		132.10	146.78	*133.98*	*158.30*	Mar		116.72	116.71	18.80	*84.08*	*56.53*
Seas_1	**9.40**	**265.39**	**1530.47**	**60.40**	**41.43**	**388.21**	**430.21**	***389.36***	***531.16***	**Seas_1**	**188.07**	**333.77**	**333.76**	**49.10**	***226.17***	***136.58***
Apr	10.29	53.66	358.93	38.50		127.99	142.23	*121.93*	*127.05*	Apr		113.36	113.36	32.50	*86.41*	*46.68*
May	4.63	23.52	322.88	27.50		132.39	147.12	*109.67*	*120.48*	May		117.48	117.48	22.30	*85.75*	*54.95*
Jun	2.56	18.09	277.08	16.10		128.22	142.49	*97.42*	*106.92*	Jun		113.97	113.96	12.60	*80.18*	*58.52*
Seas_2	**17.48**	**95.26**	**958.88**	**82.10**	**17.19**	**388.61**	**431.84**	***284.48***	***343.24***	**Seas_2**	**80.72**	**344.81**	**344.80**	**67.40**	***209.43***	***156.41***
Jul	1.89	20.15	258.09	12.80		132.58	147.34	*95.48*	*101.76*	Jul		118.01	118.00	10.10	*82.03*	*62.30*
Aug	2.59	13.33	235.60	11.40		132.62	147.42	*90.49*	*95.93*	Aug		118.21	118.20	8.45	*81.62*	*63.37*
Sep	4.50	18.16	210.95	29.20		128.43	142.68	*88.99*	*83.72*	Sep		114.56	114.56	23.60	*84.24*	*52.52*
Seas_3	**8.99**	**51.63**	**704.65**	**53.40**	**10.22**	**393.63**	**437.44**	***237.14***	***275.35***	**Seas_3**	**47.49**	**350.78**	**350.76**	**42.15**	***197.79***	***176.65***
Oct	5.82	30.96	203.74	41.40		132.72	147.53	*93.70*	*78.64*	Oct		118.53	118.52	33.80	*90.28*	*48.92*
Nov	6.22	59.88	185.88	56.80		128.46	142.78	*96.67*	*66.66*	Nov		114.83	114.82	47.50	*92.39*	*38.87*
Dec	4.39	65.20	176.63	40.50		128.54	142.77	*93.01*	*66.51*	Dec		114.94	114.93	35.20	*88.36*	*46.04*
Seas_4	**16.44**	**156.05**	**566.25**	**138.70**	**26.92**	**389.72**	**433.08**	***246.74***	***215.45***	**Seas_4**	**128.91**	**348.30**	**348.28**	**116.50**	***235.50***	***130.34***
Annual	**52.30**	**568.34**	**3760.25**	**334.60**	**95.76**	**2730.61**	**3032.07**	***1510.56***	***1594.97***	**Annual**	**445.19**	**1377.66**	**1377.60**	**275.15**	***868.90***	***591.52***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.76. *The percentage difference between calculation results on PCB-153 mass flows between the atmosphere and water: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			3.7%	64.0%	-1.3%	-1.3%	8.1%	6.4%	1.8%	-2.2%
Feb			-0.2%	63.6%	-0.9%	-0.9%	8.3%	6.6%	1.4%	-2.3%
Mar			4.6%	59.2%	-0.7%	-0.7%	8.5%	6.8%	-0.9%	-3.6%
Seas_1	**-30.5%**	**-28.8%**	**2.5%**	**62.5%**	**-1.0%**	**-1.0%**	**8.3%**	**6.6%**	**0.7%**	**-2.8%**
Apr			11.4%	54.5%	-0.5%	-0.5%	8.6%	6.9%	-1.5%	-4.4%
May			18.8%	49.8%	-0.4%	-0.4%	8.7%	7.0%	-7.1%	-10.4%
Jun			21.8%	45.2%	-0.2%	-0.2%	8.8%	7.1%	-8.0%	-11.3%
Seas_2	**-53.3%**	**-52.8%**	**15.1%**	**50.1%**	**-0.4%**	**-0.4%**	**8.7%**	**7.0%**	**-4.8%**	**-7.8%**
Jul			23.9%	40.8%	-0.1%	-0.1%	8.8%	7.2%	-9.2%	-12.2%
Aug			25.0%	36.8%	0.0%	0.0%	8.8%	7.2%	-10.2%	-14.8%
Sep			20.3%	33.2%	0.1%	0.0%	8.9%	7.2%	-9.3%	-11.9%
Seas_3	**-56.5%**	**-55.5%**	**22.9%**	**37.1%**	**0.0%**	**0.0%**	**8.9%**	**7.2%**	**-9.5%**	**-12.6%**
Oct			16.3%	29.9%	0.1%	0.1%	8.9%	7.3%	-6.1%	-8.4%
Nov			10.9%	27.0%	0.2%	0.2%	8.9%	7.3%	-1.6%	-3.7%
Dec			6.9%	24.4%	0.2%	0.2%	9.0%	7.3%	-1.7%	-3.3%
Seas_4	**-43.0%**	**-42.3%**	**10.2%**	**27.2%**	**0.2%**	**0.2%**	**9.0%**	**7.3%**	**-3.0%**	**-5.0%**
Annual	**-42.9%**	**-41.7%**	**8.2%**	**48.1%**	**-0.3%**	**-0.3%**	**90.2%**	**87.3%**	**-3.9%**	**-6.5%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-153 mass flows between the atmosphere and water: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.78.

Monthly values of PCB-153 mass flows between the atmosphere and water: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.103 a and b, respectively. Seasonal variations of gaseous exchange flows between the atmosphere and water calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions are also shown in Fig. 3.103c in more detail.

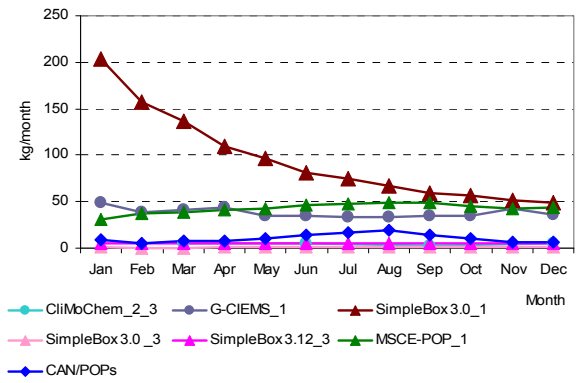


Fig. 3.103a. *PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

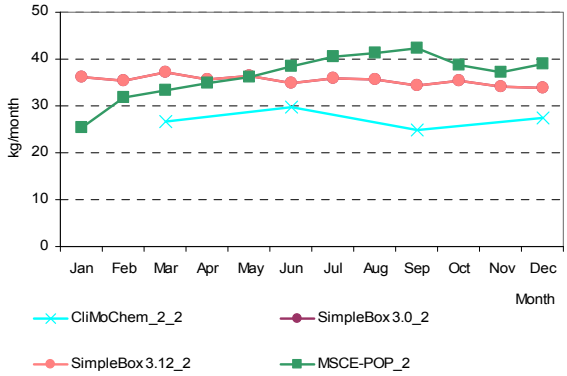


Fig. 3.103b. *PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

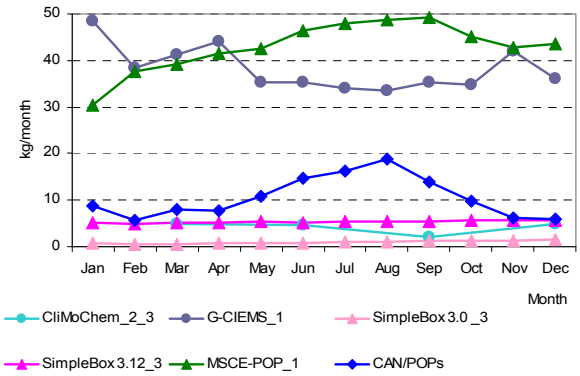


Fig. 3.103c. *PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (models with low values)*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.79.

Table 3.77. *Calculation results: PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	59.81	125.13	26.70		31.07	36.00	*55.74*	*40.84*	Jan	32.78		37.10	37.10	23.20	*32.54*	*6.55*
Feb	49.21	98.65	32.90		28.71	33.68	*48.63*	*29.03*	Feb	34.64		36.56	36.56	28.70	*34.12*	*3.72*
Mar	51.67	89.42	34.50		30.68	36.00	*48.45*	*24.26*	Mar	40.94		38.78	38.78	30.20	*37.18*	*4.76*
Seasonal_1	**160.69**	**313.20**	**94.10**	**7.00**	**90.46**	**105.67**	***128.52***	***103.02***	**Seasonal_1**	**108.36**	**32.06**	**112.44**	**112.44**	**82.10**	***89.48***	***34.51***
Apr	53.81	75.18	35.90		29.68	34.84	*45.88*	*18.75*	Apr	45.41		37.30	37.30	31.20	*37.80*	*5.83*
May	42.34	69.18	38.10		30.67	36.00	*43.26*	*15.09*	May	36.82		38.37	38.37	33.40	*36.74*	*2.34*
Jun	42.52	60.85	42.10		29.68	34.84	*42.00*	*11.82*	Jun	37.28		37.00	37.00	36.00	*36.82*	*0.56*
Seasonal_2	**138.66**	**205.21**	**116.10**	**11.66**	**90.03**	**105.67**	***111.22***	***63.25***	**Seasonal_2**	**119.51**	**55.62**	**112.67**	**112.68**	**100.60**	***100.21***	***25.84***
Jul	40.90	58.13	44.80		30.68	36.00	*42.10*	*10.41*	Jul	35.95		38.12	38.13	38.60	*37.70*	*1.19*
Aug	40.07	54.43	47.10		30.70	36.00	*41.66*	*9.32*	Aug	35.35		38.03	38.04	40.70	*38.03*	*2.18*
Sep	42.27	49.92	45.10		29.72	34.84	*40.37*	*8.08*	Sep	38.58		36.73	36.74	39.70	*37.94*	*1.46*
Seasonal_3	**123.24**	**162.49**	**137.00**	**11.00**	**91.10**	**106.83**	***105.28***	***52.33***	**Seasonal_3**	**109.89**	**54.56**	**112.89**	**112.90**	**119.00**	***101.85***	***26.64***
Oct	41.89	49.33	38.70		30.73	36.00	*39.33*	*6.93*	Oct	38.99		37.89	37.90	34.10	*37.22*	*2.14*
Nov	51.05	45.96	36.10		29.75	34.84	*39.54*	*8.71*	Nov	48.64		36.61	36.62	32.10	*38.49*	*7.09*
Dec	44.11	44.53	36.80		29.77	34.84	*38.01*	*6.31*	Dec	42.29		36.56	36.57	33.40	*37.21*	*3.70*
Seasonal_4	**137.04**	**139.82**	**111.60**	**8.54**	**90.25**	**105.67**	***98.82***	***48.12***	**Seasonal_4**	**129.92**	**40.66**	**111.07**	**111.09**	**99.60**	***98.47***	***34.10***
Annual	**559.63**	**820.72**	**458.80**	**38.20**	**361.84**	**423.84**	***443.84***	***255.87***	**Annual**	**467.68**	**182.90**	**449.07**	**449.11**	**401.30**	***390.01***	***118.36***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.78. *Calculation results: PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE- POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	8.68	48.56	203.61	30.50		0.67	5.22	*49.54*	*77.62*	Jan		36.28	36.28	25.50	*32.69*	*6.22*
Feb	5.76	38.32	157.35	37.60		0.47	4.91	*40.74*	*59.57*	Feb		35.39	35.39	31.90	*34.23*	*2.01*
Mar	7.99	41.20	136.61	39.20		0.59	5.25	*38.47*	*51.20*	Mar		37.23	37.23	33.40	*35.95*	*2.21*
Seas_1	**22.43**	**128.09**	**497.57**	**107.30**	**14.90**	**1.73**	**15.38**	***112.49***	***176.96***	**Seas_1**	**79.94**	**108.90**	**108.90**	**90.80**	***97.14***	***14.29***
Apr	7.62	44.07	109.68	41.40		0.67	5.10	*34.76*	*41.28*	Apr		35.57	35.57	35.00	*35.38*	*0.33*
May	10.70	35.24	96.37	42.40		0.78	5.31	*31.80*	*35.78*	May		36.37	36.37	36.10	*36.28*	*0.16*
Jun	14.64	35.36	81.08	46.30		0.86	5.20	*30.57*	*30.34*	Jun		34.90	34.90	38.50	*36.10*	*2.08*
Seas_2	**32.97**	**114.67**	**287.12**	**130.10**	**13.66**	**2.31**	**15.61**	***85.20***	***102.65***	**Seas_2**	**89.33**	**106.84**	**106.83**	**109.60**	***103.15***	***9.30***
Jul	16.16	33.97	74.31	47.90		0.99	5.43	*29.79*	*28.06*	Jul		35.81	35.81	40.40	*37.34*	*2.65*
Aug	18.92	33.39	66.95	48.80		1.10	5.52	*29.11*	*25.62*	Aug		35.60	35.59	41.30	*37.50*	*3.29*
Sep	13.92	35.27	59.33	49.20		1.18	5.40	*27.38*	*24.12*	Sep		34.27	34.27	42.30	*36.95*	*4.63*
Seas_3	**49.00**	**102.63**	**200.59**	**145.90**	**6.04**	**3.27**	**16.36**	***74.83***	***77.01***	**Seas_3**	**74.29**	**105.68**	**105.67**	**124.00**	***102.41***	***20.64***
Oct	9.70	34.88	56.84	45.10		1.32	5.69	*25.59*	*23.16*	Oct		35.26	35.26	38.80	*36.44*	*2.04*
Nov	6.09	42.04	51.51	42.90		1.38	5.58	*24.92*	*22.83*	Nov		33.99	33.99	37.30	*35.09*	*1.91*
Dec	5.98	36.07	48.69	43.50		1.51	5.65	*23.57*	*21.46*	Dec		33.87	33.87	38.90	*35.55*	*2.91*
Seas_4	**21.77**	**112.99**	**157.04**	**131.50**	**14.62**	**4.21**	**16.91**	***65.58***	***65.33***	**Seas_4**	**82.06**	**103.12**	**103.11**	**115.00**	***100.82***	***13.71***
Annual	**126.17**	**458.37**	**1142.32**	**514.80**	**49.22**	**11.52**	**64.25**	***338.09***	***408.75***	**Annual**	**325.62**	**424.53**	**424.52**	**439.40**	***403.52***	***52.40***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.79. *Comparison of the calculation results on PCB-153 mass flows between the atmosphere and water: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		G-CIEMS_1		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			59.81	48.56	125.13	203.61	37.10	36.28	37.10	36.28	31.07	0.67	36.00	5.22	26.70	30.50	23.20	25.50		
Feb			49.21	38.32	98.65	157.35	36.56	35.39	36.56	35.39	28.71	0.47	33.68	4.91	32.90	37.60	28.70	31.90		
Mar			51.67	41.20	89.42	136.61	38.78	37.23	38.78	37.23	30.68	0.59	36.00	5.25	34.50	39.20	30.20	33.40		
Seas_1	**7.00**	**14.90**	**160.69**	**128.09**	**313.20**	**497.57**	**112.44**	**108.90**	**112.44**	**108.90**	**90.46**	**1.73**	**105.67**	**15.38**	**94.10**	**107.30**	**82.10**	**90.80**	**32.06**	**79.94**
Apr			53.81	44.07	75.18	109.68	37.30	35.57	37.30	35.57	29.68	0.67	34.84	5.10	35.90	41.40	31.20	35.00		
May			42.34	35.24	69.18	96.37	38.37	36.37	38.37	36.37	30.67	0.78	36.00	5.31	38.10	42.40	33.40	36.10		
Jun			42.52	35.36	60.85	81.08	37.00	34.90	37.00	34.90	29.68	0.86	34.84	5.20	42.10	46.30	36.00	38.50		
Seas_2	**11.66**	**13.66**	**138.66**	**114.67**	**205.21**	**287.12**	**112.67**	**106.84**	**112.68**	**106.83**	**90.03**	**2.31**	**105.67**	**15.61**	**116.10**	**130.10**	**100.60**	**109.60**	**55.62**	**89.33**
Jul			40.90	33.97	58.13	74.31	38.12	35.81	38.13	35.81	30.68	0.99	36.00	5.43	44.80	47.90	38.60	40.40		
Aug			40.07	33.39	54.43	66.95	38.03	35.60	38.04	35.59	30.70	1.10	36.00	5.52	47.10	48.80	40.70	41.30		
Sep			42.27	35.27	49.92	59.33	36.73	34.27	36.74	34.27	29.72	1.18	34.84	5.40	45.10	49.20	39.70	42.30		
Seas_3	**11.00**	**6.04**	**123.24**	**102.63**	**162.49**	**200.59**	**112.89**	**105.68**	**112.90**	**105.67**	**91.10**	**3.27**	**106.83**	**16.36**	**137.00**	**145.90**	**119.00**	**124.00**	**54.56**	**74.29**
Oct			41.89	34.88	49.33	56.84	37.89	35.26	37.90	35.26	30.73	1.32	36.00	5.69	38.70	45.10	34.10	38.80		
Nov			51.05	42.04	45.96	51.51	36.61	33.99	36.62	33.99	29.75	1.38	34.84	5.58	36.10	42.90	32.10	37.30		
Dec			44.11	36.07	44.53	48.69	36.56	33.87	36.57	33.87	29.77	1.51	34.84	5.65	36.80	43.50	33.40	38.90		
Seas_4	**8.54**	**14.62**	**137.04**	**112.99**	**139.82**	**157.04**	**111.07**	**103.12**	**111.09**	**103.11**	**90.25**	**4.21**	**105.67**	**16.91**	**111.60**	**131.50**	**99.60**	**115.00**	**40.66**	**82.06**
Annual	**38.20**	**49.22**	**559.63**	**458.37**	**820.72**	**1142.32**	**449.07**	**424.53**	**449.11**	**424.52**	**361.84**	**11.52**	**423.84**	**64.25**	**458.80**	**514.80**	**401.30**	**439.40**	**182.90**	**325.62**

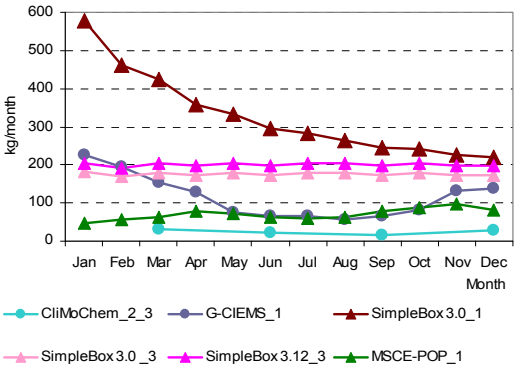
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Net mass flows between the atmosphere and water

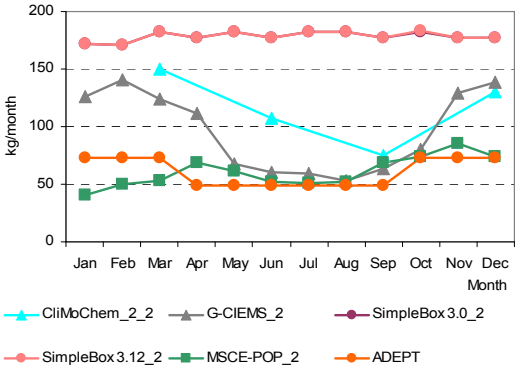
Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-153 net mass flows PCB-153 between the atmosphere and water calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.80.

Monthly values of PCB-153 net mass flows PCB-153 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.104 a and b, respectively.



a



b

Fig. 3.104a. *PCB-153 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. 3.104b. *PCB-153 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table 3.80. *Calculation results: PCB-153 net mass flows between the atmosphere and water (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT[b]		
Jan	227.43	579.45	47.33		181.42	204.31	*247.99*	*198.05*	Jan	126.11		171.50	171.50	40.31	72.80	*116.44*	*58.86*
Feb	195.89	462.80	57.94		168.18	191.13	*215.19*	*149.33*	Feb	140.36		170.88	170.89	49.55	72.80	*120.90*	*56.52*
Mar	153.35	423.92	61.31		179.78	204.31	*204.53*	*134.05*	Mar	124.10		182.67	182.68	53.45	72.80	*123.14*	*60.17*
Seas_1	**576.67**	**1466.16**	**166.58**	**96.67**	**529.37**	**599.75**	***572.53***	***488.35***	**Seas_1**	**390.56**	**449.28**	**525.05**	**525.06**	**143.31**	**218.40**	***375.28***	***160.62***
Apr	128.02	359.53	79.24		173.99	197.72	*187.70*	*106.23*	Apr	111.02		176.80	176.80	68.85	49.20	*116.53*	*59.38*
May	74.75	333.10	71.12		179.80	204.31	*172.62*	*108.04*	May	67.24		182.71	182.72	61.22	49.20	*108.62*	*67.95*
Jun	66.80	294.52	61.93		174.02	197.72	*159.00*	*97.49*	Jun	60.62		176.83	176.85	52.15	49.20	*103.13*	*67.42*
Seas_2	**269.57**	**987.15**	**212.29**	**67.88**	**527.81**	**599.75**	***444.08***	***332.23***	**Seas_2**	**238.88**	**322.86**	**536.34**	**536.37**	**182.22**	**147.60**	***327.38***	***172.39***
Jul	64.80	282.47	60.55		179.83	204.31	*158.39*	*95.26*	Jul	59.45		182.75	182.77	51.49	49.20	*105.13*	*70.97*
Aug	57.60	265.28	61.31		179.85	204.31	*153.67*	*91.47*	Aug	52.75		182.77	182.79	51.88	49.20	*103.88*	*72.04*
Sep	67.43	243.83	79.84		174.06	197.72	*152.58*	*76.43*	Sep	63.76		176.89	176.92	68.62	49.20	*107.08*	*64.14*
Seas_3	**189.84**	**791.58**	**201.70**	**46.49**	**533.75**	**606.34**	***394.95***	***290.56***	**Seas_3**	**175.96**	**223.48**	**542.42**	**542.48**	**171.99**	**147.60**	***300.66***	***188.90***
Oct	82.63	241.33	86.60		179.88	204.31	*158.95*	*71.31*	Oct	79.92		182.80	182.83	74.16	72.80	*118.50*	*58.77*
Nov	131.19	225.19	98.51		174.10	197.72	*165.34*	*50.84*	Nov	129.36		176.92	176.95	85.43	72.80	*128.29*	*49.12*
Dec	139.07	218.41	83.21		174.12	197.72	*162.51*	*53.24*	Dec	138.12		176.93	176.96	74.47	72.80	*127.86*	*51.98*
Seas_4	**352.90**	**684.92**	**268.32**	**80.54**	**528.09**	**599.75**	***419.09***	***226.68***	**Seas_4**	**347.41**	**389.63**	**536.66**	**536.74**	**234.06**	**218.40**	***377.15***	***139.73***
Annual	**1388.98**	**3929.82**	**848.89**	**291.58**	**2119.02**	**2405.59**	***1830.65***	***1292.12***	**Annual**	**1152.81**	**1385.26**	**2140.47**	**2140.66**	**731.58**	**732.00**	***1380.46***	***640.14***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates;
b - ADEPT results refer to bulk depositions (sum of dry and wet deposition mass flows).

3.4.4. Comparison of calculated values of PCB-153 mass flows transported from the atmosphere to vegetation

Dry deposition

Reference data set. Calculation results on PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.81.

Monthly values of PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.105 a and b, respectively.

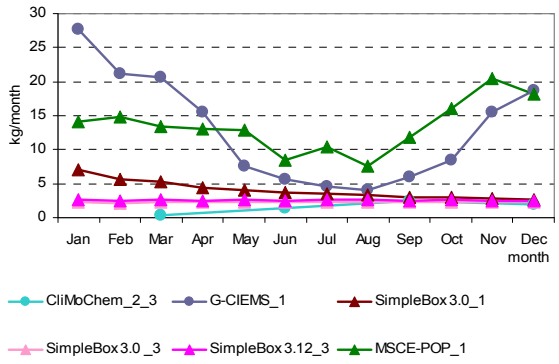


Fig. 3.105a. *PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

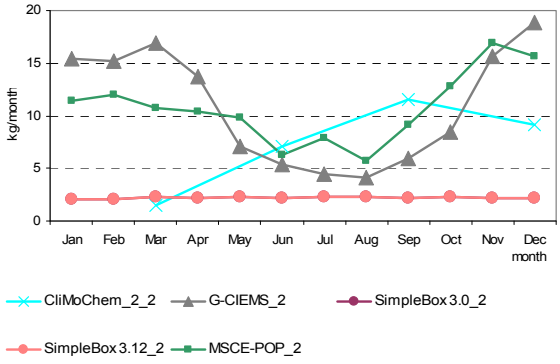


Fig. 3.105b. *PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.82.

Monthly values of PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.106 a and b, respectively.

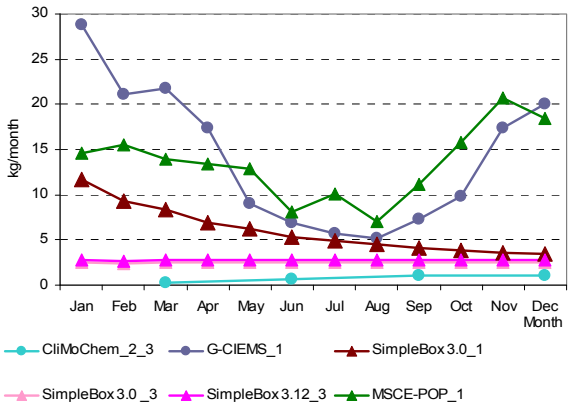


Fig. 3.106a. *PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

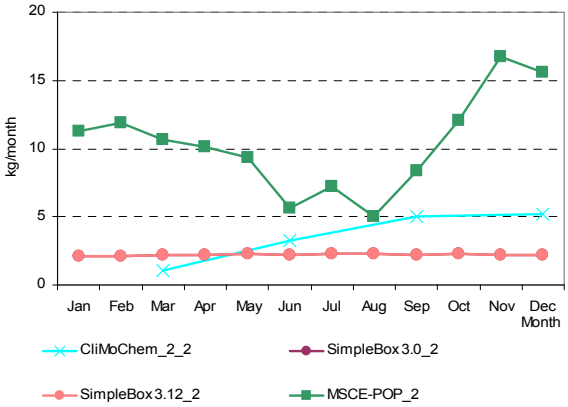


Fig. 3.106b. *PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.81 *Calculation results: PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	27.76	7.12	14.10		2.36	2.64	*10.80*	*10.61*	Jan	15.46		2.11	2.11	11.40	*7.77*	*6.74*
Feb	21.13	5.71	14.90		2.19	2.47	*9.28*	*8.39*	Feb	15.23		2.10	2.11	12.00	*7.86*	*6.77*
Mar	20.69	5.25	13.50		2.34	2.64	*8.88*	*8.00*	Mar	16.92		2.25	2.26	10.70	*8.03*	*7.14*
Seas_1	**69.58**	**18.08**	**42.50**	**0.97**	**6.88**	**7.74**	***24.29***	***26.62***	**Seas_1**	**47.61**	**4.52**	**6.47**	**6.47**	**34.10**	***19.83***	***19.79***
Apr	15.54	4.46	13.10		2.26	2.55	*7.58*	*6.27*	Apr	13.73		2.19	2.19	10.40	*7.13*	*5.86*
May	7.52	4.14	12.90		2.34	2.64	*5.91*	*4.42*	May	7.05		2.26	2.26	9.83	*5.35*	*3.74*
Jun	5.62	3.66	8.45		2.26	2.55	*4.51*	*2.57*	Jun	5.41		2.19	2.19	6.24	*4.01*	*2.13*
Seas_2	**28.68**	**12.26**	**34.45**	**4.45**	**6.86**	**7.74**	***15.74***	***12.65***	**Seas_2**	**26.20**	**21.15**	**6.64**	**6.64**	**26.47**	***17.42***	***10.07***
Jul	4.56	3.52	10.50		2.34	2.64	*4.71*	*3.35*	Jul	4.48		2.27	2.27	7.90	*4.23*	*2.66*
Aug	4.09	3.31	7.58		2.34	2.64	*3.99*	*2.12*	Aug	4.06		2.27	2.27	5.66	*3.57*	*1.63*
Sep	6.00	3.04	11.80		2.26	2.55	*5.13*	*4.02*	Sep	6.00		2.20	2.20	9.15	*4.89*	*3.36*
Seas_3	**14.65**	**9.86**	**29.88**	**7.28**	**6.94**	**7.83**	***12.74***	***8.87***	**Seas_3**	**14.54**	**34.63**	**6.73**	**6.73**	**22.71**	***17.07***	***11.84***
Oct	8.41	3.01	16.00		2.34	2.64	*6.48*	*5.88*	Oct	8.45		2.27	2.27	12.80	*6.45*	*5.14*
Nov	15.57	2.81	20.40		2.26	2.55	*8.72*	*8.63*	Nov	15.67		2.20	2.20	16.90	*9.24*	*8.15*
Dec	18.70	2.73	18.20		2.26	2.55	*8.89*	*8.73*	Dec	18.85		2.20	2.20	15.70	*9.74*	*8.80*
Seas_4	**42.69**	**8.55**	**54.60**	**5.68**	**6.86**	**7.74**	***21.02***	***21.75***	**Seas_4**	**42.97**	**27.54**	**6.67**	**6.67**	**45.40**	***25.85***	***18.80***
Annual	**155.60**	**48.76**	**161.43**	**18.38**	**27.54**	**31.06**	***73.79***	***66.39***	**Annual**	**131.32**	**87.85**	**26.51**	**26.51**	**128.68**	***80.17***	***51.93***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.82. *Calculation results: PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	28.86	11.69	14.60		2.55	2.81	*12.10*	*10.78*	Jan		2.08	2.08	11.30	*5.15*	*5.32*
Feb	21.15	9.35	15.50		2.37	2.63	*10.20*	*8.17*	Feb		2.09	2.09	11.90	*5.36*	*5.67*
Mar	21.72	8.36	14.00		2.54	2.82	*9.89*	*8.11*	Mar		2.24	2.24	10.70	*5.06*	*4.88*
Seas_1	**71.72**	**29.40**	**44.10**	**0.68**	**7.45**	**8.26**	***26.93***	***27.29***	**Seas_1**	**3.09**	**6.41**	**6.41**	**33.90**	***12.45***	***14.39***
Apr	17.39	6.89	13.40		2.46	2.73	*8.57*	*6.62*	Apr		2.18	2.18	10.10	*4.82*	*4.58*
May	8.98	6.20	12.90		2.54	2.82	*6.69*	*4.37*	May		2.25	2.25	9.30	*4.60*	*4.07*
Jun	6.90	5.32	8.13		2.46	2.73	*5.11*	*2.50*	Jun		2.19	2.19	5.68	*3.35*	*2.02*
Seas_2	**33.27**	**18.42**	**34.43**	**2.09**	**7.46**	**8.29**	***17.33***	***13.85***	**Seas_2**	**9.82**	**6.62**	**6.62**	**25.08**	***12.03***	***8.83***
Jul	5.69	4.96	10.10		2.54	2.83	*5.22*	*3.04*	Jul		2.26	2.26	7.23	*3.92*	*2.87*
Aug	5.15	4.53	7.08		2.55	2.83	*4.43*	*1.85*	Aug		2.27	2.27	5.02	*3.19*	*1.59*
Sep	7.27	4.05	11.20		2.47	2.74	*5.54*	*3.69*	Sep		2.20	2.20	8.36	*4.25*	*3.56*
Seas_3	**18.11**	**13.53**	**28.38**	**3.24**	**7.56**	**8.40**	***13.20***	***9.04***	**Seas_3**	**15.04**	**6.73**	**6.73**	**20.61**	***12.28***	***6.80***
Oct	9.84	3.91	15.80		2.55	2.83	*6.99*	*5.75*	Oct		2.27	2.27	12.10	*5.55*	*5.67*
Nov	17.33	3.57	20.70		2.47	2.74	*9.36*	*8.90*	Nov		2.20	2.20	16.70	*7.04*	*8.37*
Dec	20.06	3.39	18.50		2.47	2.74	*9.43*	*9.01*	Dec		2.21	2.21	15.60	*6.67*	*7.73*
Seas_4	**47.23**	**10.87**	**55.00**	**3.24**	**7.48**	**8.31**	***22.02***	***22.80***	**Seas_4**	**15.52**	**6.68**	**6.68**	**44.40**	***18.32***	***17.88***
Annual	**170.33**	**72.23**	**161.91**	**9.25**	**29.94**	**33.26**	***79.49***	***70.18***	**Annual**	**43.47**	**26.44**	**26.44**	**123.99**	***55.08***	***46.63***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.83.

Table 3.83. *The percentage difference between calculation results on PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			4.0%	64.1%	-1.3%	-1.3%	8.1%	6.5%	3.5%	-0.9%
Feb			0.1%	63.7%	-0.9%	-0.9%	8.4%	6.6%	4.0%	-0.8%
Mar			4.9%	59.3%	-0.7%	-0.7%	8.5%	6.8%	3.7%	0.0%
Seas_1	**-31.8%**	**-30.1%**	**3.1%**	**62.6%**	**-0.9%**	**-0.9%**	**8.3%**	**6.6%**	**3.8%**	**-0.6%**
Apr			11.9%	54.6%	-0.5%	-0.5%	8.6%	6.9%	2.3%	-2.9%
May			19.5%	49.8%	-0.3%	-0.3%	8.7%	7.0%	0.0%	-5.4%
Jun			22.6%	45.2%	-0.2%	-0.2%	8.8%	7.1%	-3.8%	-9.0%
Seas_2	**-53.5%**	**-53.0%**	**16.0%**	**50.2%**	**-0.3%**	**-0.3%**	**8.7%**	**7.0%**	**-0.1%**	**-5.3%**
Jul			24.9%	40.9%	-0.1%	-0.1%	8.9%	7.2%	-3.8%	-8.5%
Aug			26.0%	36.9%	0.0%	0.0%	8.9%	7.3%	-6.6%	-11.3%
Sep			21.0%	33.3%	0.1%	0.1%	9.0%	7.3%	-5.1%	-8.6%
Seas_3	**-56.6%**	**-55.5%**	**23.6%**	**37.2%**	**0.0%**	**0.0%**	**8.9%**	**7.2%**	**-5.0%**	**-9.2%**
Oct			16.9%	30.0%	0.2%	0.1%	9.0%	7.3%	-1.3%	-5.5%
Nov			11.3%	27.0%	0.2%	0.2%	9.0%	7.3%	1.5%	-1.2%
Dec			7.3%	24.4%	0.3%	0.3%	9.1%	7.3%	1.6%	-0.6%
Seas_4	**-43.7%**	**-43.0%**	**10.6%**	**27.2%**	**0.2%**	**0.2%**	**9.0%**	**7.3%**	**0.7%**	**-2.2%**
Annual	**-50.5%**	**-49.7%**	**9.5%**	**48.1%**	**-0.3%**	**-0.3%**	**8.7%**	**7.1%**	**0.3%**	**-3.6%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Wet deposition

Reference data set. Calculation results on PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.84.

Monthly values of PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.107 a and b, respectively.

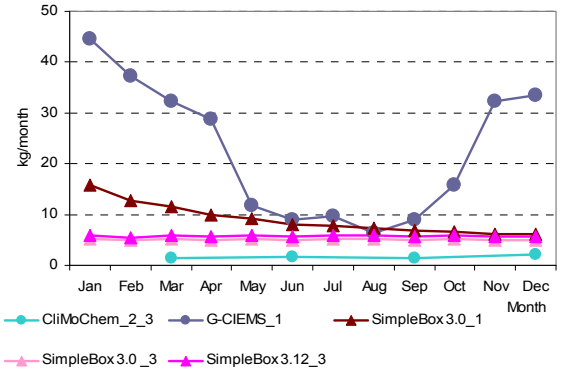


Fig. 3.107a. *PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

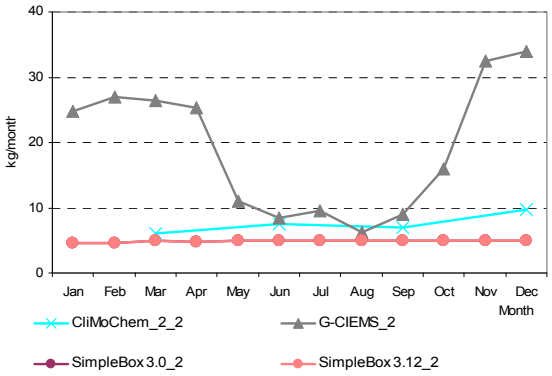


Fig. 3.107b. *PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.85.

Monthly values of PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.108 a and b, respectively.

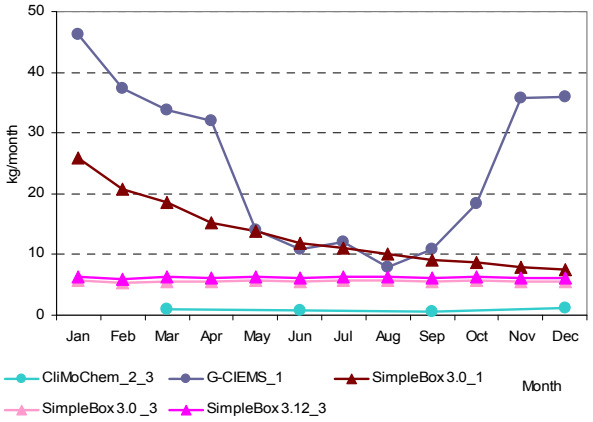


Fig. 3.108a. *PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

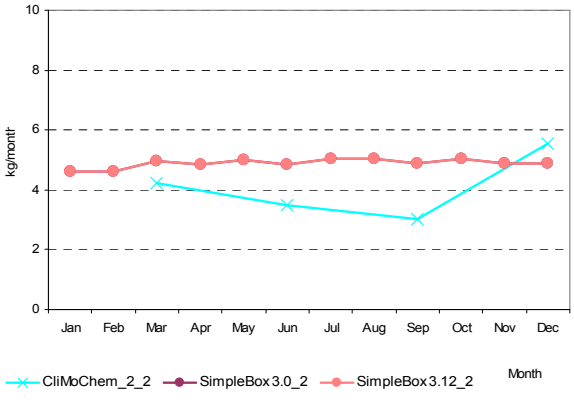


Fig. 3.108b. *PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.84. *Calculation results: PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	44.54	15.81		5.23	5.86	*17.86*	*18.43*	Jan	24.80		4.67	4.67	*11.38*	*11.62*
Feb	37.35	12.68		4.85	5.48	*15.09*	*15.26*	Feb	26.92		4.67	4.67	*12.09*	*12.84*
Mar	32.30	11.64		5.19	5.86	*13.75*	*12.70*	Mar	26.41		5.01	5.01	*12.14*	*12.36*
Seas_1	**114.18**	**40.14**	**3.94**	**15.27**	**17.19**	***38.14***	***44.49***	**Seas_1**	**78.12**	**18.32**	**14.35**	**14.35**	***31.29***	***31.28***
Apr	28.70	9.90		5.02	5.67	*12.32*	*11.13*	Apr	25.37		4.85	4.85	*11.69*	*11.84*
May	11.80	9.19		5.19	5.86	*8.01*	*3.07*	May	11.08		5.02	5.02	*7.04*	*3.50*
Jun	8.85	8.13		5.02	5.67	*6.92*	*1.86*	Jun	8.50		4.86	4.86	*6.08*	*2.10*
Seas_2	**49.34**	**27.22**	**4.70**	**15.23**	**17.19**	***22.74***	***16.89***	**Seas_2**	**44.95**	**22.34**	**14.74**	**14.74**	***24.19***	***14.29***
Jul	9.69	7.81		5.19	5.86	*7.14*	*2.03*	Jul	9.53		5.03	5.03	*6.53*	*2.60*
Aug	6.35	7.34		5.19	5.86	*6.18*	*0.91*	Aug	6.30		5.03	5.04	*5.46*	*0.73*
Sep	9.00	6.75		5.02	5.67	*6.61*	*1.74*	Sep	9.00		4.88	4.88	*6.25*	*2.38*
Seas_3	**25.04**	**21.90**	**4.38**	**15.40**	**17.38**	***16.82***	***7.91***	**Seas_3**	**24.84**	**20.83**	**14.94**	**14.94**	***18.89***	***4.84***
Oct	15.87	6.68		5.19	5.86	*8.40*	*5.02*	Oct	15.94		5.04	5.04	*8.68*	*6.29*
Nov	32.19	6.24		5.02	5.67	*12.28*	*13.29*	Nov	32.44		4.88	4.88	*14.07*	*15.91*
Dec	33.57	6.05		5.02	5.67	*12.58*	*14.00*	Dec	33.90		4.88	4.88	*14.56*	*16.75*
Seas_4	**81.63**	**18.97**	**6.03**	**15.23**	**17.19**	***27.81***	***30.50***	**Seas_4**	**82.28**	**29.21**	**14.80**	**14.81**	***35.28***	***32.07***
Annual	**270.19**	**108.22**	**19.04**	**61.13**	**68.95**	***105.51***	***97.35***	**Annual**	**230.19**	**90.70**	**58.84**	**58.84**	***109.64***	***81.76***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.
* - In MSCE-POP model wet deposition on vegetation is not taken into account since it is considered as a part of deposition directly to soil.

Table 3.85. *Calculation results: PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	46.18	25.95		5.65	6.24	*21.01*	*19.25*	Jan		4.62	4.62	*4.62*	*0.00*
Feb	37.27	20.75		5.26	5.84	*17.28*	*15.14*	Feb		4.63	4.63	*4.63*	*0.00*
Mar	33.78	18.55		5.63	6.25	*16.05*	*13.23*	Mar		4.97	4.97	*4.97*	*0.00*
Seas_1	**117.23**	**65.25**	**2.80**	**16.54**	**18.33**	***44.03***	***47.24***	**Seas_1**	**12.72**	**14.22**	**14.22**	***13.72***	***0.86***
Apr	31.98	15.30		5.45	6.06	*14.70*	*12.37*	Apr		4.83	4.83	*4.83*	*0.00*
May	14.02	13.77		5.64	6.27	*9.92*	*4.59*	May		5.00	5.00	*5.00*	*0.00*
Jun	10.78	11.81		5.46	6.07	*8.53*	*3.23*	Jun		4.86	4.85	*4.86*	*0.00*
Seas_2	**56.78**	**40.88**	**2.22**	**16.56**	**18.40**	***26.97***	***21.66***	**Seas_2**	**10.42**	**14.69**	**14.69**	***13.27***	***2.46***
Jul	12.01	11.00		5.65	6.28	*8.73*	*3.24*	Jul		5.03	5.03	*5.03*	*0.00*
Aug	7.94	10.04		5.65	6.28	*7.48*	*1.96*	Aug		5.04	5.04	*5.04*	*0.00*
Sep	10.82	8.99		5.47	6.08	*7.84*	*2.51*	Sep		4.88	4.88	*4.88*	*0.00*
Seas_3	**30.77**	**30.04**	**1.95**	**16.77**	**18.64**	***19.63***	***11.77***	**Seas_3**	**9.05**	**14.94**	**14.94**	***12.98***	***3.40***
Oct	18.45	8.69		5.65	6.29	*9.77*	*5.93*	Oct		5.05	5.05	*5.05*	*0.00*
Nov	35.69	7.92		5.47	6.08	*13.79*	*14.64*	Nov		4.89	4.89	*4.89*	*0.00*
Dec	35.89	7.53		5.48	6.08	*13.74*	*14.79*	Dec		4.90	4.90	*4.90*	*0.00*
Seas_4	**90.03**	**24.14**	**3.48**	**16.60**	**18.45**	***30.54***	***34.11***	**Seas_4**	**16.65**	**14.84**	**14.84**	***15.44***	***1.04***
Annual	**294.82**	**160.32**	**10.45**	**66.47**	**73.82**	***121.17***	***110.88***	**Annual**	**48.85**	**58.69**	**58.69**	***55.41***	***5.68***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.
* - In MSCE-POP model wet deposition on vegetation is not taken into account since it is considered as a part of deposition directly to soil.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.86.

Table 3.86. *The percentage difference between calculation results on PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	G-CIEMS_1	Simple Box 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan			3.7%	64.1%	-1.3%	-1.3%	8.1%	6.5%
Feb			-0.2%	63.7%	-0.9%	-0.9%	8.4%	6.6%
Mar			4.6%	59.3%	-0.7%	-0.7%	8.5%	6.8%
Seas_1	**-30.5%**	**-28.8%**	**2.7%**	**62.6%**	**-0.9%**	**-0.9%**	**8.3%**	**6.6%**
Apr			11.4%	54.6%	-0.5%	-0.5%	8.6%	6.9%
May			18.8%	49.8%	-0.3%	-0.3%	8.7%	7.0%
Jun			21.8%	45.2%	-0.2%	-0.2%	8.8%	7.1%
Seas_2	**-53.3%**	**-52.8%**	**15.1%**	**50.2%**	**-0.3%**	**-0.3%**	**8.7%**	**7.0%**
Jul			23.9%	40.9%	-0.1%	-0.1%	8.9%	7.2%
Aug			25.0%	36.9%	0.0%	0.0%	8.9%	7.3%
Sep			20.3%	33.3%	0.1%	0.1%	9.0%	7.3%
Seas_3	**-56.5%**	**-55.5%**	**22.9%**	**37.2%**	**0.0%**	**0.0%**	**8.9%**	**7.2%**
Oct			16.3%	30.0%	0.2%	0.1%	9.0%	7.3%
Nov			10.9%	27.0%	0.2%	0.2%	9.0%	7.3%
Dec			6.9%	24.4%	0.3%	0.3%	9.1%	7.3%
Seas_4	**-43.0%**	**-42.3%**	**10.3%**	**27.2%**	**0.2%**	**0.2%**	**9.0%**	**7.3%**
Annual	**-46.1%**	**-45.1%**	**9.1%**	**48.1%**	**-0.3%**	**-0.3%**	**8.7%**	**7.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Gaseous exchange

Reference data set. Calculation results on PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.87.

Monthly values of PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.109a and b, respectively. Seasonal variations for models with positive values of gaseous exchange flows between the atmosphere and vegetation calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. 3.109c in more detail.

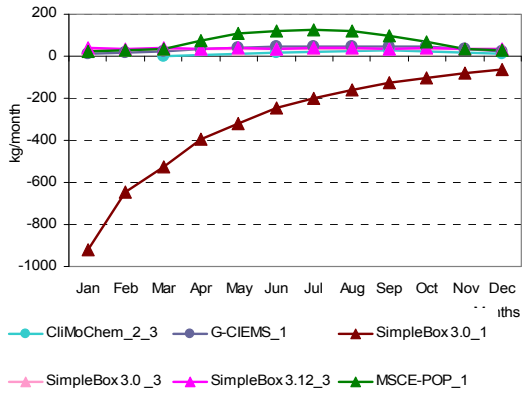


Fig. 3.109a. *PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

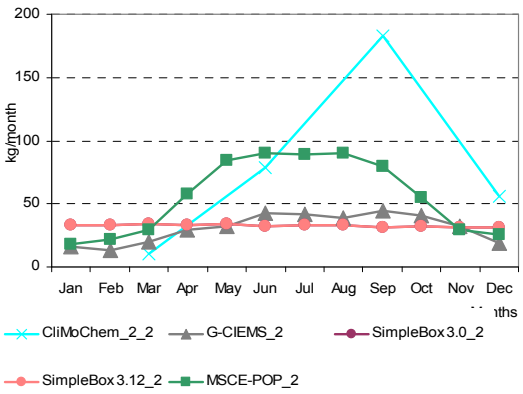


Fig. 3.109b. *PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

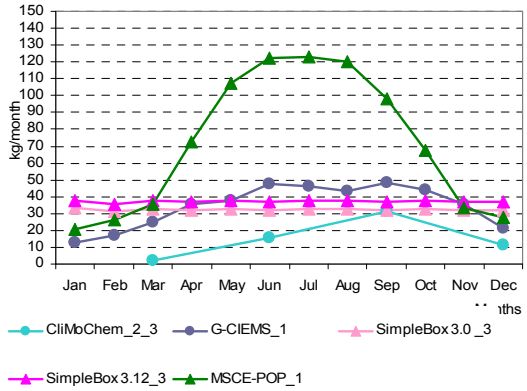


Fig. 3.109c. *PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with positive values)*

Own/alternative data set. Calculation results on PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.88.

Monthly values of PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.110a and b, respectively. Seasonal variations for models with positive values of gaseous exchange flows between the atmosphere and vegetation calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions are also shown in Fig. 3.110c in more detail.

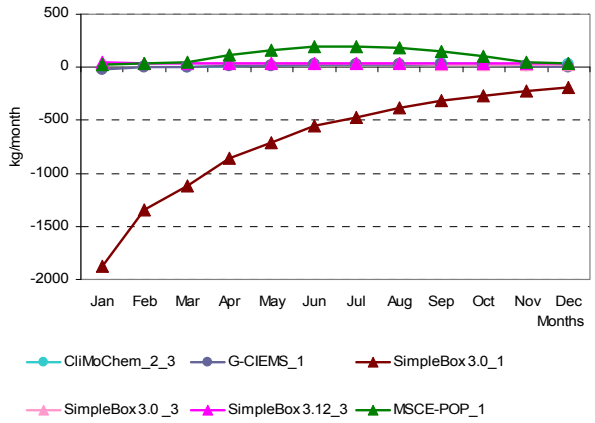


Fig. 3.110a. *PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

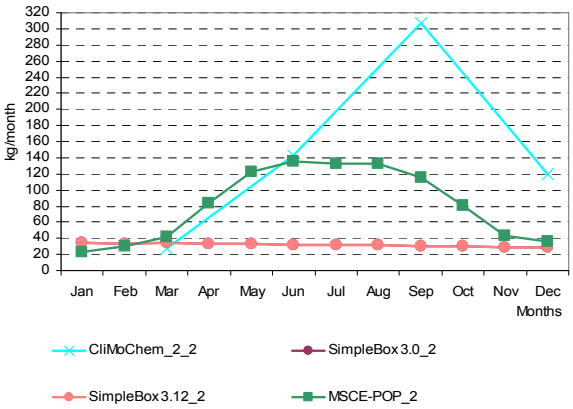


Fig. 3.110b. *PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

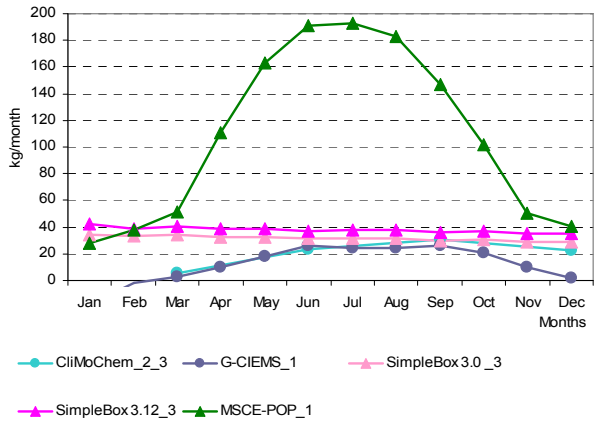


Fig. 3.110c. *PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions (models with positive values)*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.89.

Table 3.87. *Calculation results: PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	13.08	-921.76	20.70		33.45	37.94	*-163.32*	*424.10*	Jan	15.77		33.46	33.46	18.00	*25.17*	*9.61*
Feb	16.91	-646.79	26.00		30.93	35.49	*-107.49*	*301.55*	Feb	13.10		32.73	32.73	21.50	*25.01*	*9.55*
Mar	24.93	-528.35	35.30		33.01	37.94	*-79.43*	*251.00*	Mar	19.45		34.46	34.47	29.10	*29.37*	*7.08*
Seas_1	**54.92**	**-2096.89**	**82.00**	**6.67**	**97.39**	**111.36**	***-290.76***	***885.59***	**Seas_1**	**48.31**	**31.22**	**100.65**	**100.65**	**68.60**	***69.89***	***31.04***
Apr	35.81	-394.13	72.60		31.90	36.71	*-43.42*	*196.74*	Apr	29.42		32.94	32.94	57.90	*38.30*	*13.17*
May	37.82	-318.06	107.00		32.91	37.94	*-20.48*	*169.16*	May	32.57		33.69	33.69	84.00	*45.99*	*25.35*
Jun	47.76	-242.90	122.00		31.81	36.71	*-0.92*	*140.11*	Jun	42.24		32.33	32.33	90.20	*49.28*	*27.68*
Seas_2	**121.39**	**-955.09**	**301.60**	**46.39**	**96.62**	**111.36**	***-46.29***	***453.64***	**Seas_2**	**104.23**	**235.86**	**98.96**	**98.97**	**232.10**	***154.03***	***73.03***
Jul	46.28	-199.87	123.00		32.84	37.94	*8.04*	*121.87*	Jul	41.29		33.17	33.18	89.00	*49.16*	*26.83*
Aug	43.35	-159.53	120.00		32.80	37.94	*14.91*	*103.84*	Aug	39.08		32.97	32.98	89.80	*48.71*	*27.55*
Sep	48.30	-124.08	98.30		31.72	36.71	*18.19*	*83.80*	Sep	44.11		31.75	31.75	79.80	*46.85*	*22.72*
Seas_3	**137.93**	**-483.48**	**341.30**	**92.90**	**97.36**	**112.58**	***49.77***	***277.56***	**Seas_3**	**124.48**	**547.97**	**97.89**	**97.90**	**258.60**	***225.37***	***192.26***
Oct	44.19	-103.13	67.50		32.75	37.94	*15.85*	*67.82*	Oct	40.36		32.67	32.67	55.00	*40.18*	*10.53*
Nov	35.83	-80.01	33.70		31.67	36.71	*11.58*	*51.24*	Nov	32.31		31.50	31.50	29.10	*31.10*	*1.39*
Dec	21.43	-63.98	28.00		31.66	36.71	*10.76*	*42.15*	Dec	18.63		31.40	31.40	25.50	*26.73*	*6.08*
Seas_4	**101.45**	**-247.12**	**129.20**	**33.39**	**96.08**	**111.36**	***37.39***	***143.12***	**Seas_4**	**91.30**	**168.33**	**95.56**	**95.58**	**109.60**	***112.07***	***32.20***
Annual	**415.68**	**-3782.58**	**854.10**	**179.35**	**387.46**	**446.66**	***-249.89***	***1744.55***	**Annual**	**368.33**	**983.38**	**393.07**	**393.10**	**668.90**	***561.36***	***266.25***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.88. *Calculation results: PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-17.60	-1878.15	27.50		38.03	42.37	*-357.57*	*850.36*	Jan		34.68	34.68	23.00	*30.79*	*6.74*
Feb	-2.15	-1344.85	37.40		34.42	38.58	*-247.32*	*613.77*	Feb		33.33	33.33	29.70	*32.12*	*2.10*
Mar	3.02	-1123.03	51.80		36.05	40.36	*-198.36*	*517.22*	Mar		34.52	34.52	41.20	*36.75*	*3.86*
Seas_1	**-16.74**	**-4346.03**	**116.70**	**17.13**	**108.51**	**121.30**	***-666.52***	***1803.50***	**Seas_1**	**80.58**	**102.53**	**102.53**	**93.90**	***94.89***	***10.37***
Apr	9.57	-857.32	111.00		34.28	38.33	*-132.83*	*406.76*	Apr		32.52	32.51	84.30	*49.78*	*29.90*
May	17.71	-708.67	163.00		34.89	38.97	*-90.82*	*350.21*	May		32.84	32.84	122.00	*62.56*	*51.47*
Jun	25.69	-555.27	191.00		33.33	37.20	*-53.61*	*288.78*	Jun		31.18	31.17	135.00	*65.78*	*59.94*
Seas_2	**52.96**	**-2121.25**	**465.00**	**69.07**	**102.50**	**114.49**	***-219.54***	***944.24***	**Seas_2**	**427.54**	**96.53**	**96.53**	**341.30**	***240.48***	***169.90***
Jul	24.75	-469.76	193.00		34.05	37.98	*-35.99*	*252.32*	Jul		31.69	31.69	133.00	*65.46*	*58.49*
Aug	24.47	-386.87	183.00		33.71	37.58	*-21.62*	*214.46*	Aug		31.23	31.23	132.00	*64.82*	*58.18*
Sep	25.91	-311.56	147.00		32.36	36.03	*-14.05*	*173.71*	Sep		29.86	29.86	115.00	*58.24*	*49.16*
Seas_3	**75.13**	**-1168.18**	**523.00**	**93.15**	**100.12**	**111.59**	***-44.20***	***576.76***	**Seas_3**	**921.25**	**92.78**	**92.77**	**380.00**	***371.70***	***390.59***
Oct	20.69	-269.49	102.00		33.18	36.95	*-15.34*	*145.56*	Oct		30.53	30.53	80.50	*47.18*	*28.85*
Nov	9.71	-219.13	50.70		31.89	35.50	*-18.26*	*113.24*	Nov		29.27	29.27	42.70	*33.75*	*7.75*
Dec	1.81	-185.10	40.30		31.73	35.28	*-15.20*	*96.16*	Dec		29.04	29.04	35.90	*31.33*	*3.96*
Seas_4	**32.22**	**-673.73**	**193.00**	**66.60**	**96.80**	**107.73**	***-29.56***	***320.11***	**Seas_4**	**360.49**	**88.84**	**88.83**	**159.10**	***174.32***	***128.46***
Annual	**143.58**	**-8309.19**	**1297.70**	**245.94**	**407.92**	**455.11**	***-959.82***	***3623.64***	**Annual**	**1789.87**	**380.69**	**380.67**	**974.30**	***881.38***	***667.18***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table 3.89. *Comparison of the calculation results on PCB-153 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		G-CIEMS_1		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0_3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			13.1	-17.6	-921.8	-1878.2	33.46	34.68	33.46	34.68	33.45	38.03	37.94	42.37	20.7	27.5	18.00	23.00		
Feb			16.9	-2.2	-646.8	-1344.9	32.73	33.33	32.73	33.33	30.93	34.42	35.49	38.58	26.0	37.4	21.50	29.70		
Mar			24.9	3.0	-528.3	-1123.0	34.46	34.52	34.47	34.52	33.01	36.05	37.94	40.36	35.3	51.8	29.10	41.20		
Seas_1	**6.7**	**17.1**	**54.9**	**-16.7**	**-2096.9**	**-4346.0**	**100.65**	**102.53**	**100.65**	**102.53**	**97.39**	**108.51**	**111.36**	**121.30**	**82.0**	**116.7**	**68.60**	**93.90**	**31.22**	**80.58**
Apr			35.8	9.6	-394.1	-857.3	32.94	32.52	32.94	32.51	31.90	34.28	36.71	38.33	72.6	111.0	57.90	84.30		
May			37.8	17.7	-318.1	-708.7	33.69	32.84	33.69	32.84	32.91	34.89	37.94	38.97	107.0	163.0	84.00	122.00		
Jun			47.8	25.7	-242.9	-555.3	32.33	31.18	32.33	31.17	31.81	33.33	36.71	37.20	122.0	191.0	90.20	135.00		
Seas_2	**46.4**	**69.1**	**121.4**	**53.0**	**-955.1**	**-2121.2**	**98.96**	**96.53**	**98.97**	**96.53**	**96.62**	**102.50**	**111.36**	**114.49**	**301.6**	**465.0**	**232.10**	**341.30**	**235.86**	**427.54**
Jul			46.3	24.8	-199.9	-469.8	33.17	31.69	33.18	31.69	32.84	34.05	37.94	37.98	123.0	193.0	89.00	133.00		
Aug			43.3	24.5	-159.5	-386.9	32.97	31.23	32.98	31.23	32.80	33.71	37.94	37.58	120.0	183.0	89.80	132.00		
Sep			48.3	25.9	-124.1	-311.6	31.75	29.86	31.75	29.86	31.72	32.36	36.71	36.03	98.3	147.0	79.80	115.00		
Seas_3	**92.9**	**93.1**	**137.9**	**75.1**	**-483.5**	**-1168.2**	**97.89**	**92.78**	**97.90**	**92.77**	**97.36**	**100.12**	**112.58**	**111.59**	**341.3**	**523.0**	**258.60**	**380.00**	**547.97**	**921.25**
Oct			44.2	20.7	-103.1	-269.5	32.67	30.53	32.67	30.53	32.75	33.18	37.94	36.95	67.5	102.0	55.00	80.50		
Nov			35.8	9.7	-80.0	-219.1	31.50	29.27	31.50	29.27	31.67	31.89	36.71	35.50	33.7	50.7	29.10	42.70		
Dec			21.4	1.8	-64.0	-185.1	31.40	29.04	31.40	29.04	31.66	31.73	36.71	35.28	28.0	40.3	25.50	35.90		
Seas_4	**33.4**	**66.6**	**101.4**	**32.2**	**-247.1**	**-673.7**	**95.56**	**88.84**	**95.58**	**88.83**	**96.08**	**96.80**	**111.36**	**107.73**	**129.2**	**193.0**	**109.60**	**159.10**	**168.33**	**360.49**
Annual	**179.4**	**245.9**	**415.7**	**143.6**	**-3782.6**	**-8309.2**	**393.07**	**380.69**	**393.10**	**380.67**	**387.46**	**407.92**	**446.66**	**455.11**	**854.1**	**1297.7**	**668.90**	**974.30**	**983.38**	**1789.87**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Net mass flows between the atmosphere and vegetation

Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-153 net mass flows between the atmosphere and vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.90.

Monthly values of PCB-153 net mass flows between the atmosphere and vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.111 a and b, respectively. Seasonal variations for models with low positive values of net mass flows between the atmosphere and vegetation calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. 3.111c in more detail.

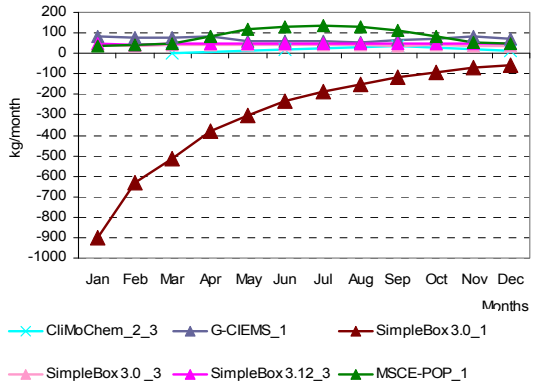


Fig. 3.111a. *PCB-153 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

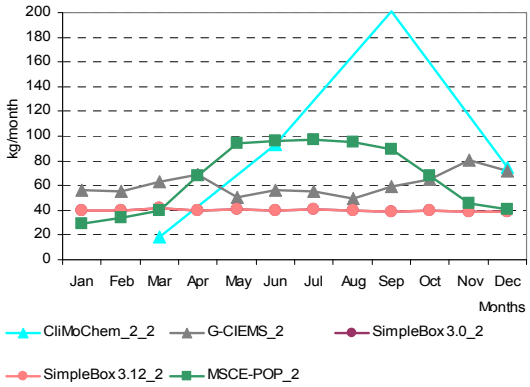


Fig. 3.111b. *PCB-153 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

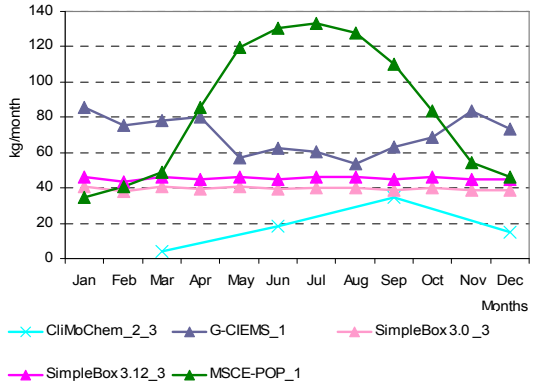


Fig. 3.111c. *PCB-153 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Table 3.90. *Calculation results: PCB-153 net mass flows between the atmosphere and vegetation (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	85.37	-898.82	34.80		41.04	46.43	*-138.24*	*425.64*	Jan	56.02		40.24	40.24	29.40	*41.47*	*10.96*
Feb	75.39	-628.40	40.90		37.97	43.43	*-86.14*	*303.51*	Feb	55.24		39.51	39.51	33.50	*41.94*	*9.31*
Mar	77.92	-511.46	48.80		40.53	46.43	*-59.56*	*253.03*	Mar	62.78		41.72	41.73	39.80	*46.51*	*10.89*
Seas_1	**238.68**	**-2038.67**	**124.50**	**11.57**	**119.54**	**136.29**	***-234.68***	***886.70***	**Seas_1**	**174.05**	**54.06**	**121.47**	**121.47**	**102.70**	***114.75***	***43.11***
Apr	80.04	-379.77	85.70		39.18	44.93	*-25.98*	*198.84*	Apr	68.52		39.98	39.98	68.30	*54.20*	*16.42*
May	57.14	-304.73	119.90		40.44	46.43	*-8.17*	*168.79*	May	50.71		40.98	40.98	93.83	*56.62*	*25.23*
Jun	62.23	-231.11	130.45		39.10	44.93	*9.12*	*139.13*	Jun	56.15		39.39	39.39	96.44	*57.84*	*26.92*
Seas_2	**199.41**	**-915.61**	**336.05**	**55.54**	**118.71**	**136.29**	***-11.60***	***452.99***	**Seas_2**	**175.38**	**279.35**	**120.34**	**120.35**	**258.57**	***190.80***	***75.17***
Jul	60.53	-188.54	133.50		40.36	46.43	*18.46*	*121.57*	Jul	55.29		40.47	40.47	96.90	*58.28*	*26.67*
Aug	53.79	-148.88	127.58		40.33	46.43	*23.85*	*102.80*	Aug	49.44		40.28	40.28	95.46	*56.36*	*26.42*
Sep	63.30	-114.29	110.10		39.00	44.93	*28.61*	*84.62*	Sep	59.12		38.82	38.83	88.95	*56.43*	*23.70*
Seas_3	**177.62**	**-451.72**	**371.18**	**104.55**	**119.70**	**137.79**	***76.52***	***276.58***	**Seas_3**	**163.85**	**603.43**	**119.57**	**119.58**	**281.31**	***257.55***	***204.36***
Oct	68.48	-93.43	83.50		40.28	46.43	*29.05*	*70.62*	Oct	64.76		39.98	39.98	67.80	*53.13*	*15.23*
Nov	83.59	-70.97	54.10		38.96	44.93	*30.12*	*59.06*	Nov	80.42		38.58	38.58	46.00	*50.89*	*19.99*
Dec	73.70	-55.20	46.20		38.94	44.93	*29.71*	*49.33*	Dec	71.38		38.48	38.49	41.20	*47.39*	*16.05*
Seas_4	**225.77**	**-219.60**	**183.80**	**45.11**	**118.17**	**136.29**	***81.59***	***159.76***	**Seas_4**	**216.55**	**225.08**	**117.03**	**117.05**	**155.00**	***166.14***	***52.35***
Annual	**841.48**	**-3625.60**	**1015.53**	**216.77**	**476.12**	**546.67**	***-88.17***	***1755.58***	**Annual**	**729.83**	**1161.93**	**478.41**	**478.45**	**797.58**	***729.24***	***281.82***

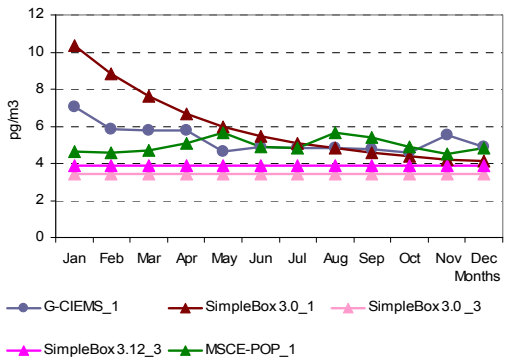
G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

3.5. Concentrations at each interface

3.5.1. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with soil

Reference data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with soil calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.91.

Monthly values of PCB-153 concentration in the atmosphere at its interface with soil calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.112 a and b, respectively.



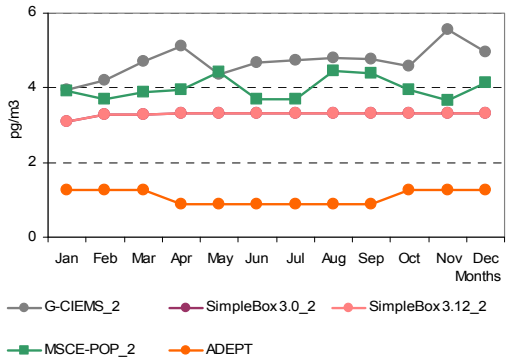
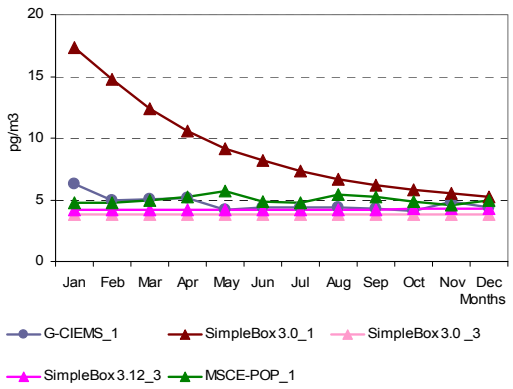


Fig. 3.112a. *PCB-153 concentration in the atmosphere at its interface with soil (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. 3.112b. *PCB-153 concentration in the atmosphere at its interface with soil (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with soil calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.92.

Monthly values of PCB-153 concentration in the atmosphere at its interface with soil calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.113 a and b, respectively.



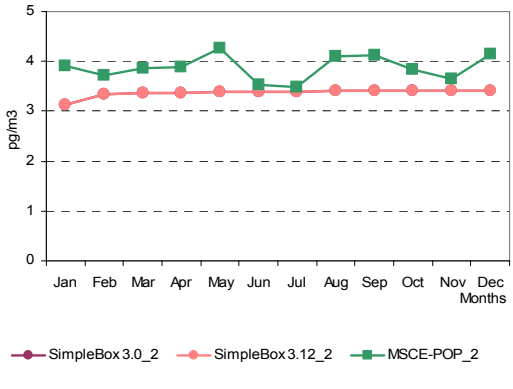


Fig. 3.113a. *PCB-153 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

Fig. 3.113b. *PCB-153 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.91. *Calculation results: PCB-153 concentration in the atmosphere at interface with soil (pg/m3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1	MSCE-POP_1	SimpleBox 3.0 _3	SimpleBox 3.12_3				G-CIEMS_2	SimpleBox 3.0_2	SimpleBox 3.12_2	MSCE-POP_2	ADEPT		
Jan	7.06	10.32	4.63	3.45	3.85	*5.86*	*2.86*	Jan	3.93	3.08	3.08	3.92	1.25	*3.05*	*1.09*
Feb	5.82	8.84	4.56	3.42	3.85	*5.30*	*2.18*	Feb	4.19	3.29	3.29	3.71	1.25	*3.15*	*1.12*
Mar	5.76	7.59	4.73	3.42	3.85	*5.07*	*1.67*	Mar	4.71	3.30	3.30	3.87	1.25	*3.29*	*1.28*
Apr	5.80	6.67	5.06	3.42	3.85	*4.96*	*1.35*	Apr	5.12	3.30	3.30	3.94	0.87	*3.31*	*1.55*
May	4.65	5.99	5.67	3.42	3.85	*4.72*	*1.12*	May	4.37	3.31	3.31	4.42	0.87	*3.26*	*1.44*
Jun	4.86	5.48	4.92	3.42	3.85	*4.51*	*0.85*	Jun	4.68	3.31	3.31	3.71	0.87	*3.18*	*1.40*
Jul	4.83	5.10	4.84	3.42	3.85	*4.41*	*0.73*	Jul	4.74	3.32	3.32	3.69	0.87	*3.19*	*1.42*
Aug	4.83	4.79	5.68	3.42	3.85	*4.51*	*0.89*	Aug	4.80	3.32	3.32	4.44	0.87	*3.35*	*1.54*
Sep	4.78	4.56	5.37	3.42	3.85	*4.39*	*0.77*	Sep	4.77	3.32	3.32	4.38	0.87	*3.33*	*1.52*
Oct	4.56	4.37	4.89	3.42	3.85	*4.22*	*0.58*	Oct	4.58	3.32	3.32	3.96	1.25	*3.29*	*1.25*
Nov	5.51	4.22	4.48	3.42	3.85	*4.29*	*0.79*	Nov	5.54	3.32	3.32	3.66	1.25	*3.42*	*1.52*
Dec	4.92	4.10	4.83	3.42	3.85	*4.22*	*0.64*	Dec	4.96	3.32	3.33	4.15	1.25	*3.40*	*1.38*
Annual	**5.28**	**6.00**	**4.97**	**3.42**	**3.85**	***4.71***	***1.06***	**Annual**	**4.70**	**3.29**	**3.29**	**3.99**	**1.06**	***3.27***	***1.36***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.92. *Calculation results: PCB-153 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.28	17.34	4.80	3.82	4.21	*7.29*	*5.70*	Jan	3.12	3.12	3.90	*3.38*	*0.45*
Feb	4.98	14.80	4.77	3.79	4.21	*6.51*	*4.66*	Feb	3.34	3.34	3.72	*3.47*	*0.22*
Mar	5.01	12.38	4.93	3.80	4.22	*6.07*	*3.56*	Mar	3.36	3.36	3.87	*3.53*	*0.29*
Apr	5.14	10.55	5.27	3.80	4.22	*5.80*	*2.73*	Apr	3.37	3.37	3.89	*3.54*	*0.30*
May	4.21	9.18	5.76	3.81	4.23	*5.44*	*2.22*	May	3.38	3.38	4.27	*3.68*	*0.51*
Jun	4.39	8.14	4.89	3.81	4.23	*5.09*	*1.75*	Jun	3.39	3.39	3.52	*3.43*	*0.08*
Jul	4.37	7.34	4.75	3.81	4.23	*4.90*	*1.41*	Jul	3.40	3.40	3.48	*3.42*	*0.05*
Aug	4.38	6.71	5.45	3.81	4.24	*4.92*	*1.17*	Aug	3.40	3.40	4.10	*3.63*	*0.40*
Sep	4.29	6.21	5.24	3.82	4.24	*4.76*	*0.96*	Sep	3.41	3.41	4.13	*3.65*	*0.42*
Oct	4.08	5.81	4.89	3.82	4.24	*4.57*	*0.80*	Oct	3.41	3.41	3.83	*3.55*	*0.24*
Nov	4.89	5.48	4.59	3.82	4.24	*4.60*	*0.63*	Nov	3.41	3.41	3.64	*3.49*	*0.13*
Dec	4.37	5.21	4.95	3.82	4.24	*4.52*	*0.56*	Dec	3.42	3.42	4.15	*3.66*	*0.42*
Annual	**4.70**	**9.10**	**5.02**	**3.81**	**4.23**	***5.37***	***2.13***	**Annual**	**3.37**	**3.37**	**3.88**	***3.54***	***0.29***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.93.

Table 3.93. *The percentage difference between calculation results on PCB-153 concentration in the atmosphere at its interface with soil obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-11.1%	68.0%	1.2%	1.2%	10.8%	9.3%	3.7%	-0.5%
Feb	-14.4%	67.5%	1.6%	1.6%	11.0%	9.4%	4.6%	0.3%
Mar	-13.0%	63.0%	1.8%	1.8%	11.2%	9.6%	4.2%	0.0%
Apr	-11.3%	58.2%	2.0%	2.0%	11.3%	9.7%	4.2%	-1.3%
May	-9.5%	53.3%	2.2%	2.2%	11.4%	9.8%	1.6%	-3.4%
Jun	-9.6%	48.5%	2.3%	2.3%	11.5%	9.9%	-0.6%	-5.1%
Jul	-9.5%	44.0%	2.4%	2.4%	11.5%	10.0%	-1.9%	-5.7%
Aug	-9.4%	39.9%	2.5%	2.5%	11.6%	10.0%	-4.0%	-7.7%
Sep	-10.2%	36.2%	2.6%	2.6%	11.6%	10.0%	-2.4%	-5.7%
Oct	-10.5%	32.8%	2.7%	2.6%	11.7%	10.1%	0.0%	-3.3%
Nov	-11.3%	29.8%	2.7%	2.7%	11.7%	10.1%	2.5%	-0.5%
Dec	-11.1%	27.1%	2.8%	2.7%	11.7%	10.1%	2.5%	0.0%
Annual	**-11.0%**	**51.5%**	**2.2%**	**2.2%**	**11.4%**	**9.8%**	**1.1%**	**-2.8%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.5.2. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with ocean

Reference data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.94.

Monthly values of PCB-153 concentration in the atmosphere at its interface with ocean calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.114 a and b, respectively.

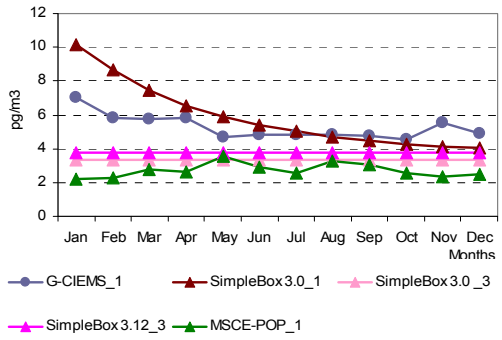


Fig. 3.114a. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

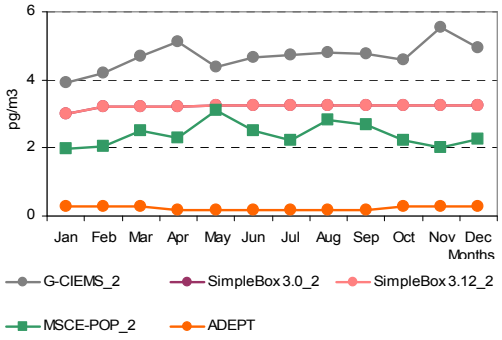


Fig. 3.114b. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.95.

Monthly values of PCB-153 concentration in the atmosphere at its interface with ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.115 a and b, respectively.

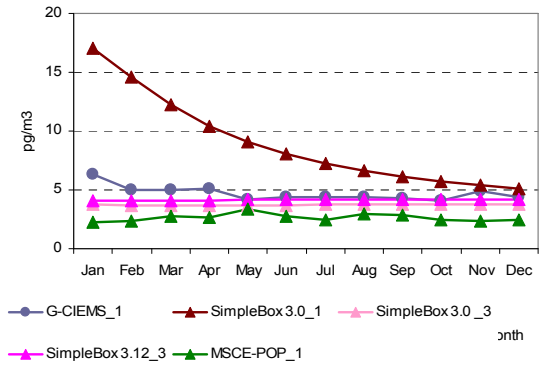


Fig. 3.115a. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

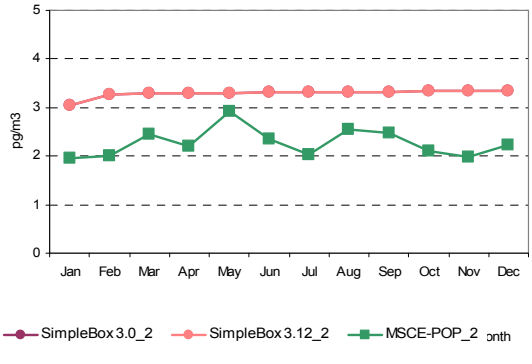


Fig. 3.115b. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.94. *Calculation results: PCB-153 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	7.06	10.15	2.22	3.37	3.77	*5.31*	*3.25*	Jan	3.93	3.01	3.01	1.98	0.30	*2.45*	*1.38*
Feb	5.82	8.70	2.29	3.34	3.77	*4.78*	*2.54*	Feb	4.19	3.21	3.21	2.04	0.30	*2.59*	*1.49*
Mar	5.76	7.47	2.80	3.34	3.77	*4.63*	*1.94*	Mar	4.71	3.22	3.22	2.50	0.30	*2.79*	*1.61*
Apr	5.80	6.57	2.62	3.34	3.77	*4.42*	*1.68*	Apr	5.12	3.23	3.23	2.28	0.19	*2.81*	*1.79*
May	4.65	5.90	3.52	3.34	3.77	*4.24*	*1.06*	May	4.37	3.23	3.23	3.12	0.19	*2.83*	*1.56*
Jun	4.86	5.40	2.91	3.34	3.77	*4.05*	*1.04*	Jun	4.68	3.23	3.24	2.52	0.19	*2.77*	*1.64*
Jul	4.83	5.01	2.57	3.34	3.77	*3.90*	*1.03*	Jul	4.74	3.24	3.24	2.22	0.19	*2.73*	*1.68*
Aug	4.83	4.71	3.24	3.34	3.77	*3.98*	*0.75*	Aug	4.80	3.24	3.24	2.82	0.19	*2.86*	*1.67*
Sep	4.78	4.48	3.04	3.34	3.77	*3.88*	*0.74*	Sep	4.77	3.24	3.24	2.68	0.19	*2.83*	*1.67*
Oct	4.56	4.29	2.58	3.34	3.77	*3.71*	*0.79*	Oct	4.58	3.24	3.24	2.23	0.30	*2.72*	*1.59*
Nov	5.51	4.14	2.34	3.34	3.77	*3.82*	*1.16*	Nov	5.54	3.25	3.25	2.02	0.30	*2.87*	*1.92*
Dec	4.92	4.02	2.49	3.34	3.77	*3.71*	*0.89*	Dec	4.96	3.25	3.25	2.26	0.30	*2.80*	*1.70*
Annual	**5.28**	**5.90**	**2.72**	**3.34**	**3.77**	***4.20***	***1.34***	**Annual**	**4.70**	**3.22**	**3.22**	**2.39**	**0.25**	***2.75***	***1.63***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.95. *Calculation results: PCB-153 concentration in the atmosphere at its interface with ocean (pg/m3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.28	17.08	2.26	3.73	4.11	*6.69*	*5.98*	Jan	3.05	3.05	1.96	*2.68*	*0.63*
Feb	4.98	14.59	2.32	3.71	4.12	*5.94*	*4.93*	Feb	3.27	3.27	2.01	*2.85*	*0.73*
Mar	5.01	12.20	2.80	3.71	4.12	*5.57*	*3.79*	Mar	3.28	3.28	2.45	*3.00*	*0.48*
Apr	5.14	10.40	2.61	3.72	4.13	*5.20*	*3.05*	Apr	3.29	3.29	2.20	*2.93*	*0.63*
May	4.21	9.06	3.39	3.72	4.13	*4.90*	*2.35*	May	3.30	3.30	2.93	*3.18*	*0.21*
Jun	4.39	8.03	2.76	3.72	4.14	*4.61*	*2.01*	Jun	3.31	3.31	2.34	*2.99*	*0.56*
Jul	4.37	7.24	2.40	3.73	4.14	*4.38*	*1.77*	Jul	3.32	3.32	2.04	*2.89*	*0.74*
Aug	4.38	6.61	2.96	3.73	4.14	*4.36*	*1.37*	Aug	3.32	3.32	2.54	*3.06*	*0.45*
Sep	4.29	6.12	2.86	3.73	4.14	*4.23*	*1.19*	Sep	3.33	3.33	2.48	*3.04*	*0.49*
Oct	4.08	5.72	2.49	3.73	4.15	*4.03*	*1.15*	Oct	3.33	3.33	2.11	*2.92*	*0.71*
Nov	4.89	5.39	2.34	3.73	4.15	*4.10*	*1.17*	Nov	3.34	3.34	1.98	*2.88*	*0.78*
Dec	4.37	5.12	2.49	3.73	4.15	*3.97*	*0.97*	Dec	3.34	3.34	2.22	*2.97*	*0.65*
Annual	**4.70**	**8.96**	**2.64**	**3.72**	**4.14**	***4.83***	***2.43***	**Annual**	**3.29**	**3.29**	**2.27**	***2.95***	***0.59***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.96.

Table 3.96. *The percentage difference between calculation results on PCB-153 concentration in the atmosphere at its interface with ocean obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-11.1%	68.2%	1.2%	1.2%	10.8%	9.2%	1.8%	-1.0%
Feb	-14.4%	67.8%	1.6%	1.6%	11.1%	9.3%	1.3%	-1.5%
Mar	-13.0%	63.3%	1.8%	1.8%	11.2%	9.5%	0.0%	-2.0%
Apr	-11.3%	58.4%	2.0%	2.0%	11.4%	9.7%	-0.4%	-3.5%
May	-9.5%	53.6%	2.2%	2.2%	11.5%	9.8%	-3.7%	-6.1%
Jun	-9.6%	48.8%	2.3%	2.3%	11.5%	9.9%	-5.2%	-7.1%
Jul	-9.5%	44.4%	2.4%	2.4%	11.6%	9.9%	-6.6%	-8.1%
Aug	-9.4%	40.2%	2.5%	2.5%	11.6%	10.0%	-8.6%	-9.9%
Sep	-10.2%	36.5%	2.6%	2.6%	11.7%	10.0%	-5.9%	-7.5%
Oct	-10.5%	33.2%	2.7%	2.7%	11.7%	10.1%	-3.5%	-5.4%
Nov	-11.3%	30.1%	2.8%	2.7%	11.7%	10.1%	0.0%	-2.0%
Dec	-11.1%	27.5%	2.8%	2.8%	11.8%	10.1%	0.0%	-1.8%
Annual	**-11.0%**	**51.8%**	**2.3%**	**2.3%**	**11.5%**	**9.8%**	**-2.9%**	**-4.9%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.5.3. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with vegetation

Reference data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.97.

Monthly values of PCB-153 concentration in the atmosphere at its interface with vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.116 a and b, respectively.

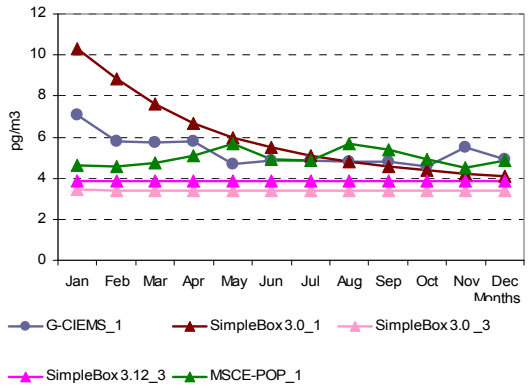


Fig. 3.116a. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

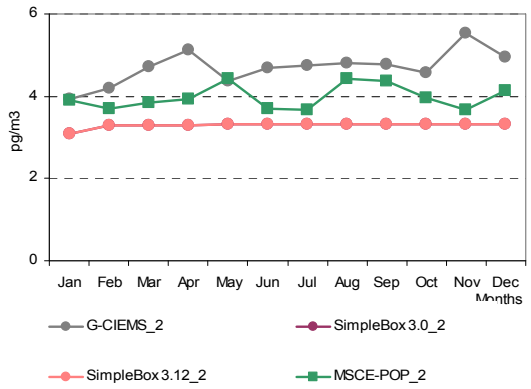


Fig. 3.116b. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.98.

Monthly values of PCB-153 concentration in the atmosphere at its interface with vegetation calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.117 a and b, respectively.

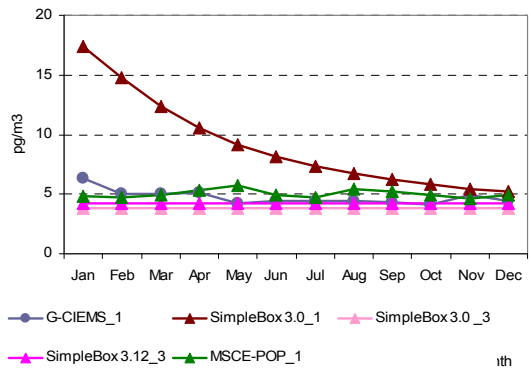


Fig. 3.117a. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

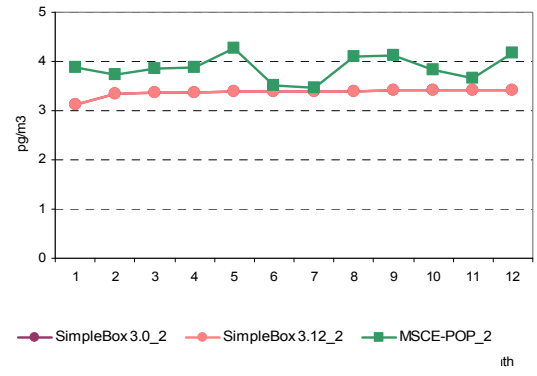


Fig. 3.117b. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.97. *Calculation results: PCB-153 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE- POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	7.06	10.32	4.62	3.45	3.85	*5.86*	*2.86*	Jan	3.93	3.08	3.08	3.91	*3.50*	*0.48*
Feb	5.82	8.84	4.56	3.42	3.85	*5.30*	*2.18*	Feb	4.19	3.29	3.29	3.71	*3.62*	*0.43*
Mar	5.76	7.59	4.72	3.42	3.85	*5.07*	*1.67*	Mar	4.71	3.30	3.30	3.85	*3.79*	*0.67*
Apr	5.80	6.67	5.07	3.42	3.85	*4.96*	*1.35*	Apr	5.12	3.30	3.30	3.94	*3.92*	*0.86*
May	4.65	5.99	5.66	3.42	3.85	*4.71*	*1.11*	May	4.37	3.31	3.31	4.42	*3.85*	*0.63*
Jun	4.86	5.48	4.91	3.42	3.85	*4.50*	*0.85*	Jun	4.68	3.31	3.31	3.70	*3.75*	*0.64*
Jul	4.83	5.10	4.83	3.42	3.85	*4.41*	*0.73*	Jul	4.74	3.32	3.32	3.68	*3.76*	*0.68*
Aug	4.83	4.79	5.68	3.42	3.85	*4.51*	*0.89*	Aug	4.80	3.32	3.32	4.43	*3.97*	*0.76*
Sep	4.78	4.56	5.36	3.42	3.85	*4.39*	*0.77*	Sep	4.77	3.32	3.32	4.37	*3.95*	*0.74*
Oct	4.56	4.37	4.89	3.42	3.85	*4.22*	*0.58*	Oct	4.58	3.32	3.32	3.96	*3.80*	*0.60*
Nov	5.51	4.22	4.48	3.42	3.85	*4.29*	*0.79*	Nov	5.54	3.32	3.32	3.66	*3.96*	*1.07*
Dec	4.92	4.10	4.84	3.42	3.85	*4.22*	*0.65*	Dec	4.96	3.32	3.33	4.15	*3.94*	*0.78*
Annual	**5.28**	**6.00**	**4.97**	**3.42**	**3.85**	***4.70***	***1.06***	**Annual**	**4.70**	**3.29**	**3.29**	**3.98**	***3.82***	***0.67***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.98. *Calculation results: PCB-153 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.28	17.34	4.80	3.82	4.21	*7.29*	*5.70*	Jan	3.12	3.12	3.89	*3.38*	*0.44*
Feb	4.98	14.80	4.77	3.79	4.21	*6.51*	*4.66*	Feb	3.34	3.34	3.72	*3.47*	*0.22*
Mar	5.01	12.38	4.92	3.80	4.22	*6.06*	*3.56*	Mar	3.36	3.36	3.85	*3.52*	*0.28*
Apr	5.14	10.55	5.28	3.80	4.22	*5.80*	*2.73*	Apr	3.37	3.37	3.89	*3.54*	*0.30*
May	4.21	9.18	5.75	3.81	4.23	*5.44*	*2.22*	May	3.38	3.38	4.26	*3.67*	*0.51*
Jun	4.39	8.14	4.89	3.81	4.23	*5.09*	*1.75*	Jun	3.39	3.39	3.51	*3.43*	*0.07*
Jul	4.37	7.34	4.75	3.81	4.23	*4.90*	*1.41*	Jul	3.40	3.40	3.47	*3.42*	*0.04*
Aug	4.38	6.71	5.44	3.81	4.24	*4.91*	*1.17*	Aug	3.40	3.40	4.09	*3.63*	*0.40*
Sep	4.29	6.21	5.23	3.82	4.24	*4.76*	*0.96*	Sep	3.41	3.41	4.12	*3.64*	*0.41*
Oct	4.08	5.81	4.89	3.82	4.24	*4.57*	*0.80*	Oct	3.41	3.41	3.83	*3.55*	*0.24*
Nov	4.89	5.48	4.60	3.82	4.24	*4.60*	*0.63*	Nov	3.41	3.41	3.65	*3.49*	*0.14*
Dec	4.37	5.21	4.96	3.82	4.24	*4.52*	*0.56*	Dec	3.42	3.42	4.16	*3.66*	*0.43*
Annual	**4.70**	**9.10**	**5.02**	**3.81**	**4.23**	***5.37***	***2.13***	**Annual**	**3.37**	**3.37**	**3.87**	***3.53***	***0.29***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.99.

Table 3.99. *The percentage difference between calculation results on PCB-153 concentration in the atmosphere at interface with vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-11.1%	68.0%	1.2%	1.2%	10.8%	9.3%	3.9%	-0.5%
Feb	-14.4%	67.5%	1.6%	1.6%	11.0%	9.4%	4.6%	0.3%
Mar	-13.0%	63.0%	1.8%	1.8%	11.2%	9.6%	4.2%	0.0%
Apr	-11.3%	58.2%	2.0%	2.0%	11.3%	9.7%	4.1%	-1.3%
May	-9.5%	53.3%	2.2%	2.2%	11.4%	9.8%	1.6%	-3.6%
Jun	-9.6%	48.5%	2.3%	2.3%	11.5%	9.9%	-0.4%	-5.1%
Jul	-9.5%	44.0%	2.4%	2.4%	11.5%	10.0%	-1.7%	-5.7%
Aug	-9.4%	39.9%	2.5%	2.5%	11.6%	10.0%	-4.2%	-7.7%
Sep	-10.2%	36.2%	2.6%	2.6%	11.6%	10.0%	-2.4%	-5.7%
Oct	-10.5%	32.8%	2.7%	2.6%	11.7%	10.1%	0.0%	-3.3%
Nov	-11.3%	29.8%	2.7%	2.7%	11.7%	10.1%	2.7%	-0.3%
Dec	-11.1%	27.1%	2.8%	2.7%	11.7%	10.1%	2.5%	0.2%
Annual	**-11.0%**	**51.5%**	**2.2%**	**2.2%**	**11.4%**	**9.8%**	**1.1%**	**-2.8%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.5.4. Comparison of calculated values of PCB-153 concentration in surface ocean layer

Reference data set. Calculation results on PCB-153 concentration in surface ocean layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.100.

Monthly values of PCB-153 concentration in surface ocean layer calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.118 a and b, respectively.

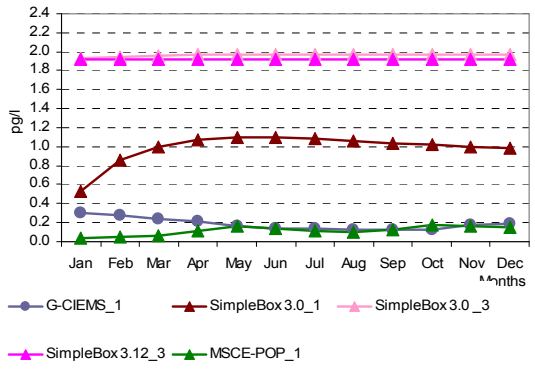


Fig. 3.118a. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

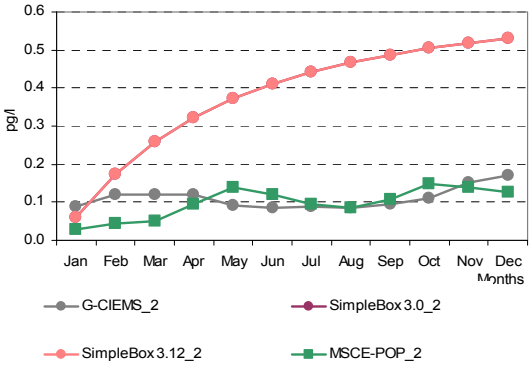


Fig. 3.118b. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in surface ocean layer calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.101.

Monthly values of PCB-153 concentration in surface ocean layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.119 a and b, respectively.

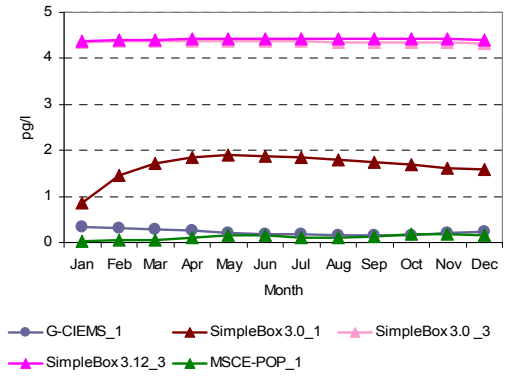


Fig. 3.119a. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

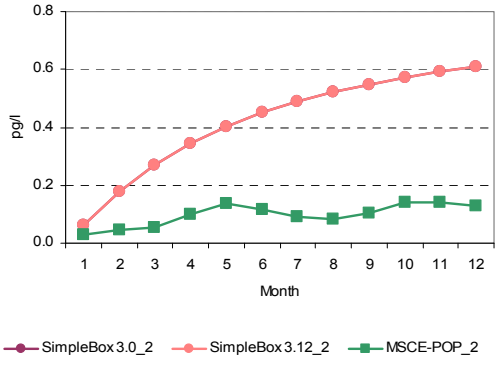


Fig. 3.119b. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.100. *Calculation results: PCB-153 concentration in surface ocean layer (pg/l) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.30	0.54	0.03	1.94	1.93	*0.95*	*0.92*	Jan	0.09	0.06	0.06	0.03	*0.06*	*0.02*
Feb	0.28	0.85	0.05	1.95	1.93	*1.01*	*0.89*	Feb	0.12	0.17	0.17	0.04	*0.13*	*0.06*
Mar	0.24	1.00	0.06	1.96	1.93	*1.04*	*0.90*	Mar	0.12	0.26	0.26	0.05	*0.17*	*0.10*
Apr	0.21	1.07	0.11	1.96	1.93	*1.06*	*0.89*	Apr	0.12	0.32	0.32	0.10	*0.22*	*0.13*
May	0.16	1.10	0.16	1.97	1.93	*1.06*	*0.89*	May	0.09	0.37	0.37	0.14	*0.24*	*0.15*
Jun	0.14	1.10	0.14	1.97	1.93	*1.06*	*0.90*	Jun	0.09	0.41	0.41	0.12	*0.26*	*0.18*
Jul	0.13	1.08	0.11	1.97	1.93	*1.05*	*0.91*	Jul	0.09	0.44	0.44	0.09	*0.27*	*0.20*
Aug	0.12	1.06	0.10	1.97	1.93	*1.04*	*0.92*	Aug	0.08	0.47	0.47	0.08	*0.28*	*0.22*
Sep	0.12	1.04	0.13	1.97	1.93	*1.04*	*0.91*	Sep	0.09	0.49	0.49	0.11	*0.29*	*0.22*
Oct	0.13	1.02	0.18	1.97	1.93	*1.05*	*0.90*	Oct	0.11	0.50	0.50	0.15	*0.32*	*0.22*
Nov	0.17	1.00	0.17	1.97	1.93	*1.05*	*0.89*	Nov	0.15	0.52	0.52	0.14	*0.33*	*0.22*
Dec	0.19	0.99	0.15	1.97	1.93	*1.04*	*0.89*	Dec	0.17	0.53	0.53	0.13	*0.34*	*0.22*
Annual	**0.18**	**0.99**	**0.12**	**1.97**	**1.93**	***1.04***	***0.90***	**Annual**	**0.11**	**0.38**	**0.38**	**0.10**	***0.24***	***0.16***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.101. *Calculation results: PCB-153 concentration in surface ocean layer (pg/l) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.34	0.86	0.04	4.36	4.37	*1.99*	*2.18*	Jan	0.06	0.06	0.03	*0.05*	*0.02*
Feb	0.31	1.45	0.06	4.37	4.39	*2.12*	*2.13*	Feb	0.18	0.18	0.05	*0.13*	*0.08*
Mar	0.28	1.72	0.06	4.37	4.41	*2.17*	*2.13*	Mar	0.27	0.27	0.05	*0.20*	*0.13*
Apr	0.25	1.85	0.12	4.37	4.42	*2.20*	*2.11*	Apr	0.35	0.35	0.10	*0.26*	*0.14*
May	0.20	1.90	0.17	4.37	4.42	*2.21*	*2.12*	May	0.40	0.40	0.14	*0.32*	*0.15*
Jun	0.18	1.89	0.15	4.37	4.43	*2.20*	*2.12*	Jun	0.45	0.45	0.12	*0.34*	*0.19*
Jul	0.17	1.85	0.12	4.36	4.43	*2.19*	*2.14*	Jul	0.49	0.49	0.09	*0.36*	*0.23*
Aug	0.15	1.80	0.10	4.36	4.43	*2.17*	*2.14*	Aug	0.52	0.52	0.08	*0.37*	*0.25*
Sep	0.16	1.74	0.13	4.35	4.42	*2.16*	*2.14*	Sep	0.55	0.55	0.10	*0.40*	*0.26*
Oct	0.17	1.68	0.18	4.35	4.42	*2.16*	*2.12*	Oct	0.57	0.57	0.14	*0.43*	*0.25*
Nov	0.21	1.63	0.17	4.34	4.42	*2.15*	*2.11*	Nov	0.59	0.59	0.14	*0.44*	*0.26*
Dec	0.23	1.58	0.16	4.33	4.41	*2.14*	*2.11*	Dec	0.61	0.61	0.13	*0.45*	*0.28*
Annual	**0.22**	**1.66**	**0.12**	**4.36**	**4.41**	***2.16***	***2.13***	**Annual**	**0.42**	**0.42**	**0.10**	***0.31***	***0.19***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.102.

Table 3.102. *The percentage difference between calculation results on PCB-153 concentration in surface ocean layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	13.2%	60.4%	0.6%	0.6%	125.3%	126.8%	8.9%	4.7%
Feb	13.6%	70.1%	2.8%	2.8%	124.1%	128.0%	8.9%	5.4%
Mar	16.5%	72.0%	4.9%	4.9%	123.3%	128.9%	7.7%	4.6%
Apr	19.8%	72.8%	6.7%	6.7%	122.6%	129.4%	5.5%	2.9%
May	23.7%	72.8%	8.3%	8.3%	122.1%	129.7%	1.2%	-1.4%
Jun	25.0%	72.2%	9.7%	9.7%	121.6%	129.9%	2.8%	-0.8%
Jul	26.3%	71.0%	10.9%	10.9%	121.3%	130.0%	1.8%	-1.4%
Aug	26.8%	69.3%	11.9%	11.9%	120.9%	129.8%	-1.0%	-3.6%
Sep	26.5%	67.2%	12.7%	12.7%	120.6%	129.7%	-0.8%	-3.7%
Oct	26.3%	65.0%	13.4%	13.4%	120.3%	129.5%	0.6%	-2.7%
Nov	22.9%	62.6%	14.0%	13.9%	120.0%	129.3%	3.0%	0.0%
Dec	21.9%	60.2%	14.4%	14.4%	119.8%	129.0%	4.7%	2.4%
Annual	**20.4%**	**68.4%**	**10.8%**	**10.8%**	**121.8%**	**129.2%**	**2.6%**	**-0.3%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.5.5. Comparison of calculated values of PCB-153 concentration in vegetation

Reference data set. Calculation results on PCB-153 concentration in vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.103.

Monthly values of PCB-153 concentration in vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.120 a and b, respectively.

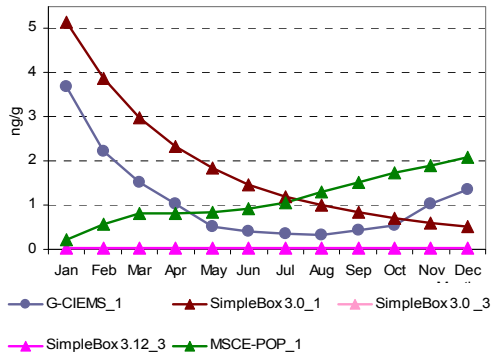


Fig. 3.120a. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

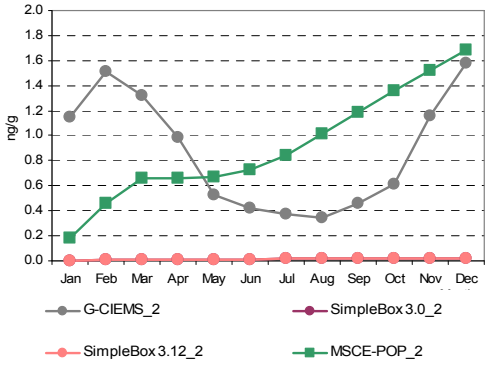


Fig. 3.120b. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.104.

Monthly values of PCB-153 concentration in vegetation calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.121 a and b, respectively.

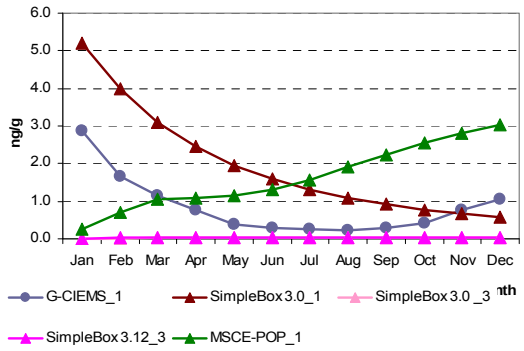


Fig. 3.121a. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

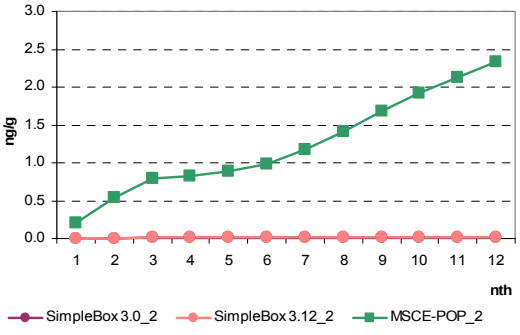


Fig. 3.121b. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.103. *Calculation results: PCB-153 concentration in vegetation (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	3.69	5.15	0.23	0.02	0.02	*1.82*	*2.43*	Jan	1.15	0.002	0.002	0.19	*0.34*	*0.55*
Feb	2.21	3.88	0.57	0.02	0.02	*1.34*	*1.68*	Feb	1.51	0.01	0.01	0.46	*0.50*	*0.71*
Mar	1.51	2.98	0.82	0.02	0.02	*1.07*	*1.24*	Mar	1.32	0.01	0.01	0.66	*0.50*	*0.63*
Apr	1.02	2.32	0.82	0.02	0.02	*0.84*	*0.94*	Apr	0.99	0.01	0.01	0.66	*0.42*	*0.49*
May	0.51	1.84	0.84	0.02	0.02	*0.65*	*0.75*	May	0.53	0.01	0.01	0.67	*0.31*	*0.34*
Jun	0.40	1.48	0.91	0.02	0.02	*0.57*	*0.63*	Jun	0.42	0.01	0.01	0.73	*0.29*	*0.35*
Jul	0.35	1.20	1.07	0.02	0.02	*0.53*	*0.57*	Jul	0.37	0.02	0.02	0.85	*0.31*	*0.39*
Aug	0.32	0.99	1.29	0.02	0.02	*0.53*	*0.58*	Aug	0.34	0.02	0.02	1.01	*0.35*	*0.47*
Sep	0.42	0.83	1.52	0.02	0.02	*0.56*	*0.63*	Sep	0.46	0.02	0.02	1.19	*0.42*	*0.55*
Oct	0.55	0.70	1.73	0.02	0.02	*0.60*	*0.70*	Oct	0.61	0.02	0.02	1.36	*0.50*	*0.64*
Nov	1.02	0.59	1.91	0.02	0.02	*0.71*	*0.79*	Nov	1.16	0.02	0.02	1.52	*0.68*	*0.78*
Dec	1.36	0.51	2.09	0.02	0.02	*0.80*	*0.91*	Dec	1.58	0.02	0.02	1.68	*0.82*	*0.93*
Annual	**1.11**	**1.87**	**1.15**	**0.02**	**0.02**	***0.84***	***0.80***	**Annual**	**0.87**	**0.01**	**0.01**	**0.91**	***0.45***	***0.51***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.104. *Calculation results: PCB-153 concentration in vegetation (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS-1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.89	5.20	0.26	0.01	0.01	*1.67*	*2.31*	Jan	0.002	0.002	0.20	*0.07*	*0.12*
Feb	1.67	3.98	0.70	0.02	0.02	*1.28*	*1.66*	Feb	0.01	0.01	0.54	*0.18*	*0.31*
Mar	1.16	3.10	1.04	0.02	0.02	*1.07*	*1.26*	Mar	0.01	0.01	0.79	*0.27*	*0.45*
Apr	0.78	2.44	1.08	0.02	0.02	*0.87*	*1.00*	Apr	0.01	0.01	0.83	*0.28*	*0.47*
May	0.38	1.95	1.16	0.02	0.02	*0.71*	*0.84*	May	0.01	0.01	0.89	*0.30*	*0.50*
Jun	0.29	1.59	1.31	0.02	0.02	*0.65*	*0.75*	Jun	0.02	0.02	0.99	*0.34*	*0.56*
Jul	0.25	1.31	1.56	0.02	0.02	*0.63*	*0.74*	Jul	0.02	0.02	1.17	*0.40*	*0.67*
Aug	0.23	1.09	1.90	0.02	0.03	*0.65*	*0.82*	Aug	0.02	0.02	1.42	*0.49*	*0.81*
Sep	0.30	0.92	2.24	0.02	0.03	*0.70*	*0.93*	Sep	0.02	0.02	1.68	*0.57*	*0.96*
Oct	0.40	0.78	2.54	0.02	0.03	*0.75*	*1.05*	Oct	0.02	0.02	1.92	*0.65*	*1.10*
Nov	0.78	0.67	2.80	0.02	0.03	*0.86*	*1.14*	Nov	0.02	0.02	2.13	*0.72*	*1.22*
Dec	1.07	0.58	3.03	0.03	0.03	*0.95*	*1.24*	Dec	0.02	0.02	2.33	*0.79*	*1.33*
Annual	**0.85**	**1.97**	**1.64**	**0.02**	**0.02**	***0.90***	***0.90***	**Annual**	**0.01**	**0.01**	**1.24**	***0.42***	***0.71***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.105.

Table 3.105. *The percentage difference between calculation results on PCB-153 concentration in vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-21.7%	0.8%	4.2%	4.2%	-37.1%	-35.3%	14.4%	9.7%
Feb	-24.3%	2.4%	5.1%	5.1%	-27.0%	-21.5%	23.6%	17.5%
Mar	-22.9%	3.9%	5.9%	5.9%	-19.0%	-10.4%	26.7%	20.9%
Apr	-23.7%	5.3%	6.5%	6.5%	-12.5%	-1.0%	32.0%	26.5%
May	-26.7%	6.5%	7.1%	7.1%	-7.3%	6.8%	38.8%	31.8%
Jun	-27.7%	7.7%	7.6%	7.6%	-3.0%	13.3%	43.5%	36.1%
Jul	-27.5%	8.7%	8.1%	8.1%	0.5%	18.8%	45.8%	38.5%
Aug	-27.9%	9.7%	8.5%	8.5%	3.5%	23.6%	47.3%	40.6%
Sep	-28.5%	10.7%	8.9%	8.9%	6.0%	27.6%	47.4%	41.2%
Oct	-27.2%	11.6%	9.2%	9.2%	8.2%	31.0%	46.8%	41.2%
Nov	-23.8%	12.4%	9.5%	9.5%	10.0%	34.0%	46.6%	40.1%
Dec	-21.7%	13.3%	9.8%	9.7%	11.5%	36.5%	45.0%	38.7%
Annual	**-23.7%**	**5.0%**	**8.2%**	**8.2%**	**-5.1%**	**10.3%**	**42.3%**	**35.9%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.5.6. Comparison of calculated values of PCB-153 concentration in surface soil layer

Reference data set. Calculation results on PCB-153 concentration in surface soil layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.106.

Monthly values of PCB-153 concentration in surface soil layer calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.122 a and b, respectively.

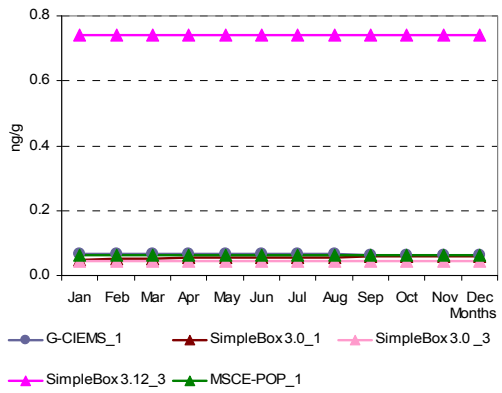


Fig.3.122a. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

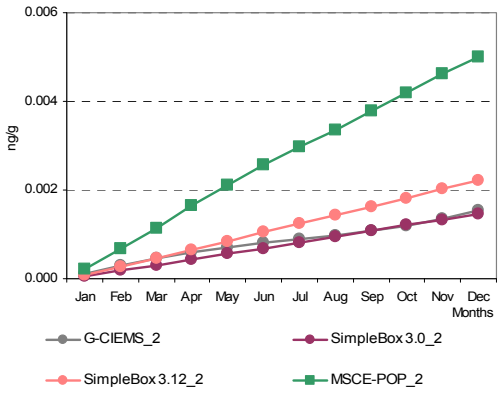


Fig.3.122b. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in surface soil layer calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.107.

Monthly values of PCB-153 concentration in surface soil layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.123a and b, respectively.

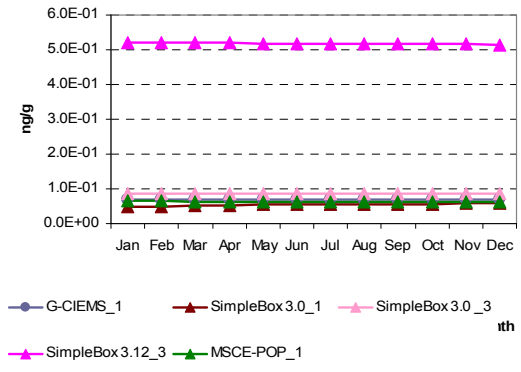


Fig. 3.123a. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

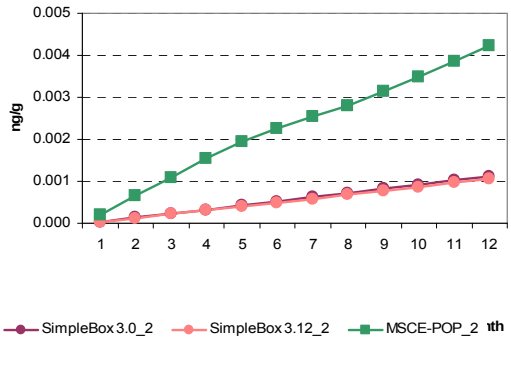


Fig. 3.123b. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.106. *Calculation results: PCB-153 concentration in surface soil layer (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.82E-02	4.70E-02	6.39E-02	4.50E-02	7.41E-01	*1.93E-01*	*3.06E-01*	Jan	1.20E-04	5.59E-05	8.54E-05	2.18E-04	*1.20E-04*	*7.05E-05*
Feb	6.78E-02	5.00E-02	6.37E-02	4.49E-02	7.41E-01	*1.93E-01*	*3.06E-01*	Feb	3.04E-04	1.78E-04	2.72E-04	6.70E-04	*3.56E-04*	*2.16E-04*
Mar	6.74E-02	5.22E-02	6.36E-02	4.48E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Mar	4.59E-04	3.03E-04	4.61E-04	1.14E-03	*5.91E-04*	*3.74E-04*
Apr	6.69E-02	5.38E-02	6.34E-02	4.47E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Apr	6.02E-04	4.31E-04	6.55E-04	1.64E-03	*8.32E-04*	*5.47E-04*
May	6.64E-02	5.50E-02	6.33E-02	4.47E-02	7.41E-01	*1.94E-01*	*3.06E-01*	May	7.08E-04	5.59E-04	8.49E-04	2.12E-03	*1.06E-03*	*7.17E-04*
Jun	6.59E-02	5.59E-02	6.31E-02	4.46E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Jun	7.99E-04	6.88E-04	1.04E-03	2.56E-03	*1.27E-03*	*8.71E-04*
Jul	6.54E-02	5.65E-02	6.28E-02	4.45E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Jul	8.93E-04	8.17E-04	1.24E-03	2.96E-03	*1.48E-03*	*1.01E-03*
Aug	6.49E-02	5.70E-02	6.26E-02	4.44E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Aug	9.77E-04	9.48E-04	1.43E-03	3.36E-03	*1.68E-03*	*1.14E-03*
Sep	6.44E-02	5.73E-02	6.24E-02	4.43E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Sep	1.07E-03	1.08E-03	1.63E-03	3.79E-03	*1.89E-03*	*1.29E-03*
Oct	6.39E-02	5.76E-02	6.23E-02	4.42E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Oct	1.19E-03	1.21E-03	1.82E-03	4.20E-03	*2.10E-03*	*1.43E-03*
Nov	6.35E-02	5.78E-02	6.21E-02	4.42E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Nov	1.35E-03	1.33E-03	2.01E-03	4.61E-03	*2.33E-03*	*1.55E-03*
Dec	6.30E-02	5.79E-02	6.20E-02	4.41E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Dec	1.54E-03	1.46E-03	2.20E-03	4.99E-03	*2.55E-03*	*1.66E-03*
Annual	**6.56E-02**	**5.48E-02**	**6.29E-02**	**4.45E-02**	**7.41E-01**	***1.94E-01***	***3.06E-01***	**Annual**	**8.35E-04**	**7.55E-04**	**1.14E-03**	**2.69E-03**	***1.35E-03***	***9.04E-04***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.107. *Calculation results: PCB-153 concentration in surface soil layer (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.86E-02	4.66E-02	6.40E-02	8.53E-02	5.22E-01	*1.57E-01*	*2.04E-01*	Jan	4.15E-05	3.96E-05	2.13E-04	*9.80E-05*	*9.96E-05*
Feb	6.88E-02	4.92E-02	6.38E-02	8.53E-02	5.22E-01	*1.58E-01*	*2.04E-01*	Feb	1.33E-04	1.27E-04	6.43E-04	*3.01E-04*	*2.96E-04*
Mar	6.89E-02	5.11E-02	6.37E-02	8.53E-02	5.21E-01	*1.58E-01*	*2.03E-01*	Mar	2.26E-04	2.15E-04	1.08E-03	*5.07E-04*	*4.96E-04*
Apr	6.89E-02	5.26E-02	6.36E-02	8.53E-02	5.20E-01	*1.58E-01*	*2.02E-01*	Apr	3.23E-04	3.07E-04	1.54E-03	*7.23E-04*	*7.07E-04*
May	6.88E-02	5.38E-02	6.34E-02	8.53E-02	5.19E-01	*1.58E-01*	*2.02E-01*	May	4.20E-04	3.99E-04	1.94E-03	*9.20E-04*	*8.84E-04*
Jun	6.88E-02	5.47E-02	6.30E-02	8.53E-02	5.18E-01	*1.58E-01*	*2.02E-01*	Jun	5.18E-04	4.92E-04	2.26E-03	*1.09E-03*	*1.01E-03*
Jul	6.87E-02	5.54E-02	6.26E-02	8.53E-02	5.18E-01	*1.58E-01*	*2.02E-01*	Jul	6.18E-04	5.85E-04	2.53E-03	*1.24E-03*	*1.11E-03*
Aug	6.86E-02	5.60E-02	6.23E-02	8.52E-02	5.18E-01	*1.58E-01*	*2.01E-01*	Aug	7.19E-04	6.81E-04	2.81E-03	*1.40E-03*	*1.22E-03*
Sep	6.86E-02	5.64E-02	6.20E-02	8.52E-02	5.17E-01	*1.58E-01*	*2.01E-01*	Sep	8.19E-04	7.75E-04	3.13E-03	*1.57E-03*	*1.35E-03*
Oct	6.86E-02	5.68E-02	6.19E-02	8.52E-02	5.16E-01	*1.58E-01*	*2.01E-01*	Oct	9.19E-04	8.69E-04	3.48E-03	*1.76E-03*	*1.49E-03*
Nov	6.86E-02	5.72E-02	6.17E-02	8.52E-02	5.16E-01	*1.58E-01*	*2.00E-01*	Nov	1.02E-03	9.64E-04	3.86E-03	*1.95E-03*	*1.66E-03*
Dec	6.86E-02	5.74E-02	6.16E-02	8.52E-02	5.15E-01	*1.58E-01*	*2.00E-01*	Dec	1.12E-03	1.06E-03	4.23E-03	*2.14E-03*	*1.81E-03*
Annual	**6.87E-02**	**5.39E-02**	**6.28E-02**	**8.53E-02**	**5.18E-01**	***1.58E-01***	***2.02E-01***	**Annual**	**5.73E-04**	**5.43E-04**	**2.31E-03**	***1.14E-03***	***1.01E-03***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.108.

Table 3.108. *The percentage difference between calculation results on PCB-153 concentration in surface soil layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	0.7%	-0.8%	-25.8%	-53.6%	89.7%	-29.5%	0.2%	-2.3%
Feb	1.4%	-1.6%	-25.6%	-53.5%	90.0%	-29.6%	0.2%	-4.0%
Mar	2.1%	-2.1%	-25.4%	-53.3%	90.4%	-29.7%	0.2%	-5.3%
Apr	2.9%	-2.2%	-25.1%	-53.1%	90.7%	-29.9%	0.3%	-6.1%
May	3.6%	-2.2%	-24.9%	-53.0%	91.0%	-30.0%	0.2%	-8.5%
Jun	4.3%	-2.2%	-24.6%	-52.8%	91.3%	-30.1%	-0.2%	-11.7%
Jul	5.1%	-2.0%	-24.4%	-52.7%	91.6%	-30.1%	-0.3%	-14.5%
Aug	5.8%	-1.8%	-24.2%	-52.5%	92.0%	-30.2%	-0.5%	-16.4%
Sep	6.6%	-1.6%	-24.0%	-52.4%	92.3%	-30.2%	-0.6%	-17.4%
Oct	7.3%	-1.3%	-23.8%	-52.3%	92.6%	-30.3%	-0.6%	-17.1%
Nov	8.1%	-1.1%	-23.6%	-52.2%	92.9%	-30.4%	-0.6%	-16.3%
Dec	8.8%	-0.8%	-23.4%	-52.0%	93.2%	-30.5%	-0.6%	-15.2%
Annual	**4.7%**	**-1.6%**	**-24.1%**	**-52.5%**	**91.5%**	**-30.0%**	**-0.2%**	**-14.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

3.5.7. Comparison of PCB-153 intermedia mass flows and concentrations at the interfaces of main environmental media

A preliminary analysis of model results on intermedia mass flows and on concentrations in the main environmental media formed at their interfaces is presented in this section. In the comparison the calculated values of PCB-153 mass flows from the atmosphere to soil, to water, to vegetation and from vegetation to soil (see Sections 3.4.1-3.4.4 above) and values of PCB-153 concentrations in the atmosphere at its interface with underlying surfaces (soil, ocean and vegetation); in the surface layer of soil, ocean and vegetation (see Sections 3.5.1–3.5.6 above) are considered.

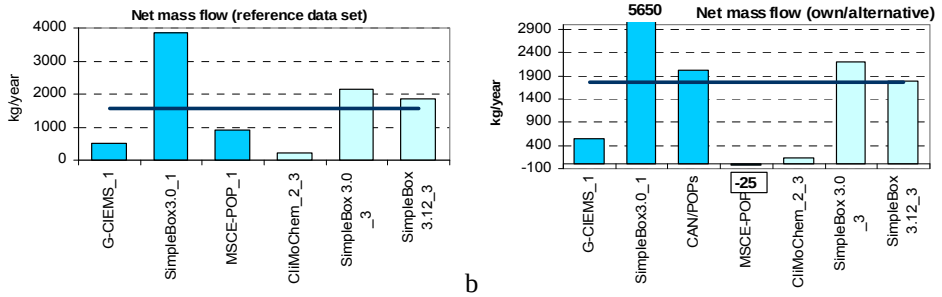
The comparison of PCB-153 mass flows transported from one compartment to another presented in Sections 3.4.1-3.4.4 includes results of one-year calculation with zero initial concentrations obtained by ADEPT, CliMoChem, G-CIEMS, MSCE-POP, SimpleBox models and with initial concentrations in media given as input data calculated by CAN/POPs, G-CIEMS, MSCE-POP and SimpleBox models; as well as results of long-term calculations for 20-year period with zero initial data with historical emissions carried out by CliMoChem and SimpleBox models. Results of CliMoChem, G-CIEMS, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of the estimates on intermedia mass flows to the variations in the input data.

The comparison of calculated concentrations presented in Sections 3.5.1–3.5.6 includes results of one-year calculations made on the basis of initial conditions (G-CIEMS, MSCE-POP, SimpleBox) and zero initial concentrations (ADEPT, G-CIEMS, MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (SimpleBox 3.0 and 3.12). The results on concentrations in the main environmental media are obtained with the use of two different physical-chemical data sets by G-CIEMS, MSCE-POP and SimpleBox models. SimpleBox and MSCE-POP predicted different values of PCB-153 concentrations in the atmosphere at its interface with different underlying surfaces. Variations in MSCE-POP air concentrations are more considerable than those in SimpleBox results.

In the section below the analysis of mass flows and concentrations in the media is presented for model results obtained on the basis of initial conditions and historical emissions. Calculated values of PCB intermedia mass flows and concentrations in the main media are presented in this section for four following interfaces: atmosphere-soil; vegetation – soil; atmosphere - seawater and atmosphere – vegetation.

Atmosphere-soil. Comparison of annual values of net exchange flow between the atmosphere and soil, which is a sum of dry and wet deposition and gaseous exchange flows, obtained on the basis of "reference" data set is presented in Table 3.67 (see Section 3.4.1). The scattering of absolute annual and monthly values between models using for calculations initial conditions and historical emissions is not large; square deviation σ_φ does not exceed the mean value of this parameter averaged between the participating models.

Annual values of net exchange flow between atmosphere and soil calculated on the basis of two data sets of physical-chemical properties are compared between different models in Fig. 3.124. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.124. *Comparison of PCB-153 annual values of net exchange flow between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The blue line in the plots shows the value of the corresponding parameter averaged between models. For calculations performed on the basis of "reference" data set, the scattering of absolute annual values between models is not large (*m* = 1582 kg/year; σ = 1348 kg/year*)*. Square deviation σ does not exceed the mean value of this parameter averaged between the participating models. In the case of results obtained with the use of "own/alternative" data sets, the difference in absolute annual values between different models' calculations is more considerable (*m* = 1760 kg/year; σ = 1946 kg/year*)*. According to the data presented, for all models' results this flow is directed from the atmosphere to soil and only in the case of MSCE-POP calculations made on the basis of initial conditions with the use of "own/alternative" data sets it is practically compensated. The highest values in both sets of calculations are characteristic of SimpleBox 3.0 results based on initial concentrations given as input data. Two groups of the participating models in terms of close results can be distinguished further: with relatively low absolute values (CliMoChem, G-CIEMS and MSCE-

POP results) and with medium values, which are close to the averaged value (CAN/POPs, and all of the rest results of SimpleBox).

Since the net exchange flow is a sum of different types of exchange flows, below the latter are considered separately. Comparison of annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.125.

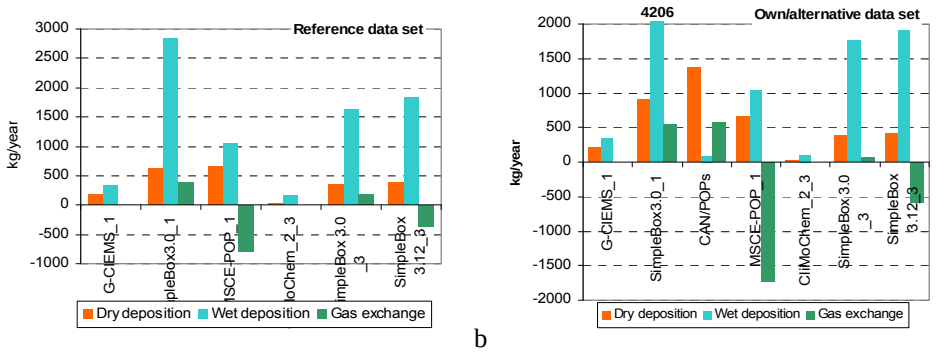
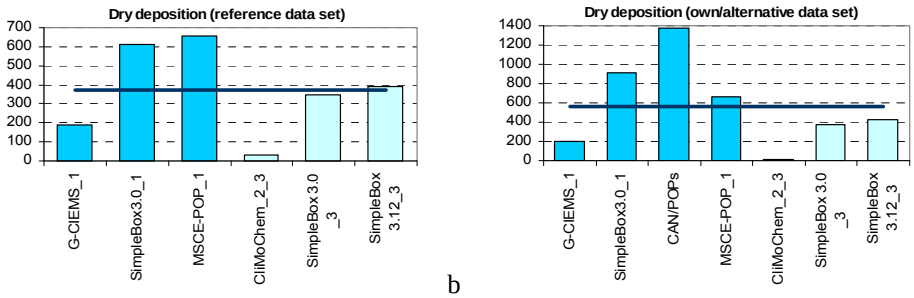


Fig.3.125. *Comparison of PCB-153 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

The absolute values of dry deposition flows from the atmosphere to soil are the most close for all models among other flows. More noticeable difference between model results is observed in absolute values of wet deposition and gaseous exchange. The maximum value of dry deposition flow among all others is obtained in CAN/POPs calculations based on initial conditions and "own/alternative" data set. The highest values of wet deposition in both sets of results are characteristic of SimpleBox 3.0 calculations performed with the use of initial conditions. G-CIEMS model provided the lowest values of gaseous exchange flows. In the case of MSCE-POP results obtained on the basis of initial conditions and SimpleBox 3.12 results based on historical emissions the gaseous flow is a re-emission flow whereas in calculations of all other models it is directed from the atmosphere to soil. The relatively low values of all considered flows are characteristic of CliMoChem model in calculations performed with "reference" and "own/alternative" data sets. Difference between results of calculations with both physical-chemical data sets is not very large for most models.

To reveal differences in calculated values obtained on "reference" and "own/alternative" data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

According to the results on dry deposition of PCB-153 from the atmosphere to soil calculated on the basis of "reference" and "own/alternative" data sets (in "reference" set of results m = 372 kg/year, σ = 242 kg/year; in "own/alternative" set of results m = 565 kg/year, σ = 458 kg/year), most models give rather close values in terms of annual and monthly absolute values (see Tables 3.58 and 3.59 in Section 3.4.1). Square deviation σ does not exceed the mean values of this parameter averaged between the participating models. Comparison of annual values of PCB-153 dry deposition from the atmosphere to soil calculated by the models on the basis of "**reference"** and "**own or alternative"** data sets is presented in Fig. 3.126. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

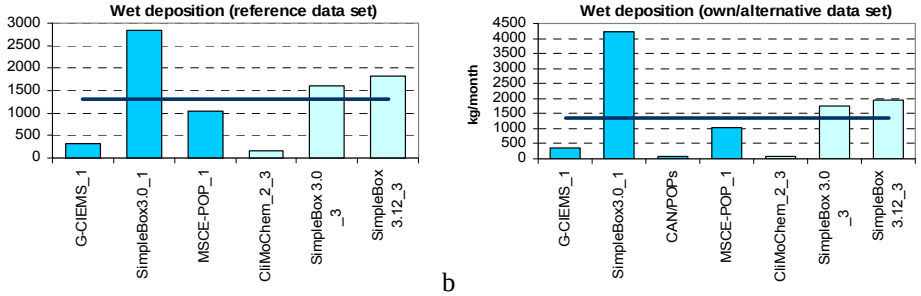


a b

Fig.3.126. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the data presented, the difference between two sets of model results varies from 0.3 to 48% depending on a model (see Table 3.60 in Section 3.4.1). The largest difference in the values obtained with "reference" and "own/alternative" data sets is characteristic of SimpleBox 3.0 results based on initial conditions. There is a negligible difference between values obtained on both data sets and presented in the results of MSCE-POP obtained with the use of initial conditions. For G-CIEMS, SimpleBox 3.0 (initial conditions) and SimpleBox 3.0 and 3.12 results based on historical emissions, the annual values of PCB-153 dry deposition mass flows transported from the atmosphere to soil obtained with the use of "own or alternative" data sets are higher than those obtained with "reference" data set; and vice versa for the rest of model results.

The scattering between different models' results on PCB-153 wet deposition mass flows from the atmosphere to soil is more considerable than that on dry depositions (Tables 3.61 and 3.62 in Section 3.4.1). However, according to the results presented (in "reference" set of results m = 1303 kg/year, σ = 1006 kg/year; in "own/alternative" set of results m = 1356 kg/year, σ = 1468 kg/year), for annual values obtained on the basis of "reference" data set square deviation is less than the averaged value. Comparison of annual values of PCB-153 wet deposition mass flows from the atmosphere to soil calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.127. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.127. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The difference between calculated annual values of PCB-153 wet deposition mass flows obtained by participating models with two data sets of physical-chemical properties lies in the range from 0.2 to 48% (Table 3.63 in Section 3.4.1). In results of G-CIEMS, SimpleBox 3.0 (initial conditions); SimpleBox (historical

emissions) and MSCE-POP (initial conditions), the annual values of calculation results obtained with the use of "own or alternative" data sets exceed those obtained with "reference" data set; and vice versa for CliMoChem results. The results of MSCE-POP model based on initial conditions show rather weak sensitivity of calculated values with respect to variations of pollutant-related parameters. Considerable difference in the results obtained with two data sets (48%) is characteristic of SimpleBox 3.0 results (initial conditions).

For two sets of results obtained, the differences in annual values of PCB-153 gaseous exchange flows between the atmosphere and soil calculated by the participating models are large (see Tables 3.64 and 3.65 given in Section 3.4.1). Square deviation of these values is considerably higher than mean values averaged between all models results (in "reference" set of results m = -93 kg/year, σ = 428 kg/year; in "own/alternative" set of results m = -162 kg/year, σ = 794 kg/year). A comparison of annual values of PCB-153 gaseous exchange between the atmosphere and soil calculated by the models on the basis of "**reference**" and "**own or alternative"** data sets is presented in Fig.3.128. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

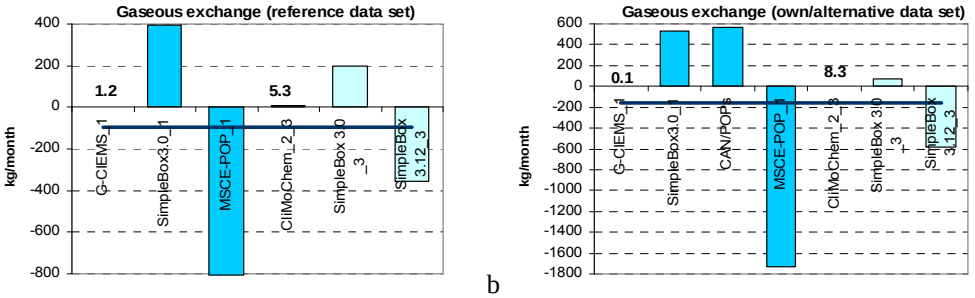


Fig.3.128. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to soil: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

Considerable difference between absolute values obtained on the basis of two different data sets is characteristic of MSCE-POP calculations made on the basis of initial concentrations (more than 115%) and of SimpleBox 3.0 and 3.12 calculations performed with the use of initial conditions and historical emissions (36 – 65%). At that in all these results, the calculated absolute values based on "own/alternative" data set are higher than those based on "reference" data set.

Thus, according to the results presented above, most participating models provide reasonable agreement in description of net intermedia mass flows from the atmosphere to soil. The results obtained on the basis of "reference" data set of pollutant-related parameters are somewhat closer than those obtained with "own or alternative" data set. The absolute values of dry deposition flows from the atmosphere to soil agree better between all models than those calculated for other types of exchange flows contributing to the net flow considered above. More noticeable difference between model results is observed in absolute values of wet deposition; the highest dispersion is characteristic of values of gaseous exchange flows. Two models calculate considerable re-emission gaseous flux from soil. Difference between results of calculations performed with the use of "reference" and "own/alternative" data sets is not very large for most models. For dry and wet depositions it does not exceed 50%, in calculations of gaseous exchange it totals approximately to 100%.

Model results on concentrations of PCB-153 in the atmosphere at its interface with soil and in the surface soil layer, which are conditioned by the considered above intermedia flows calculated with “reference” and “own/alternative” data sets are considered below.

Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with soil calculated by the models on the basis of “reference” and “own or alternative” data set (see Tables 3.91 and 3.92 in Section 3.5.1) is presented in Fig.3.129. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

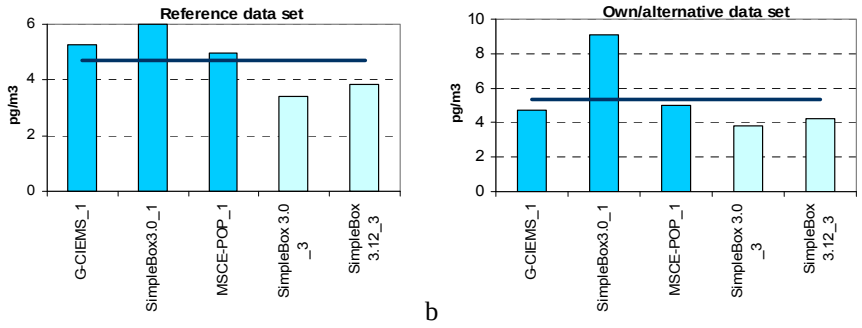
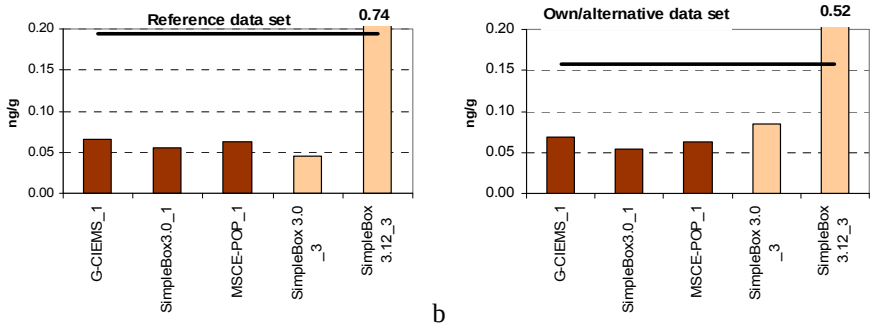


Fig.3.129. *Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

It can be seen that air concentrations values obtained on “reference” and “own/alternative” data sets are very close for all models (in “reference” set of results m = 4.71 pg/m^3, σ = 1.06 pg/m^3; in “own/alternative” set of results m = 2.13 pg/m^3, σ = 0.20 pg/m^3). Square deviation of annual values presented by different participating models does not exceed the averaged value in both cases. The difference between results obtained with two different data sets of physical-chemical properties is rather small (see Table 3.93 in Section 3.5.1). For the calculation results of G-CIEMS, the annual values of PCB-153 concentration in the atmosphere at its interface with soil obtained with the use of “own or alternative” data sets are smaller than those obtained with “reference” data set; and vice versa for SimpleBox and MSCE-POP models’ results. The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.0 calculations performed on the basis of initial conditions.

Comparison of annual values of PCB-153 concentration in surface soil layer calculated by the models on the basis of “reference” and “own/alternative” data sets (Tables 3.106 and Tables 3.107 given in Section 3.5.6) is presented in Fig.3.130. The black line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

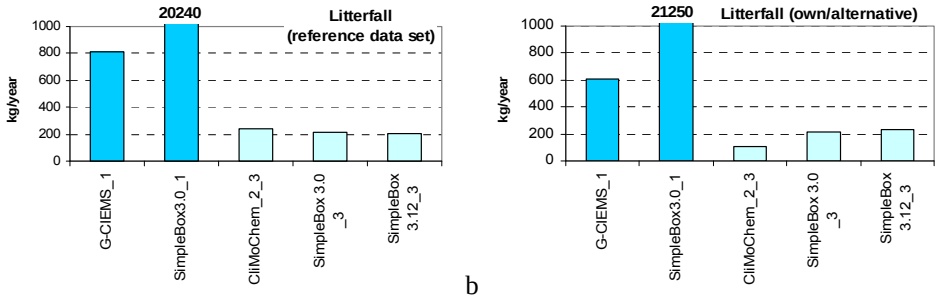
Fig.3.130. *Comparison of annual values of PCB-153 concentration in surface soil layer (ng/g) calculated by different models on the basis of "reference" (a) and "own or alternative" (b) data sets.*

According to the data presented, most models similarly describe soil concentrations. Results on PCB-153 concentration in surface soil layer calculated on the basis of "reference" and "own or alternative" data sets demonstrate reasonable agreement between most models' calculations except for results of version 3.12 of SimpleBox model. For annual values of PCB-153 concentration in surface soil layer (in "reference" set of results m = 0.19 ng/g, σ = 0.31 ng/g; in "own/alternative" set of results m = 0.16 ng/g, σ = 0.20 ng/g), square deviation is higher than the averaged value. Difference between the models' results obtained on the basis of two physical-chemical data sets varies from 0.2 to 92% (see Table 3.108 given in Section 3.5.6). For the calculation results of all models except G-CIEMS and SimpleBox 3.0 (based on historical emissions), the values of PCB-153 concentration in surface soil layer obtained with the use of "own or alternative" data sets are less than those obtained with "reference" data set. The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.12 results obtained on the basis of historical emissions. MSCE-POP results are characterised by the lowest sensitivity to the variations in physical-chemical data used.

Thus, the most part of participating models predicted close values of PCB-153 concentrations in the atmosphere at its interface with soil and in the surface soil layer taking into account the obtained estimates of intermediate flows. The high scattering in calculated values of mass flows conditioned by the gaseous exchange does not affect considerably calculated concentrations in comparison with contributions of dry and wet depositions. The difference between the maximum and minimum values of soil concentrations is higher than that for air concentrations. The difference between results obtained on the basis of "reference" and "own/alternative" physical-chemical data sets is rather small for air concentrations (50% in maximum). For soil concentrations it is about 90%.

Vegetation – soil. According to the calculation results on PCB-153 mass flows due litterfall from vegetation to soil calculated by models on the basis of both data sets of physical-chemical properties (Tables 3.68 and Tables 3.69 given in Section 3.4.2), the scattering between the maximum and minimum values obtained by different models is very high exceeding two orders of magnitude. Square deviation σ_φ between different model results in both cases considerably exceeds the averaged value (in "reference" set of results m = 4344 kg/year, σ = 9911 kg/year; in "own/alternative" set of results m = 4481 kg/year, σ = 9376 kg/year).

Comparison of annual values of PCB-153 mass flows from vegetation to soil calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.131. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).



a b

Fig.3.131. *Comparison of annual values of PCB-153 mass flows transported from vegetation to soil (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" data sets (b)*

For both set of calculation results, the maximum absolute values of PCB-153 mass flows from vegetation to soil are obtained by SimpleBox 3.0 model on the basis of initial conditions. At that the value calculated by G-CIEMS model on the basis of initial conditions is much lower than results of SimpleBox mentioned above but considerably higher than the rest of other models' results, which are relatively close to each other. Comparison of annual values of litterfall mass flows calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.132 (see also Table 3.70 given in Section 3.4.2).

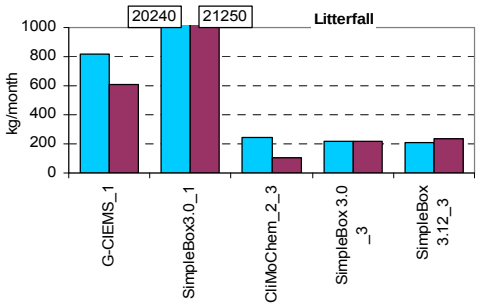
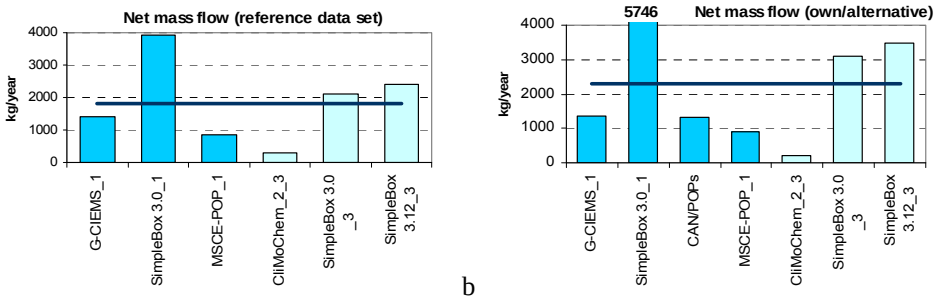


Fig.3.132. *Comparison of PCB-153 annual values of mass flows between vegetation and soil calculated by different models on the basis of two data sets*

For CliMoChem, G-CIEMS and SimpleBox 3.0 (historical emissions) results, the calculated values of PCB-153 mass flows transported from vegetation to soil obtained by the models on the basis of "reference" data set exceed those obtained with "own or alternative" data sets. According to the data presented in Table 3.70 (Section 3.4.2), the percentage difference between different models is in the range from 2 to 57%. The largest difference in the results obtained with two data sets is characteristic of CliMoChem model.

Atmosphere - seawater. Comparison of annual values of net exchange flow between the atmosphere and seawater obtained on the basis of "reference" data set is presented in Table 3.80 (see Section 3.4.3). The difference in absolute annual and monthly values obtained by the participating models is not considerable (in "reference" set of results m = 1831 kg/year, σ = 1292 kg/year; in "own/alternative" set of results m = 2298 kg/year, σ = 1922 kg/year). Square deviation σ does not exceed the mean value of this parameter averaged between the participating models in both cases.

Annual values of net exchange flow between atmosphere and seawater calculated on the basis of two data sets are compared between different models in Fig. 3.133. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.133. *Comparison of PCB-153 annual values of net exchange flow between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the results presented, all models obtained net flows directed from the atmosphere to water. There are three groups of close models' results, which can be isolated depending on magnitude of absolute values. First group of models with relatively low values includes CliMoChem, CAN/POPs, G-CIEMS and MSCE-POP models. Higher flows are calculated by SimpleBox 3.0 and 3.12 on the basis of historical emissions. Third group of results obtained on the basis of initial conditions by SimpleBox 3.0 models is characterized by the highest absolute value among others. Difference between results based on both physical-chemical data sets is rather small for all models except for SimpleBox.

Annual absolute values of dry and wet deposition and gaseous exchange flows, which formed the considered net exchange flows between the atmosphere and seawater, are compared below. Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and seawater calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.134.

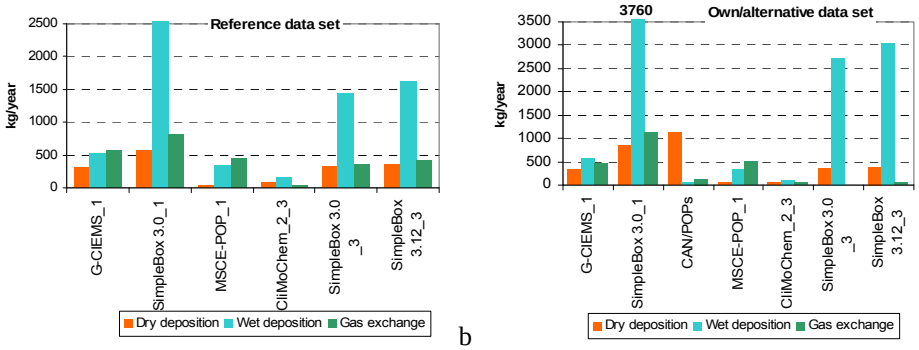


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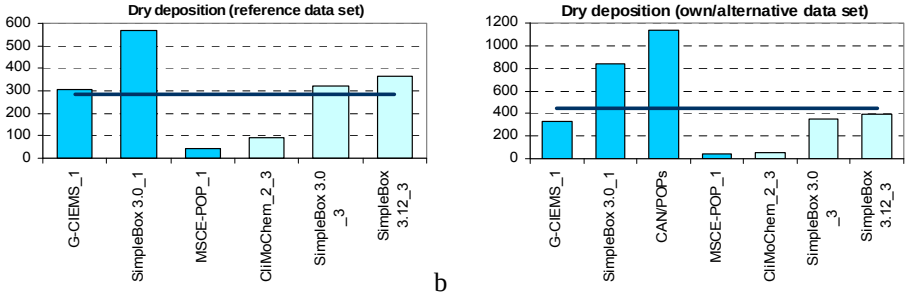
Fig.3.134. *Comparison of PCB-153 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The results on dry and wet deposition and gaseous exchange flows between these media obtained on both data sets ("reference" and "own/alternative") show that scattering of absolute values of wet deposition flows is the most noticeable in comparison with other flows. Similar to the results for atmosphere-soil interface, CAN/POPs calculations based on initial conditions and "own/alternative" data set predicted the maximum value of dry deposition flow among all others. The lowest values of dry depositions from the atmosphere to water are obtained by MSCE-POP model. The highest values of wet deposition in both sets of results are characteristic of Simple Box 3.0 calculations based on initial conditions. This model provided also the maximum values of gaseous exchange flows. Of note, most models show noticeable gaseous flows directed from the atmosphere to water. Difference between results of calculations with "reference" and "own/alternative" data sets is the most considerable for SimpleBox model.

Model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

The annual and monthly values of dry deposition of PCB-153 from the atmosphere to water calculated on the basis of "reference" and "own/alternative" data sets are in reasonable agreement for most models (see Tables 3.71 and 3.72 in Section 3.4.3). Square deviation σ in both cases does not exceed the mean values of this parameter averaged between the participating models (in "reference" set of results m = 281 kg/year, σ = 193 kg/year; in "own/alternative" set of results m = 449 kg/year, σ = 405 kg/year). Comparison of annual values of PCB-153 dry deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.135. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.135. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the data presented, the difference in absolute values obtained on the basis of both data sets ("reference" and "own/alternative") between models' results varies from 4 to 48% (Table 3.73 in Section 3.4.3). For the calculation results obtained by CliMoChem and MSCE-POP, the annual values of PCB-153 dry deposition mass flows from the atmosphere to water calculated with "own or alternative" data sets are less than those obtained with "reference" data set; and vice versa for G-CIEMS and SimpleBox model results. The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.0 calculations based on initial conditions.

According to the presented results on PCB-153 wet deposition mass flows from the atmosphere to water, the difference in results obtained on the basis of "own/alternative" data set is larger than that in results based on "reference" data set (Tables 3.74 and 3.75 in Section 3.4.3). Square deviation between participating models' results based on "reference" data set is less than the averaged value (in "reference" set of results m = 1105 kg/year, σ = 919 kg/year; in "own/alternative" set of results m = 1511 kg/year, σ = 1595 kg/year). Comparison of annual values of PCB-153 wet deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.136. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

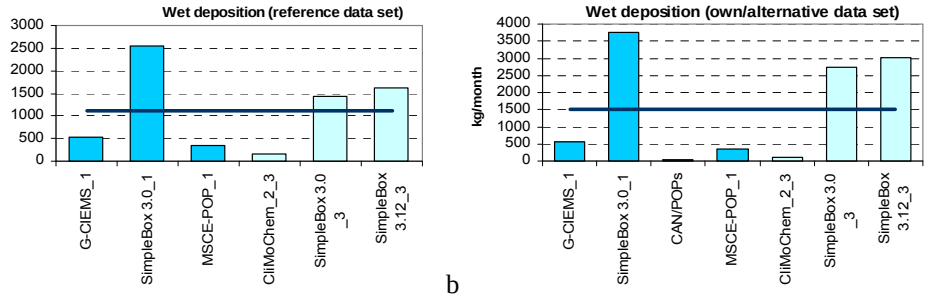


Fig.3.136. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to water: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The difference between the presented results obtained on the basis of both physical-chemical data sets varies from 4 to 90% (Table 3.76 in Section 3.4.3). The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.0 and 3.12 calculations performed on the basis of historical emissions. The lowest sensitivity to variations of pollutant-related parameters is observed in calculation results of MSCE-POP model obtained on the basis of initial conditions. Annual values of PCB-153 wet deposition mass flows from the atmosphere to water calculated by CliMoChem and MSCE-POP models with the use of "reference" data set exceed those based on "own or alternative" data sets; and vice versa for G-SIEMS and SimpleBox model results.

In comparison with the results on gaseous exchange flow obtained for the atmosphere-soil interface, the difference in values on gaseous exchange mass flows between the atmosphere and water calculated on the basis of "reference" data set is essentially lower since square deviation of these calculated values does not exceed the mean value averaged between all models (m = 444 kg/year, σ = 256 kg/year) (Tables 3.77 given in Section 3.4.3). The scattering of "own/alternative" set of results (m = 338 kg/year, σ = 409 kg/year) (Tables 3.78 given in Section 3.4.3) is noticeably higher than that for results based on "reference" data set. Comparison of annual values of PCB-153 gaseous exchange mass flows between the atmosphere and water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.137. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

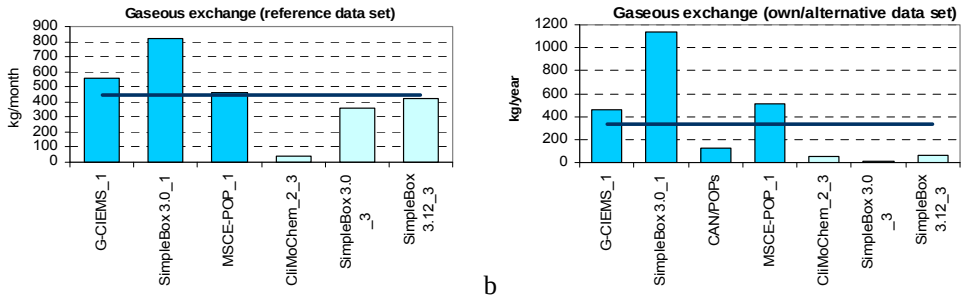


Fig.3.137. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to water: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the data presented, results of CliMoChem, SimpleBox 3.0 (initial conditions) and MSCE-POP models obtained on the basis of "own/alternative" data set are higher than those calculated with the use of

"reference" data set; and vice versa for the rest of other models' results (see also Table 3.79 in Section 3.4.3). The most considerable difference in absolute values calculated with the use of "reference" and "own/alternative" data sets is characteristic of SimpleBox 3.0 and 3.12 calculations carried out on the basis of initial conditions and historical emissions.

Thus, in the results obtained most participating models provided rather close values of net intermedia mass flows between the atmosphere and water. All models obtained net flows directed from the atmosphere to water. The scattering in results calculated by different models on the basis of "reference" data set is higher than that in the results obtained with "own or alternative" data set. The difference in absolute values of wet deposition and gaseous exchange flows is more noticeable in comparison with dry deposition flows. Maximum difference between results on all flows calculated with the use of "reference" and "own or alternative" data sets does not exceed 90%.

Model results on concentrations of PCB-153 in the atmosphere at its interface with ocean and in the surface water layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" and "own/alternative" data sets (see Tables 3.94 and 3.95 in Section 3.5.2) is presented in Fig.3.138. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

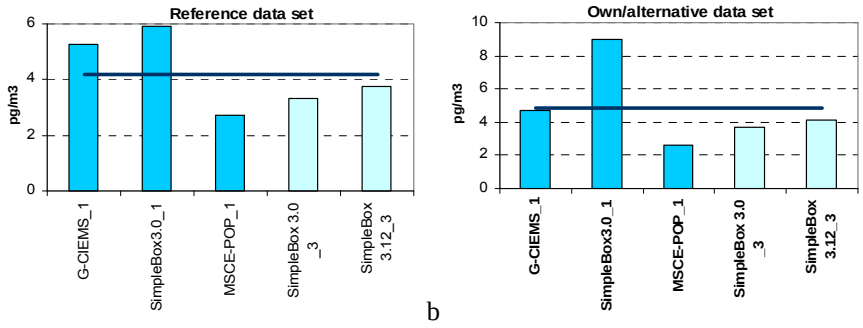


Fig.3.138. *Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Similar to the case with PCB-153 air concentrations formed at its interface with soil, in both sets of results obtained all models predicted rather close values of air concentrations formed at its interface with ocean. For both sets of results square deviation of annual values does not exceed the mean value averaged between different models (in "reference" set of results m = 4.20 pg/m^3, σ = 1.34 pg/m^3; in "own/alternative" set of results m = 4.83 pg/m^3, σ = 2.43 pg/m^3). Difference between two sets of results obtained on the basis of "reference" and "own/alternative" data sets is in the range from 3 to 52 % (results of MSCE-POP and SimpleBox 3.0 obtained on the basis of initial conditions, respectively) (see Table 3.96 in Section 3.5.2). For the calculation results of G-CIEMS and MSCE-POP models, the values of PCB-153 concentration in the atmosphere at its interface with ocean obtained with the use of "own or alternative" data sets are smaller than those obtained with "reference" data set, and vice versa for all SimpleBox results.

Comparison of annual values of PCB-153 concentration in surface ocean layer calculated by the models on the basis of “reference” and “own/alternative” data sets (see Tables 3.100 and 3.101 in Section 3.5.4) is presented in Fig.3.139. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

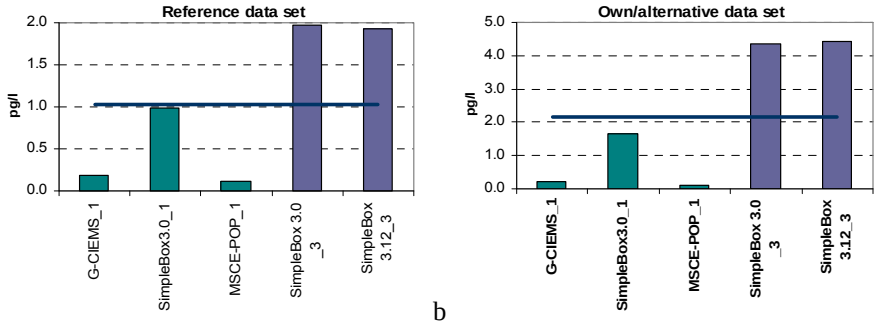


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Fig.3.139. *Comparison of annual values of PCB-153 concentration in surface ocean layer (pg/l) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

The variability of water concentrations for most models is not very large but it is higher than that for air concentrations. The maximum values are obtained by SimpleBox 3.12 model on the basis of “own/alternative” data set. MSCE-POP model’s results are characterized by the lowest values of water concentrations in both cases. At that, square deviation σ between different model results is slightly lower than the mean averaged value in the both cases (in “reference” set of results m = 1.04 pg/l, σ = 0.90 pg/l; in “own/alternative” set of results m = 2.16 pg/l, σ = 2.13 pg/l). Results of all models obtained on the basis of “reference” data set differ from those based on “own/alternative” data set in the range from 3 to 130% (see Table 3.102 given in Section 3.5.4). The maximum difference is characteristic of SimpleBox 3.12 results based on historical emissions); and the minimum difference – of MSCE-POP results. For the calculation results of all models, the values of PCB-153 concentration in surface ocean layer obtained with the use of “own or alternative” data sets exceed those obtained with “reference” data set.

The values of PCB-153 concentrations in the atmosphere at its interface with ocean are close for most participating models. The scattering in calculated values of water concentrations is more considerable. However, square deviation between different models’ results is practically equal to the mean averaged value in the both cases. The difference between absolute values of air and water concentrations obtained with both physical-chemical data sets totals to 50 and 130 %, respectively.

Atmosphere – vegetation. Comparison of annual values of net exchange flow between the atmosphere and vegetation obtained on the basis of “reference” data set is presented in Table 3.90 (see Section 3.4.4). Annual values of net exchange flow between atmosphere and vegetation calculated on the basis of two data sets (“reference” and “own/alternative”) are compared between different models in Fig. 3.140. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

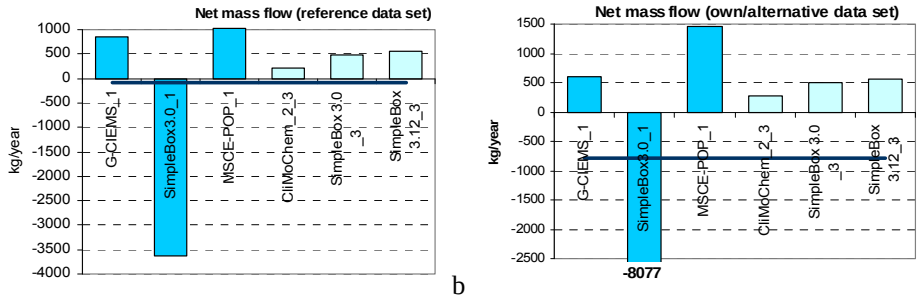

Fig.3.140. *Comparison of PCB-153 annual values of net exchange flow between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the comparison of results on net exchange flow between the atmosphere and vegetation, the difference in annual values obtained by the participating models both on the basis of "reference" (m = -88 kg/year; σ = 1756 kg/year) and "own/alternative" (m = -779 kg/year; σ = 3598 kg/year) data sets is very large. Square deviation σ of absolute annual values obtained by the participating models is much higher than the mean value of this parameter averaged between the models. That testifies a considerable discrepancy in simulation of intermedia transport between these compartments by different models. A comparison of model results on net exchange flow of PCB-153 for the atmosphere and vegetation interface demonstrates that for most models this flow is transported from the atmosphere to vegetation. Calculations made by SimpleBox 3.0 model on the basis of initial conditions show high re-emission flux from vegetation. In spite of the fact that the scattering in absolute values is very large, the most models - CliMoChem, G-CIEMS, MSCE-POP and SimpleBox 3.0 and 3.12 (historical emissions) models demonstrate relatively close results. The difference in net exchange values obtained on the basis of two data sets is noticeable for G-CIEMS, MSCE-POP, and Simple Box 3.0 (initial conditions).

Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and vegetation calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.141.

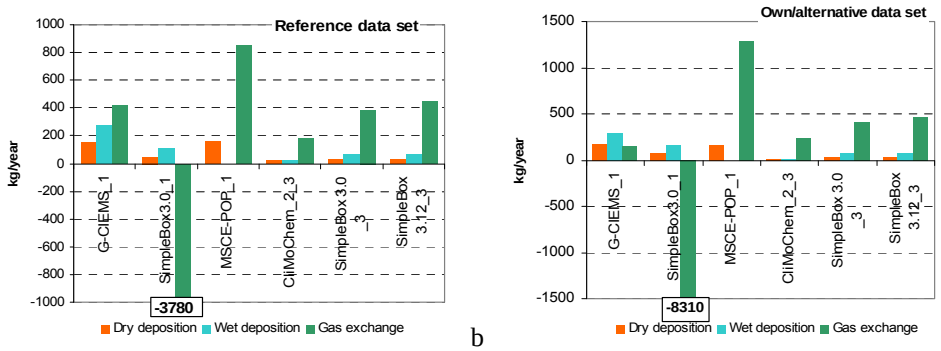

Fig.3.141. *Comparison of PCB-153 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

For model results calculated by the participating models on the basis of both physical-chemical data sets ("reference" and "own/alternative"), the absolute values of dry and wet deposition between the atmosphere and vegetation are closer to each other than those of gaseous exchange flows. The difference between results of both calculations on dry depositions is rather small for all models. Higher variability of absolute

values of wet deposition is observed. The maximum value of wet deposition flow is characteristic of G-CIEMS. It should be noted that wet deposition on vegetation is not taken into account in MSCE-POP model. For most models PCB-153 gaseous exchange flows are directed from the atmosphere to vegetation. MSCE-POP results presented the highest value of this gaseous flow among them. At that, calculations performed by SimpleBox 3.0 model on the basis of initial conditions show high re-emission flow from vegetation. For G-CIEMS, MSCE-POP and SimpleBox 3.0 (initial conditions) models noticeable difference in gaseous exchange flux between calculations on "reference" and "own/alternative" data sets can be seen.

To reveal differences in calculated values obtained on "reference" and "own/alternative" data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

According to the results on dry deposition of PCB-153 from the atmosphere to vegetation calculated on the basis of both data sets, most models predicted rather close absolute annual values (see Tables 3.81 and 3.82 in Section 3.4.4). Square deviation σ_φ does not exceed the mean values of this parameter averaged between the participating models in both cases (in "reference" set of results m = 74 kg/year, σ = 66 kg/year; in "own/alternative" set of results m = 79 kg/year, σ = 70 kg/year). Comparison of annual values of PCB-153 dry deposition mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.142. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

According to the data presented, the difference between two sets of model results varies from 0.3 to 50% depending on a model (see Table 3.83 in Section 3.4.4). The largest difference in the values obtained with two data sets is characteristic of CliMoChem results based on historical emissions. Negligible difference between values obtained on "reference" and "own/alternative" data sets is characteristic of MSCE-POP results based on initial conditions. For CliMoChem results, the annual values of PCB-153 dry deposition mass flows from the atmosphere to vegetation calculated with "own or alternative" data sets are smaller than those obtained with "reference" data set; and vice versa for G-CIEMS, MSCE-POP and all SimpleBox results.

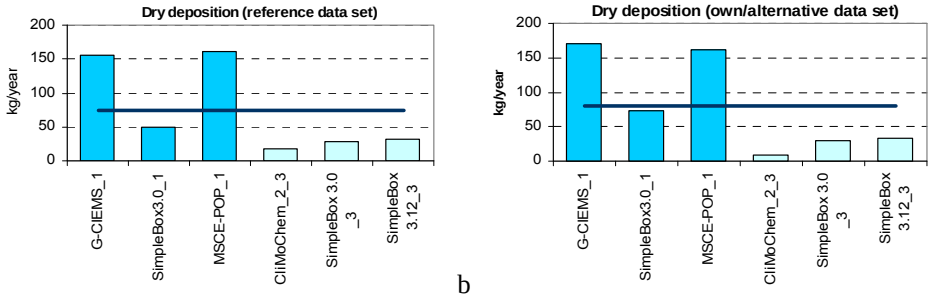

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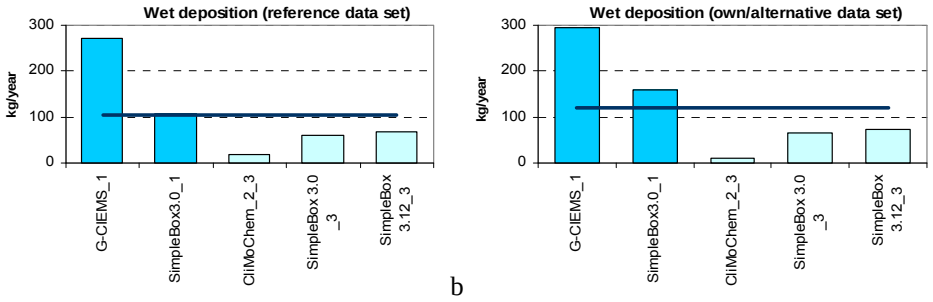
Fig.3.142. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The scattering between different models' results on PCB-153 wet deposition mass flows transported from the atmosphere to vegetation is higher than that on dry depositions (Tables 3.84 and 3.85 in Section 3.4.4). However, according to the results presented (in "reference" set of results m = 106 kg/year, σ = 97 kg/year; in "own/alternative" set of results m = 121 kg/year, σ = 111 kg/year), square deviation of this parameter values is less than the averaged value in both sets of obtained results. Comparison of annual values of PCB-153 wet

deposition mass flows transported from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.143. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

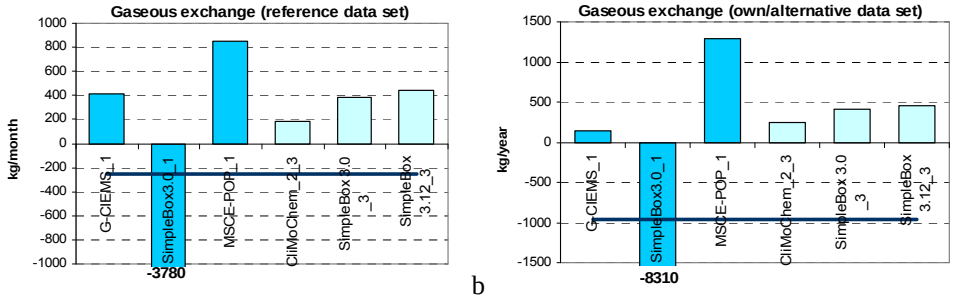


a b

Fig.3.143. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

For the calculation results of G-CIEMS and SimpleBox 3.0 and 3.12 models (initial conditions and historical emissions), the values of PCB-153 wet deposition mass flows transported from the atmosphere to vegetation obtained with the use of "own or alternative" data sets exceed those obtained with "reference" data set; and vice versa for CliMoChem model (see Table 3.86 in Section 3.4.4). The largest difference in the results obtained with two data sets making up approximately 50% is characteristic of SimpleBox 3.0 results based on initial conditions; the lowest difference equal to 9% is observed in results of MSCE-POP model.

According to the results on PCB-153 gaseous exchange flows for the atmosphere - vegetation interface calculated by the participating models on the basis of two physical-chemical data sets, the differences in both annual and monthly absolute values are very large (see Tables 3.87 and 3.88 given in Section 3.4.1). Square deviation of these values is higher than mean values averaged between all models results (in "reference" set of results m = -250 kg/year, σ = 1745 kg/year; in "own/alternative" set of results m = -960 kg/year, σ = 3624 kg/year). Comparison of annual values of PCB-153 gaseous exchange mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.144. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.144. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to vegetation: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the results presented (see also Table 3.89 in Section 3.4.4), the most considerable difference in the values obtained on "reference" and "own/alternative" data sets is characteristic of SimpleBox 3.0 model results calculated on the basis of initial conditions. The less noticeable difference among different models is obtained in the rest of this model's results. Results of MSCE-POP and CliMoChem models obtained with the use of "own/alternative" data set exceed those based on "reference" data set; and vice versa for G-CIEMS.

Thus, it can be noted that considerable scattering of net exchange flows for the atmosphere - vegetation interface obtained by different models is conditioned by the difference in gaseous exchange flows that is the most pronounced among other flows. The most participating models provided a reasonable agreement in description of dry and wet mass flows from the atmosphere to vegetation. One model predicted high re-emission flux from vegetation to the atmosphere in the case of values obtained on the basis of initial conditions. The difference between results of calculations carried out with the use of "reference" and "own/alternative" data sets is about 120%.

Model results on concentrations of PCB-153 in the atmosphere at its interface with vegetation and in vegetation, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of "reference" and 'own/alternative" data sets (see Tables 3.97 and 3.98 in Section 3.5.3) is presented in Fig.3.145. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

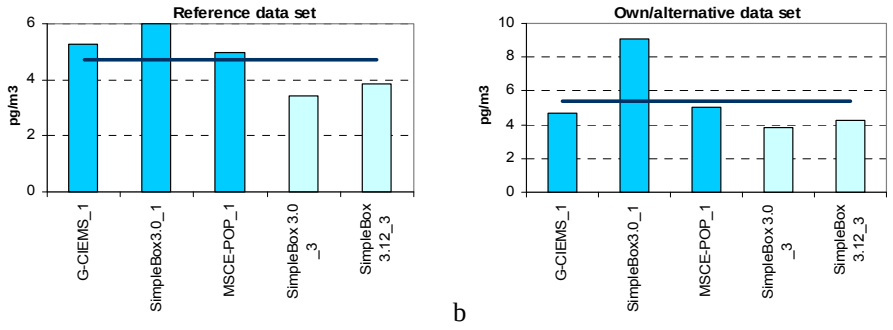
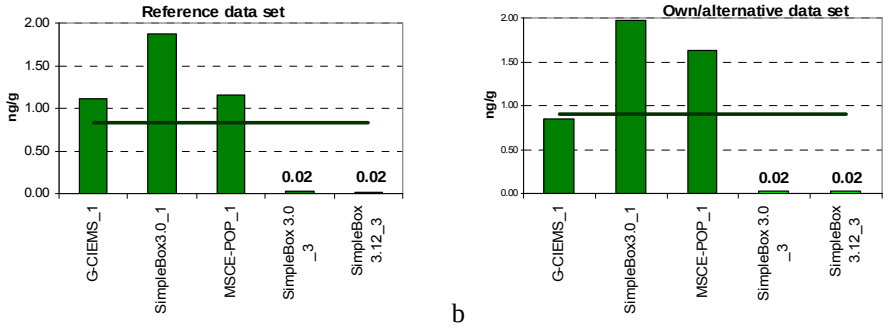


Fig.3.145. *Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with vegetation (pg/m3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the results presented, PCB-153 concentrations in the atmosphere at its interface with vegetation are close to each other for all participating models. For two sets of results obtained the differences in annual values of PCB-153 concentration in the atmosphere at its interface with vegetation are not considerable (in "reference" set of results m = 4.70 pg/m^3, σ = 1.06 pg/m^3; in "own/alternative" set of results m = 5.37 pg/m^3, σ = 2.13 pg/m^3). Square deviation of these values in all cases is lower than the mean values averaged between all models results. For the calculation results of G-CIEMS, the values of PCB-153 concentration in the atmosphere at its interface with vegetation obtained with the use of "own or alternative" data sets are smaller than those obtained with "reference" data set; and vice versa for MSCE-POP and all SimpleBox results (see Table 3.99 in Section 3.5.3). The largest difference in the results obtained with two data sets (52%) is characteristic of SimpleBox 3.0 calculations performed on the basis of initial conditions. For MSCE-POP this difference is minimum among all others and totals to 1%.

Comparison of annual values of PCB-153 concentration in vegetation calculated by the models on the basis of "reference" and 'own/alternative" data sets (see Tables 3.103 and 3.104 in Section 3.5.5) is presented in Fig.3.146. The green line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.146. *Comparison of annual values of PCB-153 concentration in vegetation (ng/g) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The differences between annual values of PCB-153 concentration in vegetation calculated by the participating models are rather considerable for two sets of results obtained (in "reference" set of results m = 0.84 pg/m^3, σ = 0.80 pg/m^3; in "own/alternative" set of results m = 0.90 pg/m^3, σ = 0.90 pg/m^3). The highest and the lowest values of the considered parameter are obtained by different versions of SimpleBox model (3.0_1 and 3.12_3). Square deviation of these values is not higher than the mean values averaged between all models results. For the calculation results of all models except G-CIEMS and SimpleBox 3.0 (historical emissions), the values of PCB-153 concentration in vegetation obtained with the use of "own or alternative data sets" exceed those obtained with "reference" data set (see Table 3.105). The largest difference in the results obtained with two data sets equal to 42% is characteristic of MSCE-POP results. Results of SimpleBox 3.0 are the less sensitive to the changes in pollutant-related parameters.

Results on PCB-153 concentrations in the atmosphere at its interface with vegetation are in good agreement for most models. The variation in values of concentrations in vegetation is higher than that in the air concentrations. The difference between absolute values of air and vegetation concentrations obtained with "reference" and "own or alternative" physical-chemical data sets totals to 50 and 42 %, respectively.

According to the comparison presented above, it can be concluded that:

- All model provide reasonable agreement in description of intermedia mass flows and concentrations in the main environmental media.

- In particular, air concentrations as the most important output of the participating models are in good agreement for all models' results. Several models predict values of PCB-153 concentrations in the atmosphere at its interface with different underlying surfaces taking into account types of these surfaces.
- The most part of participating models predict close values of PCB-153 concentrations in soil, water and vegetation. However, variability of calculated concentrations in the environmental media other than the atmosphere is higher than that for the atmosphere. According to the results obtained within Stage II calculations, the bulk of overall PCB content in the environment is accumulated in soil. In this connection, it can be noted that the difference between the maximum and minimum values of calculated soil

concentrations is higher than that for air concentrations but considerably less than that for the rest of media. Very close absolute values of soil concentrations are characteristic of most models' results.

- Most participating models provide a reasonable agreement in description of net intermedia mass flows from the atmosphere to soil and to water. The scattering in results on net intermedia mass flows between the atmosphere and vegetation is higher. The similarity in description of dry and wet deposition processes from the atmosphere to different underlying surfaces implied in the model parameterisations is testified by close results of most models based on "reference" data set. Several models calculate dry deposition to different underlying surfaces taking into account types of these surfaces. Results on dry deposition flows from the atmosphere to all of the considered underlying surfaces, wet deposition flows from the atmosphere to soil and water obtained on the basis of "reference" data set, and wet depositions from the atmosphere to vegetation obtained on the basis of both data sets are in good agreement between all models. Scattering in values of gaseous exchange is more noticeable. Two models calculate re-emission gaseous flux from soil and one – from vegetation.
- For all considered media interfaces, agreement between different models' results obtained on the basis of "reference" data set in most experiments performed is considerably better than that for results based on the "own/alternative" data set. Maximum difference between results of calculations of intermedia mass flows performed with "reference" and "own/alternative" sets of physical-chemical properties does not exceed 50% for dry and wet depositions, in calculations of gaseous exchange it is about 120%. The results of all models show rather weak sensitivity of calculated values of air concentrations with respect to variations of pollutant-related parameters. The difference in concentrations in other media than the atmosphere is more noticeable (120% in maximum).

3.6. Spatial distribution of depositions and concentrations in different compartments (optional)

Five models present results on spatial distribution of depositions and concentrations of PCB-153 in different environmental compartments: ADEPT, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox.

Calculated fields of PCB-153 concentrations in the atmosphere, soil, water and vegetation and net deposition fluxes in 2000 obtained by the participating models with the use of two different data sets ("reference" and "own or alternative") are compared below. The results on spatial distribution of PCB-153 deposition and concentrations in the main environmental media are obtained with the use of the two physical-chemical data sets by DEHM-POP, MSCE-POP and different versions of SimpleBox model.

The comparison of calculated deposition and concentration fields presented in Sections 3.6.1 and 3.6.2 below includes results of one-year calculations made on the basis of initial conditions (DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP, SimpleBox), zero initial concentrations (ADEPT, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (EVN-BETR and UK-MODEL, SimpleBox 3.0 and 3.12) (See Table 3.109). The model results obtained taking into account initial concentrations of pollutants in media and historical emissions, and on the basis of zero initial concentrations in the environmental media are compared in two different groups.

In Subsection 3.6.1 a preliminary analysis of the comparison of calculated deposition and concentration fields is made for the model results based on "reference" data set and obtained on the basis of non-zero initial conditions (initial concentrations and historical emissions).

Table 3.109. *Results on spatial distribution of PCB-153 depositions and concentrations in different compartments presented by the models*

Maps	Data set used	ADEPT[c]	DEHM-POP_1	DEHM-POP_2	EVN-BETR _1[a]	EVN-BETR _2[a]	EVN-BETR _3[a]	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Surface atmospheric concentrations, pg/m^3	ref	+	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt		+	+				+	+	+	+	+	+	+
Surface soil concentration, ng/g	ref		+	+	+	+	+	+	+	+	+	+	+	+
	own or alt		+	+				+	+	+	+	+	+	+
Surface water concentration, pg/l	ref		+	+	+	+	+	+	+	+	+	+	+	+
	own or alt		+	+				+	+	+	+	+	+	+
Concentration in vegetation, ng/g (optional)	ref				+	+	+	+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+
Net deposition flux, mg/m^2/hour	ref	+						+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+
Wet deposition of gaseous phase, mg/m^2/hour	ref												+	+
	own or alt												+	+
Wet deposition of particle phase, mg/m^2/hour	ref												+	+
	own or alt												+	+
Wet deposition total, mg/m^2/hour	ref							+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+
Dry deposition of gaseous phase, mg/m^2/hour	ref												+	+
	own or alt												+	+
Dry deposition of particle phase, mg/m^2/hour	ref												+	+
	own or alt												+	+
Dry deposition total, mg/m^2/hour	ref							+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data, the only exception was that the initial conditions for the vegetation were set to zero;

EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;

EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;

DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;

DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - EVN-BETR and UK-MODEL results were calculated with the help of a spatially resolved version of the model;

[b] – SimpleBox: results were calculated on the basis of initial concentrations given as input data. The concentrations calculated are the bulk concentrations in the compartments. Maps of concentrations are obtained on the basis of annual values of concentrations at regional and continental levels;

[c] - ADEPT results calculated on the basis of zero initial concentrations are winter averaged.

3.6.1. Comparison of results on spatial distribution of PCB-153 depositions and concentrations in different compartments obtained on the basis of "reference" data set

In this section a comparison of spatial distributions of PCB-153 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models with the use of "reference" data set on the basis of initial PCB-153 concentrations in the media, historical emissions and zero initial conditions is presented. A preliminary analysis of calculated deposition and concentration fields is made only for the model results obtained on the basis of non-zero initial conditions.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.147.

Due to different types and overall model approaches, the participating models provided calculated fields of PCB-153 air concentrations with different resolution. The finest resolution of the presented results is characteristic of DEHM-POP model. For SimpleBox model a spatial variability of results on concentration in the media is obtained by division of the cells of the calculation model domain into two types: regional and continental scales. However, it can be noted that in general all participating models describe spatial distributions of air pollution rather closely. In particular, the area of the most contaminated air with concentration equal approximately 10 pg/m^3 and higher is predicted to be over such countries as Belgium, France, Germany and Switzerland. The location of regions with relatively high, moderate and low PCB-153 concentrations in the atmosphere is similarly reproduced by EVN-BETR and UK-MODEL, DEHM-POP and MSCE-POP models. The difference between the lowest and the highest absolute values of air concentrations within the calculation domain calculated by all models is noticeable. Thus, for DEHM-POP air concentration levels in the considered region are in the range from 0.2 to 11.5 pg/m^3; for MSCE-POP – from 0.3 to 15.2 pg/m^3; for EVN-BETR and UK-MODEL (EVN-BETR_1 - initial concentrations) - from 0.0 to 15.8 pg/m^3; for EVN-BETR and UK-MODEL (EVN-BETR_3 - historical emissions) - from 0.0 to 14.3 pg/m^3; for SimpleBox 3.0 (initial concentrations) - from 5.4 to 12.8 pg/m^3; for SimpleBox 3.0 (historical emissions) - from 3.0 to 8.8 pg/m^3; for SimpleBox 3.12 (historical emissions) - from 3.4 to 9.5 pg/m^3. The maximum average value of air concentration within this domain is characteristic of SimpleBox 3.0 results obtained on the basis of initial concentrations (6 pg/m^3) and the minimum average value – of DEHM-POP results also based on initial conditions (1.4 pg/m^3). According to the results of EVN-BETR and UK-MODEL (historical emissions and initial concentrations), MSCE-POP, SimpleBox 3.0 and 3.12 (historical emissions), the annual air concentration averaged for the calculation domain varies from 2.9 to 3.8 pg/m^3.

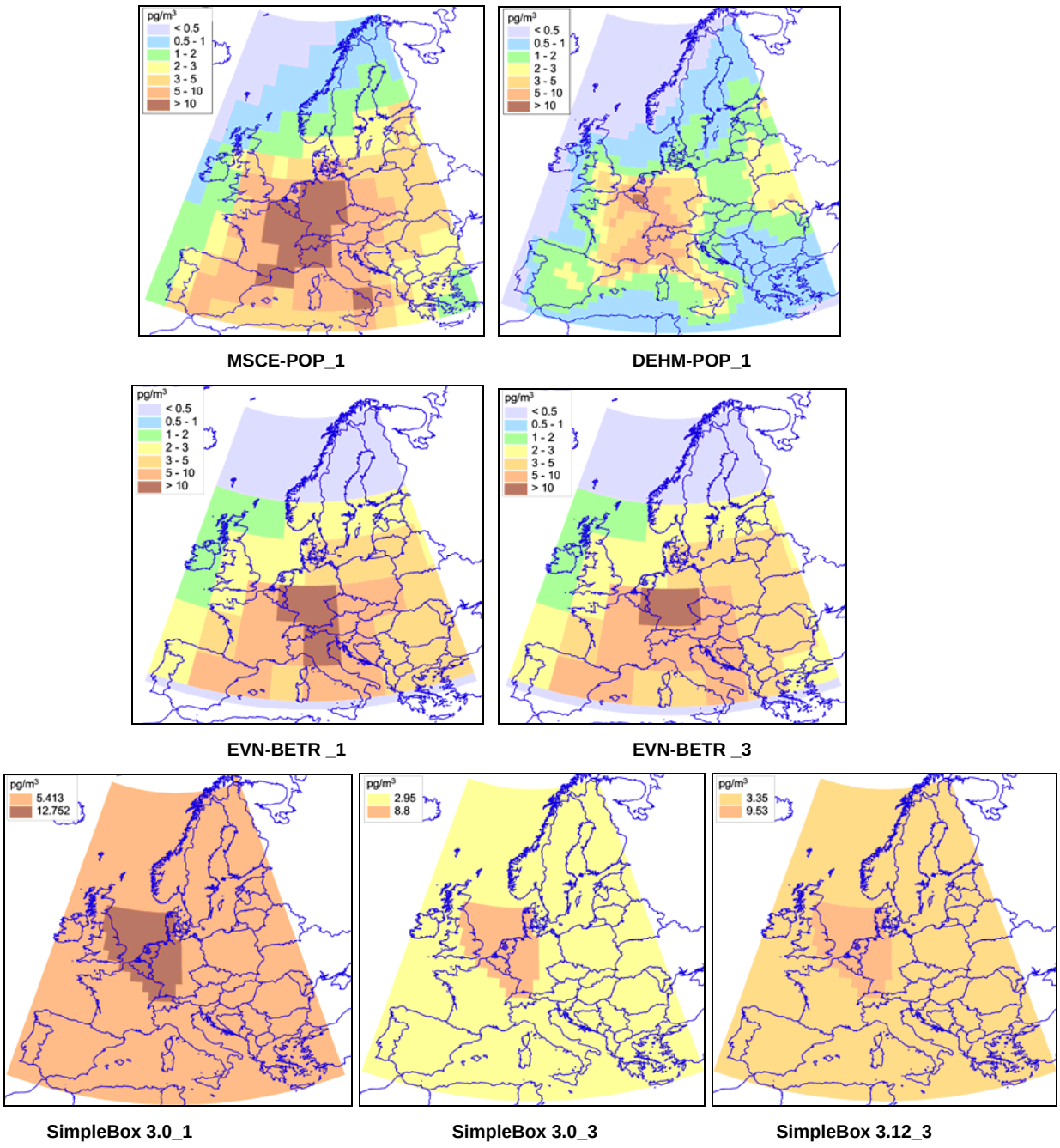


Fig. 3.147. *Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.148.

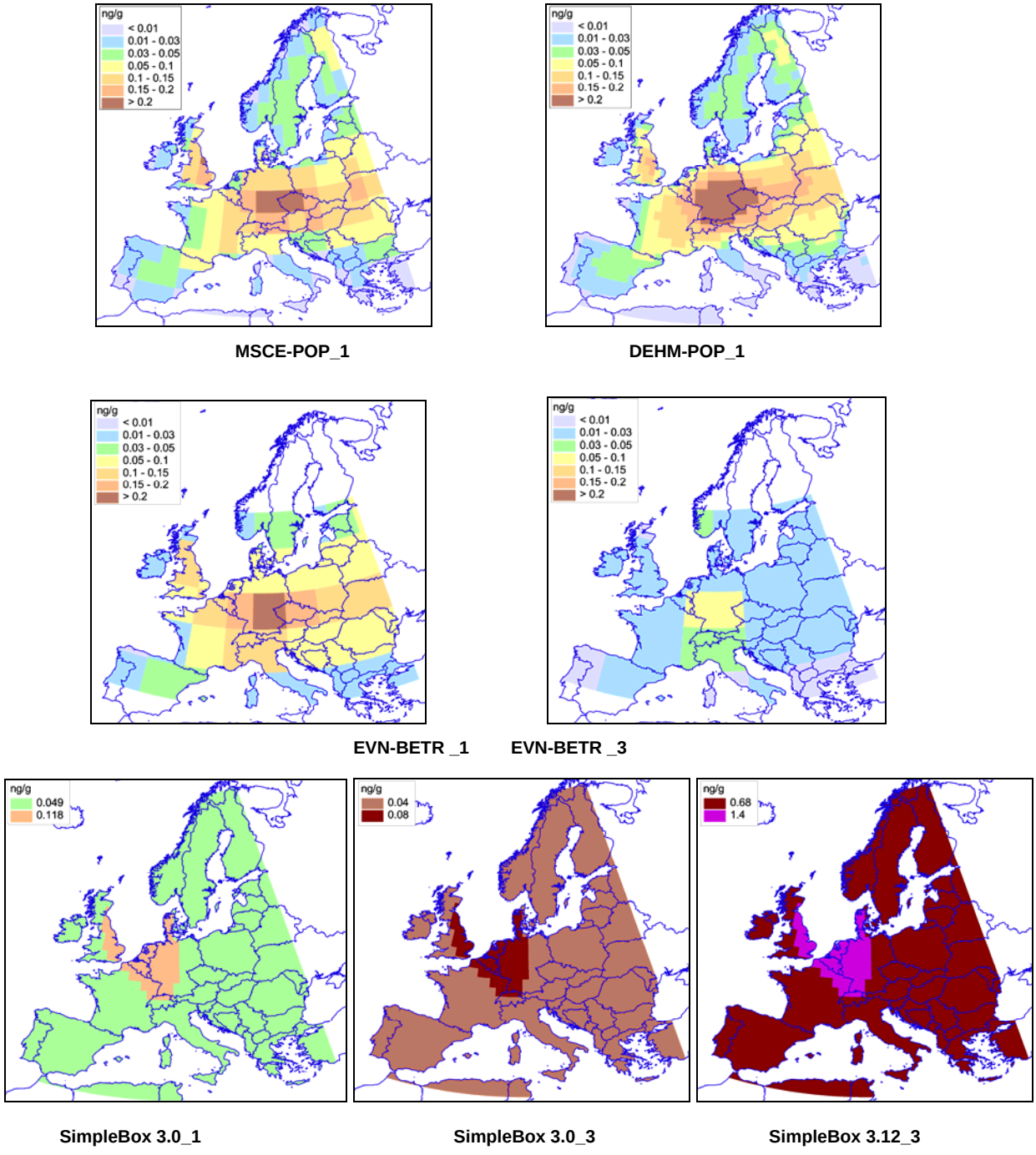


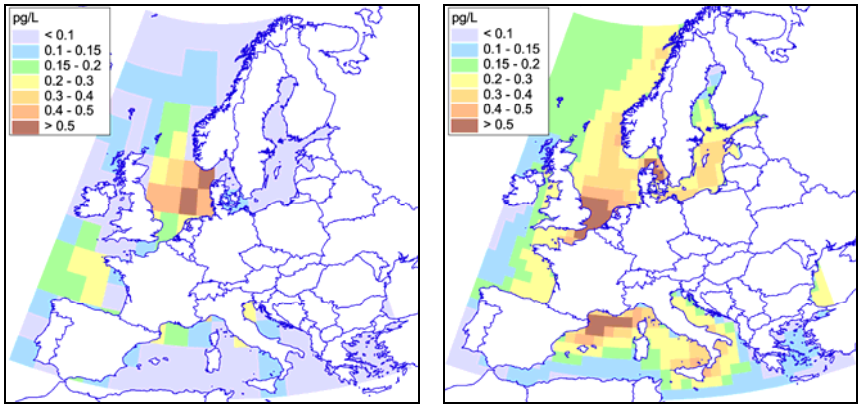
Fig. 3.148. *Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

As in the case with spatial distribution of air concentrations, the calculated fields of PCB-153 concentrations in soil calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions are in reasonable agreement between each other. EVN-BETR and UK-MODEL (initial concentrations), DEHM-POP and

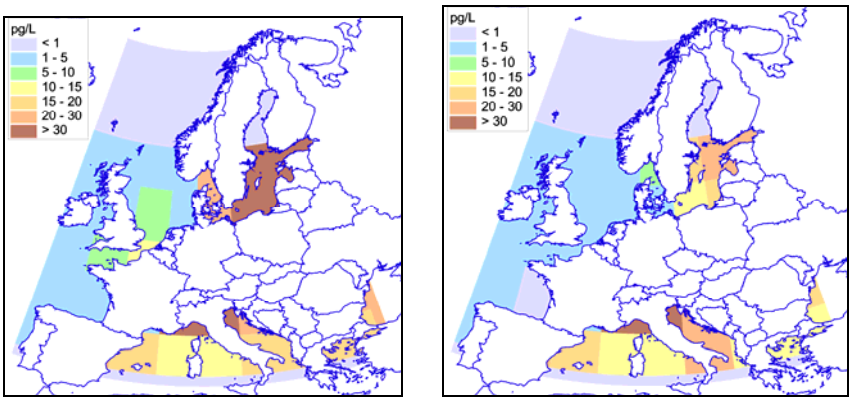
MSCE-POP models demonstrate very close results. Thus, according to these models results, considerably high PCB-153 soil concentrations (> 0.2 ng/g) in 2000 are typical for Central European countries (Germany, Austria, Poland, and the Czech Republic). In the results of different versions of SimpleBox model the region with the most contaminated soil covers not only some parts of Germany but also France, Belgium, the Netherlands and the UK. At that estimates of PCB-153 soil concentrations obtained by version 3.12 of SimpleBox model are considerably higher than those obtained by version 3.0. In general, concentrations of this pollutant in soil of Europe varied from 0.0 to 0.23 ng/g according to the results of EVN-BETR and UK-MODEL (initial concentrations); 0.0 to 0.05 ng/g according to the results of EVN-BETR and UK-MODEL (historical emissions); from $7.6 \cdot 10^{-9}$ to 0.27 ng/g according to the results of DEHM-POP model; from 0 to 0.44 ng/g according to the results of MSCE-POP; from 0.05 to 0.12 ng/g according to the results of SimpleBox 3.0 (initial concentrations); from 0.04 to 0.08 ng/g according to the results of SimpleBox 3.0 (historical emissions); and from 0.68 to 1.4 ng/g according to the results of SimpleBox 3.12 (historical emissions). The average value of soil concentration within the calculation domain obtained by the participating models is in the range from 0.01 to 0.74 ng/g.

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. 3.149.

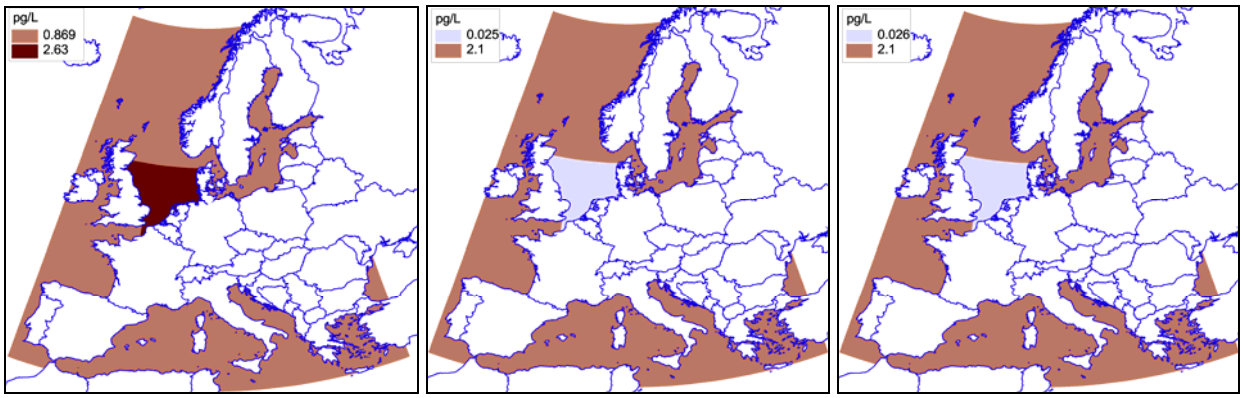
The difference in the spatial distribution of water concentrations of PCB-153 obtained by the participating models is more considerable than that in the results on concentrations in the atmosphere and soil. Thus, high values of PCB-153 seawater concentrations in the coastal waters of the North Sea vary from 1.0 to 10.0 pg/l according to the results of EVN-BETR and UK-MODEL obtained on the basis of initial concentrations and historical emissions, exceed 0.5 pg/l in the results of MSCE-POP and DEHM-POP models, and equal 0.03 and 0.87 pg/l in the results of SimpleBox 3.0 and 3.12 (historical emissions) and SimpleBox 3.0 (initial concentrations), respectively. The spatial distribution of PCB-153 water concentrations in the Mediterranean and Adriatic Seas are characterised by high values of water concentrations obtained by DEHM-POP (more than 0.5 pg/l) and EVN-BETR and UK MODEL (more than 30.0 pg/l). The latter model predicts also the highest level of water pollution for the Baltic Sea. The average value of water concentration within the calculation domain provided by EVN-BETR and UK-MODEL (initial concentrations) is equal to 11.4 pg/l, by EVN-BETR and UK-MODEL (historical emissions) - to 6.5 pg/l, by MSCE-POP – to 0.1 pg/l, by DEHM-POP – to 0.15 pg/l, by SimpleBox 3.0 (initial concentrations) – to 1.0 pg/l, by SimpleBox 3.12 (historical emissions) – to 1.9 pg/l, by SimpleBox 3.0 (historical emissions) – to 1.95 pg/l.



MSCE-POP_1 **DEHM-POP_1**



EVN-BETR _1 **EVN-BETR _3**



SimpleBox 3.0_1 **SimpleBox 3.0_3** **SimpleBox 3.12_3**

Fig. 3.149. *Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.3.150.

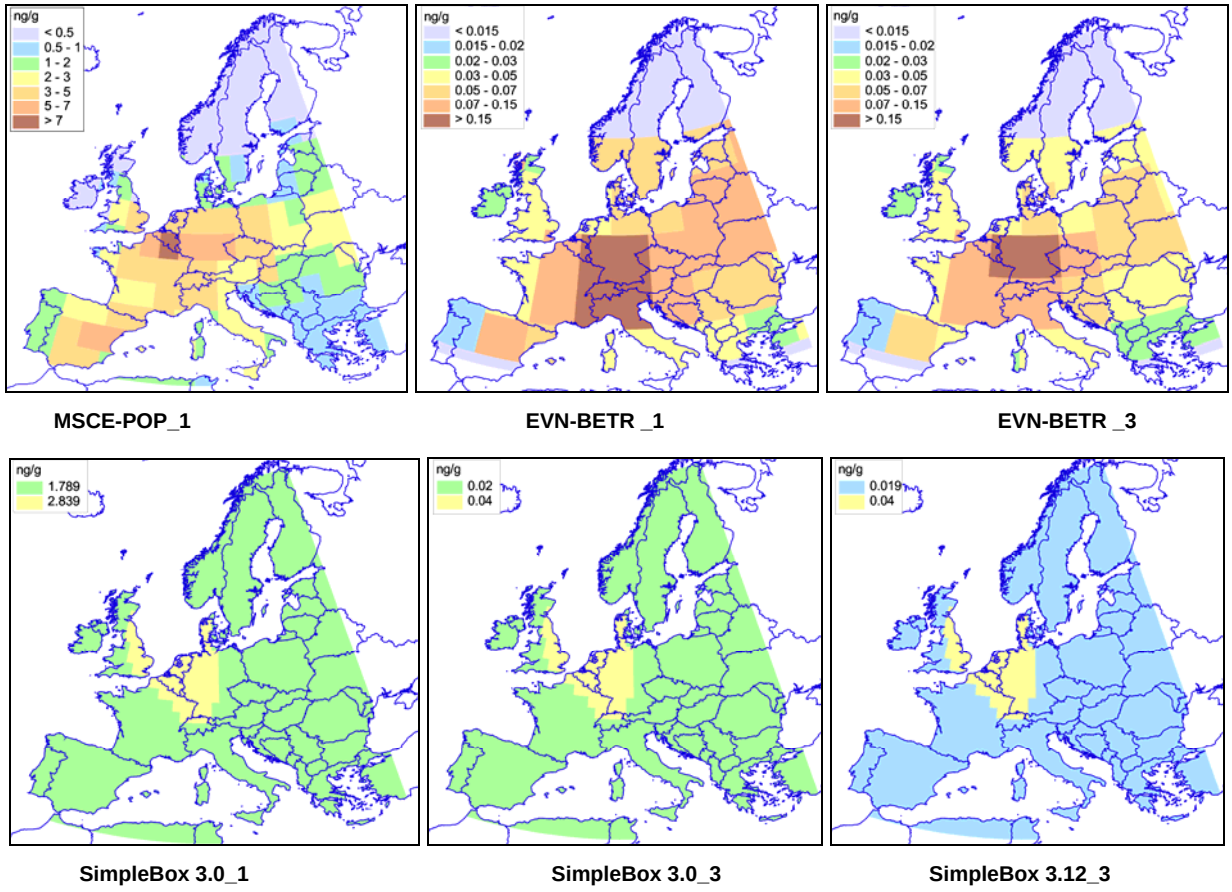


Fig. 3.150. *Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

According to the results presented, the participating models predicted rather close spatial distribution of PCB-153 concentrations in vegetation. All models results show that the highest levels of concentrations in vegetation are observed in some regions of Belgium, France, Germany and the UK. At that estimates of PCB-153 concentrations obtained by MSCE-POP and SimpleBox 3.0 (initial concentrations) are considerably higher than others. Thus, in MSCE-POP results concentration levels in vegetation of the Europe are in the range from 0.0 to 9.6 ng/g; in EVN-BETR and UK-MODEL results (initial concentrations in all media except vegetation) - from 0.0 to 0.25 ng/g; in EVN-BETR and UK-MODEL results (historical emissions) - from 0.0 to 0.19 ng/g; in SimpleBox 3.0 results (initial concentrations) - from 1.79 to 2.84 ng/g; in SimpleBox 3.0 and 3.12 results (historical emissions) - from 0.02 to 0.04 ng/g.

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.151. The values of net deposition flux include dry and wet depositions and gaseous exchange. Of note, the spatial variability of SimpleBox results in this case is higher than that in the presented above results on concentrations in the media since the deposition values in this model are dependent on the different types of underlying surfaces, which were taken into account in their calculations.

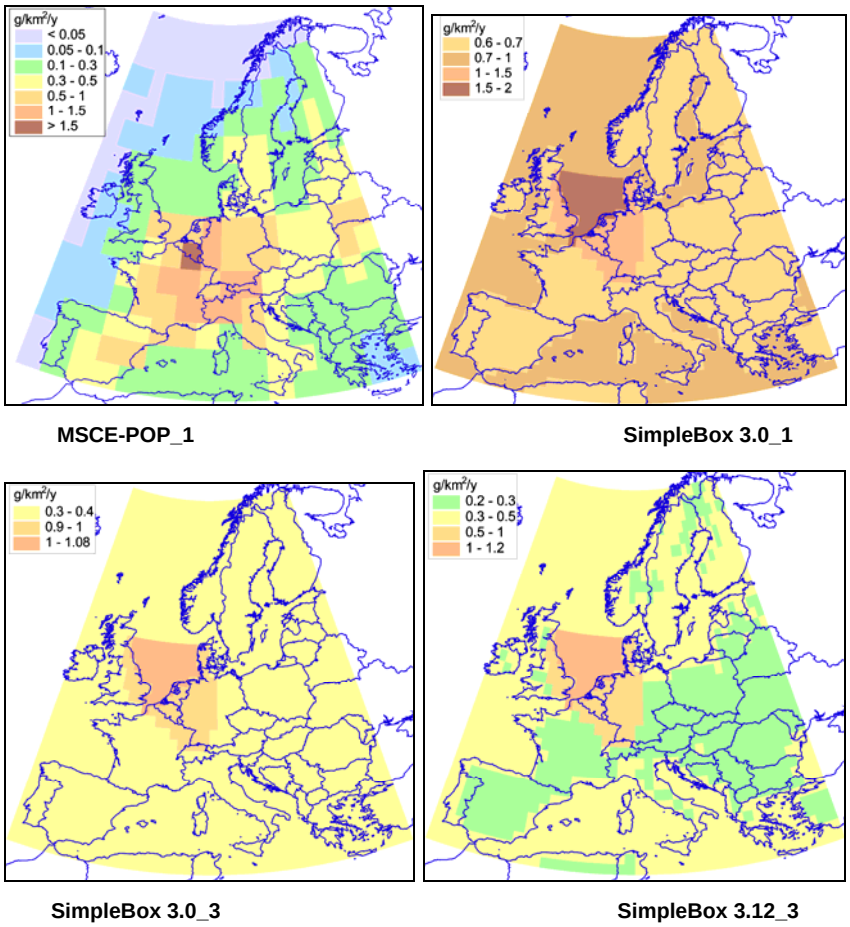


Fig. 3.151. *Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

Spatial distribution of PCB-153 net depositions obtained both by MSCE-POP and SimpleBox models shows that relatively high values of this flux within the European domain are observed in some parts of Belgium, France, Germany, the Netherlands and coastal water of the North Sea. In the results of MSCE-POP model the highest net deposition flux is directed to the territories covered by soil, but the highest flux obtained by SimpleBox model is directed to the water. For SimpleBox 3.0 (initial concentrations) the levels of depositions over different parts of the calculation domain varied from 0.6 to 2.0 g/km^2/y; for SimpleBox 3.0 (historical emissions) - from 0.3 to 1.1 g/km^2/y; for SimpleBox 3.12 (historical emissions) - from 0.2 to 1.2 g/km^2/y; and for MSCE-POP model - from 0.02 to 1.9 g/km^2/y.

Below the comparison of model results obtained on the basis of zero initial concentrations in the environmental media is presented.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by ADEPT, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.152.

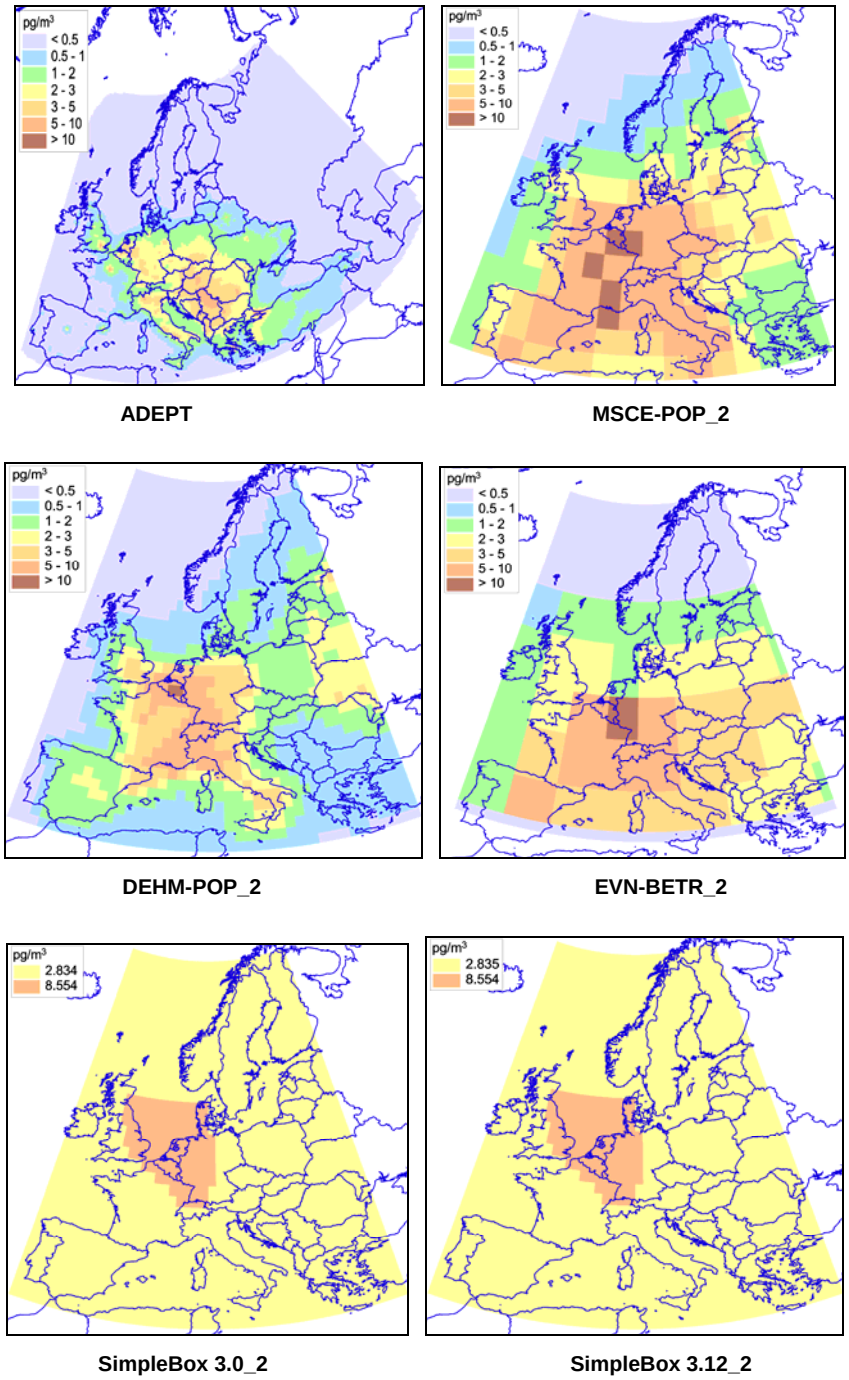


Fig. 3.152. *Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are illustrated in Fig.3.153.

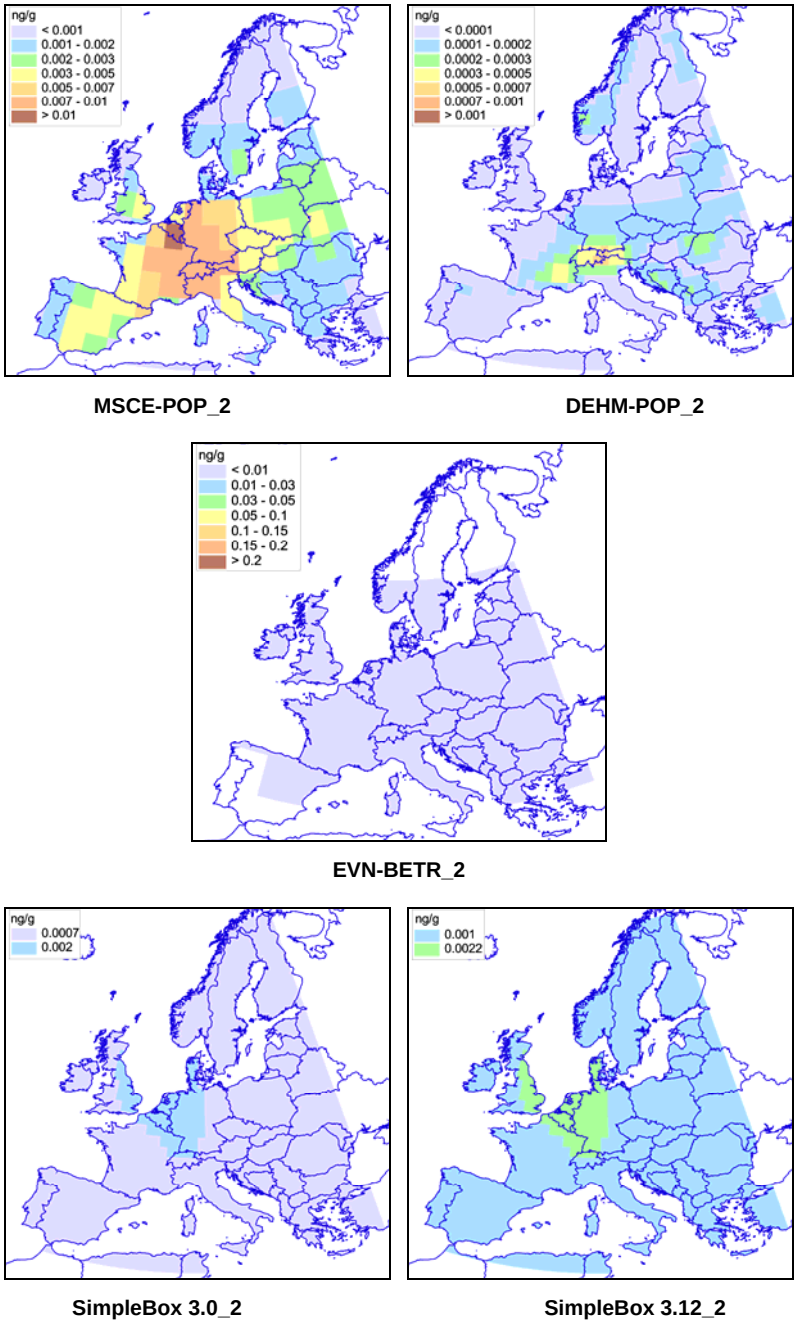


Fig. 3.153. *Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig. 3.154.

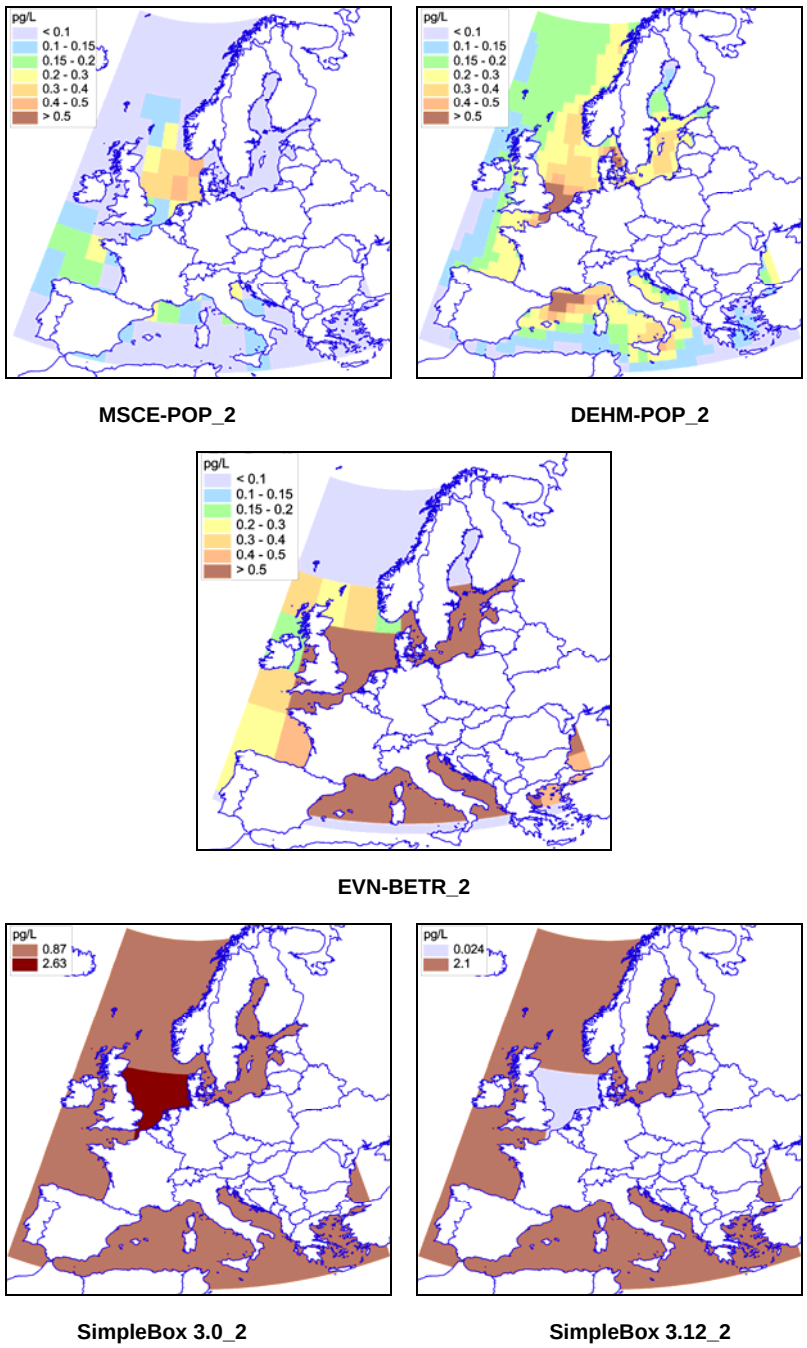


Fig. 3.154. *Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of "reference" data set and zero initial concentrations.*

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.3.155.

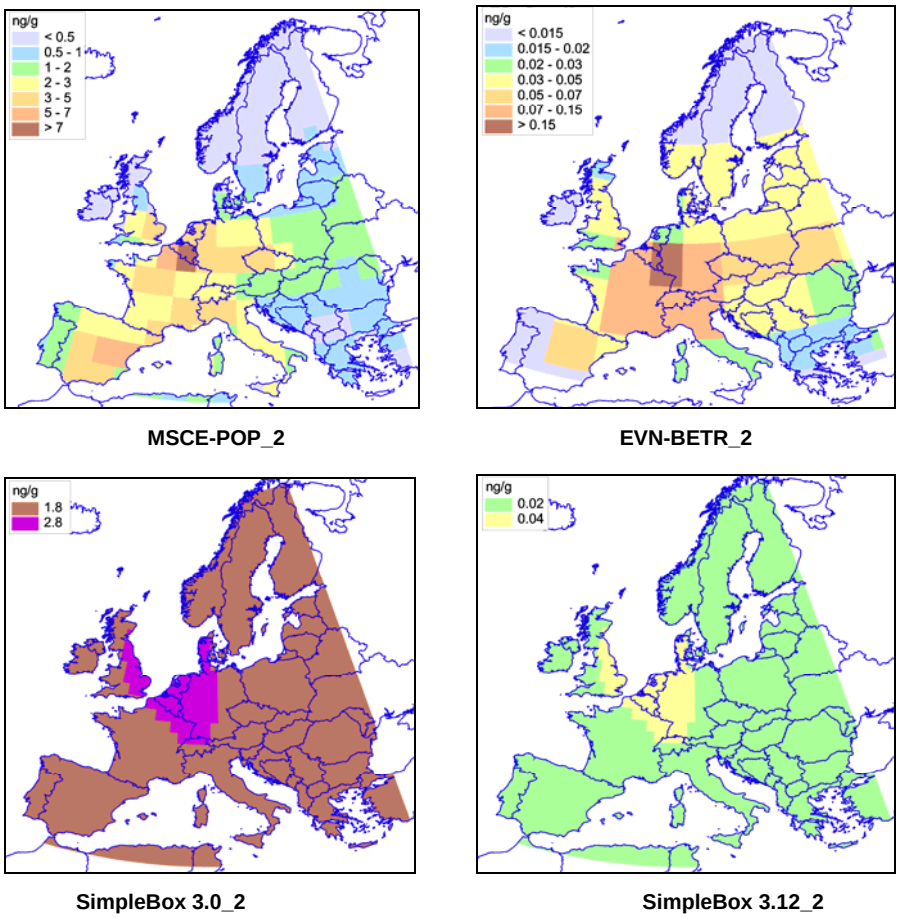


Fig. 3.155. *Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of "reference" data set and zero initial concentrations.*

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by ADEPT, MSCE-POP and SimpleBox models are shown in Fig.3.156. The values of net deposition flux include dry and wet depositions and gaseous exchange.

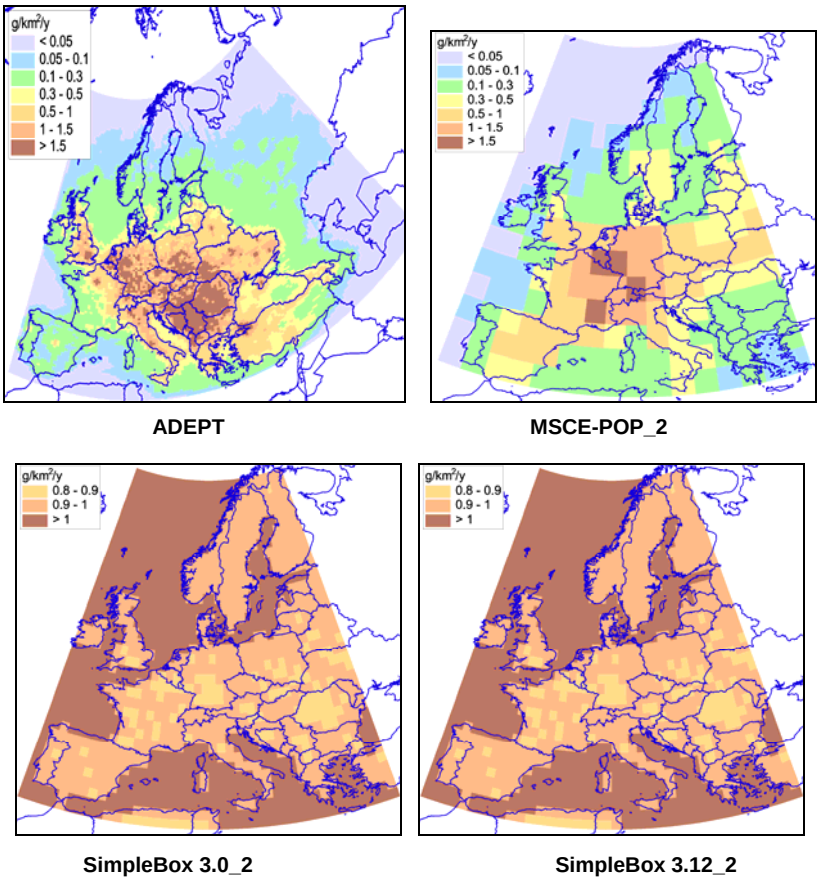


Fig. 3.156. *Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

3.6.2. Comparison of results on spatial distribution of PCB-153 depositions and concentrations in different compartments obtained on the basis of "own or alternative" data sets

In this section a comparison of spatial distributions of PCB-153 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models "own or alternative" data sets on the basis of initial concentrations of pollutants in media, historical emissions and zero initial conditions is presented.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.157.

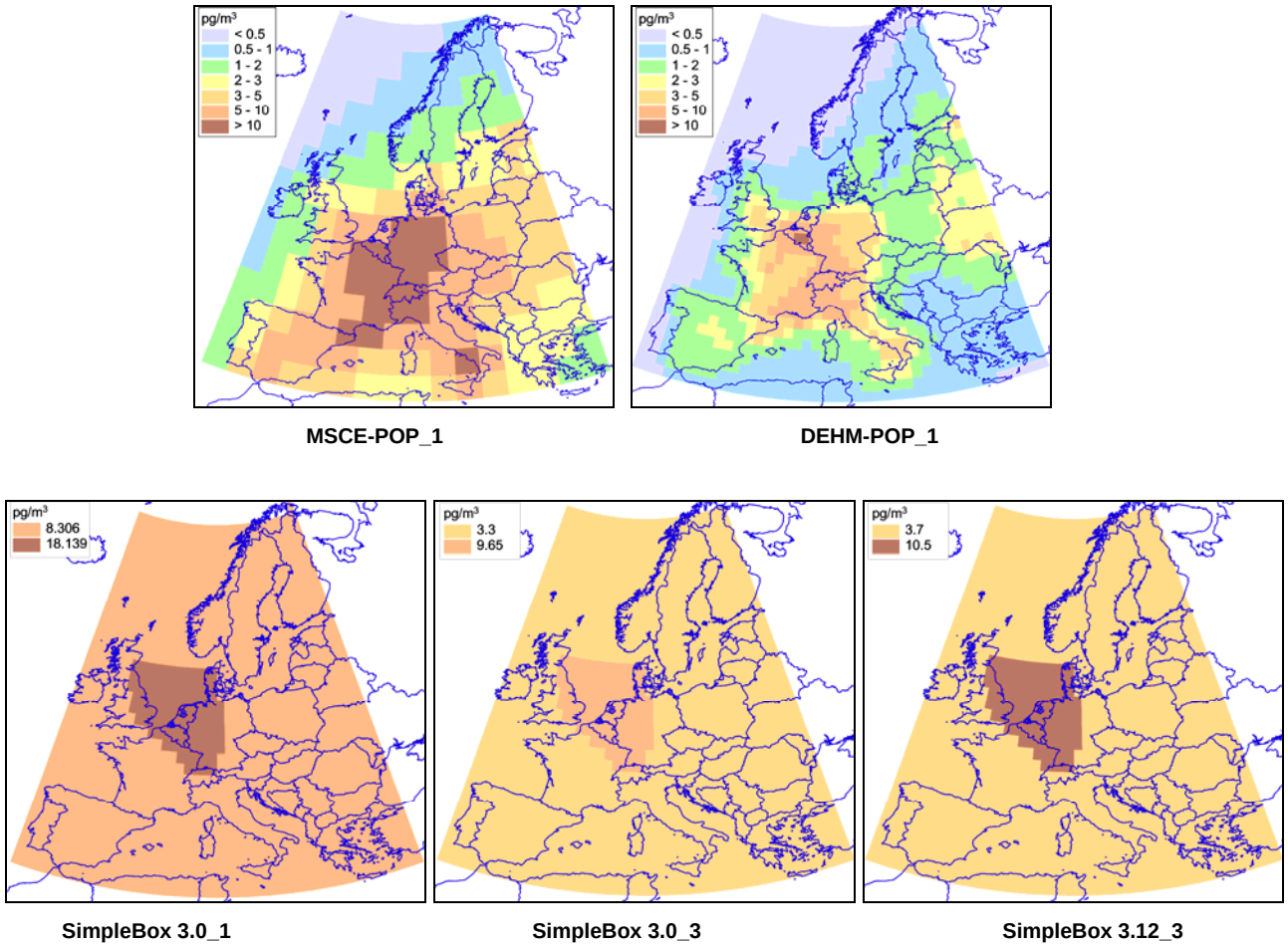


Fig. 3.157. *Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.158.

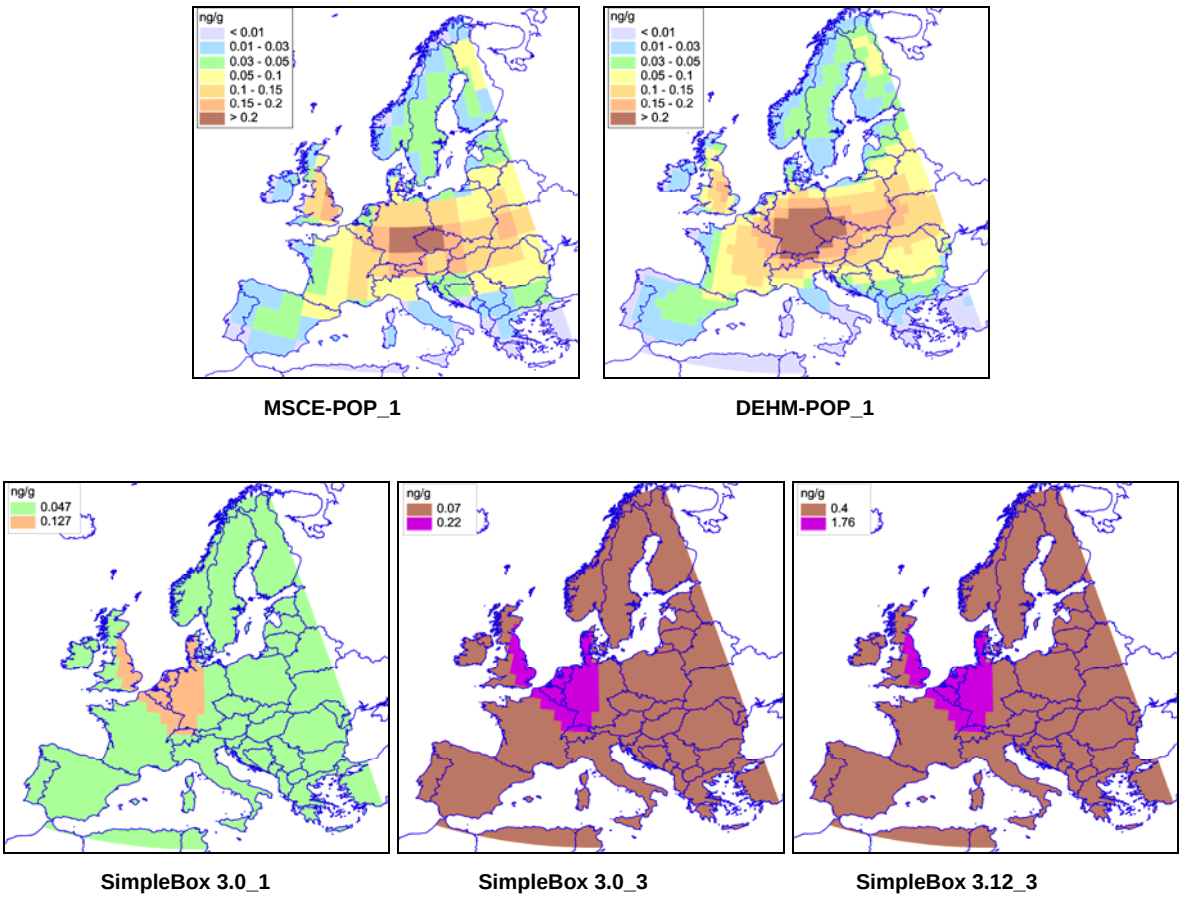


Fig. 3.158. *Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of "own or alternative" data set taking into account initial concentrations of pollutants in media or historical emissions*

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. 3.159.

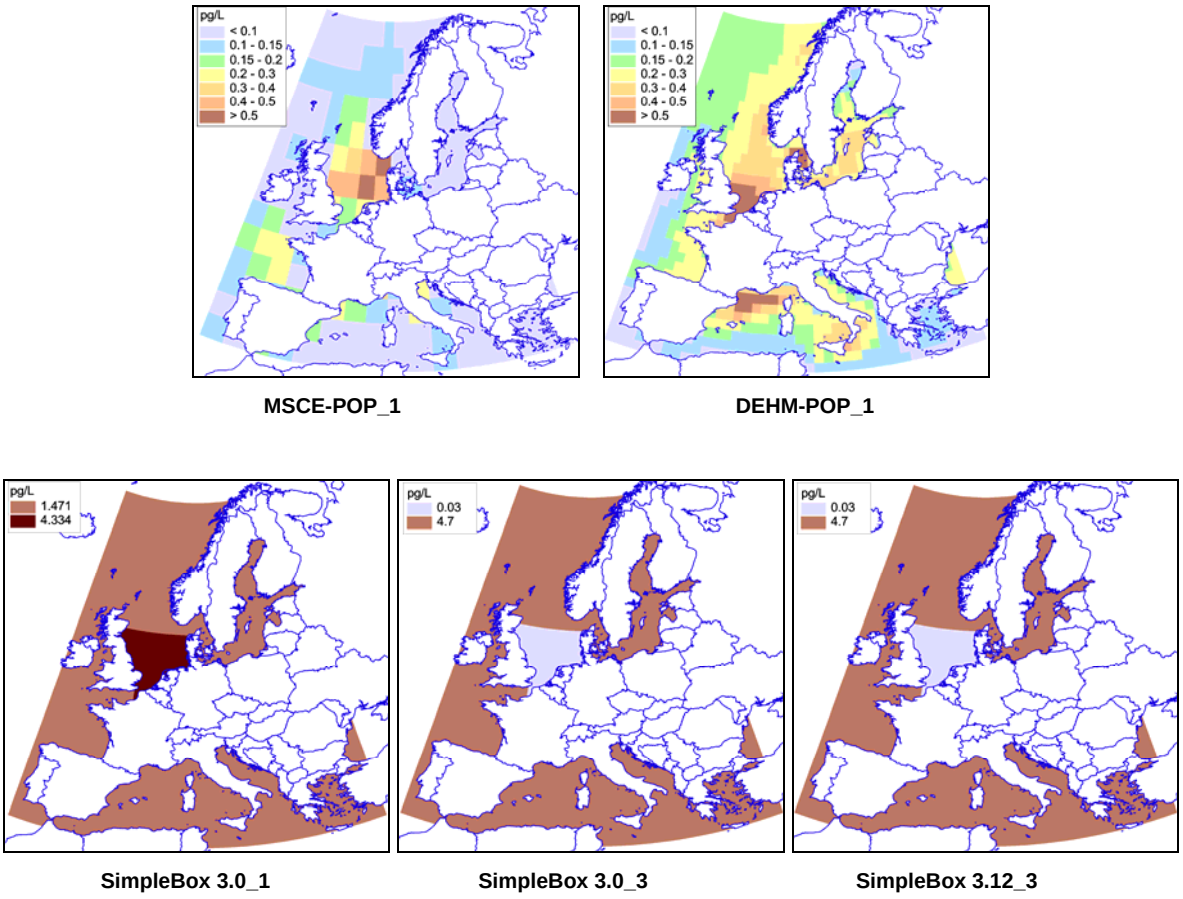


Fig. 3.159. *Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.3.160.

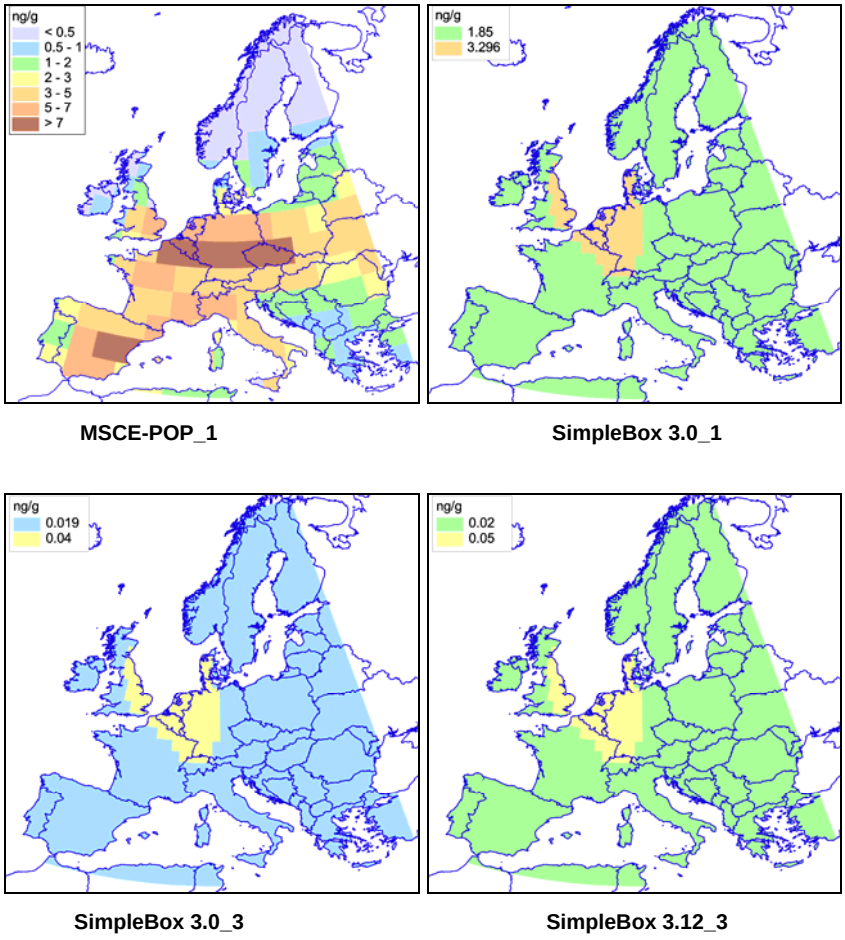


Fig. 3.160. *Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions***.**

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.161. The values of net deposition flux include dry and wet depositions and gaseous exchange.

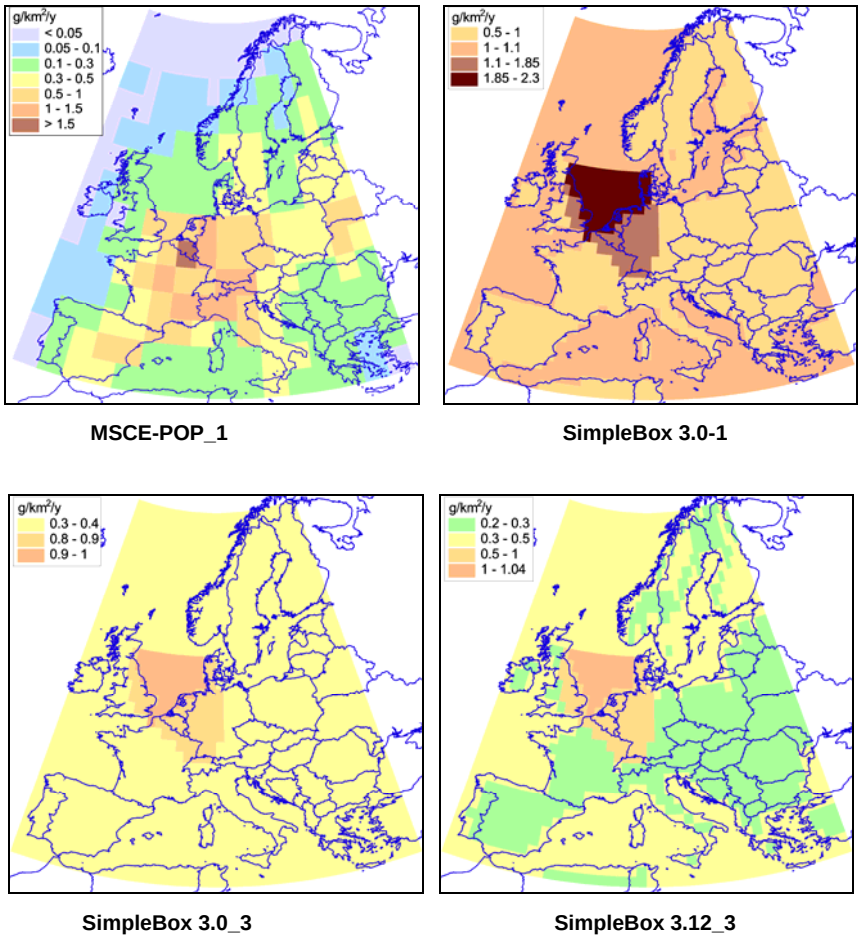


Fig. 3.161. *Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*.

The model results obtained on the basis of zero initial concentrations in the environmental media are compared below.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.162.

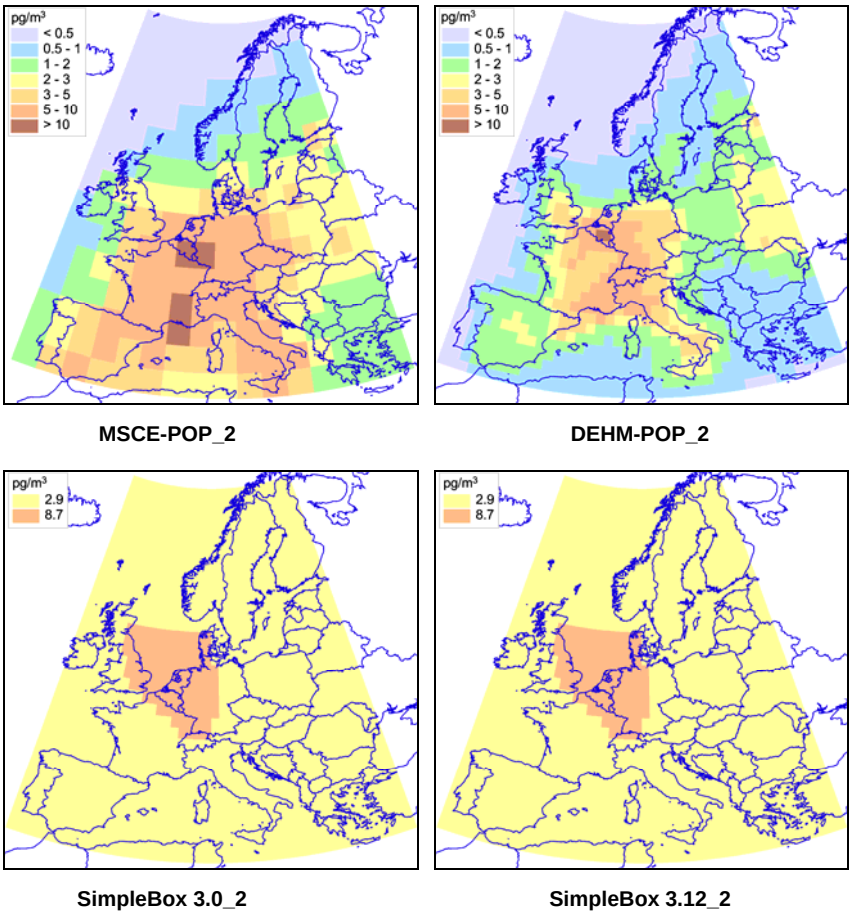


Fig. 3.162. *Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations.*

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.163.

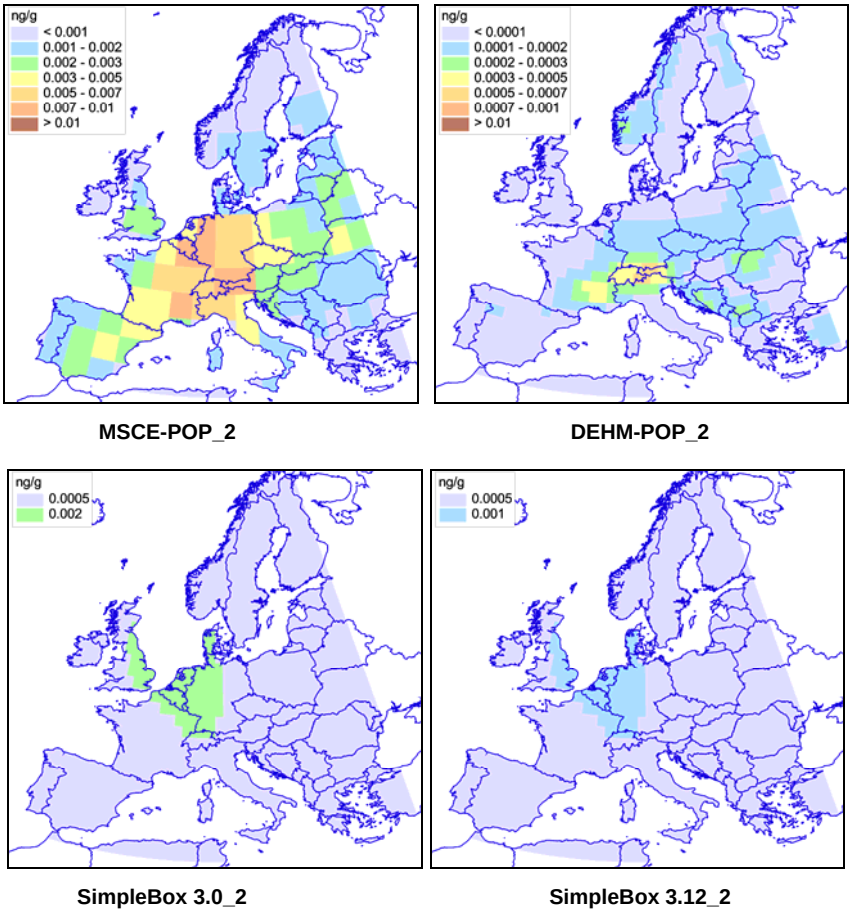


Fig. 3.163. *Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*.

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. 3.188.

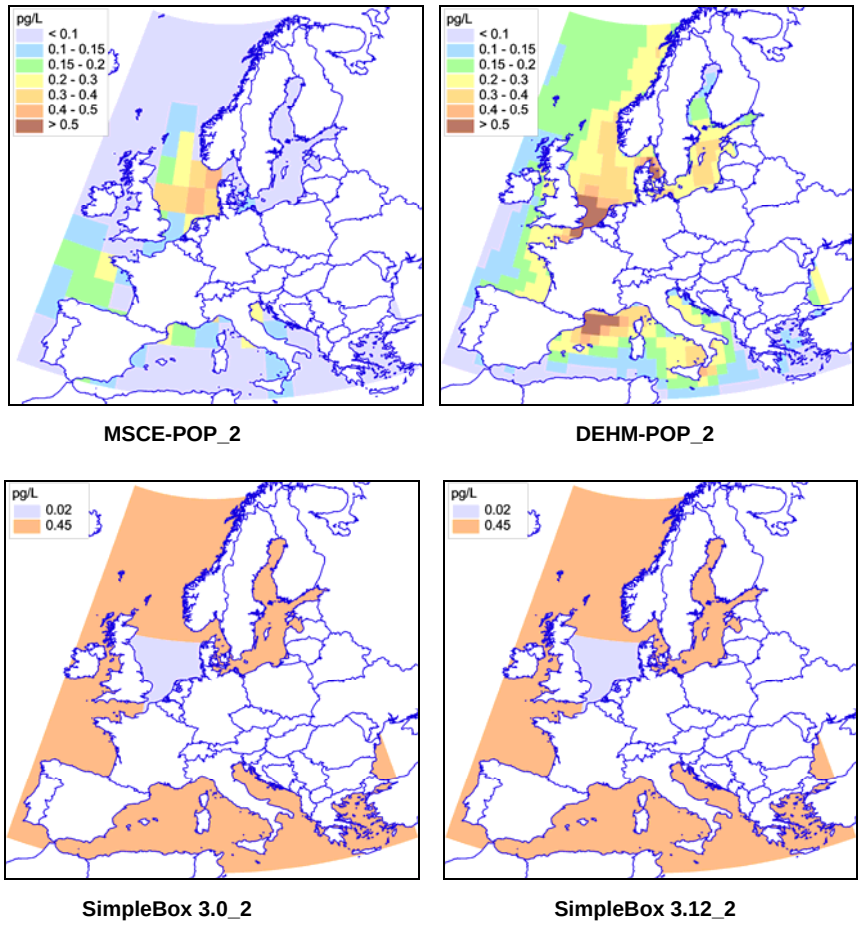
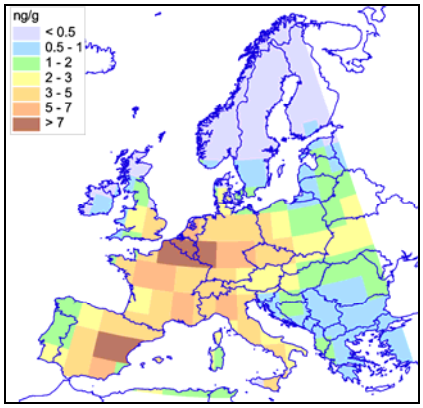
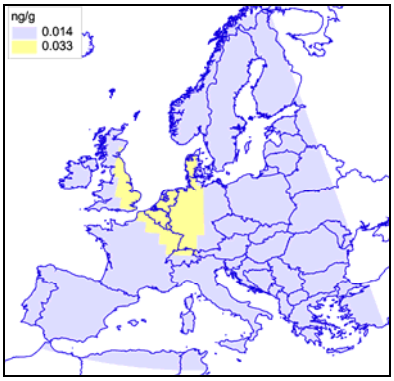


Fig. 3.164. *Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

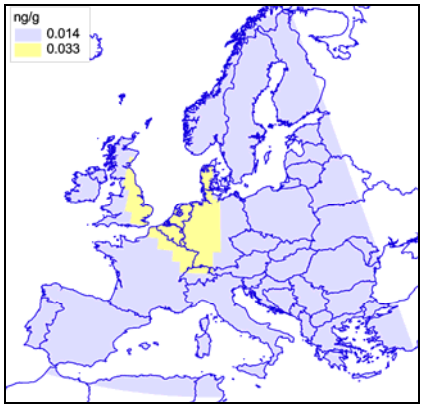
Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.3.165.



MSCE-POP_2



SimpleBox 3.0_2



SimpleBox 3.12_2

Fig. 3.165. *Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.166. The values of net deposition flux include dry and wet depositions and gaseous exchange.

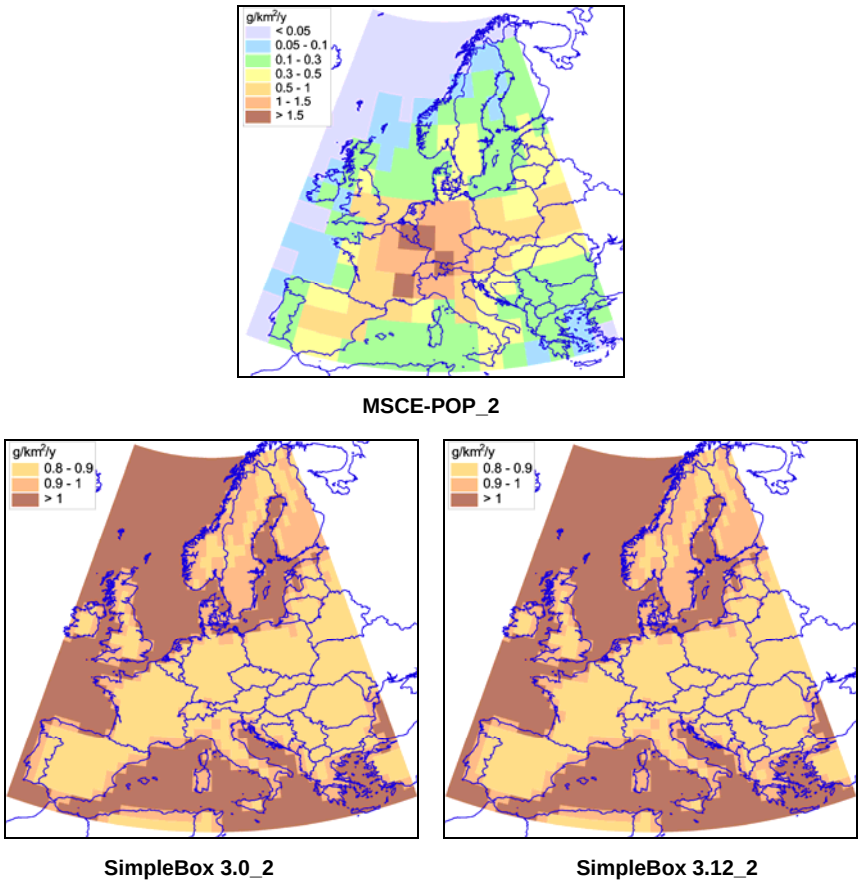


Fig. 3.166. *Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

The comparison of calculated fields of depositions and concentrations in the main environmental media obtained on the basis of "reference" and "own/alternative" data sets presented in this Section demonstrates that the models of different type and resolution closely described the spatial distribution of PCB-153 pollution.

3.7. Comparison of model results with measurements

Comparison of modelling results with available measurements of PCB air concentrations and atmosperhic depositions was carried out for 2000. Annual mean PCB concentrations obtained at 4 EMEP monitoring sites were selected: Kosetice (CZ3), Rörvik (SE2), Aspvreten (SE12), and Pallas (FI96). These sites are located (Fig. 3.167) within the modelling domain specified for the intercomparison study and reported in Berg et al. (2002). Air concentrations at all stations were sampled using conventional hi-volume air samplers, whilst atmospheric deposition at three stations (Rörvik, Aspvreten and Pallas), were sampled using bulk atmospheric deposition samplers. The samples were analyzed using conventional analytical techniques [*Berg et al*., 2002].

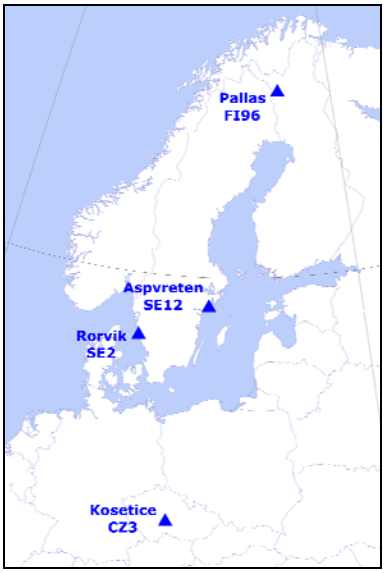
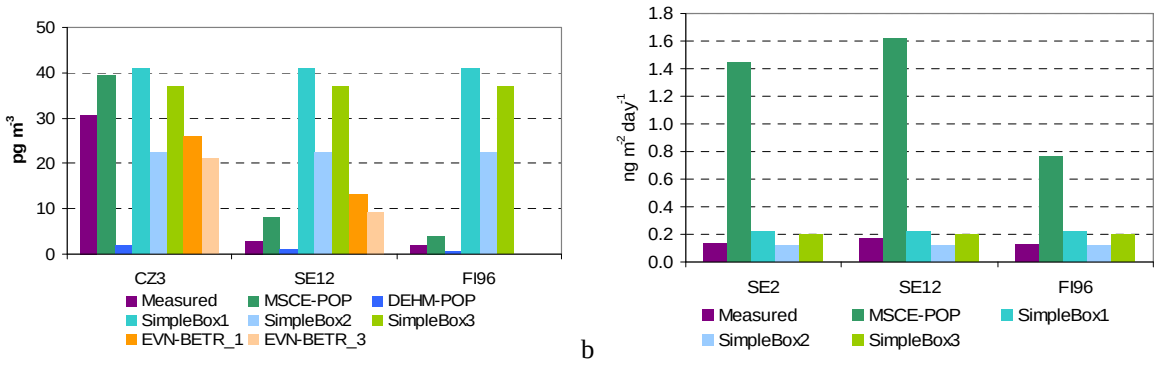


Fig. 3.167*. Location of selected monitoring sites*

It is emphasized that the intercomparison between measured and modeled atmospheric depositions should be considered with some caution. That can be mostly explained by several discrepancies existing between what is implied as measured and simulated bulk deposition values. The bulk atmospheric deposition sampling is supposed to include wet deposition of gaseous and particulate phase of POPs and also some unknown part of dry deposition. In [*Horstmann and McLachlan*, 1997] it was found that the contribution of gaseous exchange to samples is small with respect to total depositions. According to [*Guerzoni et al*., 2004] the limitation of this sampling method is mainly possible underestimation of fluxes because of the limited collection of dry gases. In models atmospheric deposition of POPs is commonly described as a combination of various advective and diffusive processes. In this study for the comparison with measured bulk deposition values the sum of dry particle deposition and overall (gas+particle) wet deposition values usually calculated in models separately (so called direct deposition values) is used without taking into account diffusive fraction of dry deposition. Despite having been suggested that the diffusive process of gaseous exchange may be a key deposition/exchange mechanism for certain POPs between the atmosphere and the underlying surface [e.g. *Wania et al*. 19998 and references therein], direct measurements of the diffusive gaseous exchange flux are still rather limited. That is why for the sake of comparison the simulated values of gaseous exchange are not included into bulk deposition values obtained by the models in this intercomparison. For all these reasons, differences between predicted and observed bulk atmospheric deposition values are indeed expected.

Comparison with measurements was mostly done for the model results obtained with “own-alternative” data set of physical-chemical properties and defined initial conditions. Thus, results of DEHM-POP and MSCE-POP models calculated on the basis of initial concentrations given as input data (MSCE-POP_1 and DEHM-POP_1) are used for comparison with measurements. SimpleBox model provided three sets of model results obtained on the basis of “alternative” data set with the help of initial concentrations given as input data or with historical emissions for 20-year period (SimpleBox 3.0_1, SimpleBox 3.0_3 and SimpleBox 3.12_3). They are presented as SimpleBox1, SimpleBox2, and SimpleBox3 in figures below. Results of EVN-BETR and UK-MODEL calculated with the use of initial concentrations (EVN-BETR_1) and historical emissions (EVN-BETR_3) were obtained on the basis of “reference” data set.

Computed and observed annual mean air concentrations and depositions of PCB-28 are presented in Fig. 3.168. Measured concentrations of PCB-28 decrease in the northern direction. This gradient is reflected in model results of EVN-BETR and UK-MODEL, MSCE-POP and DEHM-POP.



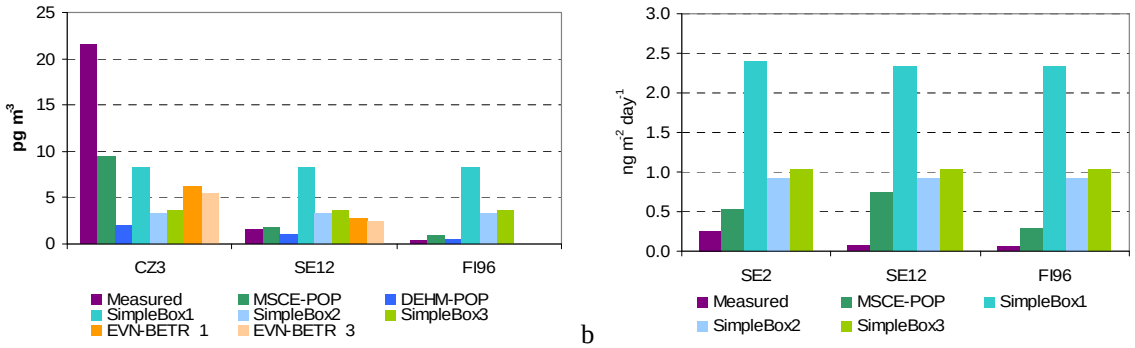
a b

Fig. 3.168. *Comparison of computed air concentrations (a) and depositions (b) of PCB-28 with measurements for 2000*

Level of PCB-28 concentrations computed by SimpleBox model is close to the one measured at Kosetice (CZ3). The same value is obtained for Aspvreten (SE12) and Pallas (FI96) overestimating observed concentrations.

Comparison of bulk deposition (wet + dry) fluxes were done for MSCE-POP and three data sets of SimpleBox. It can be seen that SimpleBox provided close values of depositions in all three cases. At the same time deposition fluxes of MSCE-POP significantly overestimate observed fluxes.

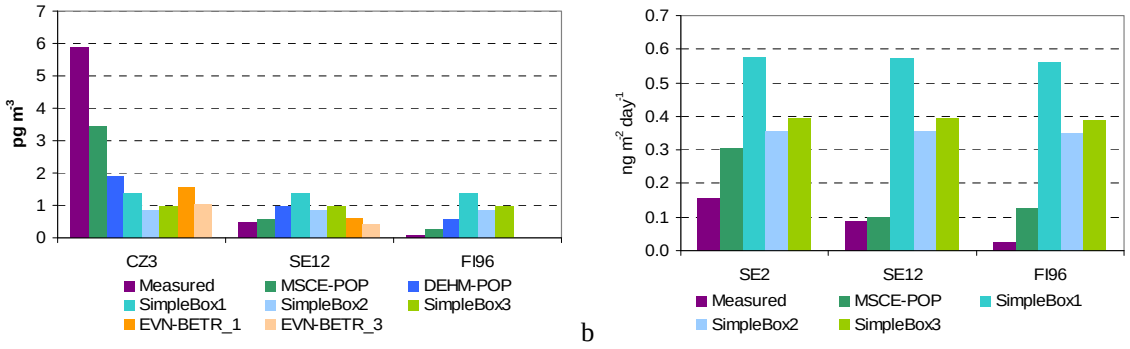
Comparison of computed and observed PCB-153 annual mean concentrations and depositions is presented in Fig. 3.169. Again similar decrease in measured concentrations of this PCB congener can be seen in northern direction. MSCE-POP and DEHM-POP also show drop of concentrations in this direction and good agreement for Aspvreten (SE12) and Pallas (FI96). Mean concentrations at Kosetice (CZ3) are underestimated by all models. In case of SimpleBox model results there is some underestimation for Kosetice (CZ3) and overestimation for other two sites. In addition to these three models data of EVN-BETR model obtained for PCB-153 on “reference” data set with the use of initial concentrations given as input data and historical emissions were also compared with measurements. Some decrease can be seen from Kosetice (CZ3) to Aspvreten (SE12) in concentrations computed by this model. Computed concentrations for Aspvreten (SE12) are in good agreement with measured and underestimated for Kosetice (CZ3).



a b

Fig. 3.169. *Comparison of computed air concentrations (a) and depositions (b) of PCB-153 with measurements for 2000*

Values of measured bulk deposition fluxes of PCB-153 were compared with the results of MSCE-POP and SimpleBox models. Computed bulk deposition fluxes of all the models overestimate measured values. It can be seen that observed spatial trend in depositions do not captured by models. Close results were obtained in comparison of PCB-180 computed and observed annual mean concentrations (Fig. 3.170).



a b

Fig. 3.170. *Comparison of computed air concentrations (a) and depositions (b) of PCB-180 with measurements for 2000*

Measured concentrations of PCB-180 in air are decreased in northern direction which is reflected in EVN-BETR and UK-MODEL, MSCE-POP and DEHM-POP model results. Mean concentrations at Kosetice (CZ3) are underestimated by all the models. Concentrations computed by MSCE-POP and EVN-BETR and UK-MODEL for Aspvreten (SE12) are in good agreement with measured value. Computed values of all other models overestimate slightly the measured value. At Pallas (FI96) for all the models more significant overestimation can be seen.

As for PCB-28 comparison of bulk deposition fluxes were done for the results of MSCE-POP and SimpleBox models. It can be seen that both models overestimate observed deposition fluxes of PCB-180 for all three sites. Results of MSCE-POP are closer to observed deposition values especially for Aspvreten (SE12).

Comparison of PCB congener composition in measured and computed air concentrations and depositions

Comparison of computed and measured congener composition in air for the selected sites is presented in Fig. 3.171.

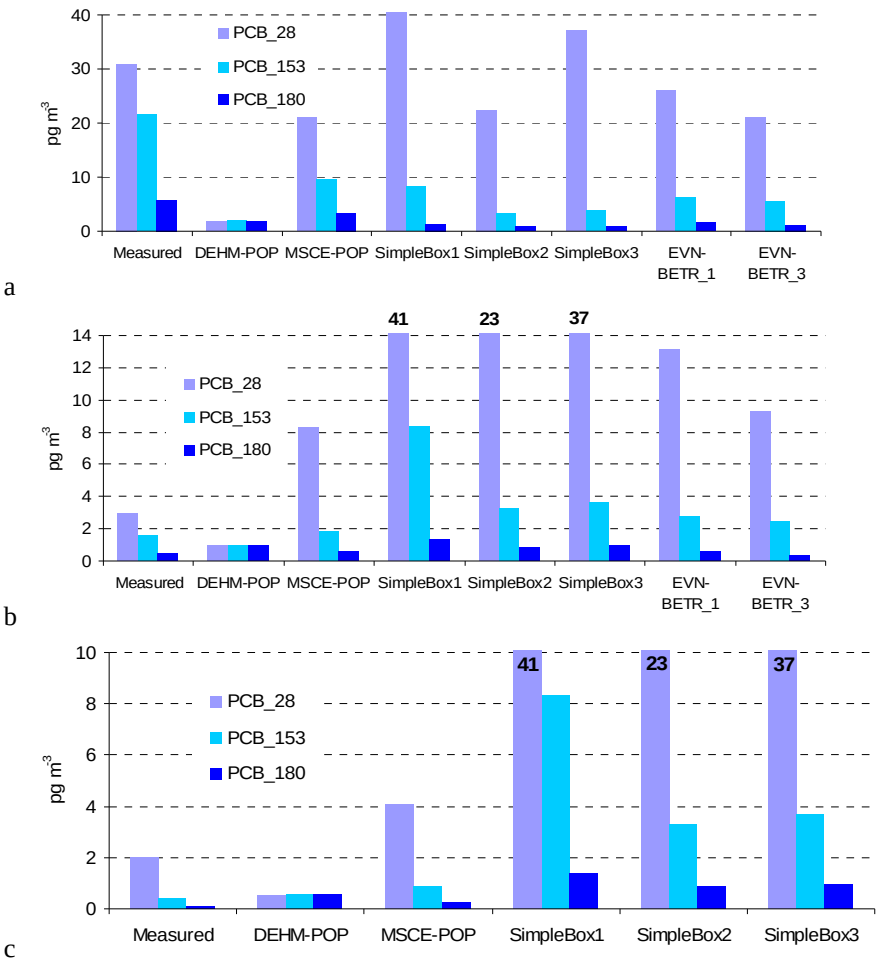


Fig.3.172. *Comparison of PCB congener composition in measured and computed air concentrations for 2000, (a) – Kosetice (CZ3), (b) – Aspvreten (SE12), (c) – Pallas (FI96)*

Practically the same composition of selected PCB congeners in air is observed at these sites. Lighter congener PCB-28 dominates for all the sites. Heavier congeners PCB-153 and PCB-180 have lower values of air concentrations. More significant difference between PCB-28 and heavier congeners is found for northern site Pallas (FI96). It can be seen that most of the models have captured measured congener composition. In case of DEHM-POP model same values of computed air concentrations of selected PCB congeners were obtained.

Comparison of computed and measured congener composition in bulk deposition fluxes for the selected sites is presented in Fig. 3.173.

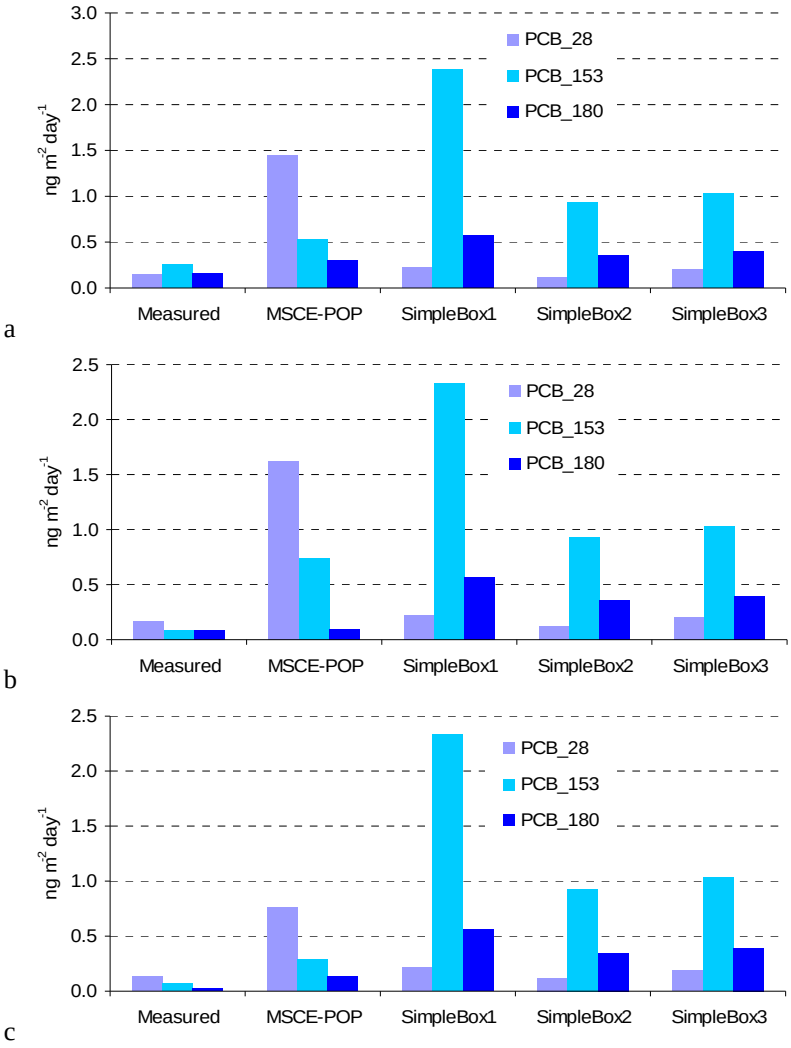


Fig. 3.174. *Comparison of PCB congener composition in measured and computed depositions for 2000, (a) – Rorvik (SE2), (b) – Aspvreten (SE12), (c) – Pallas (FI96)*

As it can be seen PCB congener composition in bulk deposition fluxes is not well captured by the models. In case of Rorvik (SE2) higher value of observed PCB-153 flux was found comparing to other two congeners. Similar composition of congeners was obtained by SimpleBox model and different by MSCE-POP model. In case of Aspvreten (SE12) both models provided different pattern of congeners in comparison to observed one. For Pallas (FI96) MSCE-POP obtained close to observed congener composition while SimpleBox obtained different results.

Conclusion remarks

Participated models reasonably reproduced observed levels and trends of PCB-153 mean annual concentrations. Comparison for other congeners has shown reasonable agreement for PCB-180 and larger differences for PCB-28. Observed levels of PCB deposition fluxes are overestimated by all the models.

PCB congener composition in air concentrations obtained by measurements is reasonably reproduced by the models. More discrepancies in found modelled and measured congener composition of PCB deposition fluxes.

Chapter 4

SENSITIVITY STUDY WITH RESPECT TO SUBSTANCE-SPECIFIC PROPERTIES USED IN THE DESCRIPTION OF BASIC PROCESSES FOR PCB-153

This chapter contains processed results of a sensitivity study with respect to physical-chemical parameter values used by the participating models for the calculations of parameters of model description of gas/particles partitioning, wet deposition and gaseous exchange between the atmosphere and soil, water and vegetation. Two sets of calculation results: obtained with "reference" data set of physical-chemical properties and with "own/alternative" data sets are presented.

For each data set used a presentation of modeling results is performed into two steps. At the first step we present the values of calculated parameters and characterize the spread in these values between models in each of the experiments. At the second step we show pairwise differences between participating models using the regression analysis.

The following statistical parameters for each experiment are used:

- the mean values *m* of the considered parameters averaged between participating models;
- the values of square deviation σ between results obtained by different models;

The analysis of pairwise differences between calculation results obtained by different models is based on the regression relation between calculated values of parameters A_T^1 and A_T^2 obtained by each two models for different experiments:

$$A_T^2 = \alpha_{12} A_T^1 + \beta_{12} + \omega_{12}, \tag{4.1}$$

where α_{12} and β_{12} are regression coefficients;

ω_{12} is the random component of the regression relation ("white noise").

For evaluation of closeness of calculated results obtained by models, we shall use regression coefficients α_{12} and β_{12} (characterizing a non-random component of the regression relation), *the residual square deviation,* that is, square deviation σ^{res}_{12} of ω_{12} (characterizing the magnitude of random component) and the correlation coefficient r_{12}.

Here numerical results for the first priority substance (PCB-153) only are presented. The corresponding results for substances of the second priority (PCB-28 and PCB-180) are presented in Annexes D and E.

4.1. Gas/particle partitioning

Reference data set. Calculation results for PCB-153 together with m_φ and σ_φ are presented in Table 4.1. For G-CIEMS calculations of gas-particle partitioning using molecular weight only (G-CIEMS 1) and using absorption scheme (G-CIEMS 2) were carried out.

Table 4.1. *Calculation results: fractions of particulate phase of PCB-153 calculated by models and statistical parameters used for evaluation ("reference" data set)*

Exp. No	T (°C)	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP	CliMoChem	SimpleBox*	m_φ	σ_φ
				1	2						
1	-12		0.81	0.96	0.78		0.88	0.11	0.98	0.75	0.32
2	-5		0.58	0.89	0.53		0.71	0.09	0.94	0.62	0.31
3	0		0.40	0.79	0.35		0.54	0.08	0.88	0.51	0.30
4	6		0.21	0.61	0.18		0.33	0.07	0.76	0.36	0.27
5	10		0.13	0.48	0.11		0.22	0.06	0.66	0.28	0.24
6	15		0.07	0.32	0.06		0.13	0.06	0.50	0.19	0.18
7	20		0.04	0.21	0.03		0.07	0.05	0.35	0.12	0.13
8	26		0.03	0.12	0.01		0.04	0.07		0.05	0.04
9	32		0.02	0.06	0.01		0.02	0.08		0.04	0.03

* - only 7 experiments for Simple Box

The plot of dependence of φ on T calculated by participating models is presented in Fig. 4.1. In addition, at the same plot the graph of average (between models) particulate fraction is given (red line). It is seen that practically all models (except CliMoChem) closely describe temperature dependence of particulate fraction. For the lower temperatures, values of fraction of particulate phase of PCB-153 calculated by CliMoChem are much lower than ones calculated by other participating models. Considering results of the first seven experiments, the highest results of this parameter are obtained by SimpleBox model.

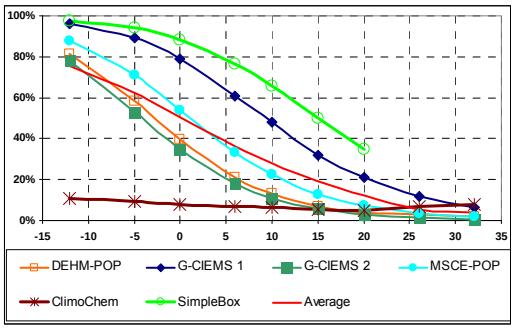


Fig. 4.1. *Calculation results of the participating models (gas-particle partitioning) obtained with reference data set*

We recall that the experiments differ mainly by ambient air temperature T (and some other parameters, see [*Shatalov et al.*, 2004]). For each temperature within the considered interval of temperatures (-12°C - 32°C), square deviation σ_φ between different model calculations (see last columns in Table 2.1) do not exceed the averaged value of particulate phase fractions. Since square deviation of particulate fraction is about 60% of the mean value, it can be concluded that most models closely describe the gas/particle partitioning process.

Calculated correlation coefficients between the results of participating models are given in Table 4.2. It is seen that these coefficients are high enough and vary from 0.7 to 1.

Table 4.2. *Correlation coefficients* r_{12}

	G-CIEMS 1	G-CIEMS 2	MSCE-POP	CliMoChem	SimpleBox*
DEHM-POP	0.92	1.00	0.99	0.88	0.89
G-CIEMS 1	–	0.91	0.97	0.70	0.99
G-CIEMS 2	–	–	0.98	0.88	0.87
MSCE-POP	–	–	–	0.83	0.93
CliMoChem	–	–	–	–	0.92

* - by 7 experiments only

The values of regression coefficients α and β calculated for all pairs of models are shown in Table 4.3.

Table 4.3. *Coefficients of regression dependence between the models (α / β)*

	G-CIEMS 1	G-CIEMS 2	MSCE-POP	CliMoChem	SimpleBox*
DEHM-POP	1.1 / 0.21	0.95 / –0.01	1.1 / 0.05	0.06 / 0.06	0.72 / 0.49
G-CIEMS 1	–	0.73 / –0.13	0. 90 / –0.12	0.04 /0.05	0.81 / 0.23
G-CIEMS 2	–	–	1.14 / 0.07	0.06 / 0.06	0.73 / 0.51
MSCE-POP	–	–	–	0.05 / 0.06	0.72 / 0.43
CliMoChem	–	–	–	–	10 / - 0.02

* - by 7 experiments only

The differences between the models are explained mainly by scaling coefficients α ranging from 0.05 to 10. For the most part of the models (not including CliMoChem results), α varies far less (from 0.72 to 1.14). Coefficients β are not very large for all pairs of models (lying in the range from – 0.13 to 0.51). This is a numerical expression of the fact that shapes of curves expressing temperature dependencies of φ (Fig. 4.1) are similar for these models.

To assess the reliability of comparative analysis given above calculations of pairwise residual square deviation σ were done (Table 4.4).

Table 4.4. *Residual square deviation,* σ^{res}_{12}

	G-CIEMS 1	G-CIEMS 2	MSCE-POP	CliMoChem	SimpleBox*
DEHM-POP	0.36	0.03	0.13	0.03	0.27
G-CIEMS 1	–	0.31	0.22	0.04	0.08
G-CIEMS 2	–	–	0.16	0.03	0.29
MSCE-POP	–	–	–	0.03	0.21
CliMoChem	–	–	–	–	0.23

* - by 7 experiments only

It is seen that the values of σ range from 0.03 to 0.36. This testifies the possibility of usage regression analysis for evaluation of the difference between model calculations.

Thus, all models describe temperature dependence of the fraction of particulate phase of PCB-153 in the atmosphere similarly. The difference of model results can be explained by difference in base values of K_{oa} or p_{ol} since the change of these values leads to scaling of calculated values of φ.

Own/altenative data set. Calculation results for PCB-153 together with m_φ and $\sigma_{.\varphi}$ are presented in Table 4.5. The data set used in calculations by each model is indicated in the first row.

Table 4.5. *Calculation results: fractions of particulate phase of PCB-153 calculated by models and statistical parameters used for evaluation own/alternative data set)*

Exp. No	T (°C)	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP	CliMoChem	SimpleBox*	m_φ	σ_φ
				1	2						
Data set		own	own		alt	own	own	own	alt		
1	-12	0.93	0.83		0.80	0.94	0.87	0.16	0.96	0.78	0.28
2	-5	0.75	0.62		0.57	0.85	0.70	0.10	0.90	0.64	0.27
3	0	0.68	0.44		0.39	0.73	0.52	0.07	0.84	0.52	0.26
4	6	0.46	0.26		0.22	0.53	0.32	0.04	0.72	0.36	0.22
5	10	0.33	0.17		0.14	0.39	0.21	0.03	0.63	0.27	0.20
6	15	0.19	0.095		0.08	0.24	0.12	0.023	0.50	0.18	0.16
7	20	0.11	0.053		0.04	0.14	0.065	0.017	0.38	0.12	0.12
8	26	0.086	0.042		0.03	0.12	0.032	0.018	0.36	0.06	0.04
9	32	0.057	0.029		0.02	0.078	0.016	0.017	0.30	0.04	0.03

The plot of dependence of φ on T calculated by participating models with "own or alternative" data set is presented in Fig. 4.2. In addition, at the same plot the graph of average (between models) particulate fraction is given (red line).

Calculated correlation coefficients between the results of participating models are given in Table 4.6. It is seen that these coefficients are high and exceed 0.9.

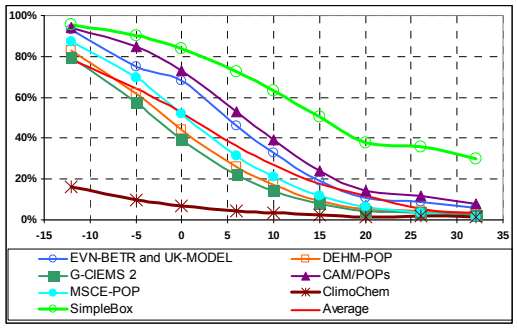


Fig. 4.2. *Calculation results of the participating models (gas-particle partitioning) obtained with "own/alternative" data set*

Table 4.6. *Correlation coefficients* r_{12}

	DEHM-POP	G-CIEMS 2	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox*
EVN-BETR and UK MODEL	0.98	0.97	1.00	0.99	0.93	0.98
DEHM-POP	–	1.00	0.97	1.00	0.98	0.93
G-CIEMS 2	–	–	0.96	0.99	0.99	0.91
CAN/POPs	–	–	–	0.98	0.91	0.99
MSCE-POP	–	–	–	–	0.97	0.95
CliMoChem	–	–	–	–	–	0.86

The values of regression coefficients α and β calculated for all pairs of models are shown in Table 4.7.

Table 4.7. *Coefficients of regression dependence between the models* (α / β)

	DEHM-POP	G-CIEMS 2	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox*
EVN-BETR and UK MODEL	0.87/ - 0.07	0.83/ - 0.07	1.02/0.04	0.96/ - 0.07	0.14/-0.004	0.76/0.32
DEHM-POP	–	0.96/ - 0.01	1.11/0/13	1.09/0.01	0.17/0.006	0.80/0.40
G-CIEMS 2	–	–	1.15/0.15	1.13/0.03	0.18/0.008	0.83/0.41
CAN/POPs	–	–	–	0.93/ - 0.10	0.14/ - 0.007	0/74/0.29
MSCE-POP	–	–	–	–	0.15/0.005	0.76/0.38
CliMoChem	–	–	–	–	–	4.34/0.39

The difference between the models' results is determined by scaling coefficient α, which varies within not very wide range (from 0.14 to 4.34). However, it is seen that this coefficients are very close to 1 for the most part of considered pairs of models (range from 0.8 to 1.3). Coefficients β are small enough compared with mean values of the considered parameter for the most part of model pairs also (lying in the range from – 0.10 to 0.41).

To assess the reliability of comparative analysis given above calculations of pairwise residual square deviation σ were done (Table 4.8).

Table 4.8. *Residual square deviation,* σ^{res}_{12}

	DEHM-POP	G-CIEMS 2	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox*
EVN-BETR and UK MODEL	0.167	0.188	0.075	0.125	0.050	0.137
DEHM-POP	–	0.031	0.237	0.069	0.027	0.260
G-CIEMS 2	–	–	0.272	0.102	0.022	0.284
CAN/POPs	–	–	–	0.161	0.058	0.100
MSCE-POP	–	–	–	–	0.036	0.214
CliMoChem	–	–	–	–	–	0.357

Values of σ vary within not very wide range also from 0.022 to 0.357.

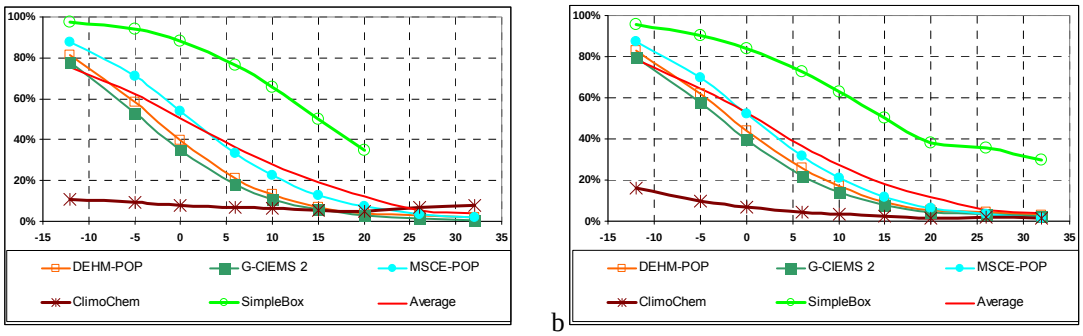
Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table 4.9.

Table 4.9. *Difference between calculations with two data sets*

Exp.No	*T* (°C)	DEHM-POP	G-CIEMS 2	MSCE-POP	CliMoChem	SimpleBox
1	-12	2%	2%	-1%	48%	-2%
2	-5	6%	8%	-2%	7%	-4%
3	0	11%	13%	-3%	-16%	-5%
4	6	23%	22%	-6%	-36%	-5%
5	10	29%	28%	-7%	-47%	-4%
6	15	35%	36%	-9%	-58%	1%
7	20	42%	41%	-10%	-66%	9%
8	26	47%	148%	-11%	-73%	
9	32	57%	236%	-12%	-79%	

This difference is visualized in Fig. 4.3.

It is seen that the difference in calculation of gas/particle partitioning caused by usage of “reference” and “own or alternative” data sets of pollutant properties is moderate. Large differences are characteristic of high temperatures where values of fractions of particulate phase are small (see Table 4.9).



a b

Fig. 4.3. *Calculation results of the participating models obtained with “reference” (a) and “own/alternative” (b) data sets (for models presented both calculations)*

Thus, for the considered interval of temperatures, most models’ results on particulate fractions of PCB-153 in the atmosphere obtained using different approaches to the description of gas/particle partitioning process are rather close to each other. Two approaches based on adsorption and absorption schemes are mainly used by the participating models.

4.2. Wet deposition

Reference data set. Calculation results for PCB-153 together with m and σ are presented in Tables 4. 4.10 and 4.11.

Table 4.10. *Calculation results: concentrations in precipitation (pg/L) ("reference" data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1		1070		805	320	1094	822	360
2	3		967		727	287	984	741	325
3	15		310		235	99	338	245	107
4	-1		1070		805	32	1094	750	496
5	3		967		727	29	984	677	448
6	15		310		235	10	338	223	149

Table 4.11. *Calculation results: wet deposition flux, ng/m^2/hour ("reference" data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1		1.07		0.80	0.32	1.09	0.82	0.36
2	3		0.97		0.73	0.29	0.98	0.74	0.32
3	15		0.31		0.24	0.099	0.34	0.24	0.11
4	-1		10.7		8.0	0.32	10.9	7.50	5.0
5	3		9.7		7.3	0.29	9.8	6.77	4.5
6	15		3.1		2.4	0.099	3.4	2.23	1.5

The comparison of calculated values of concentrations in precipitation is displayed in Fig. 4.4.

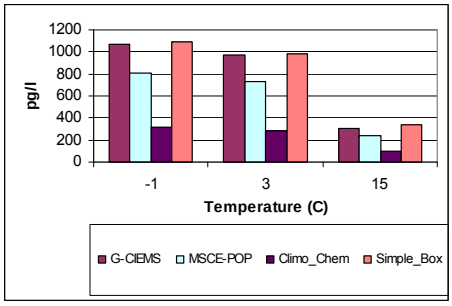


Fig. 4.4. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (reference data set)*

Pairwise regression analysis is performed only for calculated values of concentrations in precipitation since for wet deposition fluxes the results will be the same. Calculated correlation coefficients between the results of participating models are given in Table 4.12. It is seen that the correlation between models G-CIEMS, MSCE-POP and SimpleBox is very high.

Table 4.12. *Correlation coefficients r_{12}*

	MSCE-POP	CliMoChem	SimpleBox*
G-CIEMS	1.00	0.42	1.00
MSCE-POP	–	0.42	1.00
CliMoChem	–	–	0.42

The values of regression coefficients α and β calculated for all pairs of models are shown in Table 4.13.

Table 4.13. *Coefficients of regression dependence between the models (α / β)*

	MSCE-POP	CliMoChem	SimpleBox*
G-CIEMS	0.75/2.7	0.16/4.8	0.99/29.4
MSCE-POP	–	0.21/4.2	1.32/25.8
CliMoChem	–	–	1.12/660

Finally, pairwise residual square deviation σ are shown in Table 4.14. Again, these results confirm the closeness between the three above mentioned models.

Table 4.14. *Residual square deviation, σ^{res}_{12}*

	MSCE-POP	CliMoChem	SimpleBox*
G-CIEMS	1	281	8
MSCE-POP	–	281	7
CliMoChem	–	–	741

Own/alternative data set. Calculation results for PCB-153 together with *m* and σ are presented in Tables 4. 4.15 and 4.16.

Table 4.15. *Calculation results: concentrations in precipitation (pg/L) (own/alternative data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1	1870	1073	3042	808	312	1084	1365	964
2	3	1510	969	2130	729	282	978	1100	643
3	15	1480	311	3262	237	90	334	952	1238
4	-1	–	1073	–	808	31	1084	749	495
5	3	–	969	–	729	28	978	676	447
6	15	–	311	–	237	9	334	223	148

Table 4.16. *Calculation results: wet deposition flux, ng/m^2/hour (own/alternative data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1	1.870	1.073	3.042	0.808	0.312	1.084	1.365	0.964
2	3	1.510	0.969	2.130	0.729	0.282	0.978	1.100	0.643
3	15	1.480	0.311	3.262	0.237	0.090	0.334	0.952	1.238
4	-1	–	10.728	–	8.080	0.312	10.845	7.491	4.953
5	3	–	9.686	–	7.290	0.282	9.784	6.761	4.470
6	15	–	3.115	–	2.370	0.090	3.340	2.229	1.485

The comparison of calculated values of concentrations in precipitation is displayed in Fig. 4.5.

Pairwise regression analysis is performed only for calculated values of concentrations in precipitation since for wet deposition fluxes the results will be the same. Calculated correlation coefficients between the results of participating models are given in Table 4.17. The correlation between results obtained by models G-CIEMS, Climo-Chem, MSCE-POP and SimpleBox is very high.

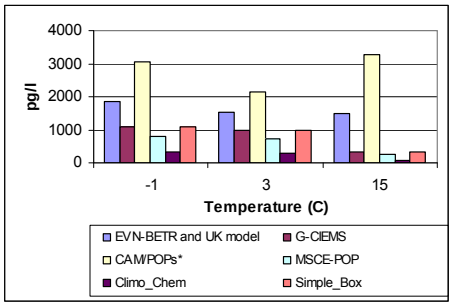


Fig. 4.5. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (own/alternative data set)*

Table 4.17. *Correlation coefficients r_{12}*

	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	0.66	0.27	0.66	0.66	0.66
G-CIEMS	–	-0.55	1.00	1.00	1.00
CAN/POPs	–	–	-0.55	-0.55	-0.55
MSCE-POP	–	–	–	1.00	1.00
CliMoChem	–	–	–	–	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table 4.18.

Table 4.18. *Coefficients of regression dependence between the models (α / β)*

	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	1.25/-1246	0.74/1616	0.94/-933	0.37/-363	1.24/-1208
G-CIEMS	–	-0.80/3438	0.75/3.5	0.29/-0.51	0.98/-1208
CAN/POPs	–	–	-0.28/1385	-0.11/538	-0.37/1837
MSCE-POP	–	–	–	0.39/-1.87	1.31/22.6
CliMoChem	–	–	–	–	3.38/29.0

Finally, pairwise residual square deviation σ are shown in Table 4.19.

Table 4.19. *Residual square deviation,* σ^{res}_{12}

	G-CIEMS	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	439	818	329	128	430
G-CIEMS	–	709	0.64	0.07	2.5
CAN/POPs	–	–	366	142	481
MSCE-POP	–	–	–	0.31	1.6
CliMoChem	–	–	–	–	2.7

Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table 4.20.

Table 4.20. *Difference between calculations with two data sets*

Exp. No	*T* (°C)	G-CIEMS	MSCE-POP	CliMoChem	SimpleBox
1	-1	0.3%	0.4%	-2.4%	-0.9%
2	3	0.2%	0.3%	-1.9%	-0.6%
3	15	0.5%	0.8%	-8.5%	-1.1%

These results are visualized in Fig. 4.6.

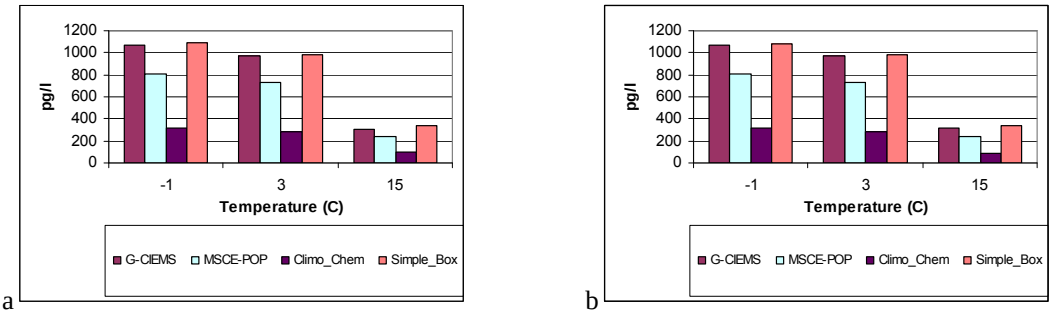


Fig. 4.6. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

Thus, the differences in wet deposition flux and concentrations in precipitation calculated by models are essential. However, square deviation does not exceed the mean value of these parameters averaged between the participating models both in the results obtained on the basis of "reference" and "own/alternative" data sets. The difference in calculation results on wet deposition caused by the usage of "reference" and "own /alternative" data sets of pollutant properties is negligible. This process needs further investigation.

4.3. Gaseous exchange between atmosphere and soil

Here we present numerical results of calculations of soil concentrations and net gaseous flux to soil obtained by the participating models and their analysis for PCB-153 with "reference" and "own/alternative" data sets.

EVN-BETR and UK model, SimpleBox, and DEHM-POP models have made calculations on these experiments using steady-state approach. CliMoChem and CAN/POPs models have obtained results under equilibrium assumption. For G-CIEMS model two versions of calculations are presented: for steady-state (G-CIEMS 1) and at equilibrium using interim calculation parameters of the model (G-CIEMS 2). For MSCE-POP model two calculation versions are presented as well: steady-state calculations (MSCE-POP 1) and calculations from dynamic model (MSCE-POP 2). In the latter case calculations for 60-year period with air concentration roughly simulating the trend of PCB air concentrations and additional two years with constant air concentrations equal to that specified in the input data. In this case soil concentrations in the end of calculation period were used for comparison. Fig. 4.7 illustrates air concentration trend used in calculations for Experiment 1.

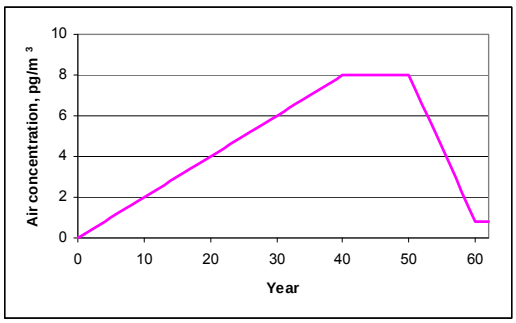


Fig. 4.7. *Air concentration trend used for calculations for MSCE-POP model (MSCE-POP 2) for Experiment 1*

In addition, the analysis of accumulation and clearance processes calculated by five models (CAN/POPs, ClimoChem, EVN-BETR and UK model, SimpleBox and MSCE-POP) is performed.

Reference data set. Calculation results for soil concentrations together with m and σ calculated with "reference" data set of PCB-153 properties are presented in Table 4.21. Net gaseous fluxes to soil of PCB-153 calculated by the models and statistical parameters used for its evaluation are given in Table 4.22.

Table 4.21. *Calculation results: soil concentrations of PCB-153 (ng/g) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAM/ POPs	MSCE-POP		CliMoChem	SimpleBox	m	σ
				1	2		1	2				
1	0.8	–	0.85	0.007	0.083	0.38	0.011	0.074	0.0004	0.0001	0.18	0.30
2	5.5	–	0.40	0.065	1.3	5.66	0.079	0.58	0.003	0.001	1.01	1.93
3	6.8	–	0.31	0.065	0.93	3.91	0.094	0.83	0.005	0.001	0.77	1.32
4	2.8	–	0.067	0.012	0.11	0.48	0.038	0.22	0.001	0.000	0.12	0.16

Table 4.22. *Calculation results: net gaseous flux to soil, of PCB-153 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox	m	σ
				1	2		1	2				
1	0.8			0.0004	0	$1.75 \cdot 10^{-13}$	0.03	0.02	0.01	0.07	0.03	0.03
2	5.5			0.002	0	$2.5 \cdot 10^{-12}$	0.24	0.21	0.10	0.49	0.21	0.19
3	6.8			0.003	0	$1.92 \cdot 10^{-12}$	0.28	0.20	0.12	0.61	0.24	0.23
4	2.8			0.001	0	$3.67 \cdot 10^{-13}$	0.10	0.03	0.05	0.25	0.09	0.10

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Pairwise regression analysis is performed only for values of soil concentrations and deposition fluxes calculated by models using steady state and dynamic approaches. In spite of the fact that numerical values of soil concentrations are highly different, the variations of the corresponding numerical values caused by change of environmental conditions between different experiments are similarly described by most of models. This can be seen from values of pairwise correlation coefficients (Table 4.23).

Table 4.23. *Correlation coefficients for soil concentrations of PCB-153 ("reference" data set)*

		G-CIEMS		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
		1	2		1	2		
DEHM-POP		-0.25	-0.17	-0.16	-0.47	-0.37	-0.38	-0.29
G-CIEMS	1		0.97	0.96	0.96	0.95	0.94	0.99
	2			1.00	0.88	0.83	0.82	0.93
CAN/POPs					0.87	0.82	0.80	0.92
MSCE-POP	1					0.98	0.98	0.98
	2						1.00	0.98
ClimoChem								0.97

Correlation coefficients for net gaseous flux are presented in Table 4.24.

Table 4.24. *Correlation coefficients for net gaseous flux to soil of PCB-153 ("reference" data set)*

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
G-CIEMS		0.91	0.76	0.94	0.94
MSCE-POP	1	–	0.96	1.00	1.00
	2	–	–	0.94	0.94
CliMoChem		–	–	–	1.00

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Tables 4.25 and 4.26, respectively.

Table 4.25. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-153 ("reference" data set)*

		G-CIEMS		CAN/POPs	MSCE-POP		ClimoChem	SimpleBox
		1	2		1	2		
DEHM-POP		-0.024/0.005	-0.316/0.74	-1.281/3.13	-0.054/0.08	-0.389/0.58	-0.002/0.003	-0.001/0.001
G-CIEMS	1	–	18.380/-0.08	78.239/-0.33	1.136/0.01	10.103/0.05	0.054/0.0003	0.021/0.00001
	2	–	–	4.283/-0.01	0.055/0.02	0.469/0.14	0.002/0.001	0.001/0.0002
CAN/POPs		–	–	–	0.013/0.02	0.108/0.14	0.001/0.001	0.0002/0.0002
MSCE-POP	1	–	–	–	–	8.882/-0.07	0.048/-0.0004	0.018/-0.0002
	2	–	–	–	–	–	0.005/-0.000001	0.002/-0.00003
ClimoChem		–	–	–	–	–	–	0.359/-0.00002

Table 4.26. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-153 ("reference" data set)*

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
G-CIEMS		118/-0.02	88/-0.02	51/-0.01	253/-0.03
MSCE-POP	1	–	0.85/-0.02	0.41/0.004	2.06/0.02
	2	–	–	0.44/0.02	2.19/0.10
CliMoChem		–	–	–	4.99/-0.001

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table 4.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-153 ("reference" data set)*

		G-CIEMS		CAN/POPs	MSCE-POP		ClimoChem	SimpleBox
		1	2		1	2		
DEHM-POP		0.05	1.04	4.47	0.06	0.55	0.003	0.001
G-CIEMS	1	–	0.27	1.25	0.02	0.19	0.001	0.0001
	2	–	–	0.10	0.03	0.33	0.002	0.0004
CAN/POPs		–	–	–	0.03	0.34	0.002	0.0005
MSCE-POP	1	–	–	–	–	0.11	0.001	0.0002
	2	–	–	–	–	–	0.0001	0.0003
ClimoChem		–	–	–	–	–	–	0.0003

Table 4.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-153 ("reference" data set)*

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
G-CIEMS		0.08	0.12	0.03	0.14
MSCE-POP	1	–	0.05	0.01	0.03
	2	–	–	0.03	0.14
CliMoChem		–	–	–	0.003

Own/alternative data set. Calculation results soil concentrations together with m and σ calculated with "own/alternative" data set of PCB-153 properties are presented in Table 4.29. Net gaseous fluxes to soil of PCB-153 calculated by the models and statistical parameters used for its evaluation are given in Table 4.30. Table 4.29 contains also the information of the data set used for calculations for each model.

Table 4.29. *Calculation results: soil concentrations of PCB-153 (ng/g) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAM/ POPs	MSCE-POP		CliMoChem	SimpleBox	m	σ
				1	2		1	2				
		own	own	alt		own	own		own	alt		
1	0.8	0.002	0.46	0.01	0.09	0.57	0.02	0.10	0.002	0.23	0.17	0.21
2	5.5	0.01	7.62	0.07	1.41	8.70	0.15	0.83	0.02	2.23	2.34	3.40
3	6.8	0.02	6.32	0.07	0.93	6.42	0.20	1.17	0.02	2.37	1.95	2.62
4	2.8	0.004	1.40	0.01	0.11	0.79	0.05	0.30	0.01	0.44	0.35	0.48

Table 4.30. *Calculation results: net gaseous flux to soil, of PCB-153 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*[*]

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox	m	σ
				1	2		1	2				
1	0.8	0.001	–	0.0004	0	$3.51 \cdot 10^{-13}$	0.030	0.009	0.014	0.003	0.010	0.011
2	5.5	0.006	–	0.002	0	$5.01 \cdot 10^{-12}$	0.229	0.157	0.097	0.202	0.115	0.097
3	6.8	0.008	–	0.003	0	$2.06 \cdot 10^{-12}$	0.254	0.082	0.120	0.094	0.093	0.092
4	2.8	0.003	–	0.001	0	$3.94 \cdot 10^{-13}$	0.077	-0.071	0.047	-0.061	-0.001	0.058

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Pairwise regression analysis is performed only for values of soil concentrations and deposition fluxes calculated by models using steady-state and dynamic approaches. In spite of the fact that numerical values of soil concentrations are highly different, the variations of the corresponding numerical values caused by change of environmental conditions between different experiments are similarly described by models. This can be seen from values of pairwise correlation coefficients (Table 4.31).

Table 4.31. *Correlation coefficients for soil concentrations of PCB-153 ("own/alternative" data set)*

		DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP		ClimoChem	SimpleBox
			1	2		1	2		
EVN-BETR and UK MODEL		0.93	0.98	0.86	0.90	1.00	1.00	1.00	0.99
DEHM-POP		–	0.99	0.98	0.99	0.90	0.90	0.91	0.98
G-CIEMS	1	–	–	0.95	0.97	0.95	0.95	0.96	1.00
	2	–	–	–	1.00	0.82	0.82	0.83	0.93
CAN/POPs		–	–	–	–	0.86	0.86	0.87	0.96
MSCE-POP	1	–	–	–	–	–	1.00	1.00	0.97
	2	–	–	–	–	–	–	1.00	0.97
ClimoChem		–	–	–	–	–	–	–	0.97

Correlation coefficients for net gaseous flux are presented in Table 4.32.

Table 4.32. *Correlation coefficients for net gaseous flux to soil of PCB-153 ("own/alternative" data set)*

		G-CIEMS 1	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.96	0.97	0.63	1.00	0.64
G-CIEMS 1		–	0.87	0.38	0.94	0.41
MSCE-POP	1	–	–	0.79	0.99	0.80
	2	–	–	–	0.68	0.99
CliMoChem		–	–	–	–	0.70

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Table 4.33 and 34, respectively.

Table 4.33. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-153 ("own/alternative" data set)*

		DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP		ClimoChem	SimpleBox
			1	2		1	2		
EVN-BETR and UK MODEL		440/ -0.19	4.15/ -0.002	74.1/ -0.06	486/ -0.46	11.3/ -0.001	64.4/ -0.01	1.23/ -0.0001	149/ -0.09
DEHM-POP		–	0.01/ 0.002	0.18/ -0.07	1.14/ -0.39	0.02/ 0.02	0.12/ 0.11	0.002/ 0.002	0.31/ 0.07
G-CIEMS	1	–	–	19.2/ -0.08	124/ -0.51	2.54/ 0.01	14.5/ 0.06	0.28/ 0.001	35.4/ -0.01
	2	–	–	–	6.26/0.14	0.11/ 0.04	0.61/ 0.21	0.01/ 0.004	1.64/0.27
CAN/POPs		–	–	–	–	0.02/ 0.03	0.10/ 0.18	0.002/0.003	0.27/ 0.21
MSCE-POP	1	–	–	–	–	–	5.71/ -0.0004	0.11/0.0001	12.9/ -0.04
	2	–	–	–	–	–	–	0.02/0.0001	2.26/ -0.04
ClimoChem		–	–	–	–	–	–	–	119/ -0.06

Table 4.34. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-153 ("own/alternative" data set)*

		G-CIEMS 1	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.29/0.0003	36.0/ -0.01	20.5/ -0.05	15.9/0.0001	24.6/ -0.05
G-CIEMS 1		–	108/ -0.02	41.9/ -0.02	50.0/ -0.01	52.1/ -0.02
MSCE-POP	1	–	–	0.69/ -0.06	0.43/0.01	0.83/ -0.06
	2	–	–	–	0.33/0.05	1.16/0.01
CliMoChem		–	–	–	–	1.67/ -0.06

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table 4.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-153 ("own/alternative" data set)*

		DEHM-POP	G-CIEMS		CAN/POPs	MSCE-POP		ClimoChem	SimpleBox
			1	2		1	2		
EVN-BETR and UK MODEL		2.18	0.01	0.57	3.10	0.01	0.07	0.001	0.33
DEHM-POP		–	0.01	0.21	0.82	0.06	0.36	0.01	0.40
G-CIEMS	1	–	–	0.35	1.63	0.04	0.25	0.004	0.10
	2	–	–	–	0.57	0.09	0.49	0.01	0.70
CAN/POPs		–	–	–	–	0.08	0.43	0.01	0.55
MSCE-POP	1	–	–	–	–	–	0.001	0.0004	0.49
	2	–	–	–	–	–	–	0.0005	0.50
ClimoChem		–	–	–	–	–	–	–	0.44

Table 4.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-153 ("own/alternative" data set)*

		G-CIEMS 1	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.0004	0.04	0.13	0.01	0.15
G-CIEMS 1		–	0.09	0.16	0.03	0.18
MSCE-POP	1	–	–	0.10	0.01	0.12
	2	–	–	–	0.06	0.03
CliMoChem		–	–	–	–	0.14

Comparison between two data sets. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table 4.29. The corresponding differences between calculated values of net flux to soil were not calculated since near the equilibrium small changes in pollutant properties can lead to essential changes of fluxes (in relative values).

Table 4.29. *Difference between calculations with two data sets*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	G-CIEMS		CAM/ POPs	MSCE-POP		CliMoChem	SimpleBox
				1	2		1	2		
1	0.8		-45.6%	0.0030%	10.2%	50.1%	61.5%	42.0%	453.8%	169141.1%
2	5.5		1807.1%	0.0010%	8.1%	53.8%	84.0%	44.2%	437.1%	170552.4%
3	6.8		1933.5%	-0.0001%	-0.4%	64.3%	116.8%	40.8%	389.0%	159125.2%
4	2.8		1999.1%	-0.0032%	-3.7%	66.3%	36.8%	35.8%	349.4%	148384.2%

Models describe gaseous flux between atmosphere and soil more closely than soil concentrations. The differences in concentrations are lower with "reference" data set than those with "own/alternative" data. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties ("reference" and "own/alternative") is considerable for most models. Model descriptions of air/soil exchange and their parameterizations need further consideration.

Accumulation/clearance dynamics of PCBs in soil. The aim of this subsection is to analyze model descriptions of long-term processes of accumulation of selected PCB congeners in soil and clearance of soil compartment at emission termination. To do this, modelling of air/soil exchange with constant air concentration for a sufficiently long period were carried out by CAN/POPs, CliMoChem, EVN-BETR and UK model, MSCE-POP, and SimpleBox models both using "reference" and "own or alternative" data sets of PCB properties.

The period under simulation was split into two periods. During the first period (accumulation) air concentrations are kept at the level defined in the corresponding input data set and initial data are assumed to be zero. Soil concentrations obtained in the end of the first period were used as initial data for the second period (clearance). During this period air concentrations are set to zero.

Fig. 4.8 shows the results of the experiment obtained by CAN/POPs, MSCE-POP, EVN-BETR and UK model, and SimpleBox models, respectively with “reference” data set. Maximum values presented on the plots correspond to the soil concentrations achieved at steady state after rather long period of accumulation.

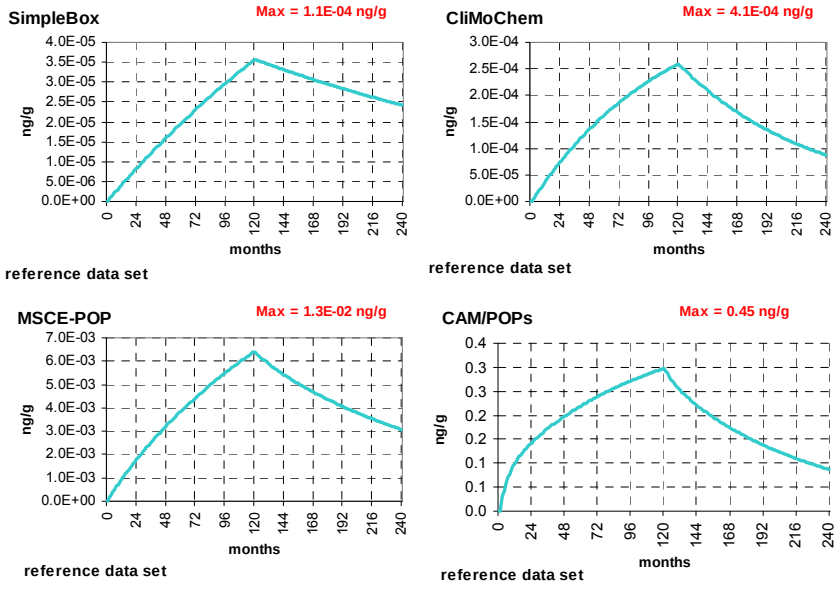


Fig. 4.8. *Long-term trends of accumulation and clearance obtained by participating models (“reference” data set)*

The results obtained with the use of “own/alternative” data sets are presented in Fig. 4.9.

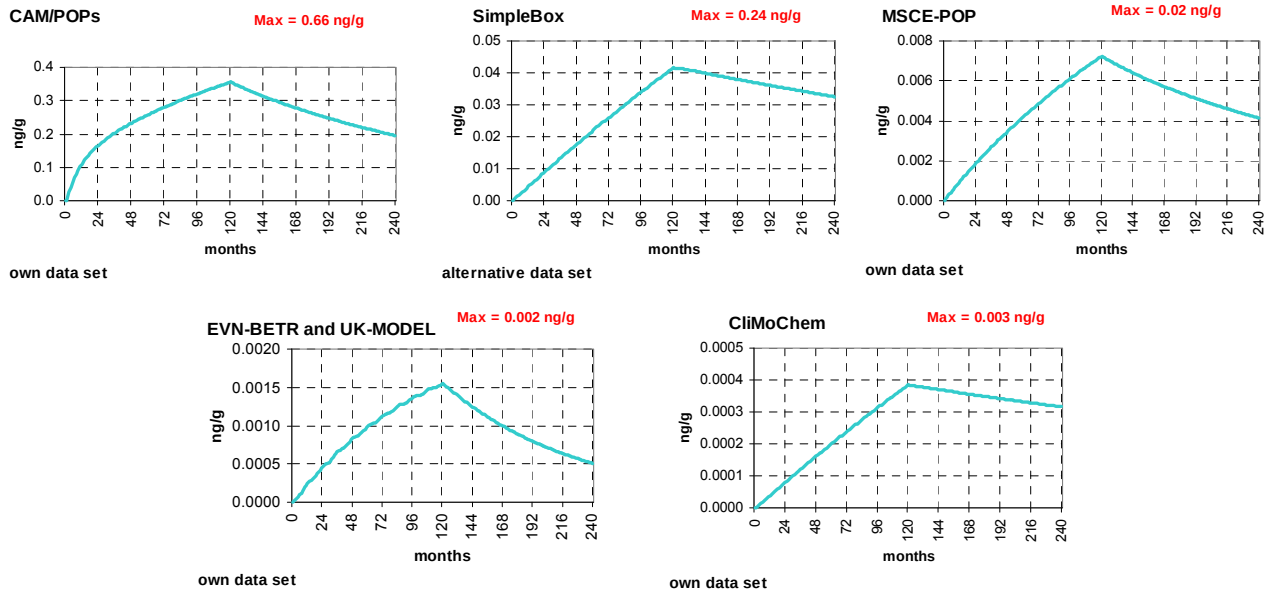


Fig. 4.9. *Long-term trends of accumulation and clearance obtained by participating models (“own/alternative” data set)*

For the analysis of calculated trends of soil concentrations at both accumulation and clearance stages bi-exponential approximation of accumulation and clearance is performed. This approximation has the form:

$$C_{soil} = C_1(1-e^{-\lambda_1 t}) + C_2(1-e^{-\lambda_2 t}), \quad \lambda_1 > \lambda_2 \qquad \text{(accumulation stage)}$$

$$C_{soil} = C_1 e^{-\lambda_1 t} + C_2 e^{-\lambda_2 t}, \quad \lambda_1 > \lambda_2 \qquad \text{(clearance stage)}$$

where t is the time, months;

λ_1 and λ_2 are exchange rate constants, month^{-1};

C_1 and C_2 are constants determining shares of concentrations involved in fast/slow process.

Such form of the dependence of soil concentrations on time is characteristic of a process with two characteristic times of exchange: fast exchange characteristic time $T_{1/2}^1 = \ln(2)/\lambda_1$ and slow exchange characteristic time $T_{1/2}^2 = \ln(2)/\lambda_2$. Calculations show that bi-exponential approximation well explains the trends of soil concentrations both at accumulation and clearance phases.

The values of characteristic times obtained by the approximation are shown in Table 4.30.

Table 4.30. *Parameters of multi-exponential approximation*

	CAN/POPs		ClimoChem		EVN-BETR and UK model		MSCE-POP		SimpleBox	
	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast
"Reference" data set										
Accumulation phase	8.3	0.58	6.9	6.9	–	–	11	1.5	18	18
Clearance phase	7.1	2.3	6.3	6.3	–	–	11	2.9	18	18
"Own/alternative" data set										
Accumulation phase	13	0.75	51	51	6.6	6.6	18	2.9	36	36
Clearance phase	14	5.8	35	35	6.2	6.0	18	5.8	28	28

As a result of this analysis all models can be split into two groups. The first group form models for which values of $T_{1/2}$ for two exponentials are close to each other (single-exponential models): Climo-Chem, EVN-BETR and UK MODEL, and SimpleBox. The second group contains models for which values of $T_{1/2}$ for slow and fast exponentials differ considerably (two-exponential models): CAN/POPs and MSCE-POP. The values of $T_{1/2}$ (for slow exponent) vary from 7 to 50 years.

The difference between results obtained with "reference" and "own/alternative" data sets (for those models which have performed both calculations) is illustrated by Fig. 4.10.

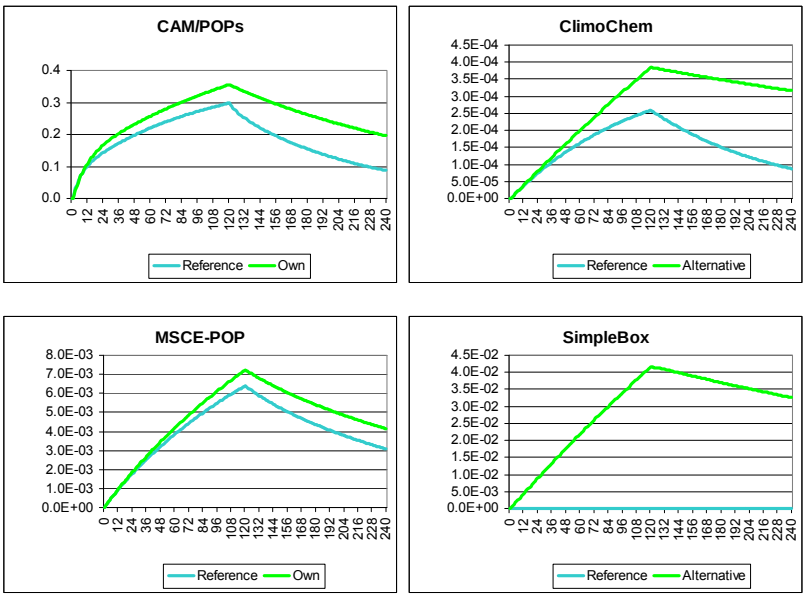


Fig. 4.10. *Difference in long-term trends due to usage of different sets of PCB properties*

4.4. Gaseous exchange between atmosphere and water

Reference data set. Calculation results for water concentrations together with m and σ calculated with "reference" data set of PCB-153 properties are presented in Table 4.31.

Table 4.31. *Calculation results: water concentrations of PCB-153 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP	m	σ
1	–	8.40	6.86	11.01	30.15	20.30	6.70	13.90	9.44
2	–	2.40	1.27	2.62	7.44	3.09	1.24	3.01	2.30
3	–	4.80	3.19	2.39	5.92	5.88	3.02	4.20	1.54
4	–	3.00	2.88	10.78	32.47	6.14	2.85	9.69	11.58

Fig. 4.11 displays the result on water concentrations of PCB-153 calculated by the participating models with the use of "reference" data set.

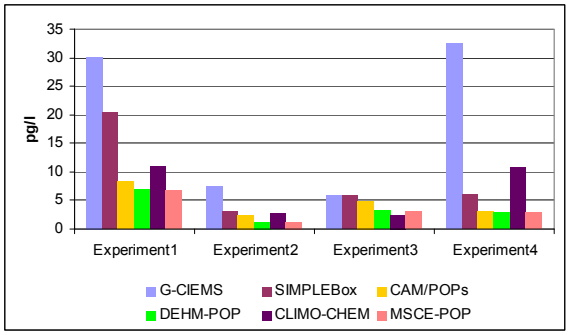


Fig. 4.11. *Calculation results of the participating models (water concentrations) obtained with "reference" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-153 calculated by the participating models are given in Table 4.32.

Table 4.32. *Calculation results: fluxes of PCB-153 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP	m	σ
Gaseous flux to water									
1	–	–	–	0.98	1.02	4.59	2.21	2.20	1.69
2	–	–	–	0.25	0.25	0.74	0.53	0.44	0.24
3	–	–	–	0.18	0.20	1.12	0.42	0.48	0.44
4	–	–	–	1.37	1.10	1.95	2.17	1.65	0.50
Gaseous flux from water									
1	–	0.39	–	0.31	0.0019	0.35	2.16	0.64	0.86
2	–	5.31	–	0.10	0.0006	0.05	0.52	1.20	2.31
3	–	0.21	–	0.03	0.0002	0.06	0.39	0.14	0.16
4	–	0.03	–	0.72	0.0053	0.10	2.15	0.60	0.91
Net gaseous flux									
1	–	0.39	–	0.67	1.02	4.24	0.05	1.27	1.69
2	–	5.31	–	0.16	0.25	0.69	0.01	1.29	2.27
3	–	0.21	–	0.14	0.20	1.07	0.02	0.33	0.42
4	–	0.03	–	0.65	1.10	1.85	0.02	0.73	0.77

Below we present parwise comparison of modelling results for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table 4.32.

Table 4.32. *Correlation coefficients for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
CAN/POPs	0.97	0.46	0.38	0.95	0.97
DEHM-POP	–	0.65	0.58	0.98	1.00
CliMoChem	–	–	1.00	0.66	0.67
G-CIEMS	–	–	–	0.59	0.60
SimpleBox	–	–	–	–	0.98

Correlation coefficients for net gaseous flux are demonstrated in Table 4.33.

Table 4.33. *Correlation coefficients for net gaseous flux ("reference" data set)*

	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
CAN/POPs	-0.56	-0.54	-0.49	-0.60
CliMoChem	–	1.00	0.79	0.67
G-CIEMS	–	–	0.74	0.60
SimpleBox	–	–	–	0.97

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4.34 and s.35, respectively.

Table 4.34. *Coefficients of regression dependence between the models (α / β) for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
CAN/POPs	0.85/ -0.40	0.82/2.88	2.00/9.72	2.74/-3.89	0.83/-0.39
DEHM-POP	–	1.34/1.95	3.52/6.50	1.06/-2.59	0.98/ -0.01
CliMoChem	–	–	2.93/ -0.64	1.06/1.76	0.32/1.32
G-CIEMS	–	–	–	0.32/2.73	0.10/1.61
SimpleBox	–	–	–	–	0.29/0.86

Table 4.35. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("reference" data set)*

	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
CAN/POPs	-0.06/0.50	-0.10/0.80	-0.31/2.42	-0.004/0.03
CliMoChem	–	1.64/ -0.02	4.31/0.22	0.04/0.01
G-CIEMS	–	–	2.43/0.40	0.02/0.01
SimpleBox	–	–	–	0.01/0.01

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.36 and 4.37.

Table 4.36. *Residual square deviation, σ for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
CAN/POPs	0.96	7.47	22.88	4.03	1.02
DEHM-POP	–	6.37	20.08	2.60	0.10
CliMoChem	–	–	2.19	10.08	2.97
G-CIEMS	–	–	–	10.83	3.20
SimpleBox	–	–	–		0.71

Table 4.37. *Residual square deviation, σ for net gaseous flux ("reference" data set)*

	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
CAN/POPs	0.42	0.70	2.39	0.02
CliMoChem	–	0.07	1.67	0.02
G-CIEMS	–	–	1.86	0.02
SimpleBox	–	–	–	0.01

Own/alternative data set. Calculation results for water concentrations together with *m* and σ calculated with "own/alternative" data set of PCB-153 properties are presented in Table 4.38. Here data set of PCB-153 properties used for calculations by each model is indicated (second row).

Table 4.38*. Calculation results: water concentrations of PCB-153 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP	*m*	σ
Set	own	own	own	own	alt	alt	own		
1	5.56	8.40	7.10	8.50	30.39	73.83	8.78	20.37	25.07
2	0.98	2.40	1.25	1.51	7.81	13.20	1.59	4.11	4.66
3	3.11	4.80	3.74	4.10	6.13	35.94	4.26	8.87	11.97
4	2.10	3.00	2.51	3.00	33.69	29.31	3.40	11.00	14.07

Fig. 4.12 displays the result on water concentrations of PCB-153 calculated by the participating models with the use of "own / alternative" data set.

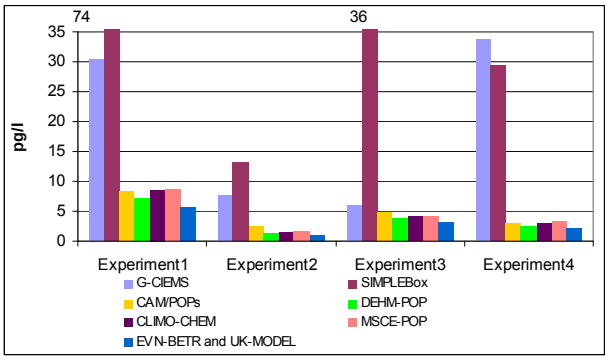


Fig. 4.12. *Calculation results of the participating models (water concentrations) obtained with "own/alternative" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-153 calculated by the models are given in Table 4.39.

Table 4.39*. Calculation results: fluxes of PCB-153 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to water									
1	2.60	2.08	–	0.86	1.02	4.37	2.27	2.20	1.27
2	0.56	0.61	–	0.21	0.26	0.71	0.55	0.48	0.20
3	0.66	0.40	–	0.17	0.02	1.08	0.42	0.46	0.37
4	1.71	1.49	–	0.86	1.12	1.99	2.33	1.59	0.54
Gaseous flux from water									
1	0.13	–	–	0.73	0.0017	2.71	2.24	1.16	1.24
2	0.03	–	–	0.18	0.0007	0.39	0.55	0.23	0.24
3	0.03	–	–	0.13	0.0000	0.84	0.41	0.28	0.35
4	0.14	–	–	0.78	0.0061	0.90	2.32	0.83	0.92
Net gaseous flux									
1	2.47	2.08	–	0.12	1.02	1.66	0.03	1.23	1.01
2	0.53	0.61	–	0.03	0.26	0.31	0.01	0.29	0.25
3	0.64	0.40	–	0.04	0.02	0.23	0.01	0.22	0.25
4	1.57	1.49	–	0.08	1.12	1.10	0.01	0.90	0.68

The parwise comparison of modelling results is done for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table 4.40.

Table 4.40. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.99	1.00	0.99	0.44	0.99	0.99
CAN/POPs	–	0.99	0.99	0.35	0.98	0.98
DEHM-POP	–	–	1.00	0.44	1.00	1.00
CliMoChem	–	–	–	0.48	1.00	1.00
G-CIEMS	–	–	–	–	0.52	0.51
SimpleBox	–	–	–	–	–	1.00

Correlation coefficients for net gaseous flux are demonstrated in Table 4.41.

Table 4.41. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.98	1.00	0.86	0.99	0.85
CAN/POPs	–	0.97	0.93	1.00	0.75
CliMoChem	–	–	0.86	0.99	0.86
G-CIEMS	–	–	–	0.91	0.47
SimpleBox	–	–	–	–	0.79

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4. 4.42 and 4.43, respectively.

Table 4.42. *Coefficients of regression dependence between the models (α / β) for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	1.37/0.63	1.29/ -0.13	1.53/ -0.22	3.25/9.94	13.1/ -0.30	1.56/ -0.06
CAN/POPs	–	0.93/-0.65	1.10/-0.85	1.91/10.64	9.34/-5.34	1.11/-0.67
DEHM-POP	–	–	1.19/ -0.08	2.54/10.2	10.2/0.96	1.21/0.09
CliMoChem	–	–	–	2. 30/ 9.67	8.53/1.59	1.02/0.16
G-CIEMS	–	–	–	–	0.92/20.1	0.11/2.41
SimpleBox	–	–	–	–	–	0.12/ -0.02

Table 4.43. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.84/0.05	0.05/0.004	0.52/ -0.07	0.74/ -0.14	0.01/0.003
CAN/POPs	–	0.06/0.003	0.65/ -0.14	0.87/ -0.17	0.01/0.004
CliMoChem	–	–	10.4/ -0.10	14.9/ -0.19	0.2/0.002
G-CIEMS	–	–	–	1.13/0.14	0.01/0.01
SimpleBox	–	–	–	–	0.01/0.01

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.44 and 4.45.

Table 4.44. *Residual square deviation, σ for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.69	0.20	0.54	22.67	5.17	0.60
CAN/POPs	–	0.50	0.70	23.57	8.49	0.94
DEHM-POP	–	–	0.33	22.65	4.29	0.47
CliMoChem	–	–	–	22.17	2.63	0.24
G-CIEMS	–	–	–	–	37.96	4.55
SimpleBox	–	–	–	–	–	0.08

Table 4.45. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.26	0.005	0.48	0.14	0.01
CAN/POPs	–	0.02	0.36	0.08	0.01
CliMoChem	–	–	0.48	0.18	0.01
G-CIEMS	–	–	–	0.50	0.02
SimpleBox	–	–	–	–	0.01

Comparison between two data sets. The difference between calculated values of concentrations in water and gaseous fluxes to/from water obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.46 and 4.47, respectively.

Table 4.46. *Difference between calculations with two data sets (water concentrations)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
1	–	0.00%	3.5%	-23%	0.78%	263%	31%
2	–	0.00%	-1.2%	-42%	4.9%	328%	28%
3	–	0.00%	17%	72%	3.7%	511%	41%
4	–	0.00%	-13%	-72%	3.8%	378%	20%

This difference is visualized in Fig. 4.13.

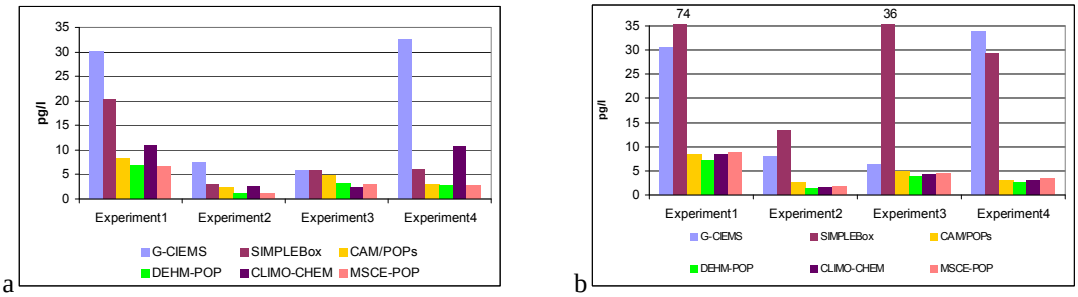


Fig. 4.13. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

Table 4.47. *Difference between calculations with two data sets (net gaseous flux)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	G-CIEMS	SimpleBox	MSCE-POP
1	–	430%	–	-81%	0.01%	-61%	-40%
2	–	-88%	–	-83%	2.8%	-55%	-42%
3	–	90%	–	-74%	-89%	-78%	-35%
4	–	5110%	–	-87%	1.66%	-41%	-45%

4.5. Gaseous exchange between atmosphere and vegetation

Reference data set. Calculation results for concentrations in vegetation together with m and σ calculated with "reference" data set of PCB-153 properties are presented in Table 4.48. Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-153 calculated by the models are given in Table 4.49.

***Table 4.48**. Calculation results: concentrations of PCB-153 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
1	–	6.4	0.40	0.10	2.31	2.91
2	–	8.7	0.48	0.23	3.15	3.95
3	–	2.5	0.16	0.05	0.89	1.12
4	–	8.6	0.53	0.21	3.10	3.87

***Table 4.49**. Calculation results: fluxes of PCB-153 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to vegetation						
1	–	0.35	0.52	0.33	0.40	0.08
2	–	1.12	1.64	0.75	1.17	0.37
3	–	0.18	0.26	0.16	0.20	0.04
4	–	0.83	1.21	0.68	0.90	0.22
Gaseous flux from vegetation						
1	–	0.35	0.12	0.0009	0.16	0.15
2	–	1.12	0.82	0.012	0.65	0.47
3	–	0.18	0.08	0.0008	0.09	0.07
4	–	0.83	0.50	0.0064	0.45	0.34
Net gaseous flux						
1	–	0	0.40	0.33	0.24	0.17
2	–	0	0.82	0.74	0.52	0.37
3	–	0	0.18	0.16	0.11	0.08
4	–	0	0.71	0.67	0.46	0.32

Below we present pairwise comparison of modelling results for concentrations in vegetation and net gaseous flux. Correlation coefficients for concentrations in vegetation are shown in Table 4.50.

***Table 4.50.** Correlation coefficients for concentrations in vegetation ("reference" data set)*

	SimpleBox	MSCE-POP
CliMoChem	0.99	0.94
SimpleBox	–	0.90

The results show that differences between concentrations are described similarly by all three models. Calculated absolute values of concentrations in vegetation differ essentially.

Correlation coefficients for net gaseous flux between SimpleBox and MSCE-POP models equals 0.997. Correlations with ClimoChem models have not been calculated since gaseous flux calculated by this model equals zero.

Values of regression coefficients α and β for concentrations in vegetation calculated for all pairs of models are given in Table 4.51.

***Table 4.51.** Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("reference" data set)*

	SimpleBox	MSCE-POP
CliMoChem	17/ -0.33	32/1.80
SimpleBox	–	0.47/ -0.04

Regression coefficients α and β between SimpleBox and MSCE-POP models equal 0.94 and –0.02, respectively. This testifies good agreement of net flux calculated by these two models.

Finally, values of residual square deviation for concentrations in vegetation are collected in Table 4.52.

Table 4.52. *Residual square deviation, σ for concentrations in vegetation ("reference" data set)*

	SimpleBox	MSCE-POP
CliMoChem	0.75	1.66
SimpleBox	–	0.06

Residual square deviation for regression dependence between net gaseous flux calculated by SimpleBox MSCE-POP models equals 0.04.

Own/alternative data set. Calculation results for concentrations in vegetation together with *m* and σ calculated with "own/alternative" data set of PCB-153 properties are presented in Table 4.53. Here data set of PCB-153 properties used for calculations by each model is indicated (second row). Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-153 calculated by the models are given in Table 4.54.

Table 4.53*. Calculation results: concentrations of PCB-153 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own	own	alt	own		
1	0.22	0.42	0.40	0.10	0.29	0.13
2	0.05	0.54	0.45	0.27	0.33	0.19
3	0.05	0.17	0.15	0.05	0.11	0.05
4	0.09	0.60	0.48	0.22	0.35	0.20

Table 4.54*. Calculation results: fluxes of PCB-153 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to vegetation						
1	4.8	0.35	0.52	0.34	1.51	1.93
2	16.5	1.12	1.64	0.88	5.04	6.62
3	2.7	0.18	0.26	0.16	0.83	1.08
4	0.12	0.83	1.21	0.72	0.72	0.39
Gaseous flux from vegetation						
1	4.92	0.05	0.26	0.0006	1.31	2.09
2	16.5	0.72	1.26	0.0097	4.63	6.88
3	2.72	0.04	0.15	0.0006	0.73	1.15
4	0.12	0.35	0.83	0.0047	0.32	0.32
Net gaseous flux						
1	-0.07	0.31	0.26	0.33	0.21	0.16
2	-0.03	0.40	0.38	0.87	0.40	0.32
3	-0.02	0.14	0.11	0.16	0.10	0.07
4	-0.0004	0.48	0.38	0.72	0.40	0.26

The parwise comparison of modelling results is done for concentrations in vegetation and net gaseous flux to vegetation. Correlation coefficients for concentrations in vegetation are shown in Table 4.55.

Table 4.55. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.08	0.25	-0.32
CliMoChem	–	0.98	0.89
SimpleBox	–	–	0.82

Correlation coefficients for net gaseous flux are demonstrated in Table 4.56.

Table 4.56. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.26	0.19	0.34
CliMoChem	–	0.98	0.88
SimpleBox	–	–	0.94

Values of regression coefficients α and β for concentrations in vegetation and net gaseous flux calculated for all pairs of models are given in Tables 4.57 and 4.58, respectively.

Table 4.57. *Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.19/ 0.42	0.48/ 0.32	-0.41/ 0.20
CliMoChem	–	1.23/ -0.02	1.65/0.17
SimpleBox	–	–	0.56/ -0.04

Table 4.58. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	1.32/0.37	0.86/ 0.31	3.81/0.64
CliMoChem	–	1.13/ 0.01	0.40/0.12
SimpleBox	–	–	2.39/ -0.15

Finally, values of residual square deviation for concentrations in vegetation and net gaseous flux are collected in Tables 4.59 and 4.60.

Table 4.59. *Residual square deviation, σ for concentrations in vegetation ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.33	0.25	0.17
CliMoChem	–	0.06	0.15
SimpleBox	–	–	0.10

Table 4.60. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.25	0.22	0.53
CliMoChem	–	0.05	0.12
SimpleBox	–	–	0.19

Comparison between two data sets. The difference between calculated values of water concentrations and net gaseous flux obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.61 – 4.64.

Table 4.61. *Difference between calculations with two data sets (concentrations in vegetation)*

N	CliMoChem	SimpleBox	MSCE-POP
1	-93%	-0.24%	1.30%
2	-94%	-7.6%	18.06%
3	-93%	-7.9%	3.11%
4	-93%	-9.9%	7.92%

Table 4.62. *Difference between calculations with two data sets (gaseous flux to vegetation)*

N	CliMoChem	SimpleBox	MSCE-POP
1	0%	0%	1.2%
2	0%	0%	18%
3	0%	0%	2.9%
4	0%	0%	6.9%

Table 4.63. *Difference between calculations with two data sets (gaseous flux from vegetation)*

N	CliMoChem	SimpleBox	MSCE-POP
1	-87%	120%	-32%
2	-36%	54%	-16%
3	-76%	86%	-32%
4	-58%	65%	-28%

Table 4.64. *Difference between calculations with two data sets (net gaseous flux)*[*]

N	SimpleBox	MSCE-POP
1	-36%	1.3%
2	-54%	18%
3	-39%	3.1%
4	-46%	7.9%

* The difference between values of net gaseous flux calculated by ClimoChem model is not calculated because for "reference" data set this flux is reported to be zero

Thus, according to the comparison of the results presented above, it can be concluded that:

- -Most models describe similarly gas/particle partitioning. The results obtained with "own" set of pollutant-related data agree better between models than those based on "reference" data set. The difference in calculation of gas/particle partitioning caused by usage of "reference" and "own or alternative" data set of pollutant properties is moderate. Large differences are characteristic of high temperatures where values of fractions of particulate phase are small. The results obtained with "own or alternative" set of pollutant-related data agree better between models.
- The differences in absolute values of wet deposition flux and concentrations in precipitation calculated by models are essential. However, square deviation does not exceed the mean value of these parameters averaged between the participating models both in the results obtained on the basis of "reference" and "own/alternative" data sets. The difference in calculation results on wet deposition caused by the usage of "reference" and "own /alternative" data sets of pollutant properties is negligible. This process needs further investigation.
- Models describe gaseous flux between atmosphere and soil more closely than soil concentrations. The differences in concentrations are lower with "reference" data set than those with "own/alternative" data. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties ("reference" and "own/alternative") is considerable for most models. Model descriptions of air/soil exchange and their parameterizations need further consideration.
- In general, most models closely describe processes of gaseous exchange between the atmosphere and water. The difference between calculated values of water concentrations and net gaseous flux from/to water obtained with two data sets of pollutant properties ("reference" and "own/alternative") is essential for some models. The same applies to the description of gaseous exchange between atmosphere and vegetation.

CONCLUSIONS

This report contains the main outcome of Stage II of the POP model intercomparison study. The following models participated in this stage: ADEPT, CAN/POPs, CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, SimpleBox, and MSCE-POP. The comparison of computed values of POP mass contained and degraded in the main environmental compartments (atmosphere, soil, water and vegetation), inflow and outflow for the specified domain, intermedia transport and spatial distribution of deposition and concentration fields in different environmental compartments is presented. Results of the sensitivity study with respect to physical-chemical parameter values used are presented. The comparison of model results on POP depositions and concentrations in the atmosphere with monitoring data is also given. In addition, the results on the sensitivity study with respect to physical-chemical parameter values used by the participating models in the description of gas/particles partitioning, wet deposition and gaseous exchange between the atmosphere and soil, water and vegetation are also considered.

The main body of this report provides a comparison of results of Stage II computational experiments for PCB-153 (first priority). The corresponding results for substances of the second priority (PCB-28 and PCB-180) are included in Annexes B, C, D and E. A preliminary analysis of the presented comparison is made for PCB-153 only.

A preliminary analysis of comparison of results for PCB-153 obtained by the participating models within Stage II shows the following:

- Most participating models provide reasonable agreement in description of mass distribution between the main environmental media. Thus, it can be concluded that:
    - The difference between the results of participating models on absolute values of PCB-153 mass contained in all considered layers of the atmosphere and soil, water and vegetation calculated on the basis of zero initial conditions (both for “reference” and “own/alternative” physical-chemical data sets) is considerably lower than that in results obtained on the basis of initial conditions. For the latter the values of PCB-153 mass contained in all considered layers of the atmosphere (except for 1 km results in “reference” data set) and 10 cm soil layer obtained by most models on the basis of both physical-chemical data sets are rather close. The difference in values of PCB-153 mass accumulated in 5cm layer of soil, 200m water layer and vegetation calculated with the use of initial conditions is more considerable than that in results obtained for the atmosphere.
    - According to the results presented by most models, PCB-153 is mainly accumulated in soil. PCB fractions in all other compartments are essentially lower and depend on type of calculations performed. The variability between PCB fractions in other environmental compartments is higher.
    - For most participating models the comparison of absolute and relative values of PCB-153 mass in the environmental media calculated with two different data sets show relatively weak sensitivity of mass balance values with respect to variations of pollutant-related parameters. Only in some cases the differences are essential.
- Model estimates of PCB-153 masses degraded in the main environmental media agree well for most models. In particular, it was noted that:
    - In calculations based on “reference” and “own/alternative” physical-chemical data sets most participating models provide rather close absolute values of PCB-153 mass degraded in the atmosphere. The difference in calculated absolute values of PCB-153 mass degraded in soil

and water is considerably higher. The limited number of models provided results on PCB-153 mass degraded in the vegetation compartment.

- Noticeable seasonal variations in computed absolute values are mostly characteristic of models that use temperature dependent degradation rates.
- The comparison of masses degraded in main environmental media calculated with “reference” and “own/alternative” data sets show that almost all models use higher degradation rates in the atmosphere in their “own or alternative” set of parameters compared with that in “reference” data set. Therefore the annual values of calculation results on PCB-153 masses degraded in the atmosphere obtained with the use of “own or alternative data sets” noticeably exceed those obtained with “reference data set”.
- Degradation rates in soil and water used by models are lower than that given in “reference” data set. Therefore, for all models’ results, the values of PCB-153 masses degraded in these media obtained with the use of “own or alternative data sets” are less than those obtained with “reference” data set.
- Analysis of relative fractions of PCB-153 mass degraded in the main environmental media that are ratios of the degraded mass and the mass contained in the considered compartment (taking into account also degraded mass) also show that most models closely describe distribution of PCB-153 mass in the environment due to degradation in the atmosphere and soil and water.

- Most models closely describe transport outside the calculation domain. Thus, it was revealed that:
  - According to the data presented for both “reference” and “own/alternative” data sets, in ADEPT, CAN/POPs and MSCE-POP model results the atmosphere is the main media of PCB-153 outside transport. Calculated fractions of overall outside transport through atmosphere considerably exceed those for other media in results of CliMoChem, G-CIEMS, and SimpleBox 3.0 and 3.12 (zero initial conditions) models. Results of SimpleBoxs 3.0 and 3.12 based on historical emissions are characterized by higher annual transport in the marine environment than in the atmosphere.
  - The most considerable contribution to the outside transport of PCB-153 due to the other considered media (sediment, soil and vegetation) than ocean and atmosphere is observed in the results of SimpleBox 3.0 model made on the basis of initial conditions.
- All model provide reasonable agreement in description of intermedia mass flows and concentrations in the main environmental media. Thus, it was obtained that:
  - Air concentrations as the most important output of the participating models are in good agreement for all models’ results. Several models predicted values of PCB-153 concentrations in the atmosphere at its interface with different underlying surfaces taking into account types of these surfaces.
  - The most part of participating models predicted close values of PCB-153 concentrations in soil, water and vegetation. However, variability of calculated concentrations in the environmental media other than the atmosphere is higher than that for the atmosphere. According to the results obtained within Stage II calculations, the bulk of overall PCB content in the environment is accumulated in soil. In this connection, it can be noted that the difference between the maximum and minimum values of calculated soil concentrations is higher than that for air concentrations but considerably less than that for the rest of media. Close absolute values of soil concentrations are characteristic of most models’ results.

- Most participating models provided reasonable agreement in description of net intermedia mass flows directed from the atmosphere to soil and to water. The scattering in results on net intermedia mass flows directed from the atmosphere to vegetation is higher. The similarity in description of dry and wet deposition processes from the atmosphere to different underlying surfaces implied in the model parameterisations is testified by close results of most models based on “reference” data set. Several models calculated dry deposition to different underlying surfaces taking into account types of these surfaces. Results on dry deposition flows from the atmosphere to all of the considered underlying surfaces, wet deposition flows from the atmosphere to soil and water obtained on the basis of “reference” data set, and wet depositions from the atmosphere to vegetation obtained on the basis of both data sets are in good agreement between all models. Scattering in values of gaseous exchange is more noticeable. Two models calculated re-emission gaseous flux from soil and one – from vegetation.

- For all considered media interfaces, agreement between different models’ results obtained on the basis of “reference” data set in most experiments performed is considerably better than that for results based on the “own/alternative” data set. Maximum difference between results of calculations of intermedia mass flows performed with both data sets of physical-chemical properties does not exceed 50% for dry and wet depositions, in calculations of gaseous exchange it is about 120%. The results of all models showed rather weak sensitivity of calculated values of air concentrations with respect to variations of pollutant-related parameters. The difference in concentrations in other media than the atmosphere is more noticeable (120% in maximum).

- The comparison of calculated fields of depositions and concentrations in the main environmental media demonstrates that the models of different type and resolution closely described the spatial distribution of PCB-153 pollution.

- The comparison of model results on PCB-153 depositions and concentrations in the atmosphere with monitoring data shows the following:

  - Participated models reasonably reproduced observed levels and trends of mean annual air concentrations. Comparison for other congeners has shown reasonable agreement for PCB-180 and larger differences for PCB-28.

  - All the models overestimate observed levels of PCB deposition fluxes.

  - The models reasonably reproduce PCB congener composition in air concentrations obtained by measurements. More discrepancies are found in the modeled and measured congener composition of PCB deposition fluxes.

- The sensitivity study with respect to physical-chemical parameter values used by the participating models in the description of gas/particles partitioning, wet deposition and gaseous exchange between the atmosphere and soil, water and vegetation performed on the basis of calculation experiments formulated at Stage I reveals that:

  - Most models describe similarly gas/particle partitioning. The results obtained with “own” set of pollutant-related data agree better between models than those based on “reference” data set. The difference in calculation of gas/particle partitioning caused by usage of “reference” and “own or alternative” data set of pollutant properties is moderate. Large differences are characteristic of high temperatures where values of fractions of particulate phase are small. The results obtained with “own or alternative” set of pollutant-related data agree better between models.

- The differences in absolute values of wet deposition flux and concentrations in precipitation calculated by models are essential. However, square deviation does not exceed the mean value of these parameters averaged between the participating models both in the results obtained on the basis of “reference” and “own/alternative” data sets. The difference in calculation results on wet deposition caused by the usage of “reference” and “own /alternative” data sets of pollutant properties is negligible. This process needs further investigation.
- Models describe gaseous flux between atmosphere and soil more closely than soil concentrations. The differences in concentrations are lower with “reference” data set than those with “own/alternative” data. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties (“reference” and “own/alternative”) is considerable for most models. Model descriptions of air/soil exchange and their parameterizations need further consideration.
- In general, most models closely describe processes of gaseous exchange between the atmosphere and water. The difference between calculated values of water concentrations and net gaseous flux from/to water obtained with two data sets of pollutant properties (“reference” and “own/alternative”) is essential for some models. The same applies to the description of gaseous exchange between atmosphere and vegetation.

A preliminary analysis of the main outcome of Stage II shows that in spite of the differences existing in the model descriptions and parameterisations, the reasonable agreement in the considered results on simulation of the basic processes of PCB behaviour in the environment is observed for most models. More detailed analysis of similarities and distinctions between different participating models in description of main processes is planned to be made in the framework of scientific publication.

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Annex A

ALTERNATIVE DATA SET OF PHYSICAL-CHEMICAL PROPERTIES OF PCB-153, PCB-28 AND PCB-180

For models using “reference data sets” as own sets of physical-chemical properties, it is proposed to carry out sensitivity studies of Stage II with the use of alternative data sets. Data on physical-chemical properties (including degradation rate constants) are mostly taken from CliMoChem and DEHM-POP models.

Description		Numerical values			**Comments**	**Reference**
		PCB-153	PCB-28	PCB-180		
Air/water partition coefficient, K_{AW} (dimensionless)						
Temperature dependent: $K_{AW} = K^0_{AW} \exp (- a_{KAW}(1/T - 1/T_0))$ where T - temperature (K); K^0_{AW} is the value at the reference temperature T_0; a_{KAW} is a parameter of temperature dependence.	K^0_{AW} (T_0), dimensionless	2.01E-03	4.63E-03	1.83E-03	$K_{AW}(T) = K_{AW}(T_{ref}) \exp(\mathrm{d}HK_{AW}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{AW}(T_{ref})$ = Henry 's law constant at T_{ref} (dimensionless) PCB 153: $9.18 \cdot 10^{-3}$; PCB 28: $1.27 \cdot 10^{-2}$; PCB 180: $8.92 \cdot 10^{-3}$ $\mathrm{d}HK_{AW}$ = phase transfer enthalpy (J/mol) PCB 153: 71000; PCB 28: 47200; PCB 180: 74100 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{KAW}	8536	5680	8917		
Subcooled liquid vapour pressure, p_{OL} (Pa)						
Temperature dependent: $p_{OL} = p^0_{OL} \exp (- a_p(1/T - 1/T_0))$ where T - temperature (K); p^0_{OL} is the value at the reference temperature T_0; a_p is a parameter of temperature dependence.	p^0_{OL} (T_0),	6.89E-05	6.26E-03	1.77E-05	Not used in DEHM-POP and CliMoChem models $p_{OL}(T) = p_{OL}(T_{ref}) \exp(\mathrm{d}Hp_{OL}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $p_{OL}(T_{ref})$ = Subcooled liquid vapour pressure at T_{ref} (Pa) PCB 153: $4.62 \cdot 10^{-4}$; PCB 28: $3.15 \cdot 10^{-2}$; PCB 180: $1.32 \cdot 10^{-4}$ $\mathrm{d}Hp_{OL}$ = phase transfer enthalpy (J/mol) PCB 153: 89030; PCB 28: 75620; PCB 180: 94140 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_p	10707.8	9095.0	11322.4		
Octanol/water partition coefficient, K_{OW} (dimensionless)						
Temperature dependent: $K_{OW} = K^0_{OW} \exp (a_{KOW}(1/T - 1/T_0))$ where T - temperature (K); K^0_{OW} is the value at the reference temperature T_0; a_{KOW} is a parameter of temperature dependence.	K^0_{OW} (T_0), dimensionless	8.17E+06	9.41E+05	1.84E+07	$K_{OW}(T) = K_{OW}(T_{ref}) \exp((\mathrm{d}HK_{OW}/R)(1/T_{ref}-1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{OW}(T_{ref})$ = octanol/water partitioning coefficient at T_{ref} PCB 153: $5.62 \cdot 10^6$; PCB 28: $5.13 \cdot 10^5$; PCB 180: $1.54 \cdot 10^7$ $\mathrm{d}HK_{OW}$ = phase transfer enthalpy (J/mol) PCB 153: -17500; PCB 28: -28400; PCB 180: -8270 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{KOW}	2102.4	3414.5	994.6		
Octanol/air partition coefficient, K_{OA} (dimensionless)						
Temperature dependent: $K_{OA} = K^0_{OA} \exp (a_{KOA}(1/T - 1/T_0))$ where T – temperature, K; K^0_{OA} is the value at the reference temperature T_0; a_{KOA} is a parameter of temperature dependence.	K^0_{OA} (T_0), dimensionless	2.74E+10	5.84E+08	9.78E+10	Not used in CliMoChem model $K_{OA}(T) = K_{OA}(T_{ref}) \exp((\mathrm{d}HK_{OA}/R)(1/T_{ref} - 1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{OA}(T_{ref})$ = octanol/water partitioning coefficient at T_{ref} PCB 153: $4.14 \cdot 10^9$; PCB 28: $1.16 \cdot 10^8$; PCB 180: $1.68 \cdot 10^{10}$ $\mathrm{d}HK_{OA}$ = phase transfer enthalpy (J/mol) PCB 153: -88440; PCB 28: -75620; PCB 180: -82410 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{KOA}	10636.8	9095.0	9911.6		

Description		Numerical values			Comments	Reference
		PCB-153	PCB-28	PCB-180		
Organic carbon/water partition coefficient, K_{OC} (dimensionless)						
Regression relation: $K_{OC} = regc\ K_{OW}^{b}$	*regc*	0.35	0.35	0.35	K_{OC} is calculated from K_{OW}, where K_{OW} is the temperature dependent octanol-water partition coefficient	*Seth et al.,* 1999
where *regc* and b are regression coefficients	*b*	1	1	1		
Water solubility, S_{WL} (mol/m^3)						
Temperature independent	$S_{WL}(T)$, mol/m^3	1.38E-05	5.45E-04	3.88E-06	Not used in DEHM-POP and CliMoChem models. Values are calculated for T = 283.15 with the help of the following temperature dependence: $S_{WL}(T) = S_{WL}(T_{ref})\ \exp(d_{HS_{WL}}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K); $S_{WL}(T_{ref})$ = water solubility at T_{ref} (mol/m^3) PCB 153: $2.03 \cdot 10^{-5}$; PCB 28: $1.00 \cdot 10^{-3}$; PCB 180: $5.95 \cdot 10^{-6}$ $d_{HS_{WL}}$ = phase transfer enthalpy (J/mol) PCB 153: 18060; PCB 28: 28390; PCB 180: 20000 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
Degradation rate constants, k_d (1/s)						
Degradation in atmosphere: Temperature independent	$k_{air}(T)$, 1/s	9.78E-08	6.53E-07	5.93E-08	The rate constants of the second order degradation process in air used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe. Then multiplying the second order rate constants by mean annual OH-radical concentration in the surface layer of 2 km depth at the latitude of 450N (0.8·106 molec/cm^3) [*Yu Lu and Khall,* 1991], the first order degradation rate constants were calculated.	*This study*
Degradation in soil: Temperature independent	$k_{soil}(T)$, 1/s	7.29E-10	4.62E-09	3.64E-10	The rate constants of the first order degradation process in soil used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*
Degradation in water: Temperature independent	$k_{water}(T)$, 1/s	8.27E-10	6.85E-08	4.13E-10	The rate constants of the first order degradation process in water used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*
Degradation in vegetation: Temperature independent	$K_{veg}(T)$, 1/s	1.18E-07	7.92E-07	7.19E-08	The rate constants of the first order degradation process in vegetation used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here for the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

COMPARISON OF RESULTS OF STAGE II COMPUTATIONAL EXPERIMENTS FOR PCB-28

A comparison of results on computational experiments of Stage II for PCB-28 obtained by the participating models is presented in this Annex. Five models participated in this comparison: CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, SimpleBox, and MSCE-POP.

B.1. Distribution of PCB-28 mass between environmental compartments

B.1.1. Comparison of calculated values of PCB-28 mass in the atmosphere

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-28 contained in the atmosphere within layers of 1 km, 5 km and 10 km height.

Reference data set. Calculation results on PCB-28 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.1.

Monthly values of PCB-28 mass contained in 1 km layer of the atmosphere calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.1 a and b, respectively.

Calculation results on PCB-28 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.2.

Monthly values of PCB-28 mass contained in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. B.2.

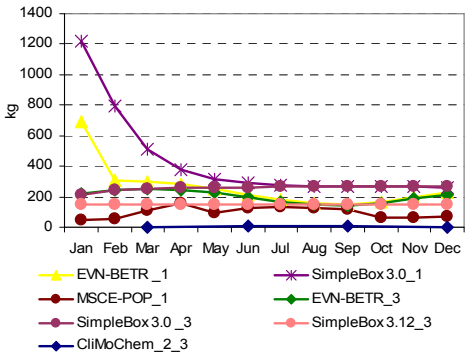


Fig. B.1a. *PCB-28 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

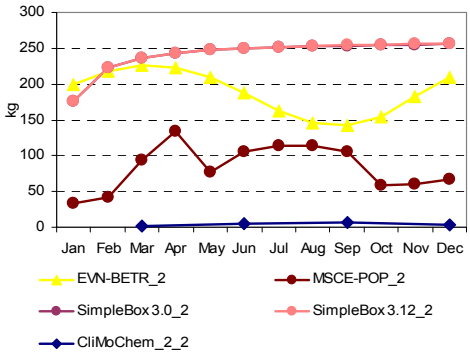


Fig. B.1b. *PCB-28 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

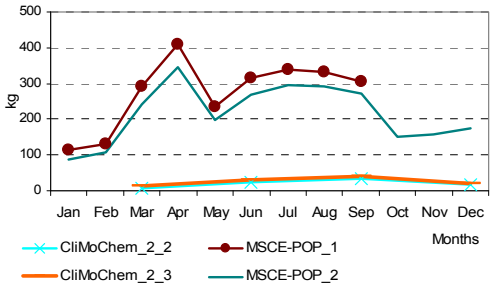


Fig. B.2. *PCB-28 mass in the 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

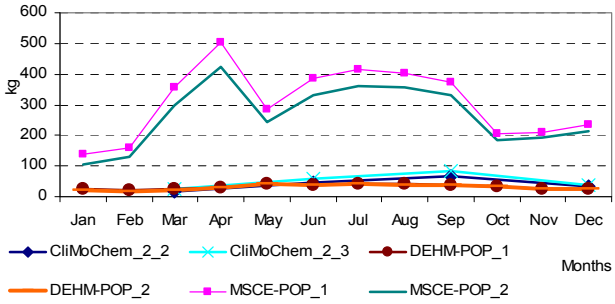


Fig. B.3. *PCB-28 mass in the 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference data set*

Table B.1. *Calculation results: PCB-28 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	EVN-BETR_1[a]	SimpleBox 3.0_1[b]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	689.41	1222.01	44.30	220.95		215.00	148.55	*423.37*	*449.94*	Jan	199.39		176.62	176.62	33.39	*146.51*	*76.17*
Feb	308.66	790.77	51.37	243.35		245.23	148.55	*297.99*	*257.63*	Feb	218.53		223.03	223.10	41.94	*176.65*	*89.83*
Mar	297.92	507.60	113.91	252.19		254.19	148.55	*262.39*	*138.97*	Mar	226.21		236.46	236.60	94.50	*198.44*	*69.47*
Seas_1	**432.00**	**840.13**	**69.86**	**238.83**	**2.45**	**238.14**	**148.55**	***281.42***	***282.47***	**Seas_1**	**214.71**	**1.57**	**212.04**	**212.10**	**56.61**	***139.41***	***102.57***
Apr	284.85	375.13	159.78	246.53		258.94	148.55	*245.63*	*84.00*	Apr	223.64		243.52	243.75	134.58	*211.37*	*52.05*
May	254.78	314.98	91.04	226.57		261.59	148.55	*216.25*	*82.04*	May	209.77		247.42	247.74	77.04	*195.49*	*80.96*
Jun	215.75	287.25	122.23	197.66		263.24	148.55	*205.78*	*63.81*	Jun	187.17		249.82	250.24	104.83	*198.02*	*68.83*
Seas_2	**251.79**	**325.79**	**124.35**	**223.58**	**6.02**	**261.26**	**148.55**	***191.62***	***106.71***	**Seas_2**	**206.86**	**4.63**	**246.92**	**247.24**	**105.48**	***162.23***	***105.42***
Jul	179.77	274.47	132.04	168.96		264.37	148.55	*194.69*	*60.26*	Jul	162.89		251.46	251.97	114.54	*195.22*	*68.16*
Aug	156.46	268.44	128.82	149.57		265.24	148.55	*186.18*	*63.16*	Aug	145.78		252.70	253.32	113.26	*191.27*	*72.53*
Sep	150.15	265.66	118.65	144.76		265.93	148.55	*182.28*	*65.69*	Sep	141.78		253.70	254.41	105.45	*188.84*	*76.76*
Seas_3	**162.13**	**269.53**	**126.51**	**154.43**	**8.19**	**265.18**	**148.55**	***162.07***	***88.85***	**Seas_3**	**150.15**	**6.90**	**252.62**	**253.24**	**111.08**	***154.80***	***103.76***
Oct	163.70	264.35	65.98	158.06		266.51	148.55	*177.86*	*76.56*	Oct	154.90		254.55	255.35	59.09	*180.97*	*93.95*
Nov	194.05	263.74	66.80	186.57		267.02	148.55	*187.79*	*75.19*	Nov	182.27		255.29	256.19	60.93	*188.67*	*91.94*
Dec	**226.56**	263.46	74.40	**215.74**		267.46	148.55	*199.36*	*74.77*	Dec	209.17		255.93	256.93	67.67	*197.43*	*89.33*
Seas_4	**194.77**	**263.85**	**69.06**	**186.79**	**3.80**	**267.00**	**148.55**	***161.97***	***97.41***	**Seas_4**	**182.12**	**3.37**	**255.26**	**256.16**	**62.56**	***151.89***	***114.57***
Annual	**260.17**	**424.82**	**97.44**	**200.91**	**5.11**	**257.89**	**148.55**	***199.27***	***134.57***	**Annual**	**188.46**	**4.12**	**241.71**	**242.19**	**83.93**	***152.08***	***104.90***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.
[b] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.2. *Calculation results: PCB-28 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	113.82				Jan		85.81		
Feb	132.01				Feb		107.76		
Mar	292.69				Mar		242.81		
Seas_1	**179.51**	**12.26**	***95.88***	***118.26***	**Seas_1**	**7.87**	**145.46**	***76.66***	***97.29***
Apr	410.57				Apr		345.81		
May	233.92				May		197.95		
Jun	314.07				Jun		269.37		
Seas_2	**319.52**	**30.08**	***174.80***	***204.66***	**Seas_2**	**23.14**	**271.04**	***147.09***	***175.30***
Jul	339.29				Jul		294.32		
Aug	331.01				Aug		291.03		
Sep	304.88				Sep		270.96		
Seas_3	**325.06**	**40.94**	***183.00***	***200.91***	**Seas_3**	**34.49**	**285.44**	***159.97***	***177.44***
Oct	169.54				Oct		151.83		
Nov	171.64				Nov		156.55		
Dec	191.16				Dec		173.87		
Seas_4	**177.45**	**19.00**	***98.22***	***112.04***	**Seas_4**	**16.84**	**160.75**	***88.79***	***101.76***
Annual	**250.38**	**25.57**	***137.98***	***158.97***	**Annual**	**20.58**	**215.67**	***118.13***	***137.95***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Calculation results on PCB-28 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table B.3.

Monthly values of PCB-28 mass contained in 10 km layer of the atmosphere calculated by the participating models on the basis of “reference” data set are compared in Fig. B.3.

Own/alternative data set. Calculation results on PCB-28 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data sets together with statistical parameters used for evaluation are presented in Table B.4.

Monthly values of PCB-28 mass contained in 1 km layer of the atmosphere calculated by participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.4a and b, respectively.

Calculation results on PCB-28 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data set together with statistical parameters used for evaluation are presented in Table B.5.

Monthly values of PCB-28 mass contained in 5 km layer of the atmosphere calculated by the models on the basis of “own or alternative” data sets are compared in Fig. B.5.

Calculation results on PCB-28 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data sets together with statistical parameters used for evaluation are presented in Table B.6.

Monthly values of PCB-28 mass contained in 10 km layer of the atmosphere calculated by the participating models on the basis of “own or alternative” data sets are compared in Fig. B.6.

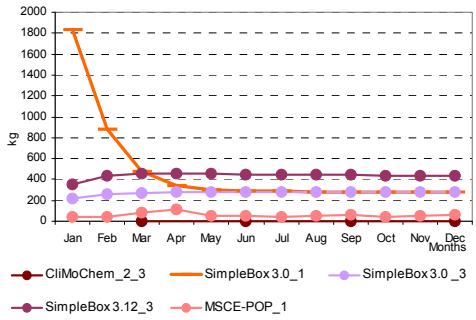


Fig.B.4a. *PCB-28 mass contained in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data set and non-zero initial conditions*

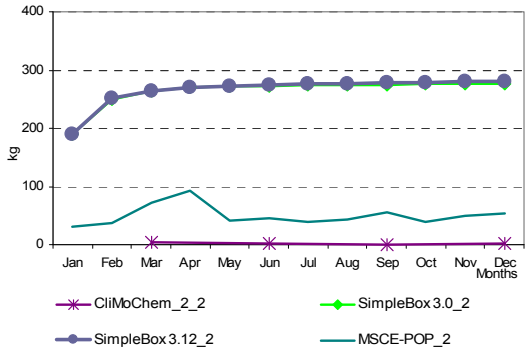


Fig. B.4b. *PCB-28 mass contained in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets and zero initial conditions*

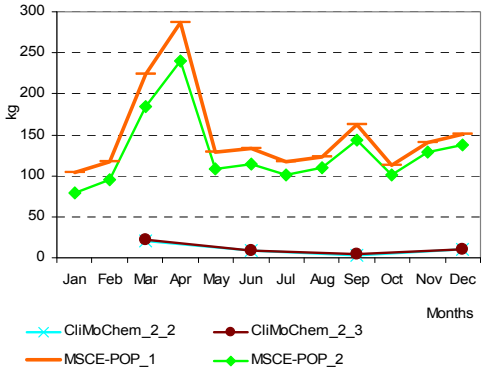


Fig. 3.5. *PCB-28 mass in 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets*

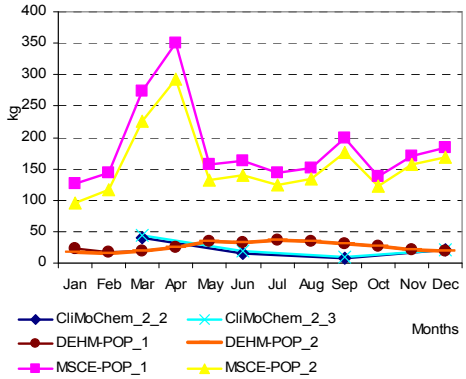


Fig. 3.6. *PCB-28 mass contained in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets*

Table B.3. *Calculation results: PCB-28 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	26.00	139.19		*82.60*	*80.04*	Jan		19.52	104.94	*62.23*	*60.40*
Feb	19.36	161.43		*90.40*	*100.46*	Feb		18.79	131.78	*75.29*	*79.90*
Mar	23.33	357.94		*190.64*	*236.61*	Mar		23.06	296.94	*160.00*	*193.66*
Seas_1	**22.90**	**219.52**	**24.51**	***88.98***	***113.06***	**Seas_1**	**15.74**	**20.46**	**177.89**	***71.36***	***92.28***
Apr	30.32	502.10		*266.21*	*333.60*	Apr		30.10	422.90	*226.50*	*277.75*
May	40.33	286.07		*163.20*	*173.76*	May		40.12	242.08	*141.10*	*142.80*
Jun	37.32	384.09		*210.71*	*245.21*	Jun		37.12	329.42	*183.27*	*206.69*
Seas_2	**35.99**	**390.75**	**60.16**	***162.30***	***198.21***	**Seas_2**	**46.28**	**35.78**	**331.47**	***137.84***	***167.77***
Jul	41.89	414.93		*228.41*	*263.78*	Jul		41.67	359.93	*200.80*	*225.05*
Aug	39.88	404.80		*222.34*	*258.04*	Aug		39.66	355.91	*197.79*	*223.63*
Sep	36.92	372.85		*204.89*	*237.54*	Sep		36.77	331.36	*184.07*	*208.31*
Seas_3	**39.56**	**397.53**	**81.87**	***172.99***	***195.61***	**Seas_3**	**68.99**	**39.37**	**349.07**	***152.48***	***170.90***
Oct	32.87	207.34		*120.10*	*123.37*	Oct		32.81	185.67	*109.24*	*108.09*
Nov	25.84	209.91		*117.87*	*130.15*	Nov		25.81	191.45	*108.63*	*117.13*
Dec	23.54	233.78		*128.66*	*148.66*	Dec		23.52	212.64	*118.08*	*133.73*
Seas_4	**27.42**	**217.01**	**38.00**	***94.14***	***106.54***	**Seas_4**	**33.67**	**27.38**	**196.59**	***85.88***	***95.93***
Annual	**31.47**	**306.20**	**51.14**	***129.60***	***153.26***	**Annual**	**41.17**	**30.75**	**263.75**	***111.89***	***131.62***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
* - data of DEHM-POP are given for 15 km layer of the atmosphere.

Table B.4. *Calculation results: PCB-28 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_ 2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1830.78	40.34		213.55	351.00	*608.92*	*824.43*	Jan		190.62	190.68	30.55	*137.28*	*92.44*
Feb	879.30	45.55		259.62	435.86	*405.08*	*354.14*	Feb		250.28	250.60	37.21	*179.36*	*123.11*
Mar	472.26	86.98		271.14	451.74	*320.53*	*180.02*	Mar		264.01	264.69	71.95	*200.22*	*111.09*
Seas_1	**1060.78**	**57.62**	**4.46**	**248.10**	**412.87**	***356.77***	***425.50***	**Seas_1**	**3.98**	**234.97**	**235.33**	**46.57**	***130.21***	***122.41***
Apr	342.50	111.46		275.48	454.51	*295.99*	*143.48*	Apr		269.19	270.26	93.41	*210.95*	*101.79*
May	302.61	49.90		277.41	453.13	*270.76*	*166.43*	May		271.48	272.95	42.20	*195.54*	*132.80*
Jun	289.81	51.88		278.50	450.65	*267.71*	*163.97*	Jun		272.78	274.65	44.62	*197.35*	*132.27*
Seas_2	**311.64**	**71.08**	**1.89**	**277.13**	**452.76**	***222.90***	***184.08***	**Seas_2**	**1.62**	**271.15**	**272.62**	**60.08**	***151.37***	***141.20***
Jul	285.48	45.38		279.26	447.91	*264.51*	*165.64*	Jul		273.70	275.96	39.44	*196.36*	*135.91*
Aug	283.80	47.91		279.86	445.16	*264.18*	*163.46*	Aug		274.44	277.09	42.52	*198.01*	*134.67*
Sep	283.04	63.13		280.35	442.54	*267.26*	*155.79*	Sep		275.04	278.06	56.00	*203.03*	*127.34*
Seas_3	**284.11**	**52.14**	**0.90**	**279.82**	**445.20**	***212.43***	***183.24***	**Seas_3**	**0.67**	**274.39**	**277.03**	**45.98**	***149.52***	***146.89***
Oct	282.61	43.61		280.77	440.02	*261.75*	*163.47*	Oct		275.56	278.94	39.06	*197.85*	*137.53*
Nov	282.35	54.46		281.13	437.62	*263.89*	*157.78*	Nov		276.01	279.75	50.00	*201.92*	*131.58*
Dec	282.18	58.51		281.45	435.35	*264.37*	*155.16*	Dec		276.41	280.49	53.45	*203.45*	*129.92*
Seas_4	**282.38**	**52.19**	**2.18**	**281.12**	**437.67**	***211.11***	***180.42***	**Seas_4**	**2.08**	**275.99**	**279.73**	**47.50**	***151.33***	***147.29***
Annual	484.73	58.26	2.36	271.54	437.12	***250.80***	***217.18***	**Annual**	2.09	264.13	266.18	**50.03**	***145.61***	***139.42***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.5. *Calculation results: PCB-28 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	103.64				Jan		78.49		
Feb	117.05				Feb		95.60		
Mar	223.50				Mar		184.88		
Season_1	**148.06**	**22.30**	***85.18***	***88.92***	**Season_1**	**19.91**	**119.66**	***69.78***	***70.53***
Apr	286.40				Apr		240.03		
May	128.22				May		108.45		
Jun	133.30				Jun		114.65		
Season_2	**182.64**	**9.45**	***96.05***	***122.46***	**Season_2**	**8.08**	**154.38**	***81.23***	***103.45***
Jul	116.60				Jul		101.33		
Aug	123.12				Aug		109.25		
Sep	162.21				Sep		143.89		
Season_3	**133.98**	**4.48**	***91.57***	***91.57***	**Season_3**	**3.35**	**118.16**	***81.18***	***81.18***
Oct	112.06				Oct		100.36		
Nov	139.94				Nov		128.48		
Dec	150.34				Dec		137.34		
Season_4	**134.11**	**10.92**	***87.11***	***87.11***	**Season_4**	**10.41**	**122.06**	***78.95***	***78.95***
Annual	**149.70**	**11.79**	***80.74***	***97.51***	**Annual**	**10.44**	**128.56**	***69.50***	***83.53***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table B.6. *Calculation results: PCB-28 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	*σ*	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	22.63	126.75		*74.69*	*73.62*	Jan		17.26	95.98	*56.62*	*55.67*
Feb	16.50	143.14		*79.82*	*89.55*	Feb		16.18	116.92	*66.55*	*71.23*
Mar	19.39	273.32		*146.36*	*179.56*	Mar		19.23	226.10	*122.66*	*146.28*
Seas_1	**19.51**	**181.07**	**44.61**	***81.73***	***86.94***	**Seas_1**	**39.82**	**17.56**	**146.33**	***67.90***	***68.83***
Apr	25.48	350.25		*187.86*	*229.65*	Apr		25.35	293.54	*159.45*	*189.64*
May	35.03	156.80		*95.92*	*86.11*	May		34.90	132.62	*83.76*	*69.10*
Jun	32.27	163.01		*97.64*	*92.45*	Jun		32.15	140.21	*86.18*	*76.41*
Seas_2	**30.93**	**223.36**	**18.91**	***91.06***	***114.73***	**Seas_2**	**16.15**	**30.80**	**188.79**	***78.58***	***95.73***
Jul	35.95	142.60		*89.27*	*75.41*	Jul		35.80	123.92	*79.86*	*62.31*
Aug	34.40	150.56		*92.48*	*82.14*	Aug		34.26	133.60	*83.93*	*70.25*
Sep	31.41	198.37		*114.89*	*118.06*	Sep		31.33	175.97	*103.65*	*102.27*
Seas_3	**33.92**	**163.85**	**8.97**	***68.91***	***83.16***	**Seas_3**	**6.70**	**33.80**	**144.50**	***61.67***	***73.00***
Oct	27.60	137.04		*82.32*	*77.38*	Oct		27.57	122.73	*75.15*	*67.29*
Nov	20.85	171.13		*95.99*	*106.27*	Nov		20.83	157.12	*88.98*	*96.38*
Dec	19.41	183.85		*101.63*	*116.28*	Dec		19.40	167.96	*93.68*	*105.04*
Seas_4	**22.62**	**164.01**	**21.85**	***69.49***	***81.85***	**Seas_4**	**20.82**	**22.60**	**149.27**	***64.23***	***73.65***
Annual	**26.74**	**183.07**	**23.58**	***77.80***	***91.18***	**Annual**	**20.87**	**26.19**	**157.22**	***68.10***	***77.23***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - data of DEHM-POP are given for 15 km layer of the atmosphere.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-28 mass contained in 1, 5 and 10 km layers of the atmosphere obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables B.7-B.9.

Table B.7. *The percentage difference between calculation results on PCB-28 mass contained in 1 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			49.8%	7.9%	8.0%	-0.7%	136.3%	-8.9%	-8.5%
Feb			11.2%	12.2%	12.3%	5.9%	193.4%	-11.3%	-11.3%
Mar			-7.0%	11.7%	11.9%	6.7%	204.1%	-23.6%	-23.9%
Season_1	**153.0%**	**82.0%**	**26.3%**	**10.8%**	**10.9%**	**4.2%**	**177.9%**	**-17.5%**	**-17.7%**
Apr			-8.7%	10.5%	10.9%	6.4%	206.0%	-30.2%	-30.6%
May			-3.9%	9.7%	10.2%	6.0%	205.0%	-45.2%	-45.2%
Jun			0.9%	9.2%	9.8%	5.8%	203.4%	-57.6%	-57.4%
Season_2	**-65.1%**	**-68.6%**	**-4.3%**	**9.8%**	**10.3%**	**6.1%**	**204.8%**	**-42.8%**	**-43.0%**
Jul			4.0%	8.8%	9.5%	5.6%	201.5%	-65.6%	-65.6%
Aug			5.7%	8.6%	9.4%	5.5%	199.7%	-62.8%	-62.5%
Sep			6.5%	8.4%	9.3%	5.4%	197.9%	-46.8%	-46.9%
Season_3	**-90.3%**	**-89.0%**	**5.4%**	**8.6%**	**9.4%**	**5.5%**	**199.7%**	**-58.8%**	**-58.6%**
Oct			6.9%	8.3%	9.2%	5.4%	196.2%	-33.9%	-33.9%
Nov			7.1%	8.1%	9.2%	5.3%	194.6%	-18.5%	-17.9%
Dec			7.1%	8.0%	9.2%	5.2%	193.1%	-21.4%	-21.0%
Season_4	**-38.2%**	**-42.5%**	**7.0%**	**8.1%**	**9.2%**	**5.3%**	**194.6%**	**-24.4%**	**-24.1%**
Annual	**-49.3%**	**-53.9%**	**14.1%**	**9.3%**	**9.9%**	**5.3%**	**194.3%**	**-40.2%**	**-40.4%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data; SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations; SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table B.8.*The percentage difference between calculation results on PCB-28 mass contained in 5 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			-8.9%	-8.5%
Feb			-11.3%	-11.3%
Mar			-23.6%	-23.9%
Season_1	**153.0%**	**82.0%**	**-17.5%**	**-17.7%**
Apr			-30.2%	-30.6%
May			-45.2%	-45.2%
Jun			-57.6%	-57.4%
Season_2	**-65.1%**	**-68.6%**	**-42.8%**	**-43.0%**
Jul			-65.6%	-65.6%
Aug			-62.8%	-62.5%
Sep			-46.8%	-46.9%
Season_3	**-90.3%**	**-89.0%**	**-58.8%**	**-58.6%**
Oct			-33.9%	-33.9%
Nov			-18.5%	-17.9%
Dec			-21.4%	-21.0%
Season_4	**-38.2%**	**-42.5%**	**-24.4%**	**-24.1%**
Annual	**-49.3%**	**-53.9%**	**-40.2%**	**-40.4%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table B.9. *The percentage difference between calculation results on PCB-28 mass contained in 10 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_ 2_2	CliMoChem _2_3	DEHM-POP_1	DEHM-POP_2	MSCE-POP_1	MSCE-POP_2
Jan			-13.0%	-11.6%	-8.9%	-8.5%
Feb			-14.8%	-13.9%	-11.3%	-11.3%
Mar			-16.9%	-16.6%	-23.6%	-23.9%
Season_1	**153.0%**	**82.0%**	**-14.8%**	**-14.2%**	**-17.5%**	**-17.7%**
Apr			-16.0%	-15.8%	-30.2%	-30.6%
May			-13.1%	-13.0%	-45.2%	-45.2%
Jun			-13.5%	-13.4%	-57.6%	-57.4%
Season_2	**-65.1%**	**-68.6%**	**-14.1%**	**-13.9%**	**-42.8%**	**-43.0%**
Jul			-14.2%	-14.1%	-65.6%	-65.6%
Aug			-13.7%	-13.6%	-62.8%	-62.5%
Sep			-14.9%	-14.8%	-46.8%	-46.9%
Season_3	**-90.3%**	**-89.0%**	**-14.3%**	**-14.1%**	**-58.8%**	**-58.6%**
Oct			-16.0%	-16.0%	-33.9%	-33.9%
Nov			-19.3%	-19.3%	-18.5%	-17.9%
Dec			-17.5%	-17.5%	-21.4%	-21.0%
Season_4	**-38.2%**	**-42.5%**	**-17.5%**	**-17.5%**	**-24.4%**	**-24.1%**
Annual	**-49.3%**	**-53.9%**	**-15.0%**	**-14.8%**	**-40.2%**	**-40.4%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data; DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data. MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

B.1.2. Comparison of calculated values of PCB-28 mass in soil

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-28 contained in soil within 5 cm and 10 cm depth.

Reference data set. Calculation results on PCB-28 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.10.

Monthly values of PCB-28 mass contained in 5cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.3.7a and b, respectively.

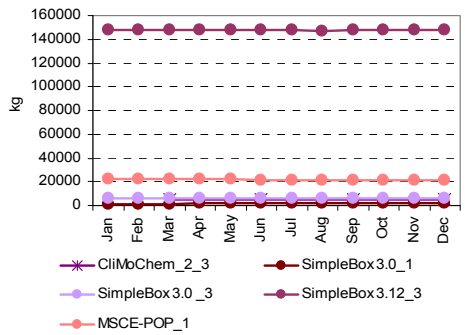


Fig. B.7a. *PCB-28 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

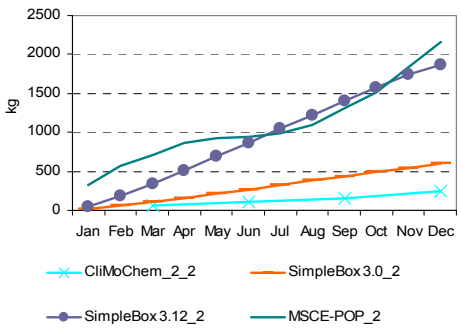


Fig. B.7b. *PCB-28 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Calculation results on PCB-28 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table B.11.

Monthly values of PCB-28 mass contained in 10 cm layer of soil calculated by the participating models on the basis of “reference” data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.8a and b, respectively.

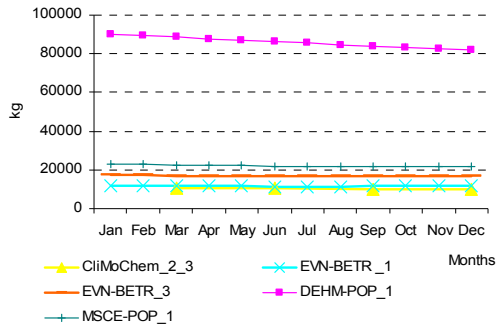


Fig. B.8a. *PCB-28 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and non-zero initial conditions*

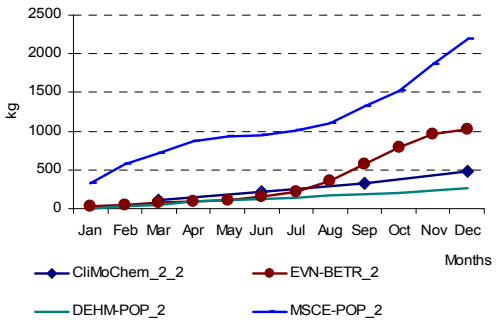


Fig. B.8b. *PCB-28 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and zero initial conditions*

Table B.10. *Calculation results: PCB-28 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	Simple Box 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	923.8	22699.2		5956.0	148110.7	*44422.4*	*69749.4*	Jan		15.6	49.7	324.7	*130.0*	*169.5*
Feb	1239.6	22582.2		5970.0	148110.7	*44475.6*	*69693.6*	Feb		58.3	186.4	572.9	*272.5*	*267.9*
Mar	1414.2	22365.0		5988.6	148110.7	*44469.6*	*69677.0*	Mar		107.6	345.0	713.6	*388.8*	*305.4*
Seas_1	**1192.55**	**22548.8**	**5213.5**	**5971.5**	**148110.7**	***36607.4***	***62866.8***	**Seas_1**	**57.9**	**60.5**	**193.7**	**537.1**	***212.3***	***225.6***
Apr	1524.0	22200.5		6009.4	148110.7	*44461.2*	*69668.0*	Apr		160.7	508.8	859.9	*509.8*	*349.6*
May	1601.5	21953.5		6031.3	148110.7	*44424.2*	*69674.5*	May		215.0	690.4	922.3	*609.2*	*360.6*
Jun	1664.1	21671.5		6053.9	148110.7	*44375.0*	*69688.0*	Jun		270.0	866.7	933.9	*690.2*	*365.4*
Seas_2	**1596.54**	**21941.8**	**5128.0**	**6031.6**	**148110.7**	***36561.7***	***62848.3***	**Seas_2**	**107.0**	**215.2**	**688.6**	**905.4**	***479.1***	***380.2***
Jul	1719.6	21456.0		6076.4	148110.7	*44340.7*	*69696.1*	Jul		325.1	1043.4	995.2	*787.9*	*401.5*
Aug	1772.5	21300.4		6099.7	147330.3	*44125.7*	*69310.8*	Aug		381.2	1225.7	1090.8	*899.2*	*453.7*
Sep	1822.7	21306.3		6122.6	148110.7	*44340.6*	*69683.1*	Sep		436.3	1398.9	1305.7	*1047.0*	*530.9*
Seas_3	**1771.60**	**21354.2**	**5043.7**	**6099.6**	**147850.5**	***36423.9***	***62745.6***	**Seas_3**	**159.7**	**380.9**	**1222.7**	**1130.6**	***723.4***	***532.3***
Oct	1871.9	21305.9		6145.1	148110.7	*44358.4*	*69669.0*	Oct		491.2	1574.3	1512.6	*1192.7*	*608.3*
Nov	1920.5	21462.1		6168.1	148110.7	*44415.3*	*69637.7*	Nov		546.0	1749.0	1839.1	*1378.1*	*722.0*
Dec	1967.8	21622.0		6190.7	148110.7	*44472.8*	*69606.4*	Dec		599.7	1873.8	2165.6	*1546.4*	*832.7*
Seas_4	**1920.08**	**21463.3**	**4994.7**	**6168.0**	**148110.7**	***36531.3***	***62832.0***	**Seas_4**	**242.2**	**545.7**	**1732.4**	**1839.1**	***1089.8***	***814.2***
Annual	**1620.2**	**21827.1**	**5095.0**	**6067.7**	**148045.6**	***36531.1***	***62822.6***	**Annual**	**141.7**	**300.6**	**959.3**	**1103.0**	***626.2***	***475.8***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-28 mass contained in 5cm layer of soil (kg) calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation. are presented in Table B.12.

Monthly values of PCB-28 mass contained in 5cm layer of soil calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.9a and b, respectively.

Calculation results on PCB-28 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.13.

Monthly values of PCB-28 mass contained in 10 cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.10a and b, respectively.

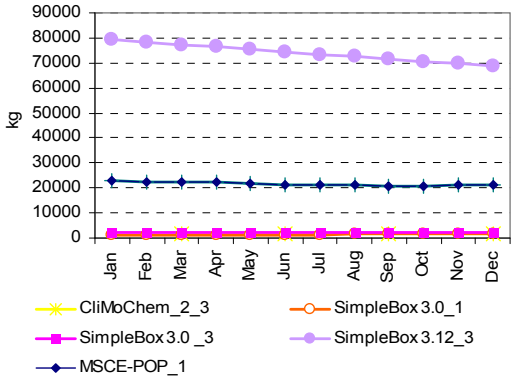


Fig. 3.9a. *PCB-28 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

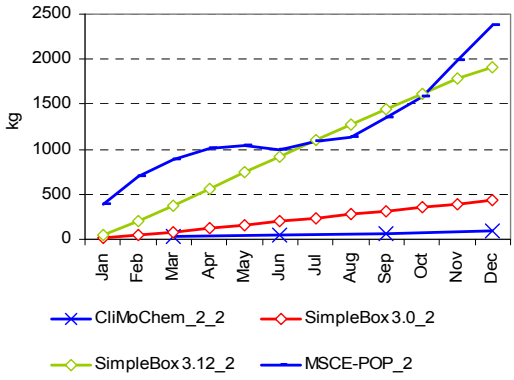


Fig. 3.9b. *PCB-28 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

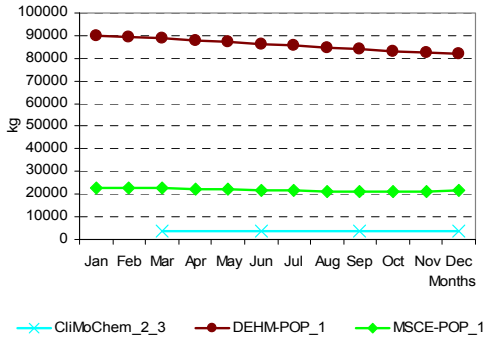


Fig. B.10a. *PCB-28 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

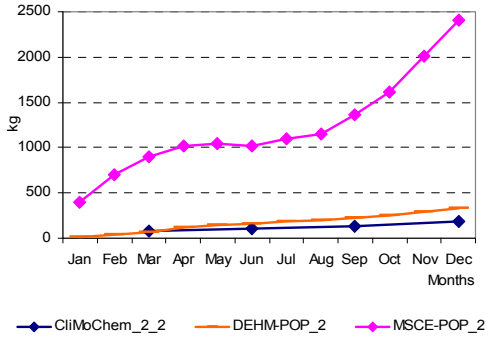


Fig. B.10b. *PCB-28 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table B.11. *Calculation results: PCB-28 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	EVN-BETR _1[b]	EVN-BETR_3[b]	CliMo Chem_2_3				EVN-BETR_2[a]	CliMo Chem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	90190.0	22947.3	11828.5	17248.3		*35553.6*	*36706.1*	Jan	24.9		6.6	328.2	*119.9*	*180.6*
Feb	89390.0	22829.0	11767.9	17111.3		*35274.6*	*36358.6*	Feb	49.5		24.4	579.1	*217.7*	*313.3*
Mar	88600.0	22609.5	11683.3	16971.0		*34965.9*	*36033.3*	Mar	70.2		48.2	721.4	*279.9*	*382.5*
Seas_1	**89393.3**	**22795.3**	**11759.9**	**17110.2**	**10427.1**	***30297.2***	***33395.3***	**Seas_1**	**48.2**	**115.8**	**26.4**	**542.9**	***183.3***	***242.7***
Apr	87830.0	22443.2	11598.8	16832.1		*34676.1*	*35711.6*	Apr	90.9		87.5	869.3	*349.2*	*450.4*
May	87020.0	22193.5	11520.0	16699.5		*34358.3*	*35377.3*	May	115.7		108.1	932.4	*385.4*	*473.7*
Jun	86240.0	21908.3	11453.4	16579.5		*34045.3*	*35057.3*	Jun	150.8		125.4	944.1	*406.8*	*465.5*
Seas_2	**87030.0**	**22181.7**	**11524.1**	**16703.7**	**10255.9**	***29539.1***	***32482.5***	**Seas_2**	**119.1**	**214.1**	**107.0**	**915.3**	***338.9***	***387.2***
Jul	85460.0	21690.6	11421.1	16493.1		*33766.2*	*34716.6*	Jul	216.9		145.1	1006.1	*456.0*	*477.7*
Aug	84680.0	21533.2	11473.1	16488.5		*33543.7*	*34337.4*	Aug	361.7		163.3	1102.7	*542.6*	*495.1*
Sep	83920.0	21539.2	11596.6	16555.4		*33402.8*	*33921.9*	Sep	576.1		178.7	1320.0	*691.6*	*579.3*
Seas_3	**84686.7**	**21587.6**	**11496.9**	**16512.3**	**10087.4**	***28874.2***	***31527.2***	**Seas_3**	**384.9**	**319.3**	**162.4**	**1142.9**	***502.4***	***437.1***
Oct	83170.0	21538.8	11726.1	16629.7		*33266.2*	*33509.5*	Oct	797.0		200.8	1529.1	*842.3*	*665.3*
Nov	82430.0	21696.7	11790.8	16641.8		*33139.8*	*33108.1*	Nov	955.5		233.6	1859.2	*1016.1*	*814.5*
Dec	81700.0	21858.4	11764.7	16566.2		*32972.3*	*32745.7*	Dec	1026.4		260.1	2189.3	*1158.6*	*971.4*
Seas_4	**82433.3**	**21698.0**	**11760.5**	**16612.6**	**9989.3**	***28498.7***	***30492.8***	**Seas_4**	**926.3**	**484.3**	**231.5**	**1859.2**	***875.3***	***716.0***
Annual	**85885.8**	**22065.6**	**11635.4**	**16734.7**	**10189.9**	***29302.3***	***31974.3***	**Annual**	**369.6**	**283.4**	**131.8**	**1115.1**	***475.0***	***437.9***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - data of DEHM-POP are given for 15 cm layer of soil;
[b] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.

Table B.12. *Calculation results: PCB-28 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	859.1	22735.9		1989.1	79437.1	*26255.3*	*36853.3*	Jan		11.4	53.1	386.1	*150.2*	*205.3*
Feb	1111.4	22636.4		2006.7	78322.6	*26019.3*	*36258.7*	Feb		43.9	204.4	694.1	*314.1*	*338.8*
Mar	1213.3	22427.7		2028.5	77281.4	*25737.7*	*35736.4*	Mar		81.2	378.1	888.0	*449.1*	*408.0*
Seas_1	**1061.3**	**22600.0**	**1861.4**	**2008.1**	**78347.0**	***21175.6***	***33225.1***	**Seas_1**	**37.6**	**45.5**	**211.9**	**656.1**	***237.8***	***290.2***
Apr	1268.0	22181.0		2051.8	76347.7	*25462.2*	*35277.5*	Apr		120.5	552.9	1010.7	*561.4*	*445.2*
May	1306.9	21840.0		2075.5	75279.0	*25125.4*	*34760.1*	May		160.1	741.1	1036.0	*645.7*	*445.6*
Jun	1340.7	21459.5		2099.2	74320.6	*24805.0*	*34298.3*	Jun		199.7	920.7	1001.3	*707.2*	*441.4*
Seas_2	**1305.2**	**21826.8**	**1829.9**	**2075.5**	**75315.8**	***20470.6***	***31870.8***	**Seas_2**	**54.0**	**160.1**	**738.2**	**1016.0**	***492.1***	***460.9***
Jul	1372.6	21228.2		2122.8	73384.7	*24527.1*	*33842.9*	Jul		239.0	1098.0	1084.4	*807.1*	*492.1*
Aug	1404.2	20986.9		2146.8	72526.0	*24266.0*	*33425.0*	Aug		278.8	1280.5	1140.7	*900.0*	*542.5*
Sep	1434.8	20946.4		2170.2	71563.3	*24028.7*	*32951.0*	Sep		317.6	1447.9	1344.9	*1036.8*	*625.0*
Seas_3	**1403.9**	**21053.8**	**1778.3**	**2146.6**	**72491.3**	***19774.8***	***30630.0***	**Seas_3**	**65.7**	**278.5**	**1275.5**	**1190.0**	***702.4***	***619.5***
Oct	1465.1	20955.7		2193.5	70687.9	*23825.5*	*32518.0*	Oct		356.2	1617.5	1590.2	*1188.0*	*720.4*
Nov	1495.0	21155.9		2216.6	69828.5	*23674.0*	*32087.9*	Nov		394.6	1784.5	1983.8	*1387.6*	*865.8*
Dec	1524.1	21359.6		2239.2	69005.6	*23532.1*	*31677.0*	Dec		432.0	1907.9	2378.1	*1572.7*	*1015.5*
Seas_4	**1494.7**	**21157.0**	**1775.9**	**2216.5**	**69840.7**	***19297.0***	***29469.4***	**Seas_4**	**93.1**	**394.2**	**1770.0**	**1984.0**	***1060.3***	***955.0***
Annual	**1316.3**	**21659.4**	**1811.4**	**2111.7**	**73998.7**	***20179.5***	***31298.4***	**Annual**	**62.6**	**219.6**	**998.9**	**1211.5**	***623.1***	***567.0***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.13. *Calculation results: PCB-28 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	90190.0	22984.4		*56587.2*	*47521.6*	Jan		10.5	390.3	*200.4*	*268.6*
Feb	89400.0	22883.8		*56141.9*	*47034.1*	Feb		34.4	701.7	*368.1*	*471.9*
Mar	88630.0	22672.8		*55651.4*	*46638.8*	Mar		65.4	897.7	*481.5*	*588.5*
Seas_1	**89406.7**	**22847.0**	**3722.8**	***38658.8***	***44977.1***	**Seas_1**	**75.3**	**36.7**	**663.2**	***258.4***	***351.1***
Apr	87880.0	22423.5		*55151.7*	*46284.7*	Apr		118.3	1021.8	*570.0*	*638.9*
May	87090.0	22078.8		*54584.4*	*45969.9*	May		143.4	1047.3	*595.3*	*639.1*
Jun	86300.0	21694.0		*53997.0*	*45683.3*	Jun		162.8	1012.2	*587.5*	*600.6*
Seas_2	**87090.0**	**22065.4**	**3659.8**	***37605.1***	***43832.2***	**Seas_2**	**107.9**	**141.5**	**1027.1**	***425.5***	***521.3***
Jul	85540.0	21460.2		*53500.1*	*45311.2*	Jul		184.2	1096.3	*640.2*	*644.9*
Aug	84760.0	21216.3		*52988.1*	*44932.2*	Aug		202.8	1153.1	*678.0*	*672.0*
Sep	83990.0	21175.4		*52582.7*	*44416.7*	Sep		220.0	1359.6	*789.8*	*805.8*
Seas_3	**84763.3**	**21283.9**	**3556.6**	***36534.6***	***42697.4***	**Seas_3**	**131.3**	**202.3**	**1203.0**	***512.2***	***599.3***
Oct	83240.0	21184.7		*52212.4*	*43879.7*	Oct		250.2	1607.5	*928.9*	*959.8*
Nov	82520.0	21387.1		*51953.6*	*43227.5*	Nov		295.4	2005.4	*1150.4*	*1209.2*
Dec	81790.0	21593.1		*51691.5*	*42565.7*	Dec		333.0	2404.1	*1368.5*	*1464.5*
Seas_4	**82516.7**	**21388.3**	**3551.7**	***35818.9***	***41413.1***	**Seas_4**	**186.1**	**292.9**	**2005.7**	***828.2***	***1021.1***
Annual	**85944.2**	**21896.2**	**3622.7**	***37154.4***	***43229.8***	**Annual**	**125.2**	**168.4**	**1224.8**	***506.1***	***622.8***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] – data of DEHM-POP are given for 15 cm layer of soil;
[b] - in CAN/POPs results the second layer of soil is applied as 5cm.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-28 masses contained in soil within 5 and 10 cm layers obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables B.14-B.15.

Table B.14. *The percentage difference between calculation results on PCB-28 masses contained within 5 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-7.0%	-26.9%	6.8%	-66.6%	-46.4%	0.2%	18.9%
Feb			-10.3%	-24.8%	9.6%	-66.4%	-47.1%	0.2%	21.2%
Mar			-14.2%	-24.5%	9.6%	-66.1%	-47.8%	0.3%	24.4%
Season_1	-35.0%	-64.3%	-11.0%	-24.8%	9.4%	-66.4%	-47.1%	0.2%	22.2%
Apr			-16.8%	-25.0%	8.6%	-65.9%	-48.5%	-0.1%	17.5%
May			-18.4%	-25.5%	7.3%	-65.6%	-49.2%	-0.5%	12.3%
Jun			-19.4%	-26.0%	6.2%	-65.3%	-49.8%	-1.0%	7.2%
Season_2	-49.6%	-64.3%	-18.2%	-25.6%	7.2%	-65.6%	-49.1%	-0.5%	12.2%
Jul			-20.2%	-26.5%	5.2%	-65.1%	-50.5%	-1.1%	9.0%
Aug			-20.8%	-26.9%	4.5%	-64.8%	-50.8%	-1.5%	4.6%
Sep			-21.3%	-27.2%	3.5%	-64.6%	-51.7%	-1.7%	3.0%
Season_3	-58.9%	-64.7%	-20.8%	-26.9%	4.3%	-64.8%	-51.0%	-1.4%	5.3%
Oct			-21.7%	-27.5%	2.7%	-64.3%	-52.3%	-1.6%	5.1%
Nov			-22.2%	-27.7%	2.0%	-64.1%	-52.9%	-1.4%	7.9%
Dec			-22.5%	-28.0%	1.8%	-63.8%	-53.4%	-1.2%	9.8%
Season_4	-61.6%	-64.4%	-22.2%	-27.7%	2.2%	-64.1%	-52.8%	-1.4%	7.9%
Annual	-55.8%	-64.4%	-18.8%	-26.9%	4.1%	-65.2%	-50.0%	-0.8%	9.8%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table B.15. *The percentage difference between calculation results on PCB-28 mass contained within 10 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	DEHM-POP_1	DEHM-POP_2	MSCE-POP_1	MSCE-POP_2
Jan			0.00%	58.4%	0.2%	18.9%
Feb			0.01%	40.9%	0.2%	21.2%
Mar			0.03%	35.7%	0.3%	24.4%
Season_1	**-35.0%**	**-64.3%**	**0.01%**	**39.2%**	**0.2%**	**22.2%**
Apr			0.06%	35.3%	-0.1%	17.5%
May			0.08%	32.7%	-0.5%	12.3%
Jun			0.07%	29.8%	-1.0%	7.2%
Season_2	**-49.6%**	**-64.3%**	**0.07%**	**32.3%**	**-0.5%**	**12.2%**
Jul			0.09%	26.9%	-1.1%	9.0%
Aug			0.09%	24.2%	-1.5%	4.6%
Sep			0.08%	23.1%	-1.7%	3.0%
Season_3	**-58.9%**	**-64.7%**	**0.09%**	**24.6%**	**-1.4%**	**5.3%**
Oct			0.08%	24.6%	-1.6%	5.1%
Nov			0.11%	26.5%	-1.4%	7.9%
Dec			0.11%	28.0%	-1.2%	9.8%
Season_4	**-61.6%**	**-64.4%**	**0.10%**	**26.5%**	**-1.4%**	**7.9%**
Annual	**-55.8%**	**-64.4%**	**0.07%**	**27.7%**	**-0.8%**	**9.8%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.

B.1.3. Comparison of calculated values of PCB-28 mass in water

According to the programme of Stage II model results of computational experiments on mass balance include masses of PCB-28 contained in sea within a layer of 200 m depth.

Reference data set. Calculation results on PCB-28 mass contained in 200 m layer of seawater (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.16.

Monthly values of PCB-28 mass contained in 200 m layer of seawater calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.11a and b, respectively.

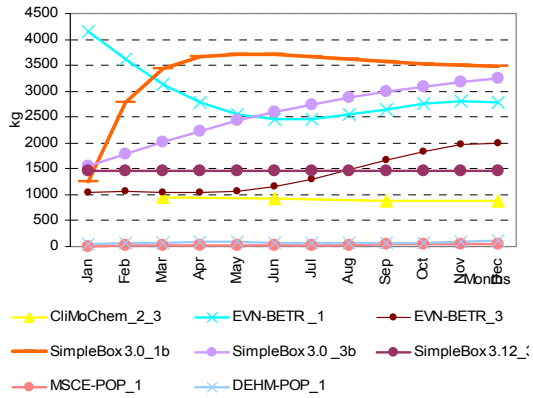


Fig. B.11a. *PCB-28 mass contained in 200 m layer of seawater (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

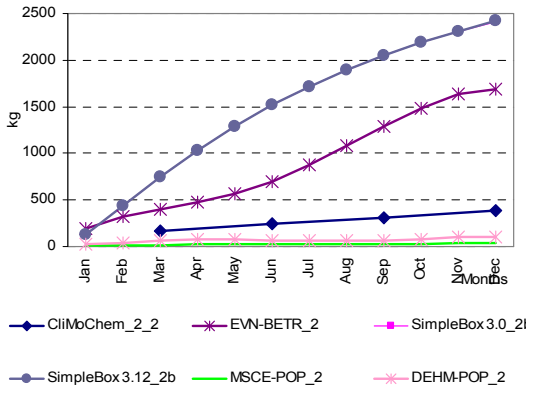
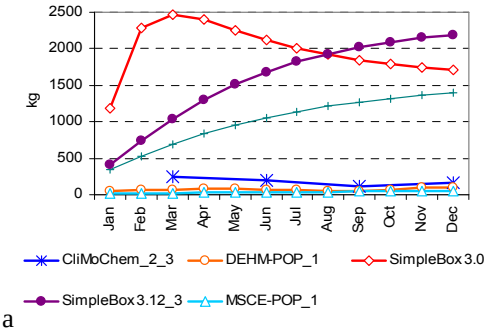


Fig. B.11b. *PCB-28 mass contained in 200 m layer of seawater (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

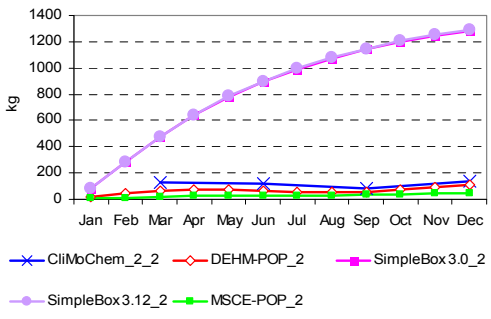
Own/alternative data set. Calculation results on PCB-28 mass contained in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.17.

Monthly values of PCB-28 mass contained in 200 m layer of water calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.12a and b, respectively.



a

Fig. B.12a. *PCB-28 mass contained in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*



b

Fig. B.12b. *PCB-28 mass contained in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table B.16. *Calculation results: PCB-28 mass contained in 200 m layer of seawater (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	DEHM-POP_1	MSCE-POP_1	EVN-BETR_1[a]	SimpleBox 3.0_1[b]	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	DEHM-POP_2	MSCE-POP_2		
Jan	43.36	10.20	4142.35	1263.44	1047.47		1559.78	1459.29	*1360.84*	*1381.65*	Jan	189.63		126.72	126.70	20	7.73	*94.16*	*77.79*
Feb	60.10	12.21	3623.45	2781.32	1068.35		1796.66	1459.29	*1543.05*	*1335.46*	Feb	322.27		439.17	439.15	44.74	9.73	*251.01*	*210.14*
Mar	70.90	16.25	3139.81	3426.74	1054.85		2025.44	1459.29	*1599.04*	*1357.22*	Mar	404.07		746.53	746.64	60.77	13.48	*394.30*	*355.16*
Seas_1	**58.12**	**12.89**	**3635.20**	**2490.50**	**1056.89**	**960.71**	**1793.96**	**1459.29**	***1433.44***	***1217.17***	**Seas_1**	**305.32**	**163.28**	**437.47**	**437.50**	**41.84**	**10.31**	***232.62***	***189.66***
Apr	84.56	23.64	2781.34	3665.44	1047.65		2237.17	1459.29	*1614.16*	*1364.58*	Apr	475.10		1032.88	1033.17	77.85	19.91	*527.78*	*493.38*
May	82.25	29.20	2551.89	3719.85	1076.08		2425.59	1459.29	*1620.59*	*1362.83*	May	565.02		1288.66	1289.34	78.01	24.89	*649.18*	*620.85*
Jun	71.20	27.70	2450.71	3700.80	1159.94		2592.01	1459.29	*1637.38*	*1362.24*	Jun	695.66		1515.21	1516.35	68.59	23.67	*763.89*	*735.98*
Seas_2	**79.34**	**26.85**	**2594.65**	**3695.36**	**1094.55**	**926.00**	**2418.26**	**1459.29**	***1536.79***	***1283.65***	**Seas_2**	**578.59**	**247.95**	**1278.92**	**1279.62**	**74.82**	**22.82**	***580.45***	***575.13***
Jul	63.86	25.57	2460.53	3656.73	1301.56		2738.31	1459.29	*1672.26*	*1364.87*	Jul	872.74		1714.79	1716.48	62.13	21.92	*877.61*	*836.93*
Aug	59.62	24.85	2544.69	3607.61	1482.96		2869.04	1459.29	*1721.15*	*1373.44*	Aug	1081.99		1893.44	1895.79	58.41	21.29	*990.18*	*928.90*
Sep	61.06	36.47	2654.78	3563.82	1671.14		2982.31	1459.29	*1775.55*	*1384.56*	Sep	1293.79		2048.45	2051.54	60.23	31.84	*1097.17*	*1008.04*
Seas_3	**61.51**	**28.96**	**2553.33**	**3609.39**	**1485.22**	**884.22**	**2863.22**	**1459.29**	***1618.14***	***1304.93***	**Seas_3**	**1082.84**	**309.34**	**1885.56**	**1887.94**	**60.26**	**25.01**	***875.16***	***871.40***
Oct	76.61	35.74	2756.66	3526.79	1842.13		3082.15	1459.29	*1825.62*	*1398.62*	Oct	1486.44		2185.51	2189.42	76.04	31.26	*1193.73*	*1079.50*
Nov	98.50	40.71	2815.52	3497.57	1968.42		3170.24	1459.29	*1864.32*	*1408.09*	Nov	1634.24		2307.22	2311.98	98.04	35.95	*1277.49*	*1139.11*
Dec	109.80	38.14	2781.98	3476.20	2005.78		3248.24	1459.29	*1874.21*	*1411.39*	Dec	1694.47		2413.98	2419.62	109.4	34.00	*1334.30*	*1190.01*
Seas_4	**94.97**	**38.20**	**2784.72**	**3500.19**	**1938.78**	**872.06**	**3166.88**	**1459.29**	***1731.88***	***1346.90***	**Seas_4**	**1605.05**	**387.57**	**2302.24**	**2307.01**	**94.49**	**33.74**	***1121.68***	***1077.96***
Annual	**73.49**	**26.72**	**2891.98**	**3323.86**	**1393.86**	**910.75**	**2560.58**	**1459.29**	***1580.06***	***1248.04***	**Annual**	**892.95**	**277.03**	**1476.05**	**1478.02**	**67.85**	**22.97**	***702.48***	***675.52***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
[b] - SimpleBox data presented here are masses calculated for continental level.

Table B.17. *Calculation results: PCB-28 mass contained in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	DEHM-POP_1	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	DEHM-POP_2	MSCE-POP_2		
Jan	46.09	1189.88	11.60		350.03	411.89	*401.90*	*475.04*	Jan		80.62	80.61	22.74	8.79	*48.19*	*37.87*
Feb	60.49	2286.01	14.35		527.27	738.51	*725.33*	*925.02*	Feb		282.24	282.35	46.46	11.47	*155.63*	*146.96*
Mar	68.58	2473.31	19.31		693.63	1041.02	*859.17*	*999.54*	Mar		473.65	474.16	59.70	16.07	*255.90*	*252.37*
Seas_1	**58.39**	**1983.07**	**15.09**	**248.72**	**523.64**	**730.48**	***593.23***	***734.07***	**Seas_1**	**129.37**	**278.84**	**279.04**	**42.97**	**12.11**	***148.47***	***126.62***
Apr	81.18	2393.25	29.47		838.68	1299.92	*928.50*	*976.95*	Apr		640.85	642.17	75.49	25.00	*345.88*	*341.99*
May	77.55	2255.64	34.86		959.64	1510.98	*967.73*	*950.86*	May		780.44	782.68	74.00	29.86	*416.75*	*421.64*
Jun	65.57	2123.47	31.93		1059.95	1681.74	*992.53*	*940.82*	Jun		896.26	899.68	63.43	27.42	*471.70*	*492.44*
Seas_2	**74.77**	**2257.45**	**32.09**	**192.09**	**952.76**	**1497.55**	***834.45***	***906.88***	**Seas_2**	**122.60**	**772.52**	**774.84**	**70.97**	**27.43**	***353.67***	***384.89***
Jul	59.41	2011.38	28.25		1143.02	1819.06	*1012.22*	*941.07*	Jul		992.16	996.95	57.97	24.27	*517.84*	*550.64*
Aug	55.66	1918.83	28.31		1213.01	1931.21	*1029.40*	*947.16*	Aug		1073.09	1079.39	54.66	24.43	*557.89*	*598.67*
Sep	55.94	1846.25	43.28		1270.40	2019.88	*1047.15*	*951.95*	Sep		1139.46	1147.36	55.30	38.17	*595.07*	*633.21*
Seas_3	**57.00**	**1925.49**	**33.28**	**118.62**	**1208.81**	**1923.39**	***877.76***	***923.44***	**Seas_3**	**83.55**	**1068.24**	**1074.57**	**55.98**	**28.96**	***462.26***	***556.41***
Oct	71.22	1788.93	44.26		1318.37	2091.15	*1062.79*	*957.96*	Oct		1195.03	1204.63	70.81	39.13	*627.40*	*661.12*
Nov	94.16	1743.85	50.76		1358.90	2148.67	*1079.27*	*960.70*	Nov		1242.00	1253.29	93.82	45.18	*658.57*	*680.51*
Dec	106.00	1709.37	48.92		1392.71	2194.34	*1090.27*	*967.85*	Dec		1281.24	1294.23	105.70	43.99	*681.29*	*700.74*
Seas_4	**90.46**	**1747.38**	**47.98**	**158.61**	**1356.66**	**2144.72**	***924.30***	***938.44***	**Seas_4**	**133.86**	**1239.42**	**1250.72**	**90.11**	**42.77**	***551.38***	***634.08***
Annual	**70.15**	**1978.35**	**32.11**	**179.51**	**1010.47**	**1574.03**	***807.44***	***841.30***	**Annual**	**117.35**	**839.75**	**844.79**	**65.01**	**27.81**	***378.94***	***424.16***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.18.

Table B.18. *The percentage difference between calculation results on PCB-28 mass in water (kg) obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	DEHM-POP_1	DEHM-POP_2	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			6.3%	13.7%	-5.8%	-36.4%	-36.4%	-77.6%	-71.8%	13.7%	13.8%
Feb			0.6%	3.8%	-17.8%	-35.7%	-35.7%	-70.7%	-49.4%	17.5%	17.9%
Mar			-3.3%	-1.8%	-27.8%	-36.6%	-36.5%	-65.8%	-28.7%	18.8%	19.2%
Season_1	**-20.8%**	**-74.1%**	**0.5%**	**2.7%**	**-20.4%**	**-36.3%**	**-36.2%**	**-70.8%**	**-49.9%**	**17.1%**	**17.4%**
Apr			-4.0%	-3.0%	-34.7%	-38.0%	-37.8%	-62.5%	-10.9%	24.6%	25.5%
May			-5.7%	-5.1%	-39.4%	-39.4%	-39.3%	-60.4%	3.5%	19.4%	20.0%
Jun			-7.9%	-7.5%	-42.6%	-40.8%	-40.7%	-59.1%	15.2%	15.3%	15.8%
Season_2	**-50.6%**	**-79.3%**	**-5.8%**	**-5.1%**	**-38.9%**	**-39.6%**	**-39.4%**	**-60.6%**	**2.6%**	**19.5%**	**20.2%**
Jul			-7.0%	-6.7%	-45.0%	-42.1%	-41.9%	-58.3%	24.7%	10.4%	10.7%
Aug			-6.6%	-6.4%	-46.8%	-43.3%	-43.1%	-57.7%	32.3%	13.9%	14.8%
Sep			-8.4%	-8.2%	-48.2%	-44.4%	-44.1%	-57.4%	38.4%	18.7%	19.9%
Season_3	**-73.0%**	**-86.6%**	**-7.3%**	**-7.1%**	**-46.7%**	**-43.3%**	**-43.1%**	**-57.8%**	**31.8%**	**14.9%**	**15.8%**
Oct			-7.0%	-6.9%	-49.3%	-45.3%	-45.0%	-57.2%	43.3%	23.9%	25.2%
Nov			-4.4%	-4.3%	-50.1%	-46.2%	-45.8%	-57.1%	47.2%	24.7%	25.7%
Dec			-3.5%	-3.4%	-50.8%	-46.9%	-46.5%	-57.1%	50.4%	28.2%	29.4%
Season_4	**-65.5%**	**-81.8%**	**-4.7%**	**-4.6%**	**-50.1%**	**-46.2%**	**-45.8%**	**-57.2%**	**47.0%**	**25.6%**	**26.8%**
Annual	**-57.6%**	**-80.3%**	**-4.5%**	**-4.2%**	**-40.5%**	**-43.1%**	**-42.8%**	**-60.5%**	**7.9%**	**20.1%**	**21.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

B.1.4. Comparison of calculated values of PCB-28 mass in vegetation

Reference data set. Calculation results on PCB-28 mass in vegetation (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.19.

Monthly values of PCB-28 mass in vegetation calculated by participating models on the basis of "reference" data set are compared in Fig. B.13.

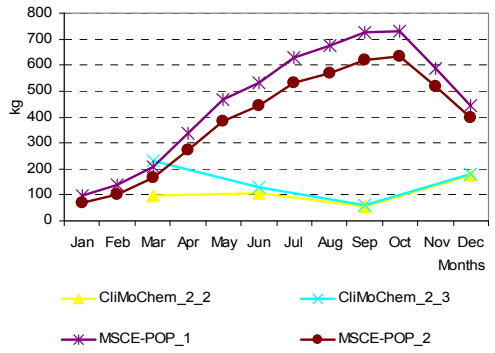


Fig. B.13. *PCB-28 mass in vegetation (kg) calculated by the participating models on the basis of "reference" data set*

Own/alternative data set. Calculation results on PCB-28 mass in vegetation (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.20.

Monthly values of PCB-28 mass in vegetation calculated by participating models on the basis of "own or alternative" data sets are compared in Fig. B.14.

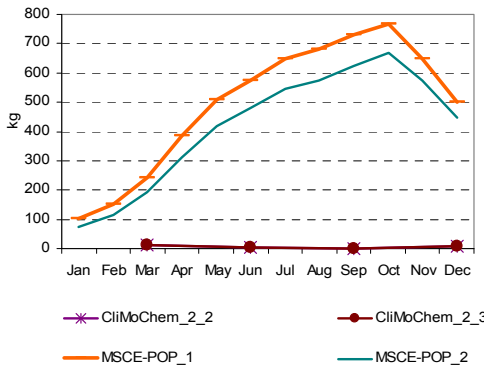


Fig. B.14. *PCB-28 mass in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets*

Table B.19. *Calculation results: PCB-28 mass in vegetation (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	97.1				Jan		68.4		
Feb	136.5				Feb		102.6		
Mar	209.9				Mar		164.5		
Season_1	**147.85**	**230.42**	***189.1***	***58.4***	**Season_1**	**96.0**	**111.82**	***103.9***	***11.2***
Apr	335.4				Apr		272.1		
May	466.2				May		385.4		
Jun	531.2				Jun		442.7		
Season_2	**444.24**	**131.20**	***287.7***	***221.4***	**Season_2**	**104.6**	**366.75**	***235.7***	***185.3***
Jul	629.8				Jul		530.0		
Aug	673.9				Aug		569.2		
Sep	723.7				Sep		619.0		
Season_3	**675.83**	**60.92**	***368.4***	***434.8***	**Season_3**	**54.4**	**572.73**	***313.6***	***366.5***
Oct	731.0				Oct		634.0		
Nov	588.9				Nov		518.0		
Dec	445.7				Dec		396.2		
Season_4	**588.51**	**182.15**	***385.3***	***287.3***	**Season_4**	**175.0**	**516.08**	***345.5***	***241.2***
Annual	**464.1**	**151.17**	***307.6***	***221.3***	**Annual**	**107.5**	**391.8**	***249.7***	***201.1***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.20. *Calculation results: PCB-28 mass in vegetation (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	104.61				Jan		75.05		
Feb	153.15				Feb		116.55		
Mar	243.23				Mar		192.42		
Season_1	**166.99**	**11.31**	***89.15***	***110.09***	**Season_1**	**10.58**	**128.01**	***69.29***	***83.04***
Apr	384.87				Apr		313.22		
May	507.94				May		420.08		
Jun	572.90				Jun		478.02		
Season_2	**488.57**	**2.76**	***245.66***	***343.52***	**Season_2**	**2.47**	**403.77**	***203.12***	***283.76***
Jul	649.24				Jul		546.17		
Aug	680.84				Aug		574.97		
Sep	730.32				Sep		624.68		
Season_3	**686.80**	**0.75**	***343.77***	***485.11***	**Season_3**	**0.58**	**581.94**	***291.26***	***411.08***
Oct	767.65				Oct		667.22		
Nov	649.13				Nov		573.41		
Dec	501.65				Dec		448.58		
Season_4	**639.48**	**7.65**	***323.56***	***446.77***	**Season_4**	**7.47**	**563.07**	***285.27***	***392.87***
Annual	**495.46**	**5.62**	***250.54***	***346.37***	**Annual**	**5.27**	**419.20**	***212.24***	***292.69***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.21.

Table B.21. *The percentage difference between calculation results on PCB-28 mass in vegetation (kg) obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_ 2_2	CliMoChem_ 2_3	MSCE-POP_1	MSCE-POP_2
Jan			7.7%	9.7%
Feb			12.2%	13.6%
Mar			15.9%	17.0%
Season_ 1	**-89.0%**	**-95.1%**	**12.9%**	**14.5%**
Apr			14.8%	15.1%
May			9.0%	9.0%
Jun			7.9%	8.0%
Season_ 2	**-97.6%**	**-97.9%**	**10.0%**	**10.1%**
Jul			3.1%	3.1%
Aug			1.0%	1.0%
Sep			0.9%	0.9%
Season_ 3	**-98.9%**	**-98.8%**	**1.6%**	**1.6%**
Oct			5.0%	5.2%
Nov			10.2%	10.7%
Dec			12.6%	13.2%
Season_ 4	**-95.7%**	**-95.8%**	**8.7%**	**9.1%**
Annual	**-95.1%**	**-96.3%**	**6.8%**	**7.0%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

B.1.5. Comparison of distribution of PCB-28 mass between environmental media

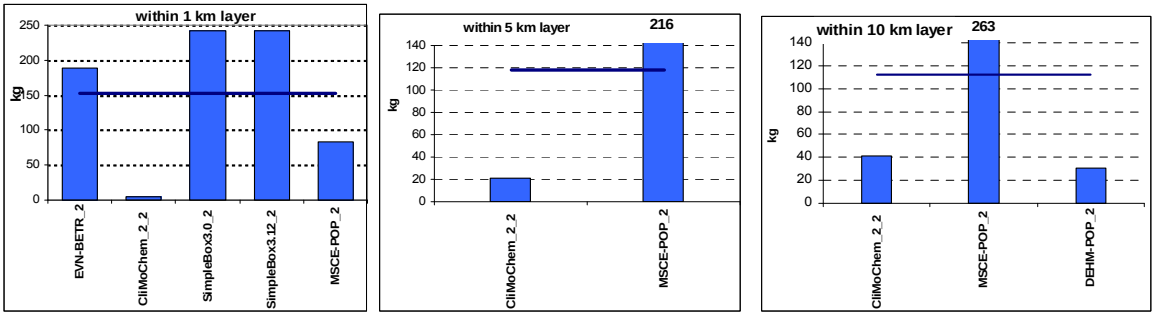
Mass balance estimates presented in Sections B.1.1-B.1.4 comprise masses of PCB-28 contained in different environmental compartments calculated by the participating models. The considered estimates of mass distribution in 2000 include results of one-year calculation with zero initial concentrations obtained by DEHM-POP, MSCE-POP, SimpleBox 3.0 and 3.12 models and with initial concentrations in media given as input data calculated by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP, and SimpleBox 3.0 models; as well as results of long-term calculations for 20-year period with zero initial data with historical emissions carried out by CliMoChem and SimpleBox 3.0 and 3.12 models. Results of CliMoChem, DEHM-POP, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of these models' calculations to the variations in the input data.

A comparison of absolute values and relative fractions of PCB-28 mass contained in the main environmental compartments is presented in this section. The comparison is made separately for results calculated on the basis of initial concentrations or historical emissions (non-zero initial conditions) and for results based on zero initial conditions.

Atmosphere. Comparison of annual values of PCB-28 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "reference" data set is presented in Fig. B.15a. Fig. B.15b shows the same results but

obtained on the basis of initial concentrations or historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

a



b

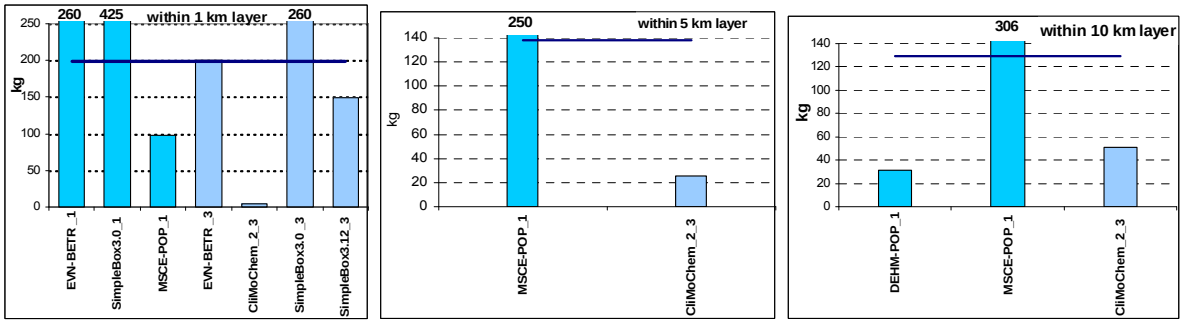


Fig. B.15. *Comparison of annual values of PCB-28 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of air content profiles of annual values of PCB-28 mass calculated by MSCE-POP and CliMoChem models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set is presented in Fig. B.16.

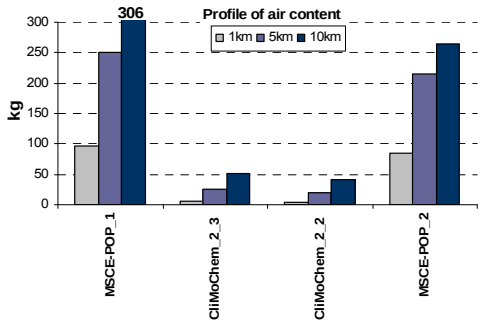


Fig. B.16. *Comparison of air content profiles of annual values of PCB-28 mass calculated by four models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set*

Comparison of annual values of PCB-28 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig. B.17a. Fig. B.17b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

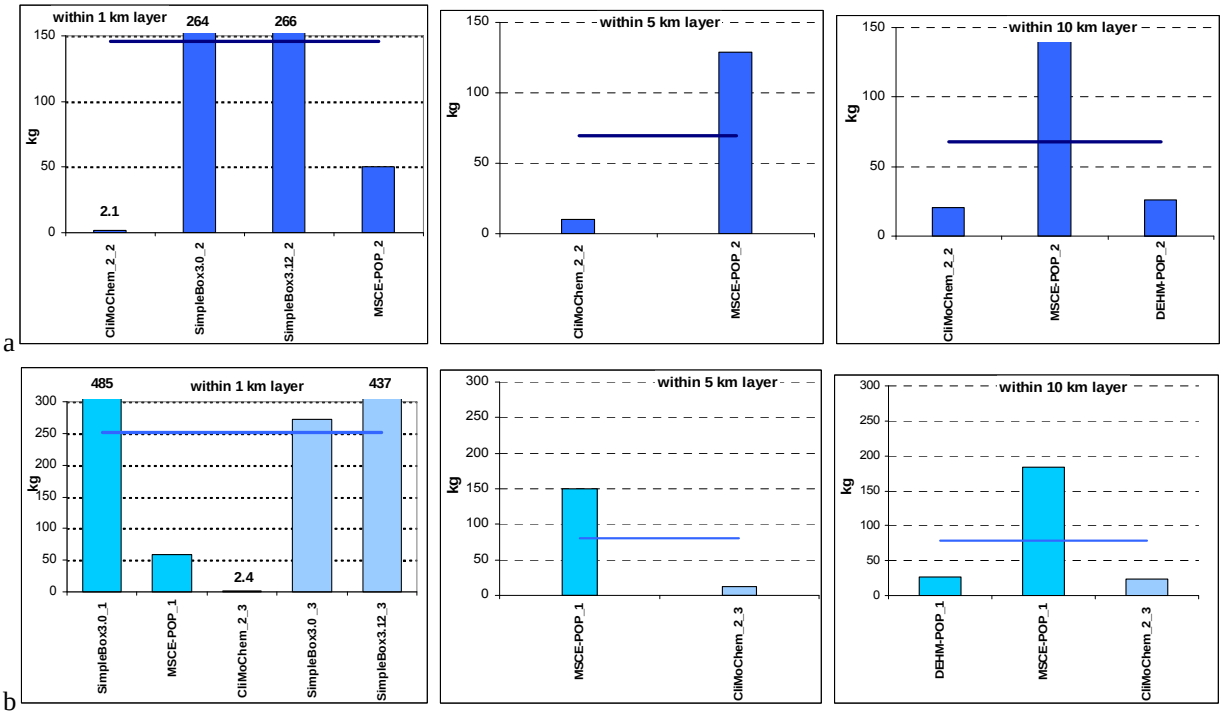


Fig. B.17. *Comparison of annual values of PCB-28 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of air content profiles of annual values of PCB-28 mass calculated by MSCE-POP and CliMoChem models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative" data sets is presented in Fig. B.18.

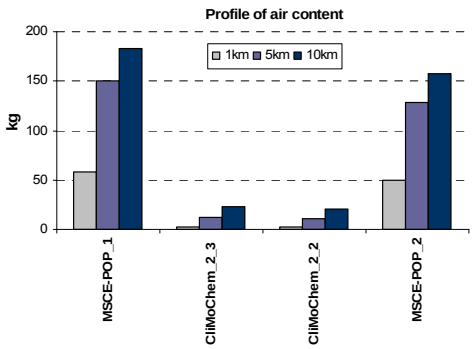


Fig. B.18. *Comparison of air content profiles of annual values of PCB-28 mass calculated by five models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative data sets"*

Comparison of annual values of PCB-28 mass contained in 1, 5 and 10 km layers of the atmosphere obtained by the participating models with the use of "reference" and "own/alternative" data sets is presented in Fig. B.19.

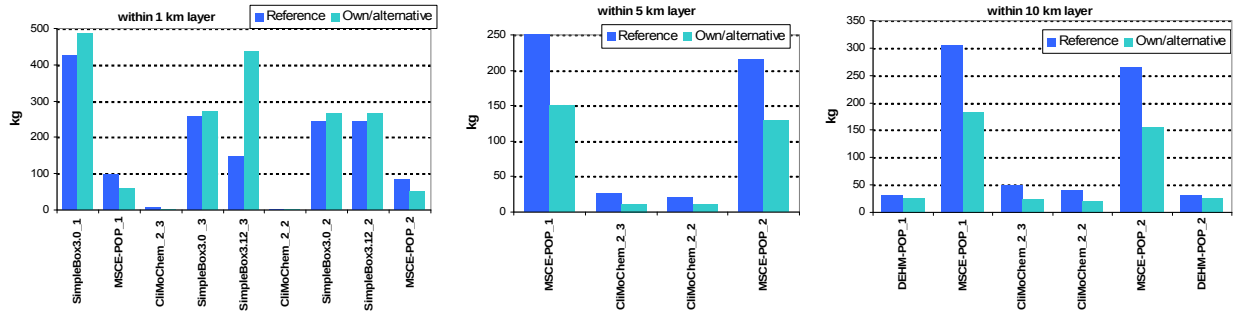


Fig. B.19. *Comparison of PCB-28 mass contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of two data set*

Soil. Comparison of annual values of PCB-28 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "reference" data set is presented in Fig. B.20a. Fig. B.20b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

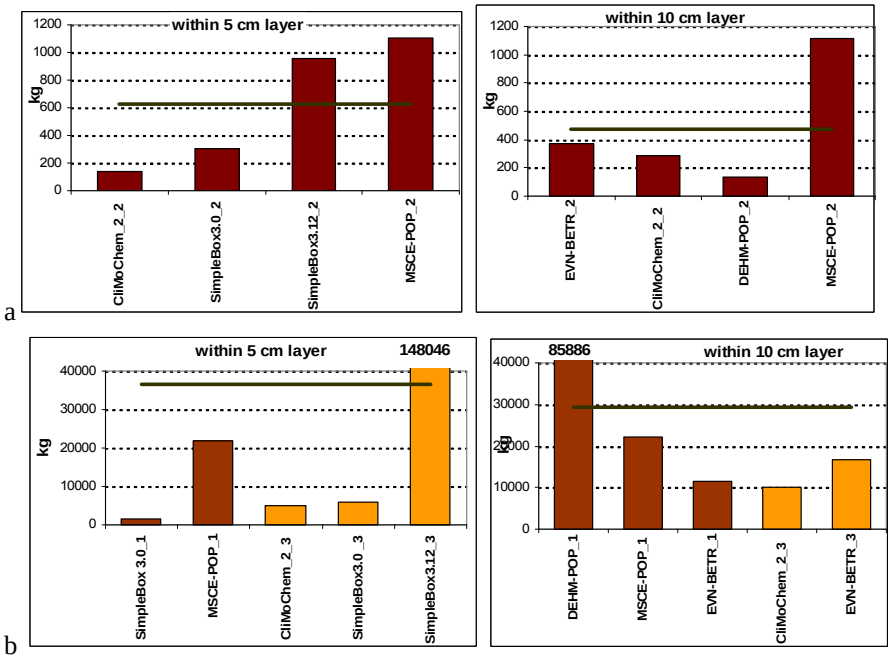


Fig. B.20. *Comparison of annual values of PCB-28 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of soil content profiles of annual values of PCB-28 mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set is presented in Fig. B.21.

Comparison of annual values of PCB-28 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig. B.22a. Fig. B.22b shows the same results but obtained on the basis of initial concentrations or historical emissions. Different color of columns corresponds to the

different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

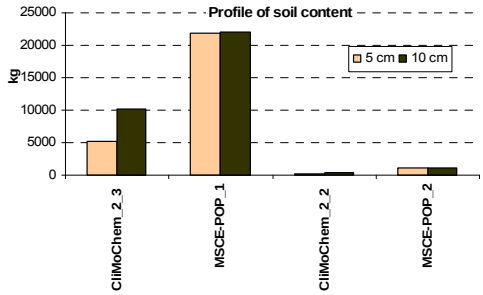


Fig. B.21. *Comparison of soil content profiles of annual values of PCB-28 mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set*

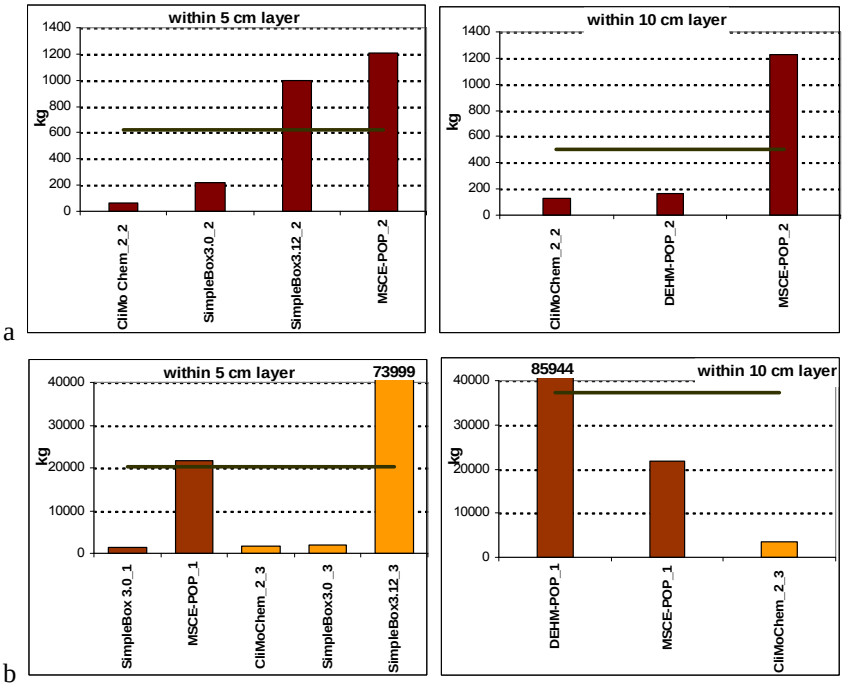


Fig. B.22. *Comparison of annual values of PCB-28 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non- zero initial conditions)*

Comparison of soil content profiles of annual values of PCB-28 mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets is presented in Fig. B.23.

Comparison of annual values of PCB-28 mass contained in the considered different layers of soil obtained with "reference" and "own/alternative" data sets is presented in Fig. B.24.

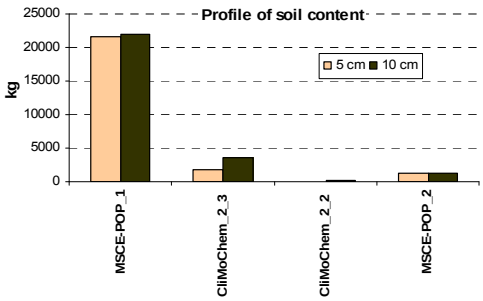


Fig. B.23. *Comparison of soil content profiles of annual values of PCB-28 mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets*

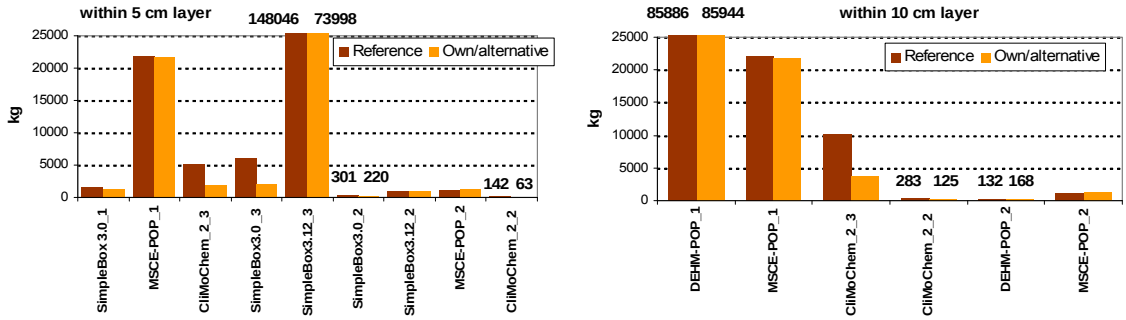


Fig. B.24. *Comparison of PCB-28 mass contained within 5 and 10 cm soil layers calculated by different models on the basis of two data set*

Water. Comparison of annual values of PCB-28 water content calculated by different models on the basis of zero initial concentrations and with the use of "***reference"*** data set is presented in Fig. B.25a. Fig. B.25b shows the same results but obtained on the basis of initial concentrations or historical emissions. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plot shows the value of the corresponding parameter averaged between models.

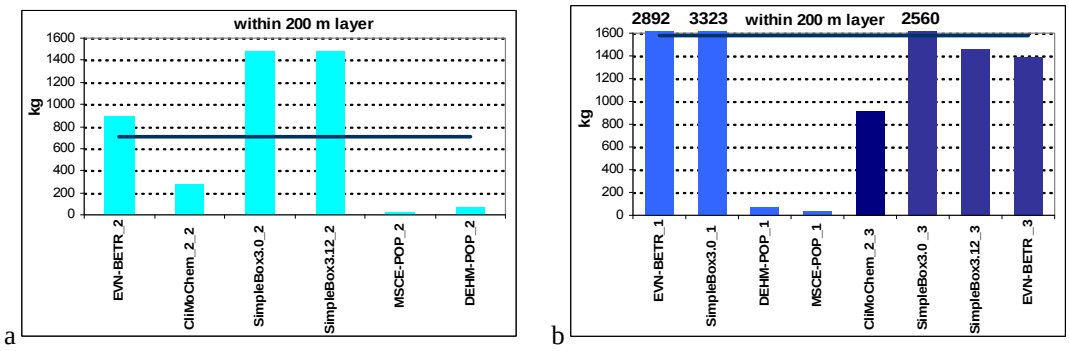


Fig. B.25. *Comparison of annual values of PCB-28 masses contained in water within 200 m layer calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Figs.3.26a and B.26b show the annual values of PCB-28 masses contained in water layer of 200 m and calculated by different models on the basis of "***own or alternative***" data set and zero and non-zero initial conditions, respectively (blue line corresponds to the averaged value). Different color of columns corresponds to the different types of calculations (a - one-year calculations on the basis of zero initial conditions; b - one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

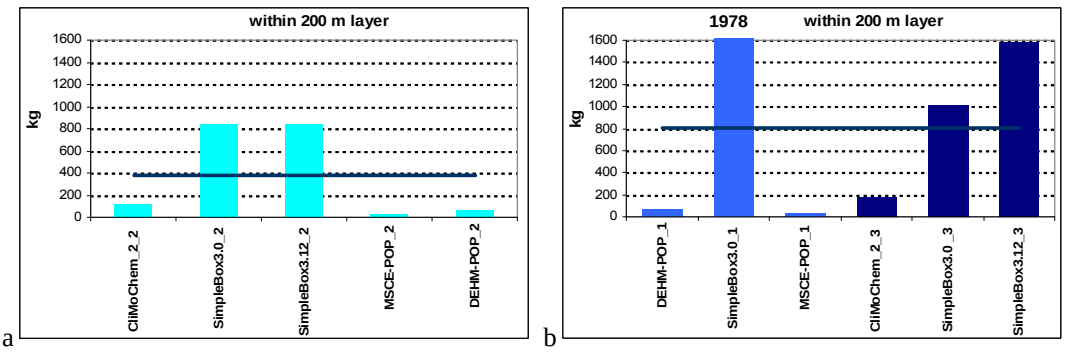


Fig. B.26. *Comparison of annual values of PCB-28 masses contained in water within 200 m layer calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-28 mass contained in the 200m layer of water obtained by the participating models on the basis of "reference" and "own/alternative" data sets is presented in Fig. B.27.

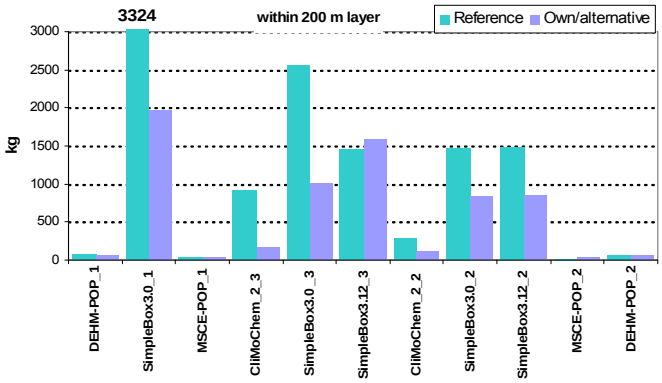


Fig. B.27. *Comparison of PCB-28 mass contained within 200 m water layer calculated by different models on the basis of two data sets*

Vegetation. Annual values of PCB-28 mass contained in vegetation obtained on the basis of zero initial conditions and with the use of "reference" and "own/alternative" data sets are presented in Fig. B.28a.

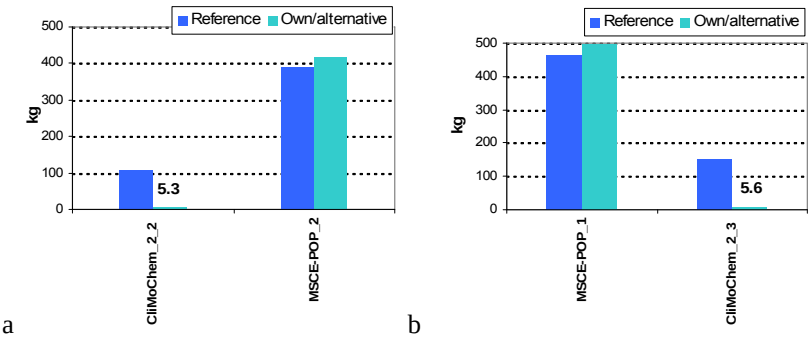


Fig. B.28. *Comparison of PCB-28 mass contained in vegetation calculated by different models on the basis of "reference" and "own/alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Relative distribution of PCB mass. The distribution of PCB-28 mass between main environmental compartments averaged for the results obtained by the participating models on the basis of zero and non-zero initial conditions is presented in Fig. B.29a and b, respectively. In this figure results calculated with the use of “reference” and “own/alternative” data sets are given. Of note, absolute values of averaged mass of PCB-28 in each media calculated with two different data sets of physical-chemical properties could not be directly compared since calculation results of different participating models are enclosed in these averaged figures.

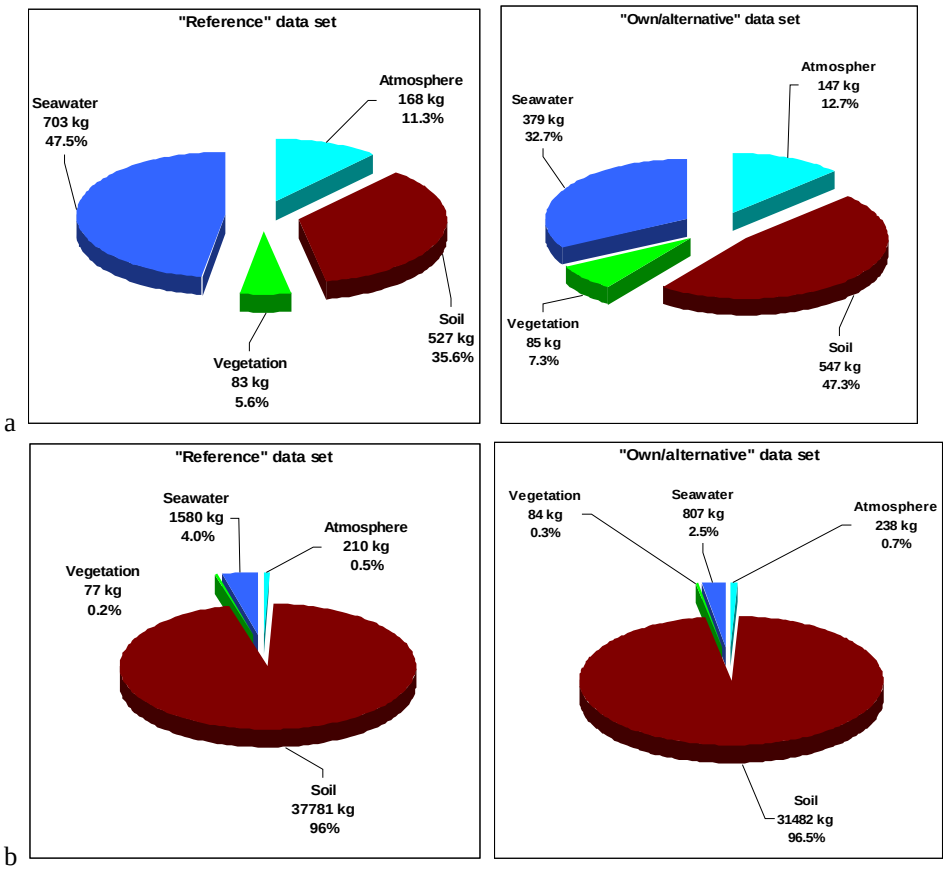
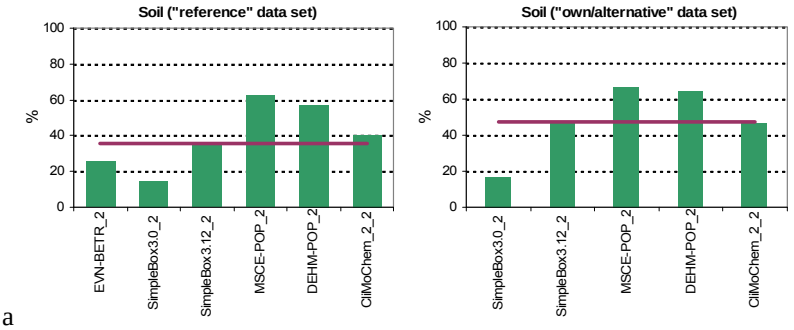
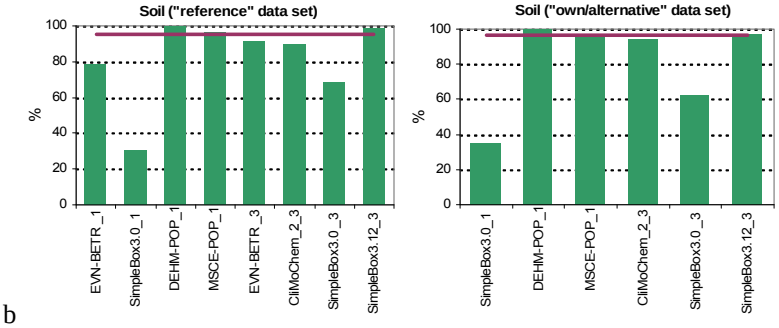


Fig. B.29. *Distribution of PCB-28 mass between environmental compartments (kg) averaged for all participating models and calculated on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

To show redistribution of the pollutant between main environmental compartments for each participating model in more detail, plots of PCB-28 fractions in different environmental compartments calculated by the models on the basis of zero and non-zero initial conditions are presented in Figs. B.30a and b, respectively. In these figures fractions of PCB-28 mass in soil calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.



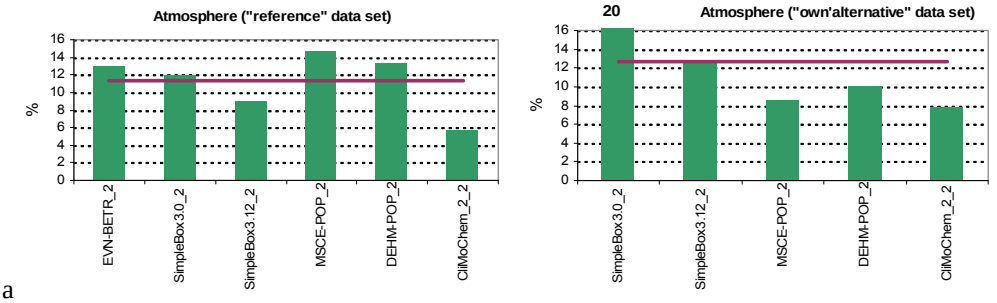
a



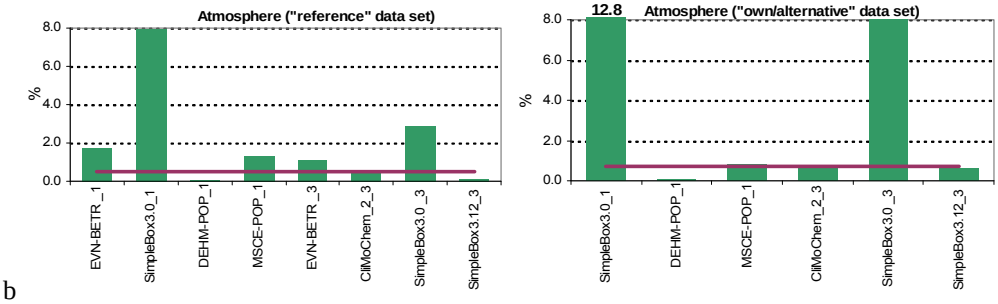
b

Fig. B.30. *Fractions of PCB-28 mass in soil calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of PCB-28 mass in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. B.31a and b, respectively. In these figures fractions of PCB-28 mass in the atmosphere calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.



a



b

Fig. B.31. *Fractions of PCB-28 mass in the atmosphere calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of PCB-28 mass in seawater calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. B.32a and b, respectively. In these figures fractions of PCB-28 mass in seawater calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.

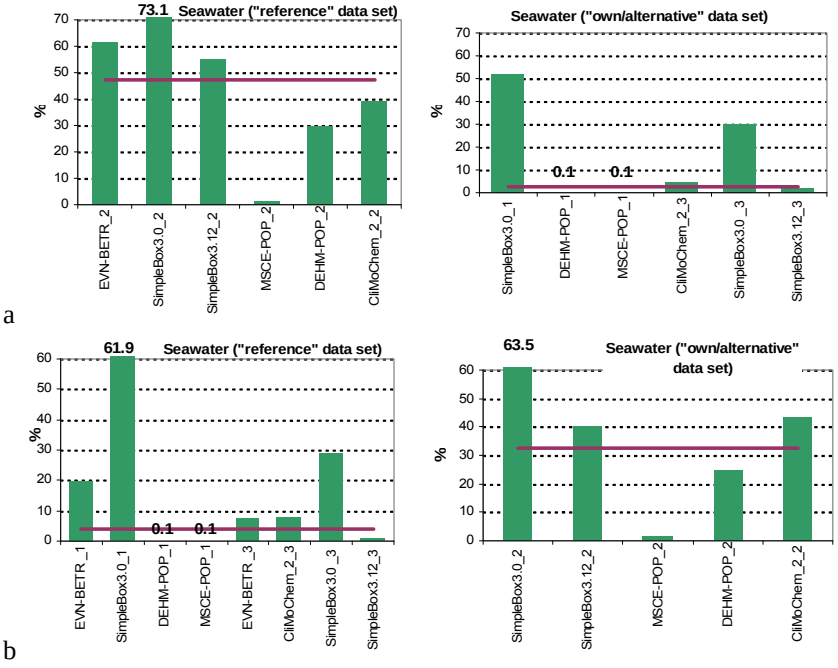


Fig. B.32. *Fractions of PCB-28 mass in seawater calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of total environmental mass of PCB-28 contained in vegetation calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. B.33a and b, respectively. In these figures fractions of PCB-28 mass in vegetation calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models. Of note, the models, for which vegetation compartment was not included into calculations of mass balance, are also shown in the plots.

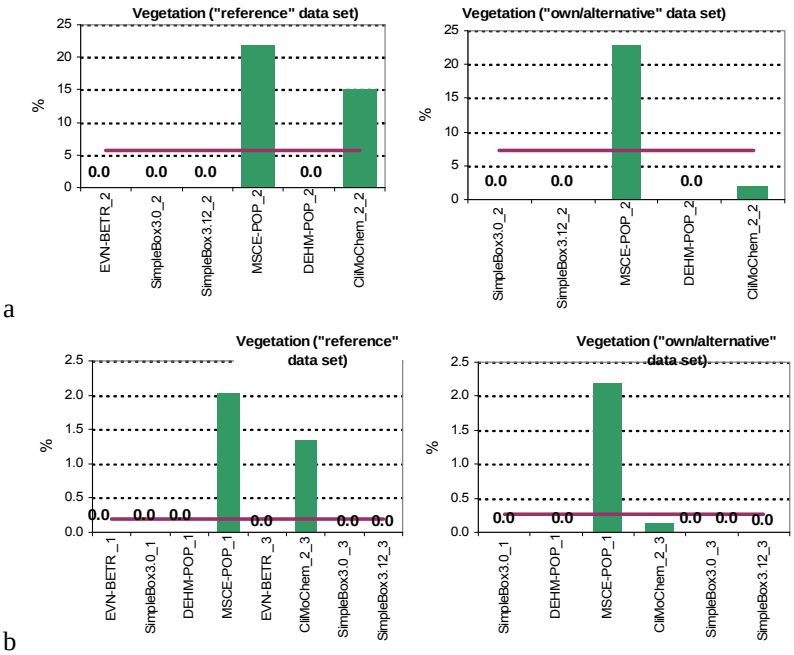


Fig. B.33. *Fractions of PCB-28 mass in vegetation calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

B.2. Masses degraded in the environmental compartments

B.2.1. Comparison of calculated values of PCB-28 mass degraded in the atmosphere

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-28 degraded in the atmosphere within layers of 1 km, 5 km and 10 km height.

Reference data set. Calculation results on PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.22.

Monthly values of PCB-28 mass degraded in 1 km layer of the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.34 a and b, respectively. Seasonal variations of low values of mass contained in 1 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. B.34c in more detail.

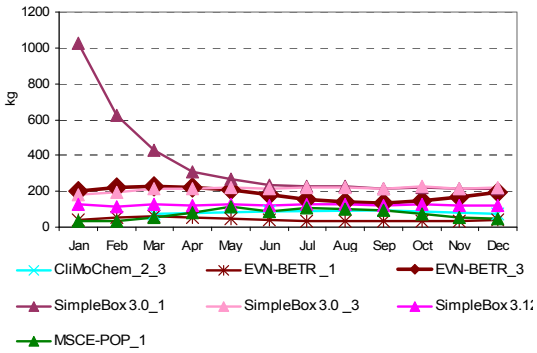


Fig. B.34a. *PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

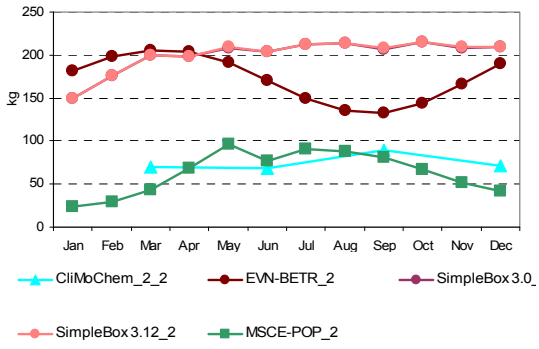


Fig. B.34b. *PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

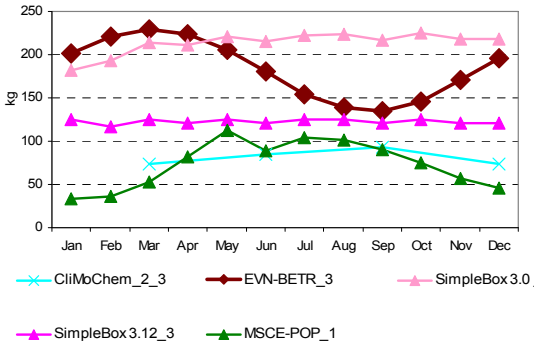


Fig. B.34c. *PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Calculation results on PCB-28 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.23.

Monthly values of PCB-28 mass degraded in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. B.35.

Calculation results on PCB-28 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.24.

Monthly values of PCB-28 mass degraded in 10 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set are compared in Fig. B.36.

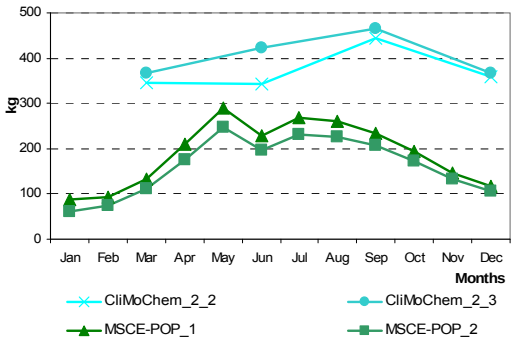


Fig. B.35. *PCB-28 mass degraded in 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

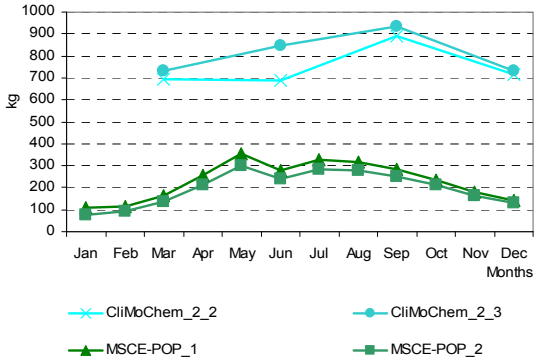


Fig. B.36. *PCB-28 mass degraded in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

Table B.22. *Calculation results: PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	MSCE-POP_1	EVN-BETR_1[a]	SimpleBox 3.0_1[b]	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0_3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	34.02	42.83	1026.38	201.04		181.46	125.40	*268.52*	*377.60*	Jan	181.49		149.24	149.25	24.05	*126.01*	*69.65*
Feb	36.10	55.24	621.15	221.39		193.51	117.31	*207.45*	*215.49*	Feb	198.90		176.09	176.14	28.85	*144.99*	*78.17*
Mar	52.10	59.18	426.51	229.43		214.37	125.40	*184.50*	*140.15*	Mar	205.89		199.50	199.61	43.32	*162.08*	*79.23*
Seas_1	**122.22**	**157.25**	**2074.03**	**651.86**	**73.17**	**589.34**	**368.10**	***576.57***	***698.49***	**Seas_1**	**586.28**	**69.33**	**524.82**	**524.99**	**96.22**	***360.33***	***254.78***
Apr	81.55	54.36	305.34	224.27		211.30	121.35	*166.36*	*96.39*	Apr	203.54		198.79	198.97	68.44	*167.43*	*66.03*
May	112.81	45.19	265.17	206.16		220.56	125.40	*162.55*	*81.76*	May	190.93		208.67	208.94	95.75	*176.07*	*54.21*
Jun	89.48	37.24	234.16	180.04		214.78	121.35	*146.18*	*76.54*	Jun	170.52		203.88	204.22	76.51	*163.78*	*60.29*
Seas_2	**283.85**	**136.78**	**804.68**	**610.47**	**84.70**	**646.63**	**368.10**	***419.32***	***273.70***	**Seas_2**	**564.98**	**68.71**	**611.34**	**612.13**	**240.70**	***419.57***	***250.05***
Jul	104.41	33.88	231.28	154.62		222.88	125.40	*145.41*	*74.81*	Jul	149.06		212.05	212.48	90.12	*165.93*	*58.67*
Aug	101.47	34.41	226.24	138.46		223.61	125.40	*141.60*	*73.84*	Aug	134.92		213.09	213.61	88.15	*162.44*	*61.80*
Sep	90.96	34.73	216.70	135.03		216.95	121.35	*135.95*	*71.50*	Sep	132.23		207.03	207.60	80.59	*156.86*	*61.95*
Seas_3	**296.84**	**103.01**	**674.23**	**428.12**	**93.21**	**663.43**	**372.14**	***375.86***	***236.31***	**Seas_3**	**416.21**	**89.01**	**632.17**	**633.68**	**258.86**	***405.99***	***237.29***
Oct	75.45	34.63	222.83	146.10		224.67	125.40	*138.18*	*76.85*	Oct	143.17		214.63	215.31	67.48	*160.14*	*70.44*
Nov	56.96	35.04	215.15	170.47		217.83	121.35	*136.13*	*78.49*	Nov	166.53		208.31	209.04	51.52	*158.85*	*74.26*
Dec	45.15	40.50	214.92	196.42		218.19	121.35	*139.42*	*82.65*	Dec	190.46		208.83	209.64	41.41	*162.59*	*81.27*
Seas_4	**177.56**	**110.17**	**652.89**	**513.00**	**73.14**	**660.69**	**368.10**	***365.08***	***250.83***	**Seas_4**	**500.16**	**71.67**	**631.77**	**633.98**	**160.40**	***399.60***	***266.32***
Annual	**880.47**	**507.22**	**4205.83**	**2203.45**	**324.22**	**2560.09**	**1476.44**	***1736.82***	***1372.35***	**Annual**	**2067.63**	**298.72**	**2400.10**	**2404.79**	**756.19**	***1585.49***	***988.79***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;

[b] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.23. *Calculation results: PCB-28 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	87.40				Jan		61.80		
Feb	92.77				Feb		74.13		
Mar	133.87				Mar		111.32		
Seas_1	**314.05**	**365.87**	***339.96***	***36.64***	**Seas_1**	**346.64**	**247.25**	***296.95***	***70.28***
Apr	209.54				Apr		175.86		
May	289.88				May		246.02		
Jun	229.93				Jun		196.59		
Seas_2	**729.36**	**423.49**	***576.42***	***216.28***	**Seas_2**	**343.57**	**618.48**	***481.02***	***194.39***
Jul	268.29				Jul		231.56		
Aug	260.73				Aug		226.51		
Sep	233.72				Sep		207.08		
Seas_3	**762.75**	**466.07**	***614.41***	***209.78***	**Seas_3**	**445.06**	**665.16**	***555.11***	***155.63***
Oct	193.88				Oct		173.38		
Nov	146.36				Nov		132.37		
Dec	116.00				Dec		106.41		
Seas_4	**456.25**	**365.69**	***410.97***	***64.03***	**Seas_4**	**358.34**	**412.16**	***385.25***	***38.06***
Annual	**2262.40**	**1621.12**	***1941.76***	***453.45***	**Annual**	**1493.61**	**1943.05**	***1718.33***	***317.80***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

Table B.24. *Calculation results: PCB-28 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	106.89				Jan		75.58		
Feb	113.45				Feb		90.65		
Mar	163.72				Mar		136.14		
Seas_1	**384.06**		***557.90***	***245.85***	**Seas_1**	**693.29**	**302.37**	***497.83***	***276.42***
Apr	256.26	**731.74**			Apr		215.07		
May	354.51				May		300.87		
Jun	281.19				Jun		240.42		
Seas_2	**891.96**		***869.47***	***31.80***	**Seas_2**	**687.14**	**756.36**	***721.75***	***48.94***
Jul	328.11	**846.98**			Jul		283.18		
Aug	318.85				Aug		277.01		
Sep	285.83				Sep		253.25		
Seas_3	**932.79**		***932.46***	***0.47***	**Seas_3**	**890.11**	**813.44**	***851.78***	***54.21***
Oct	237.11	**932.13**			Oct		212.04		
Nov	178.99				Nov		161.88		
Dec	141.87				Dec		130.14		
Seas_4	**557.96**		***644.68***	***122.63***	**Seas_4**	**716.68**	**504.05**	***610.36***	***150.35***
Annual	**2766.77**	**731.39**	***3004.51***	***336.21***	**Annual**	**2987.22**	**2376.23**	***2681.72***	***432.03***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Own/alternative data set. Calculation results on PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.25.

Monthly values of PCB-28 mass degraded in 1 km layer of the atmosphere calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.37 a and b, respectively. Seasonal variations of low values of mass contained in 1 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. B.37c in more detail.

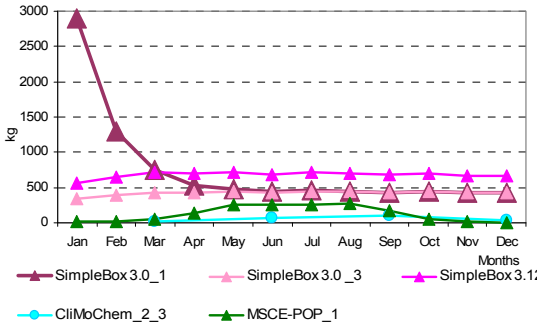


Fig. B.37a. *PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own/alternative" data set and non-zero initial conditions (all models)*

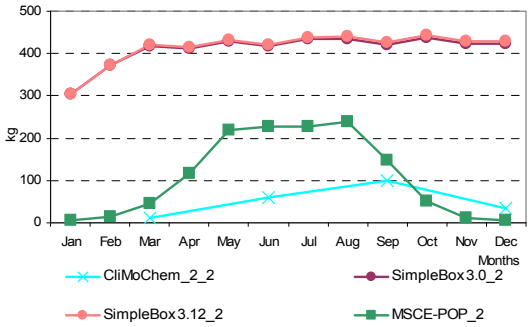


Fig. B.37b. *PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own/alternative" data set and zero-initial conditions*

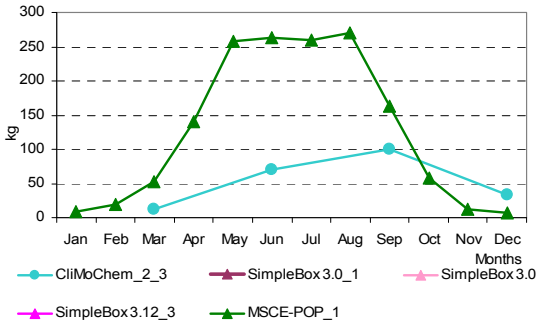


Fig. B.37c. *PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Calculation results on PCB-28 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data set together with statistical parameters used for evaluation are presented in Table B.26.

Monthly values of PCB-28 mass degraded in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. B.38.

Calculation results on PCB-28 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative data sets” together with statistical parameters used for evaluation are presented in Table B.27.

Monthly values of PCB-28 mass degraded in 10 km layer of the atmosphere calculated by the participating models on the basis of “own or alternative” data sets are compared in Fig. B.39.

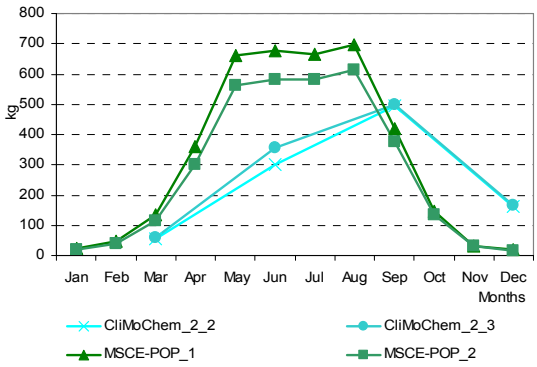


Fig. B.38. *PCB-28 mass degraded in 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own/alternative” data set*

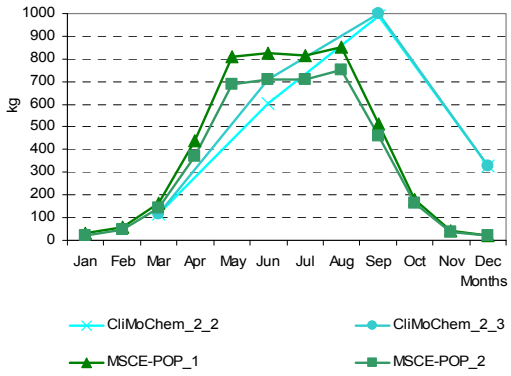


Fig. B.39. *PCB-28 mass degraded in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own/alternative” data set*

Table B.25. *Calculation results: PCB-28 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMo Chem_ 2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	9.45	2889.68		338.79	555.28	*948.30*	*1313.57*	Jan		302.59	302.69	7.10	*204.13*	*170.63*
Feb	18.62	1297.97		384.96	644.60	*586.54*	*539.34*	Feb		371.17	371.65	15.24	*252.69*	*205.63*
Mar	52.89	746.14		429.66	714.07	*485.69*	*321.69*	Mar		418.41	419.48	44.73	*294.21*	*216.06*
Seas_1	**81.0**	**4933.8**	**11.65**	**1153.4**	**1914.0**	***1618.75***	***2014.99***	**Seas_1**	**11.39**	**1092.17**	**1093.82**	**67.07**	***566.11***	***608.82***
Apr	140.40	524.38		422.41	695.25	*445.61*	*232.54*	Apr		412.79	414.43	117.74	*314.99*	*170.82*
May	257.90	479.10		439.51	716.25	*473.19*	*188.50*	May		430.15	432.47	218.63	*360.42*	*122.79*
Jun	263.00	444.17		427.00	689.37	*455.88*	*175.77*	Jun		418.26	421.11	225.87	*355.08*	*111.91*
Seas_2	**661.3**	**1447.7**	**71.02**	**1288.9**	**2100.9**	***1113.95***	***775.98***	**Seas_2**	**60.27**	**1261.21**	**1268.01**	**562.25**	***787.94***	***587.33***
Jul	258.79	452.17		442.42	708.03	*465.36*	*184.63*	Jul		433.65	437.20	226.00	*365.62*	*120.93*
Aug	271.05	449.53		443.37	703.71	*466.91*	*178.22*	Aug		434.81	438.98	238.73	*370.84*	*114.43*
Sep	162.74	433.88		429.82	677.01	*425.86*	*210.07*	Sep		421.70	426.30	146.91	*331.64*	*159.99*
Seas_3	**692.6**	**1335.6**	**99.95**	**1315.6**	**2088.8**	***1106.50***	***749.25***	**Seas_3**	**98.93**	**1290.16**	**1302.48**	**611.64**	***825.80***	***582.25***
Oct	57.76	447.67		444.81	695.61	*411.46*	*263.48*	Oct		436.58	441.90	52.53	*310.34*	*223.28*
Nov	12.81	432.83		431.00	669.52	*386.54*	*273.17*	Nov		423.18	428.88	11.85	*287.97*	*239.15*
Dec	6.99	432.58		431.48	666.05	*384.28*	*274.66*	Dec		423.78	430.01	6.54	*286.78*	*242.72*
Seas_4	**77.6**	**1313.1**	**32.90**	**1307.3**	**2031.2**	***952.40***	***870.44***	**Seas_4**	**32.79**	**1283.54**	**1300.80**	**70.91**	***672.01***	***716.30***
Annual	**1512.40**	**9030.11**	**215.51**	**5065.23**	**8134.77**	***4791.60***	***3902.25***	**Annual**	**203.38**	**4927.08**	**4965.10**	**1311.87**	***2851.86***	***2460.24***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.26. *Calculation results: PCB-28 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	24.28				Jan		18.23		
Feb	47.85				Feb		39.17		
Mar	135.90				Mar		114.93		
Seas_1	**208.03**	**58.24**	***133.14***	***105.91***	**Seas_1**	**56.96**	**172.34**	***114.65***	***81.58***
Apr	360.75				Apr		302.55		
May	662.68				May		561.79		
Jun	675.80				Jun		580.39		
Seas_2	**1699.23**	**355.08**	***1027.15***	***950.46***	**Seas_2**	**301.37**	**1444.72**	***873.05***	***808.47***
Jul	664.98				Jul		580.70		
Aug	696.48				Aug		613.44		
Sep	418.16				Sep		377.49		
Seas_3	**1779.62**	**499.77**	***1139.69***	***904.99***	**Seas_3**	**494.64**	**1571.63**	***1033.14***	***761.55***
Oct	148.43				Oct		134.98		
Nov	32.91				Nov		30.44		
Dec	17.96				Dec		16.79		
Seas_4	**199.29**	**164.48**	***181.89***	***24.62***	**Seas_4**	**163.93**	**182.21**	***173.07***	***12.93***
Annual	**3886.17**	**1077.57**	***2481.87***	***1985.98***	**Annual**	**1016.90**	**3370.91**	***2193.90***	***1664.53***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table B.27. *Calculation results: PCB-28 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	sults obtained n the basis of initial oncentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	MSCE-POP_2		
Jan	29.69				Jan		22.30		
Feb	58.52				Feb		47.90		
Mar	166.19				Mar		140.56		
Seas_1	**254.41**	**116.49**	***185.45***	***97.52***	**Seas_1**	**113.92**	**210.76**	***162.34***	***68.48***
Apr	441.18				Apr		370.00		
May	810.42				May		687.03		
Jun	826.46				Jun		709.78		
Seas_2	**2078.06**	**710.15**	***1394.10***	***967.25***	**Seas_2**	**602.75**	**1766.81**	***1184.78***	***823.12***
Jul	813.23				Jul		710.17		
Aug	851.75				Aug		750.19		
Sep	511.39				Sep		461.65		
Seas_3	**2176.36**	**999.55**	***1587.95***	***832.13***	**Seas_3**	**989.28**	**1922.01**	***1455.64***	***659.54***
Oct	181.52				Oct		165.07		
Nov	40.25				Nov		37.23		
Dec	21.96				Dec		20.54		
Seas_4	**243.72**	**328.96**	***286.34***	***60.27***	**Seas_4**	**327.86**	**222.83**	***275.35***	***74.27***
Annual	**4752.54**	**2155.14**	***3453.84***	***1836.64***	**Annual**	**2033.80**	**4122.41**	***3078.11***	***1476.87***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-28 mass degraded in 1, 5 and 10 km layers of obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables B.28 – B.30.

Table B.28. *The percentage difference between calculation results on PCB-28 mass degraded in 1 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			182%	103%	103%	87%	343%	-72%	-70%
Feb			109%	111%	111%	99%	450%	-48%	-47%
Mar			75%	110%	110%	100%	469%	2%	3%
Seas_1	**-84%**	**-84%**	**138%**	**108%**	**108%**	**96%**	**420%**	**-34%**	**-30%**
Apr			72%	108%	108%	100%	473%	72%	72%
May			81%	106%	107%	99%	471%	129%	128%
Jun			90%	105%	106%	99%	468%	194%	195%
Seas_2	**-12%**	**-16%**	**80%**	**106%**	**107%**	**99%**	**471%**	**133%**	**134%**
Jul			96%	105%	106%	99%	465%	148%	151%
Aug			99%	104%	106%	98%	461%	167%	171%
Sep			100%	104%	105%	98%	458%	79%	82%
Seas_3	**11%**	**7%**	**98%**	**104%**	**106%**	**98%**	**461%**	**133%**	**136%**
Oct			101%	103%	105%	98%	455%	-23%	-22%
Nov			101%	103%	105%	98%	452%	-78%	-77%
Dec			101%	103%	105%	98%	449%	-85%	-84%
Seas_4	**-54%**	**-55%**	**101%**	**103%**	**105%**	**98%**	**452%**	**-56%**	**-56%**
Annual	**-32%**	**-34%**	**115%**	**105%**	**106%**	**98%**	**451%**	**72%**	**73%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations; SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data; SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations; SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Table B.29. *The percentage difference between calculation results on PCB-28 mass degraded in 5 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			-72%	-70%
Feb			-48%	-47%
Mar			2%	3%
Seas_1	**-84%**	**-84%**	**-34%**	**-30%**
Apr			72%	72%
May			129%	128%
Jun			194%	195%
Seas_2	**-12%**	**-16%**	**133%**	**134%**
Jul			148%	151%
Aug			167%	171%
Sep			79%	82%
Seas_3	**11%**	**7%**	**133%**	**136%**
Oct			-23%	-22%
Nov			-78%	-77%
Dec			-85%	-84%
Seas_4	**-54%**	**-55%**	**-56%**	**-56%**
Annual	**-32%**	**-34%**	**72%**	**73%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and

with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table B.30. *The percentage difference between calculation results on PCB-28 mass degraded in 10 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			-72%	-70%
Feb			-48%	-47%
Mar			2%	3%
Seas_1	**-84%**	**-84%**	**-34%**	**-30%**
Apr			72%	72%
May			129%	128%
Jun			194%	195%
Seas_2	**-12%**	**-16%**	**133%**	**134%**
Jul			148%	151%
Aug			167%	171%
Sep			79%	82%
Seas_3	**11%**	**7%**	**133%**	**136%**
Oct			-23%	-22%
Nov			-78%	-77%
Dec			-85%	-84%
Seas_4	**-54%**	**-55%**	**-56%**	**-56%**
Annual	**-32%**	**-34%**	**72%**	**73%**

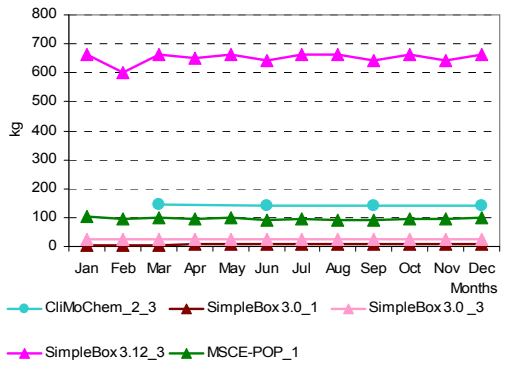
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

3.2.2. Comparison of calculated values of PCB-28 mass degraded in soil

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-28 degraded in soil within 5 cm and 10 cm depth.

Reference data set. Calculation results on PCB-28 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.31.

Monthly values of PCB-28 mass degraded in soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.40a and b, respectively.



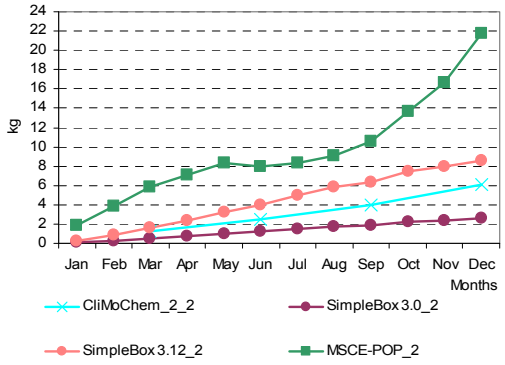
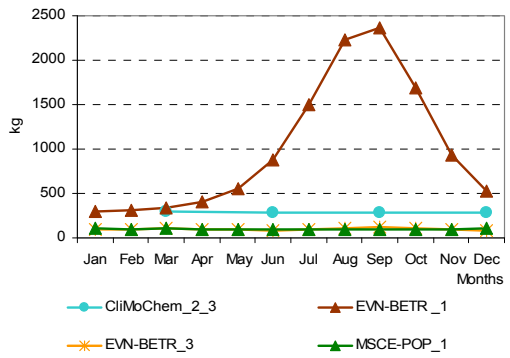


Fig. B.40a. *PCB-28 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. B.40b. *PCB-28 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Calculation results on PCB-28 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.32.

Monthly values of PCB-28 mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.41a and b, respectively. Seasonal variations of low values of mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. B.41c in more detail.



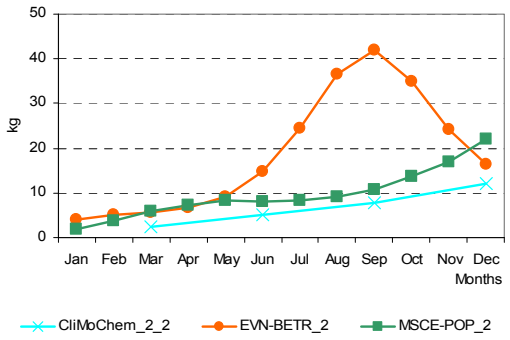


Fig. B.41a. *PCB-28 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

Fig. B.41b. *PCB-28 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

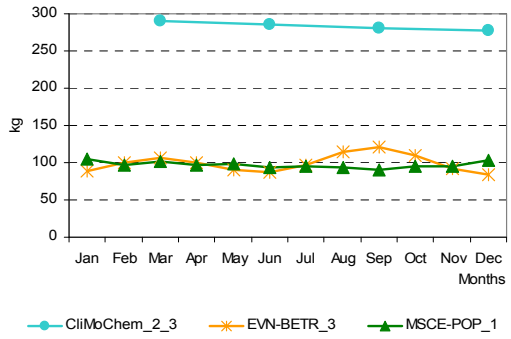


Fig. B.41c. *PCB-28 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Table B.31. *Calculation results: PCB-28 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	103.11	3.95		25.45	664.98	*199.38*	*313.31*	Jan		0.07	0.24	1.80	*0.71*	*0.95*
Feb	94.98	4.98		23.86	600.63	*181.11*	*282.35*	Feb		0.25	0.81	3.85	*1.64*	*1.93*
Mar	100.41	6.08		25.59	664.98	*199.27*	*313.13*	Mar		0.49	1.65	5.89	*2.68*	*2.84*
Seas_1	**298.50**	**15.02**	**145.29**	**74.91**	**1930.59**	***492.86***	***810.66***	**Seas_1**	**1.23**	**0.82**	**2.70**	**11.54**	***4.07***	***5.04***
Apr	96.07	6.35		24.85	649.02	*194.07*	*305.75*	Apr		0.71	2.34	7.07	*3.37*	*3.30*
May	97.90	6.90		25.76	664.98	*198.89*	*313.19*	May		0.98	3.28	8.27	*4.18*	*3.73*
Jun	92.42	6.94		25.02	643.53	*191.98*	*303.27*	Jun		1.19	3.98	7.93	*4.37*	*3.39*
Seas_2	**286.39**	**20.19**	**142.91**	**75.63**	**1957.53**	***496.53***	***822.76***	**Seas_2**	**2.50**	**2.88**	**9.61**	**23.27**	***9.56***	***9.70***
Jul	93.60	7.42		25.95	664.98	*197.99*	*313.52*	Jul		1.48	4.94	8.35	*4.92*	*3.44*
Aug	92.55	7.65		26.05	662.01	*197.06*	*312.10*	Aug		1.73	5.80	9.06	*5.53*	*3.67*
Sep	89.98	7.62		25.30	643.53	*191.61*	*303.35*	Sep		1.91	6.40	10.51	*6.28*	*4.30*
Seas_3	**276.13**	**22.70**	**140.60**	**77.30**	**1970.52**	***497.45***	***828.88***	**Seas_3**	**3.94**	**5.12**	**17.14**	**27.92**	***13.53***	***11.30***
Oct	94.70	8.10		26.24	664.98	*198.50*	*313.21*	Oct		2.22	7.44	13.66	*7.77*	*5.73*
Nov	94.28	8.04		25.48	643.53	*192.83*	*302.76*	Nov		2.39	7.99	16.65	*9.01*	*7.19*
Dec	101.48	8.33		25.76	664.98	*200.14*	*312.52*	Dec		2.64	8.62	21.82	*11.03*	*9.81*
Seas_4	**290.46**	**24.47**	**139.07**	**77.48**	**1973.49**	***500.99***	***829.15***	**Seas_4**	**6.09**	**7.25**	**24.04**	**52.13**	***22.38***	***21.46***
Annual	**1151.49**	**82.39**	**567.87**	**305.32**	**7832.12**	***1987.84***	***3291.39***	**Annual**	**13.77**	**16.06**	**53.49**	**114.86**	***49.54***	***47.20***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table B.32. *Calculation results: PCB-28 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	EVN-BETR_1[a]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3				EVN-BETR_2[a]	CliMo Chem_2_2	MSCE-POP_2		
Jan	300.05	104.24	87.97		*164.09*	*118.03*	Jan	4.13		1.82	*2.98*	*1.63*
Feb	305.06	96.01	100.41		*167.16*	*119.44*	Feb	5.21		3.89	*4.55*	*0.93*
Mar	344.02	101.51	106.49		*184.01*	*138.60*	Mar	5.58		5.95	*5.77*	*0.27*
Seas_1	**949.13**	**301.76**	**294.88**	**290.58**	***459.09***	***326.72***	**Seas_1**	**14.92**	**2.47**	**11.67**	***9.68***	***6.46***
Apr	412.13	97.12	100.40		*203.22*	*180.93*	Apr	6.68		7.15	*6.92*	*0.33*
May	555.66	98.97	90.03		*248.22*	*266.29*	May	9.24		8.36	*8.80*	*0.62*
Jun	879.82	93.43	87.46		*353.57*	*455.76*	Jun	14.65		8.01	*11.33*	*4.69*
Seas_2	**1847.61**	**289.53**	**277.89**	**285.83**	***675.21***	***781.61***	**Seas_2**	**30.57**	**5.00**	**23.52**	***19.70***	***13.21***
Jul	1498.57	94.63	97.56		*563.59*	*809.72*	Jul	24.53		8.44	*16.49*	*11.38*
Aug	2228.00	93.56	114.44		*812.00*	*1226.34*	Aug	36.66		9.16	*22.91*	*19.45*
Sep	2370.98	90.96	121.66		*861.20*	*1307.60*	Sep	41.95		10.63	*26.29*	*22.15*
Seas_3	**6097.55**	**279.15**	**333.67**	**281.20**	*1747.89*	*2899.88*	**Seas_3**	**103.15**	**7.88**	**28.22**	*46.42*	*50.17*
Oct	1695.86	95.74	110.09		*633.90*	*919.72*	Oct	35.04		13.81	*24.43*	*15.02*
Nov	936.01	95.31	92.64		*374.65*	*486.15*	Nov	24.08		16.83	*20.46*	*5.13*
Dec	524.59	102.59	83.70		*236.96*	*249.27*	Dec	16.51		22.06	*19.28*	*3.92*
Seas_4	**3156.46**	**293.64**	**286.43**	**278.14**	***1003.67***	***1435.21***	**Seas_4**	**75.64**	**12.19**	**52.70**	***46.84***	***32.13***
Annual	**12050.75**	**1164.07**	**1192.87**	**1135.74**	***3885.86***	***5443.31***	**Annual**	**224.28**	**27.53**	**116.11**	***122.64***	***98.54***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
a - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.

Own/alternative data set. Calculation results on PCB-28 mass degraded in 5cm layer of soil (kg) calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.33.

Monthly values of PCB-28 mass degraded in 5cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.42a and b, respectively.

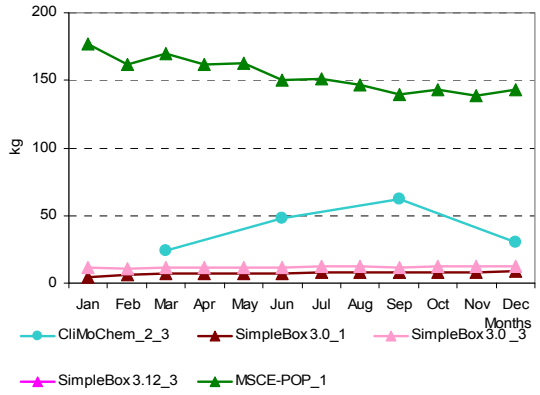


Fig. B.42a. *PCB-28 mass degraded in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

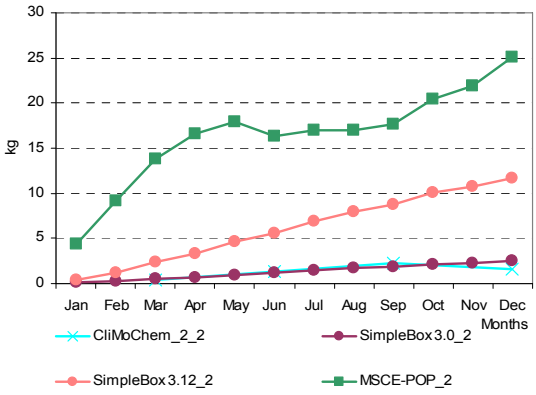


Fig. B.42b. *PCB-28 mass degraded in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table B.33. *Calculation results: PCB-28 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	176.87	4.88		11.32	468.35	*165.36*	*217.12*	Jan		0.07	0.34	4.36	*1.59*	*2.40*
Feb	162.14	5.92		10.68	416.83	*148.89*	*192.79*	Feb		0.25	1.17	9.22	*3.55*	*4.93*
Mar	170.15	6.91		11.55	455.06	*160.92*	*210.27*	Mar		0.49	2.39	13.74	*5.54*	*7.17*
Seas_1	**509.15**	**17.72**	23.95	**33.55**	**1340.24**	***384.92***	***573.73***	**Seas_1**	**0.39**	**0.81**	**3.90**	**27.32**	***8.10***	***12.90***
Apr	162.07	6.99		11.30	438.87	*154.81*	*202.64*	Apr		**0.70**	3.36	16.61	*6.89*	*8.52*
May	162.38	7.45		11.82	442.66	*156.08*	*204.18*	May		**0.96**	4.65	17.97	*7.86*	*8.94*
Jun	150.65	7.40		11.57	422.63	*148.06*	*194.77*	Jun		**1.16**	5.58	16.33	*7.69*	*7.80*
Seas_2	**475.10**	**21.84**	47.71	**34.69**	**1304.16**	***376.70***	***552.49***	**Seas_2**	**1.37**	**2.82**	**13.60**	**50.90**	***17.17***	***23.14***
Jul	151.08	7.83		12.09	430.91	*150.48*	*198.44*	Jul		**1.43**	6.87	17.05	*8.45*	*7.93*
Aug	146.72	8.02		12.23	425.49	*148.11*	*195.82*	Aug		**1.67**	8.00	16.97	*8.88*	*7.69*
Sep	139.79	7.93		11.96	406.06	*141.44*	*186.74*	Sep		**1.84**	8.75	17.64	*9.41*	*7.92*
Seas_3	**437.59**	**23.78**	62.46	**36.27**	**1262.47**	***364.51***	***530.74***	**Seas_3**	**2.32**	**4.94**	**23.62**	**51.66**	***20.63***	***22.75***
Oct	143.54	8.37		12.49	414.17	*144.64*	*190.33*	Oct		**2.13**	10.09	20.39	*10.87*	*9.16*
Nov	138.41	8.27		12.22	395.65	*138.64*	*181.69*	Nov		**2.28**	10.77	21.89	*11.65*	*9.84*
Dec	143.20	8.53		12.44	403.73	*141.97*	*185.38*	Dec		**2.51**	11.65	25.11	*13.09*	*11.37*
Seas_4	**425.15**	**25.17**	30.45	**37.15**	**1213.54**	***346.29***	***514.00***	**Seas_4**	**1.60**	**6.92**	**32.52**	**67.39**	***27.11***	***30.06***
Annual	**1846.98**	**88.51**	**164.57**	**141.66**	**5120.41**	***1472.43***	***2170.52***	**Annual**	**5.67**	**15.49**	**73.64**	**197.27**	***73.02***	***88.10***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Calculation results on PCB-28 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.34.

Table 3.34. *Calculation results: PCB-28 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	MSCE- POP_2		
Jan	178.80				Jan		4.40		
Feb	163.91				Feb		9.32		
Mar	172.01				Mar		13.90		
Seas_1	**514.72**	**47.90**	***281.31***	***330.09***	**Seas_1**	**0.77**	**27.61**	***14.19***	***18.98***
Apr	163.84				Apr		16.79		
May	164.15				May		18.16		
Jun	152.30				Jun		16.51		
Seas_2	**480.29**	**95.43**	***287.86***	***272.14***	**Seas_2**	**2.74**	**51.46**	***27.10***	***34.45***
Jul	152.73				Jul		17.23		
Aug	148.32				Aug		17.16		
Sep	141.32				Sep		17.83		
Seas_3	**442.37**	**124.91**	***283.64***	***224.48***	**Seas_3**	**4.64**	**52.22**	***28.43***	***33.65***
Oct	145.10				Oct		20.62		
Nov	139.93				Nov		22.13		
Dec	144.76				Dec		25.38		
Seas_4	**429.79**	**60.90**	***245.35***	***260.85***	**Seas_4**	**3.20**	**68.13**	***35.66***	***45.91***
Annual	**1867.17**	**329.14**	***1098.15***	***1087.56***	**Annual**	**11.34**	**199.43**	***105.38***	***132.99***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
a - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model on the basis of initial concentrations given as input data;
[b]– in CAN/POPs results the second layer of soil is applied as 5cm;

Monthly values of PCB-28 mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.43a and b, respectively.

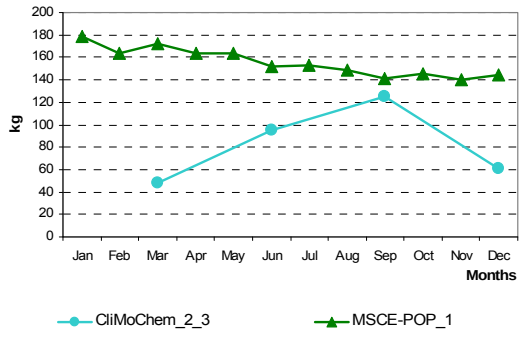


Fig. B.43a. *PCB-28 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

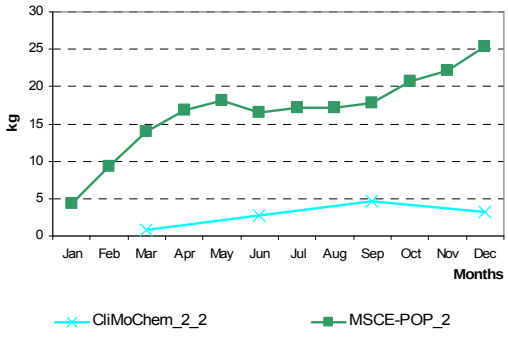


Fig. B.43b. *PCB-28 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-28 mass degraded in soil within 5 and 10 cm layers obtained with two different data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables B.35-B.36.

Table B.35. *The percentage difference between calculation results on PCB-28 mass degraded within 5 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			24%	-3%	42%	-56%	-30%	72%	141%
Feb			19%	-1%	45%	-55%	-31%	71%	140%
Mar			14%	0%	45%	-55%	-32%	69%	133%
Seas_1	**-69%**	**-84%**	**18%**	**-1%**	**44%**	**-55%**	**-31%**	**71%**	**137%**
Apr			10%	-1%	44%	-55%	-32%	69%	135%
May			8%	-2%	42%	-54%	-33%	66%	117%
Jun			7%	-2%	40%	-54%	-34%	63%	106%
Seas_2	**-45%**	**-67%**	**8%**	**-2%**	**42%**	**-54%**	**-33%**	**66%**	**119%**
Jul			6%	-3%	39%	-53%	-35%	61%	104%
Aug			5%	-3%	38%	-53%	-36%	59%	87%
Sep			4%	-4%	37%	-53%	-37%	55%	68%
Seas_3	**-41%**	**-56%**	**5%**	**-4%**	**38%**	**-53%**	**-36%**	**58%**	**85%**
Oct			3%	-4%	36%	-52%	-38%	52%	49%
Nov			3%	-5%	35%	-52%	-39%	47%	31%
Dec			2%	-5%	35%	-52%	-39%	41%	15%
Seas_4	**-74%**	**-78%**	**3%**	**-5%**	**35%**	**-52%**	**-39%**	**46%**	**29%**
Annual	**-59%**	**-71%**	**7%**	**-4%**	**38%**	**-54%**	**-35%**	**60%**	**72%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations; SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data; SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations; SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Table B.36. *The percentage difference between calculation results on PCB-28 mass degraded within 10 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			72%	141%
Feb			71%	140%
Mar			69%	133%
Seas_1	**-69%**	**-84%**	**71%**	**137%**
Apr			69%	135%
May			66%	117%
Jun			63%	106%
Seas_2	**-45%**	**-67%**	**66%**	**119%**
Jul			61%	104%
Aug			59%	87%
Sep			55%	68%
Seas_3	**-41%**	**-56%**	**58%**	**85%**
Oct			52%	49%
Nov			47%	31%
Dec			41%	15%
Seas_4	**-74%**	**-78%**	**46%**	**29%**
Annual	**-59%**	**-71%**	**60%**	**72%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

3.2.3. Comparison of calculated values of PCB-28 mass degraded in water

According to the programme of Stage II model results of computational experiments on mass balance include masses of PCB-28 degraded in sea within a layer of 200 m depth.

Reference data set. Calculation results on PCB-28 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.37.

Monthly values of PCB-28 mass degraded in 200 m layer of water calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.44a and b, respectively. Seasonal variations of low values of mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "reference" data set and -zero initial conditions are also shown in Fig. B.44c in more detail.

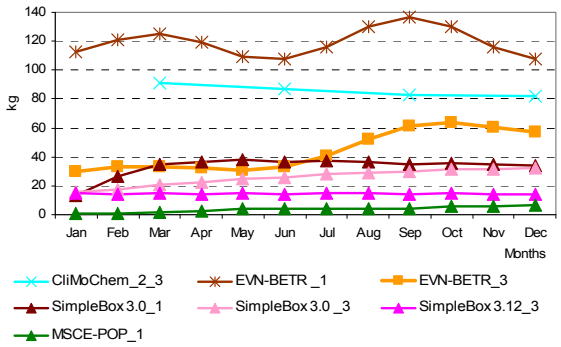


Fig. B.44a. *PCB-28 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

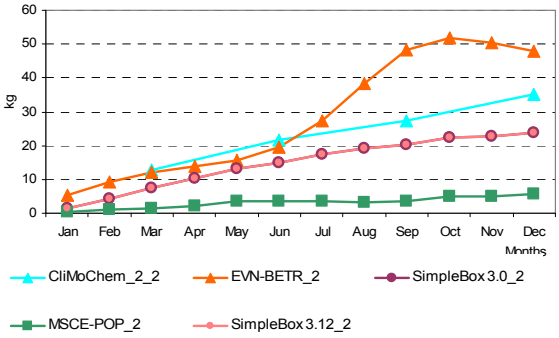


Fig. B.44b. *PCB-28 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

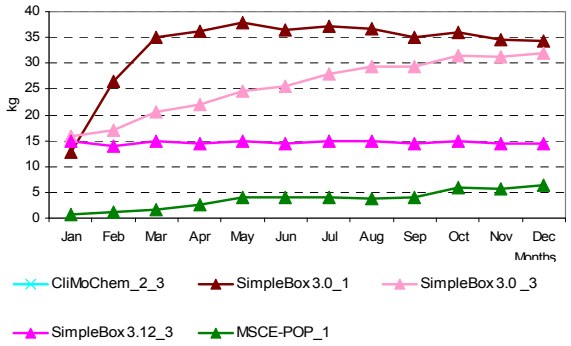


Fig. B.44c. *PCB-28 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions (models with low values)*

Table B.37. *Calculation results: PCB-28 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	SimpleBox 3.0_1[b]	MSCE-POP_1	EVN-BETR_1[a]	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0_3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	12.87	0.60	112.58	30.19		15.89	14.87	*31.17*	*40.98*	Jan	5.28		1.29	1.29	0.42	*2.07*	*2.18*
Feb	26.51	1.24	120.90	32.80		17.13	13.91	*35.42*	*43.26*	Feb	9.32		4.19	4.19	0.95	*4.66*	*3.46*
Mar	34.92	1.71	125.08	33.46		20.64	14.87	*38.45*	*44.19*	Mar	12.03		7.61	7.61	1.36	*7.15*	*4.39*
Seas_1	**74.31**	**3.56**	**358.56**	**96.45**	**91.14**	**53.66**	**43.65**	***103.05***	***117.02***	**Seas_1**	**26.63**	**12.93**	**13.09**	**13.09**	**2.72**	***13.69***	***8.50***
Apr	36.15	2.61	119.09	31.99		22.06	14.39	*37.72*	*41.66*	Apr	13.79		10.19	10.19	2.16	*9.08*	*4.92*
May	37.91	4.01	109.68	30.86		24.72	14.87	*37.01*	*37.55*	May	15.72		13.13	13.14	3.40	*11.35*	*5.44*
Jun	36.50	4.05	107.31	33.14		25.56	14.39	*36.82*	*36.57*	Jun	19.70		14.94	14.95	3.42	*13.25*	*6.93*
Seas_2	**110.55**	**10.66**	**336.08**	**95.99**	**87.21**	**72.34**	**43.65**	***108.07***	***106.06***	**Seas_2**	**49.21**	**21.64**	**38.26**	**38.28**	**8.98**	***31.27***	***15.89***
Jul	37.26	3.98	115.73	40.55		27.90	14.87	*40.05*	*39.54*	Jul	27.35		17.47	17.49	3.37	*16.42*	*9.86*
Aug	36.76	3.86	129.69	51.92		29.24	14.87	*44.39*	*45.02*	Aug	38.32		19.29	19.32	3.26	*20.05*	*14.34*
Sep	35.14	4.10	136.98	61.58		29.41	14.39	*46.93*	*48.30*	Sep	48.21		20.20	20.23	3.50	*23.03*	*18.54*
Seas_3	**109.17**	**11.94**	**382.40**	**154.05**	**83.14**	**86.55**	**44.13**	***124.48***	***122.41***	**Seas_3**	**113.87**	**27.46**	**56.97**	**57.04**	**10.13**	***53.09***	***39.46***
Oct	35.94	5.89	130.08	63.84		31.41	14.87	*47.01*	*45.33*	Oct	51.90		22.27	22.31	5.12	*25.40*	*19.43*
Nov	34.49	5.74	116.20	60.38		31.26	14.39	*43.75*	*40.18*	Nov	50.26		22.75	22.80	5.00	*25.20*	*18.69*
Dec	34.28	6.34	107.38	56.80		32.03	14.39	*41.87*	*36.57*	Dec	47.92		23.81	23.86	5.59	*25.29*	*17.36*
Seas_4	**104.71**	**17.97**	**353.66**	**181.03**	**82.41**	**94.70**	**43.65**	***125.45***	***113.02***	**Seas_4**	**150.08**	**35.32**	**68.83**	**68.97**	**15.71**	***67.78***	***51.33***
Annual	**398.74**	**44.13**	**1430.70**	**527.52**	**343.89**	**307.26**	**175.09**	***461.05***	***454.88***	**Annual**	**339.78**	**97.35**	**177.14**	**177.38**	**37.55**	***165.84***	***113.65***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
b - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-28 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.38.

Monthly values of PCB-28 mass degraded in 200 m layer of water calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.45a and b, respectively.

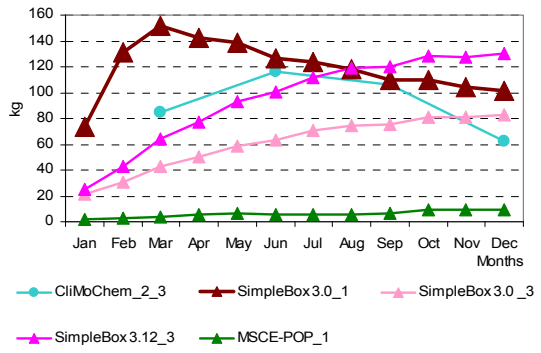


Fig. B.45a. *PCB-28 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

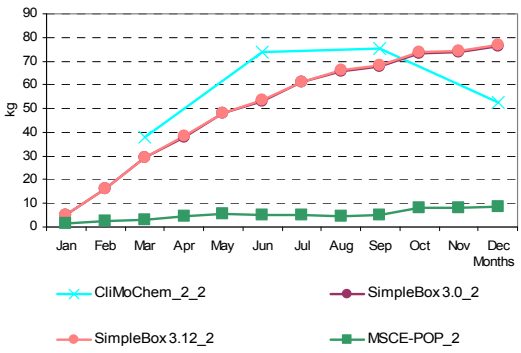


Fig. B.45b. *PCB-28 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table B.38. *Calculation results: PCB-28 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_ 2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	73.15	1.96		21.52	25.32	*30.49*	*30.23*	Jan		4.96	4.96	1.42	*3.78*	*2.04*
Feb	131.46	2.99		30.32	42.47	*51.81*	*55.61*	Feb		16.23	16.24	2.40	*11.62*	*7.99*
Mar	152.04	3.61		42.64	64.00	*65.57*	*62.84*	Mar		29.12	29.15	2.97	*20.41*	*15.10*
Seas_1	**356.65**	**8.55**	**84.33**	**94.48**	**131.79**	***135.16***	***131.66***	**Seas_1**	**37.67**	**50.30**	**50.34**	**6.79**	***36.28***	***20.54***
Apr	**142.38**	5.14		49.89	77.33	*68.68*	*57.44*	Apr		38.12	38.20	4.38	*26.90*	*19.51*
May	**138.66**	6.42		58.99	92.89	*74.24*	*55.77*	May		47.98	48.11	5.52	*33.87*	*24.55*
Jun	**126.33**	5.95		63.06	100.05	*73.85*	*52.18*	Jun		53.32	53.52	5.11	*37.32*	*27.89*
Seas_2	**407.37**	**17.50**	**116.30**	**171.94**	**270.27**	***196.68***	***149.15***	**Seas_2**	**73.72**	**139.42**	**139.84**	**15.01**	***92.00***	***60.00***
Jul	**123.65**	5.68		70.27	111.83	*77.86*	*53.28*	Jul		60.99	61.29	4.89	*42.39*	*32.48*
Aug	**117.96**	5.32		74.57	118.72	*79.14*	*53.36*	Aug		65.97	66.35	4.58	*45.63*	*35.56*
Sep	**109.83**	6.06		75.58	120.16	*77.91*	*51.55*	Sep		67.79	68.26	5.29	*47.11*	*36.22*
Seas_3	**351.44**	**17.06**	**105.63**	**220.41**	**350.71**	***209.05***	***148.35***	**Seas_3**	**75.16**	**194.75**	**195.90**	**14.75**	***120.14***	***90.25***
Oct	**109.97**	9.12		81.05	128.55	*82.17*	*52.48*	Oct		73.46	74.05	8.08	*51.86*	*37.92*
Nov	**103.74**	9.20		80.84	127.83	*80.40*	*51.20*	Nov		73.89	74.56	8.18	*52.21*	*38.13*
Dec	**101.69**	9.74		82.85	130.54	*81.21*	*51.52*	Dec		76.22	76.99	8.75	*53.99*	*39.18*
Seas_4	**315.41**	**28.06**	**62.63**	**244.74**	**386.92**	***207.55***	***156.85***	**Seas_4**	**52.72**	**223.57**	**225.61**	**25.01**	***131.73***	***107.83***
Annual	**1430.87**	**71.18**	**368.90**	**731.58**	**1139.68**	***748.44***	***552.68***	**Annual**	**239.27**	**608.04**	**611.69**	**61.56**	***380.14***	***275.01***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.39.

Table B.39. *The percentage difference between calculation results on PCB-28 mass degraded in 200 m layer of water obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	Simple Box 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			468%	284%	284%	35%	70%	226%	237%
Feb			396%	288%	288%	77%	205%	140%	153%
Mar			335%	283%	283%	107%	330%	110%	119%
Seas_1	**191%**	**-7%**	**380%**	**284%**	**285%**	**76%**	**202%**	**140%**	**149%**
Apr			294%	274%	275%	126%	437%	97%	103%
May			266%	265%	266%	139%	525%	60%	63%
Jun			246%	257%	258%	147%	595%	47%	49%
Seas_2	**241%**	**33%**	**268%**	**264%**	**265%**	**138%**	**519%**	**64%**	**67%**
Jul			232%	249%	250%	152%	652%	43%	45%
Aug			221%	242%	243%	155%	698%	38%	40%
Sep			213%	236%	237%	157%	735%	48%	51%
Seas_3	**174%**	**27%**	**222%**	**242%**	**243%**	**155%**	**695%**	**43%**	**46%**
Oct			206%	230%	232%	158%	764%	55%	58%
Nov			201%	225%	227%	159%	788%	60%	63%
Dec			197%	220%	223%	159%	807%	54%	57%
Seas_4	**49%**	**-24%**	**201%**	**225%**	**227%**	**158%**	**786%**	**56%**	**59%**
Annual	**146%**	**7%**	**259%**	**243%**	**245%**	**138%**	**551%**	**61%**	**64%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.2.4. Comparison of calculated values of PCB-28 mass degraded in vegetation

Reference data set. Values of PCB-28 mass degraded in vegetation (kg) obtained by CliMoChem_2_2 and CliMoChem_2_3 models on the basis of "reference" data set are equal to zero.

Own/alternative data set. Calculation results on PCB-28 mass degraded in vegetation (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.40.

Table B.40. *Calculation results: PCB-28 mass degraded in vegetation (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of historical emissions	Results obtained on the basis of zero initial concentrations	*m*	σ
	CliMoChem_2_3	CliMoChem_2_2		
Jan				
Feb				
Mar				
Seas_1	**97.59**	**91.57**	***94.58***	***3.01***
Apr				
May				
Jun				
Seas_2	**160.84**	**158.83**	***159.83***	***1.01***
Jul				
Aug				
Sep				
Seas_3	**140.64**	**138.87**	***139.75***	***0.89***
Oct				
Nov				
Dec				
Seas_4	**228.58**	**227.56**	***228.07***	***0.51***
Annual	**627.65**	**616.82**	***622.24***	***5.41***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
* - In MSCE-POP model degradation in vegetation is not taken into account.

Monthly values of PCB-28 mass degraded in vegetation calculated by the participating models on the basis of "own or alternative" data sets are compared in Fig. B.46.

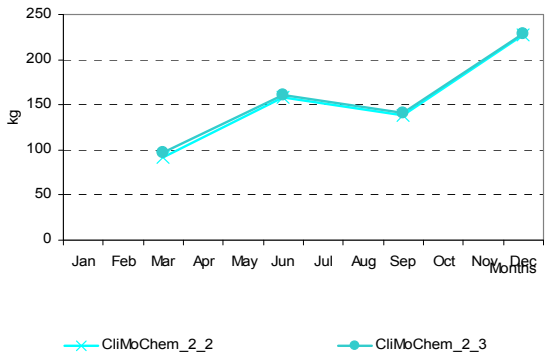


Fig. B.46. *PCB-28 mass degraded in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets*

3.2.5. Comparison of distribution of PCB-28 mass degraded in the environment

Sections from B.2.1 to B.2.4 above are devoted to the comparison between the results of participating models on PCB-28 mass degraded in the main environmental compartments (atmosphere, soil, water and vegetation). The comparison includes results of one-year calculations made on the basis of initial conditions (EVN-BETR and UK-MODEL, MSCE-POP, SimpleBox) and zero initial concentrations (CliMoChem, MSCE-POP and SimpleBox) along with results of long-term calculations performed with historical emissions (EVN-BETR and UK-MODEL, CliMoChem and SimpleBox). Calculation results obtained with the use of two different physical-chemical data sets are submitted by CliMoChem, MSCE-POP and SimpleBox models.

A preliminary analysis of the main results on comparison of absolute and relative values of PCB-28 mass degraded in the main environmental compartments is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions and for results based on zero-initial conditions.

Atmosphere.Comparison of annual values of PCB-28 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. B.47a. Fig. B.47b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

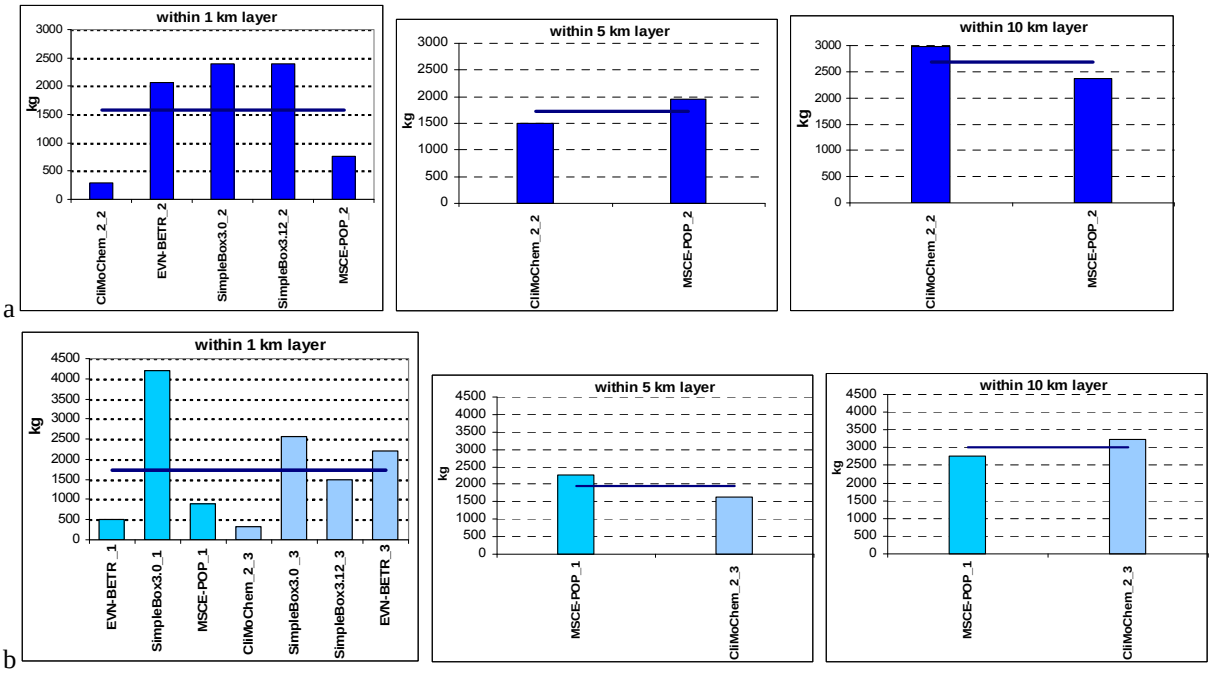


Fig. B.47. *Comparison of annual values of PCB-28 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-28 degraded mass calculated by CliMoChem and MSCE-POP models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set is presented in Fig. B.48.

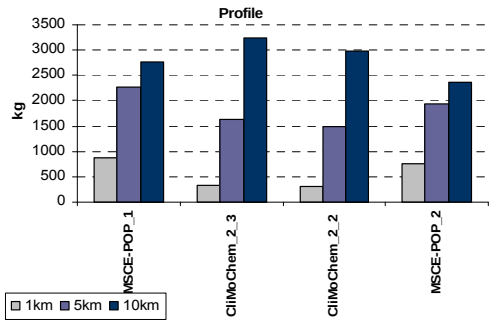


Fig. 3.48. *Comparison of profiles of annual values of PCB-28 degraded mass calculated by the models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference data set»*

Comparison of annual values of PCB-28 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative***" data sets is presented in Fig. B.49a. Fig. B.49b shows the same results but obtained on the basis of initial concentrations or historical

emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

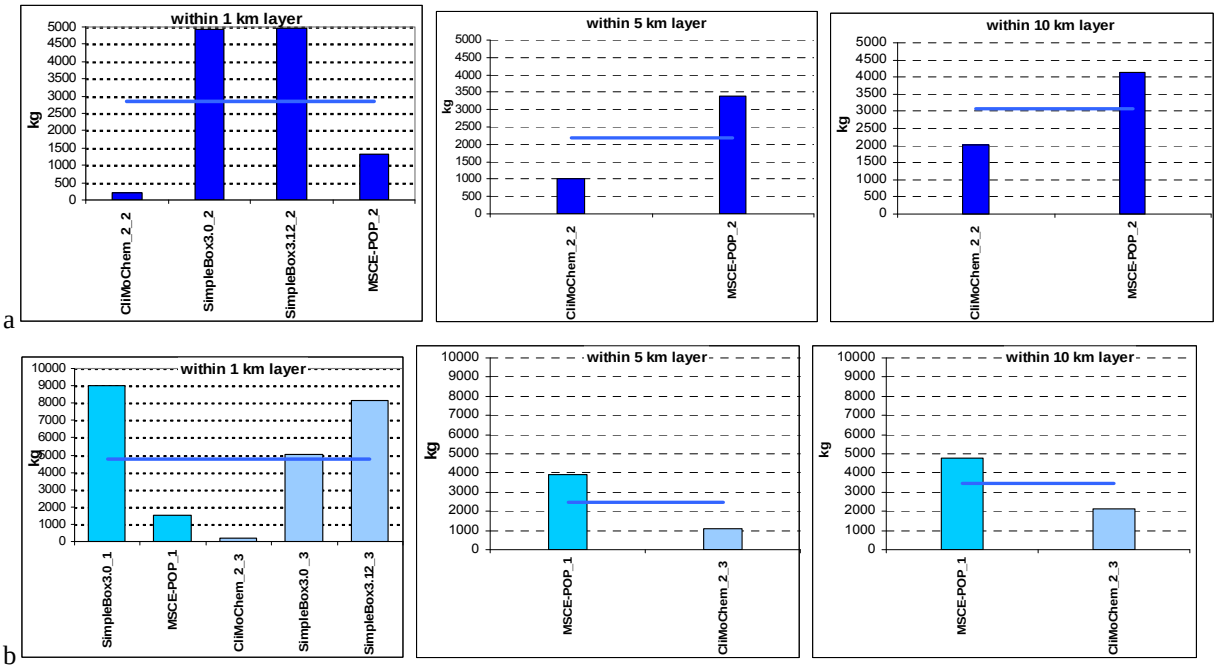


Fig. B.49. *Comparison of annual values of PCB-28 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-28 degraded mass calculated by CliMoChem and MSCE-POP models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative" data sets is presented in Fig. B.50.

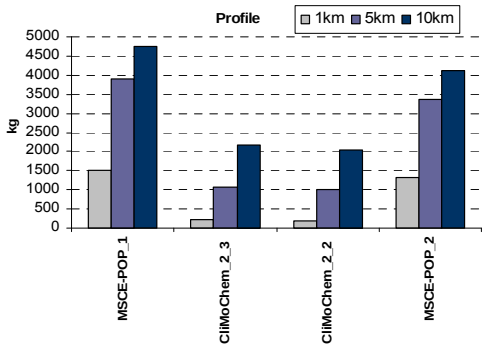


Fig. B.50. *Comparison of profiles of annual values of PCB-28 degraded mass calculated by the models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative data sets"*

Comparison of annual values of PCB-28 mass degraded in the considered different layers of the atmosphere obtained with "reference" and "own/alternative" data sets is presented in Fig. B.51.

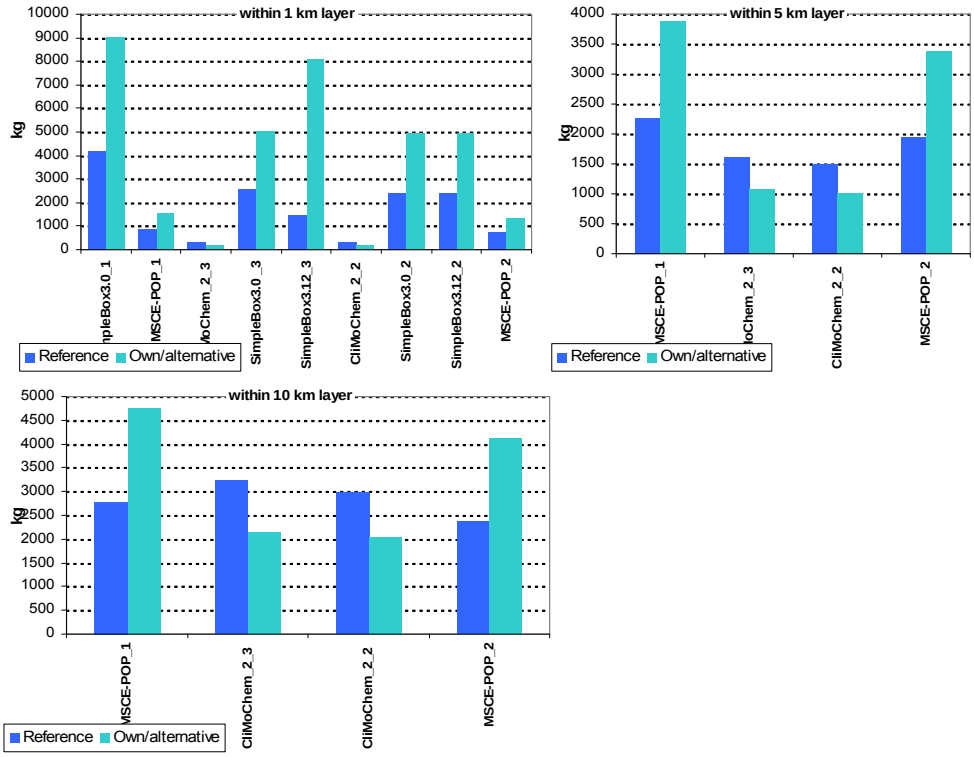


Fig. B.51. *Comparison of PCB-28 mass degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of two data set*

Soil. Comparison of annual values of PCB-28 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. B.52a. Fig. B.52b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

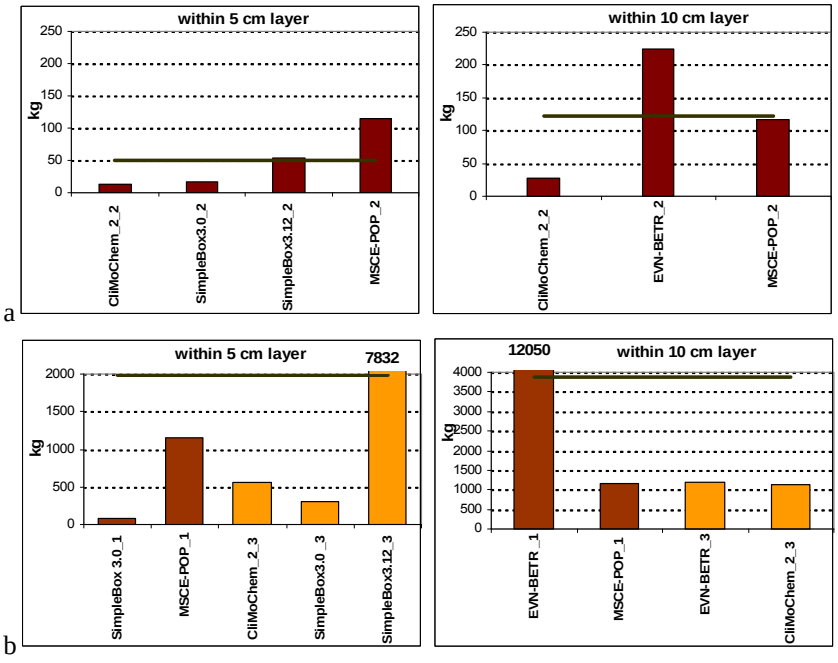


Fig. B.52. *Comparison of annual values of PCB-28 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

A comparison of profiles of annual values of PCB-28 degraded mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of “reference” data set is presented in Fig. B.53.

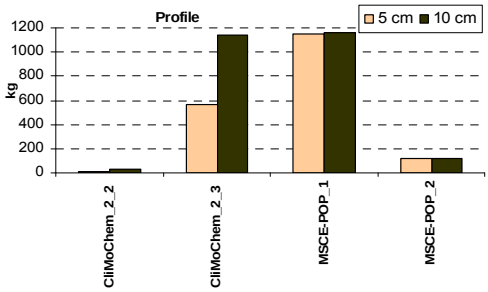
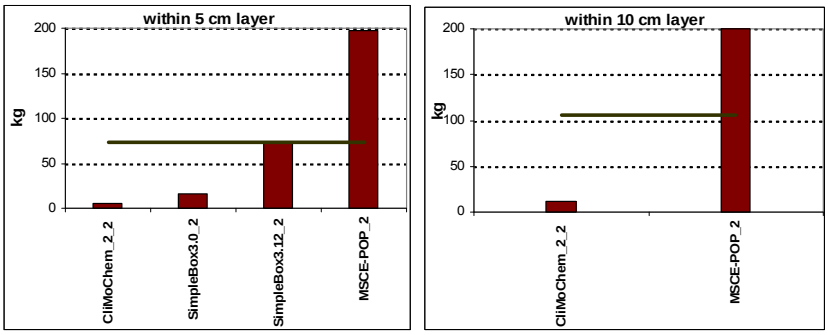


Fig. 3.53. *Comparison of profiles of annual values of PCB-28 degraded mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of “reference data set”*

Comparison of annual values of PCB-28 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of “***own or alternative***” data sets is presented in Fig. B.54a. Fig. B.54b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

a



b

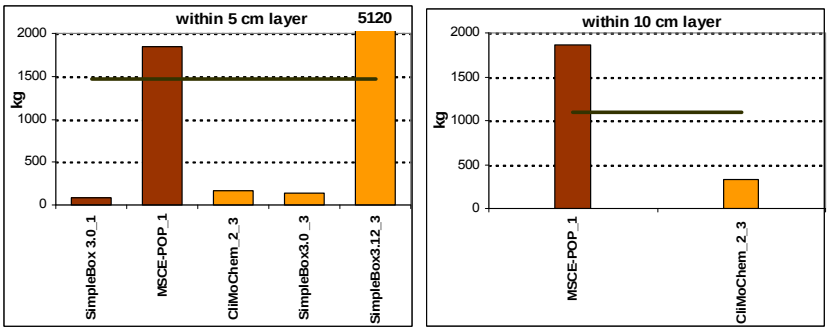


Fig. B.54. *Comparison of annual values of PCB-28 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-28 degraded mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of “own or alternative” data sets is presented in Fig. B.55.

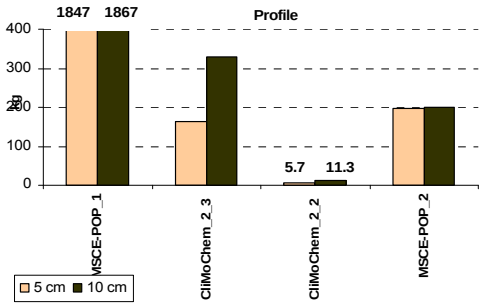


Fig. B.55. *Comparison of profiles of annual values of PCB-28 degraded mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative data sets"*

Comparison of annual values of PCB-28 mass degraded in the considered different layers of soil obtained with "reference" and "own/alternative" data sets is presented in Fig. B.56.

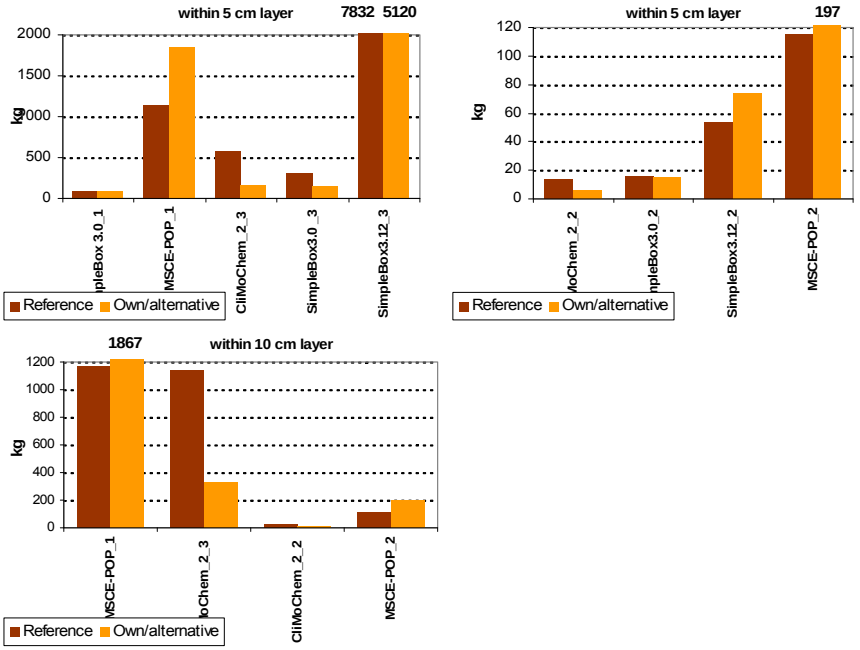


Fig. B.56. *Comparison of PCB-28 mass degraded within 5 and 10 cm soil layers calculated by different models on the basis of two data set*

Water. A comparison of annual values of PCB-28 masses degraded in water layer of 200 m calculated by different models on the basis of zero initial concentrations and with the use of "***reference"*** data set is presented in Fig. B.57a. Fig. B.57b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plot shows the value of the corresponding parameter averaged between models.

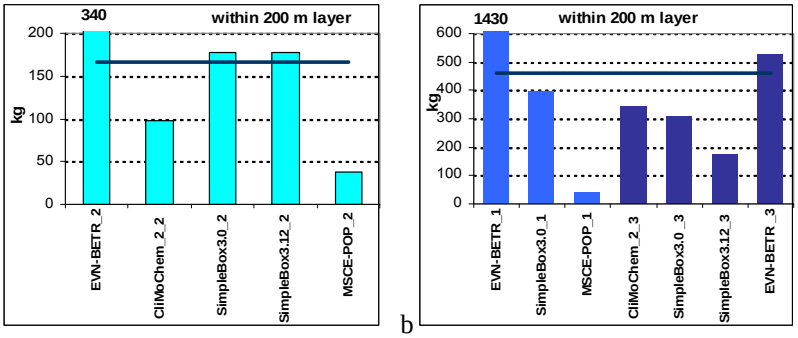


Fig. B.57. *Comparison of annual values of PCB-28 masses degraded in water within 200 m layer calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-28 masses degraded in water layer of 200 m calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative"*** data sets is presented in Fig. B.58a (blue line corresponds to the averaged value). Fig. B.58b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

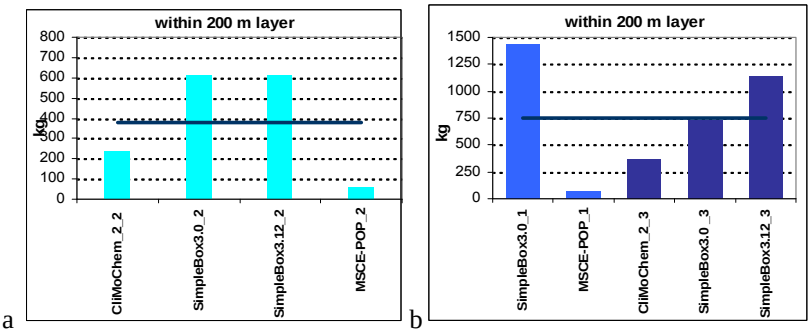


Fig. B.58. *Comparison of annual values of PCB-28 masses degraded in water within 200 m layer calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Annual values of PCB-28 mass degraded in the 200m layer of water obtained by the participating models on the basis of "reference" and "own/alternative" data sets are compared in Fig. B.59.

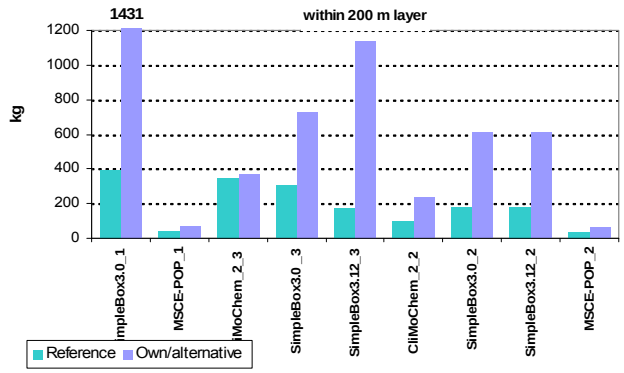


Fig. B.59. *Comparison of PCB-28 mass degraded within 200 m water layer calculated by different models on the basis of two data sets*

Vegetation. Annual values of PCB-28 mass degraded in vegetation obtained by the participating models on the basis of "reference" and "own/alternative" data sets are shown in Fig. B.60.

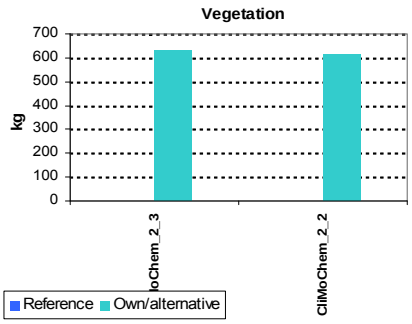


Fig. B.60. *Comparison of PCB-28 mass degraded in vegetation calculated by different models on the basis of two data sets*

Relative distribution of PCB mass degraded in the environmental compartments

The presented estimates of PCB-28 masses degraded in the main environmental compartments allow one to reveal the relative contributions of degradation process occurs in this or that media to the overall mass of PCB-28 in the whole environment. Below, the comparison of relative fractions of PCB-28 mass degraded in the main environmental media in relation to the mass balance estimates is presented. Of note, here and hereinafter fractions of mass degraded in different media are the ratios of the degraded mass and the mass contained in the considered compartment (taking into account also degraded mass).

Fractions of PCB-28 mass degraded in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Figs. B.61a and b, respectively. In these figures fractions of PCB-28 mass degraded in the atmosphere calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.

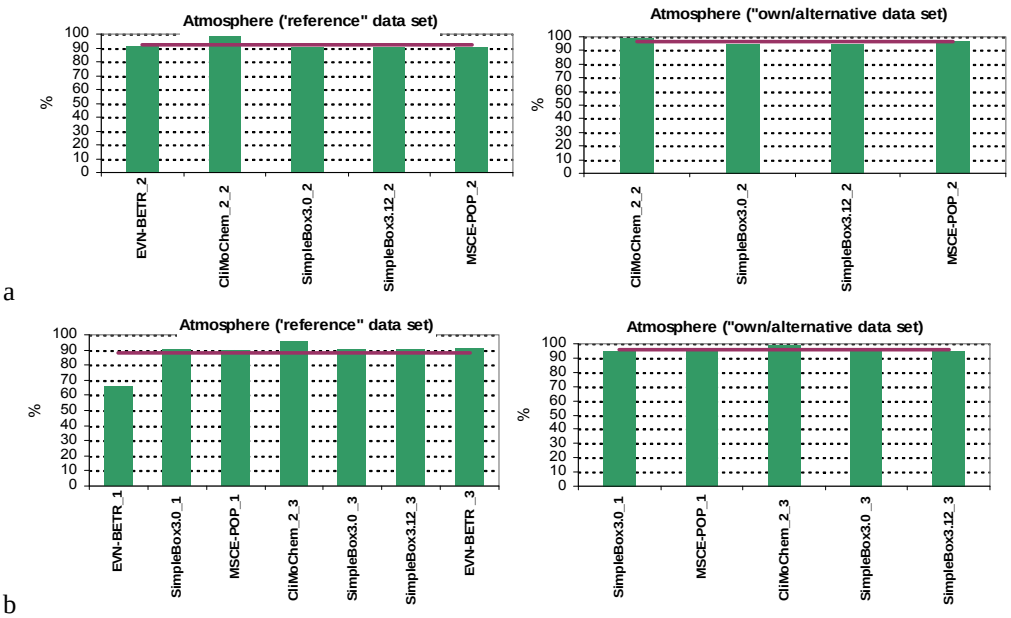


Fig. B.61. *Fractions of PCB-28 mass degraded in the atmosphere calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

In Fig. B.62 a and b fractions of PCB-28 mass degraded in soil calculated by the different models on the basis of zero and non-zero initial conditions are presented, respectively. In these figures fractions of PCB-28 mass degraded in soil calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared.

Fractions of PCB-28 mass degraded in seawater calculated by the participating on the basis of zero and non-zero initial conditions are presented in Figs. B.63a and b, respectively. In these figures fractions of PCB-28 mass degraded in the atmosphere calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared.

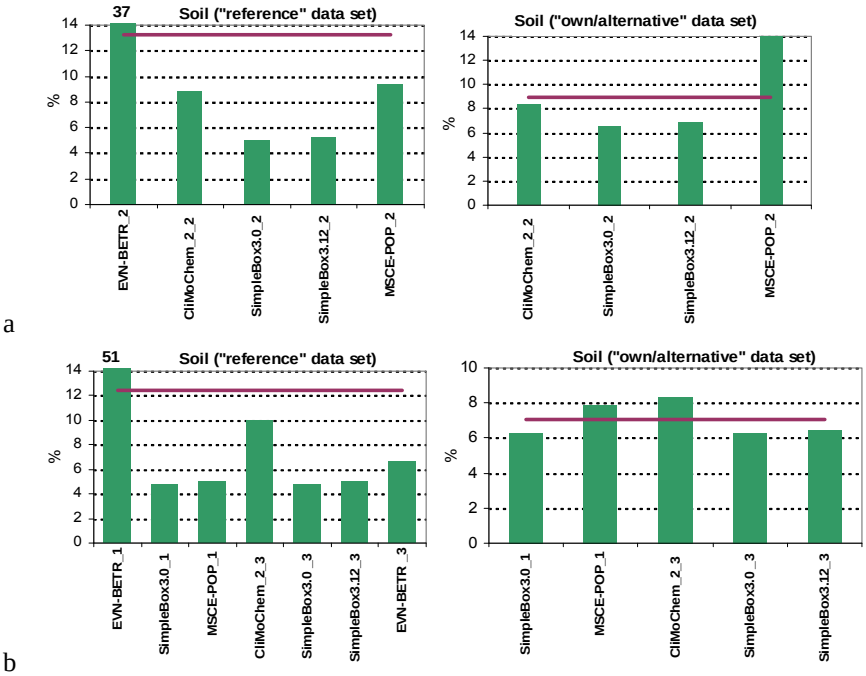


Fig. B.62. *Fractions of PCB-28 mass degraded in soil calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

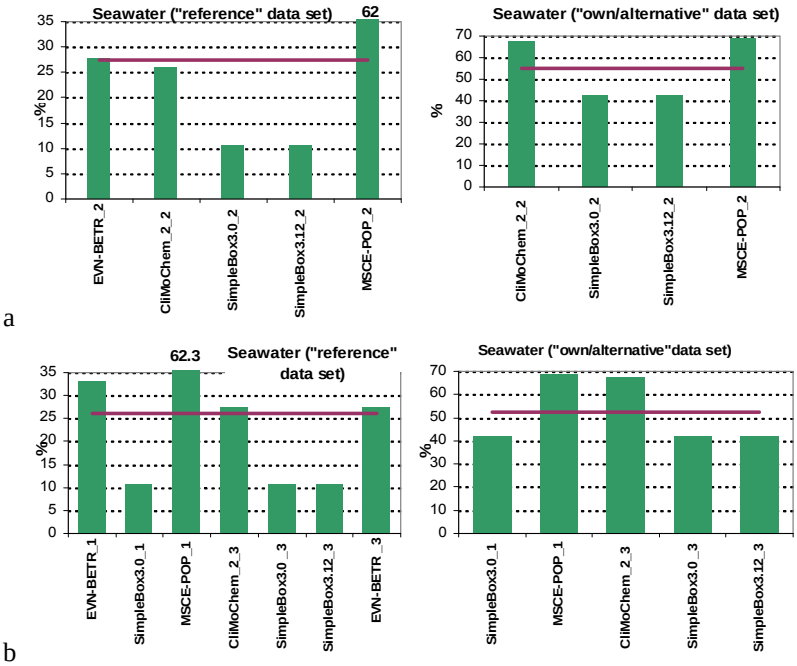


Fig. B.63. *Fractions of PCB-28 mass degraded in seawater calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

For the participating models, which consider process of degradation in vegetation, fractions of PCB-28 mass degraded in vegetation calculated on the basis of zero and non-zero initial conditions are presented in Figs. B.64a and b, respectively.

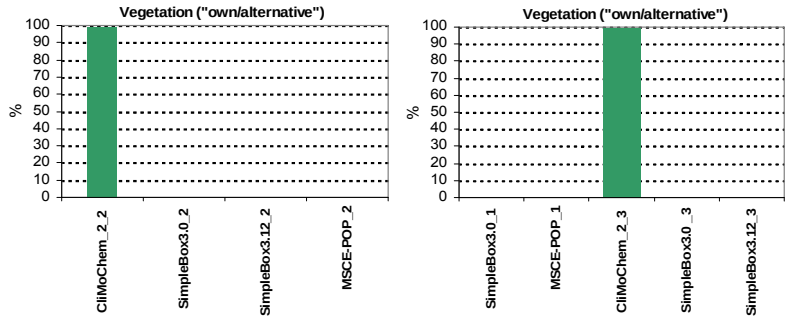


Fig. B.64. *Fractions of PCB-28 mass degraded in vegetation calculated by the participating models on the basis of "own or alternative" data sets*

3.2.6. Comparison of calculated values of PCB-28 mass deposited into deep sea

In this section a comparison of results calculated by CliMoChem model with historical emission scenario on the basis of their own Land Cover Data [*DeFries and Townshend*, 1994] and Land Cover Data given as input data for this intercomparison study [*Guo and Chen*, 1994] is presented. Of note, contrary to the calculations discussed in the previous and subsequent sections in this simulation, PCB-28 is emitted as pulse emission into air each year at the beginning of season one.

Reference data set. Two sets of calculated values of PCB-28 mass deposited into deep sea (kg) obtained by CliMoChem model on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.41.

Table B.41. *Calculation results: PCB-28 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "reference" data set and statistical parameters used for evaluation*

Month	CliMoChem_1_3	CliMoChem_2_3	*m*	σ
Season_1	119.45	139.78	*129.62*	*14.38*
Season_2	68.66	79.19	*73.93*	*7.45*
Season_3	47.38	53.77	*50.57*	*4.52*
Season_4	63.48	73.07	*68.27*	*6.78*
Annual	**298.96**	**345.81**	***322.38***	***33.13***

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

Seasonal values of PCB-28 mass deposited into deep sea calculated by CliMoChem model on the basis of "reference" data set are compared in Fig. B.65.

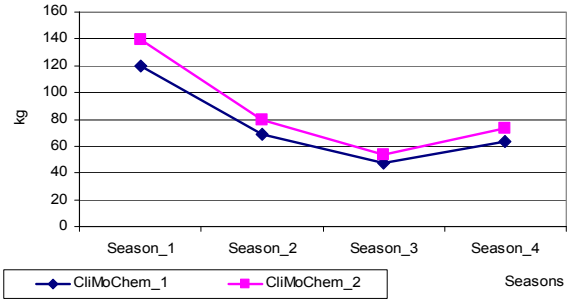


Fig. B.65. *PCB-28 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "reference" data sets*

Own/alternative data set. Two versions of calculation results on PCB-28 mass deposited into deep sea (kg) obtained by CliMoChem model on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.42.

Table B.42. *Calculation results: PCB-28 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	CliMoChem_1_3	CliMoChem_2_3	*m*	σ
Season_1	28.32	35.24	*31.78*	*4.89*
Season_2	12.50	15.91	*14.21*	*2.41*
Season_3	4.68	6.07	*5.37*	*0.98*
Season_4	4.24	5.76	*5.00*	*1.08*
Annual	**49.74**	**62.98**	***56.36***	***9.36***

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

Seasonal values of PCB-28 mass deposited into deep sea calculated by CliMoChem model on the basis of "own or alternative" data sets are compared in Fig. B.66.

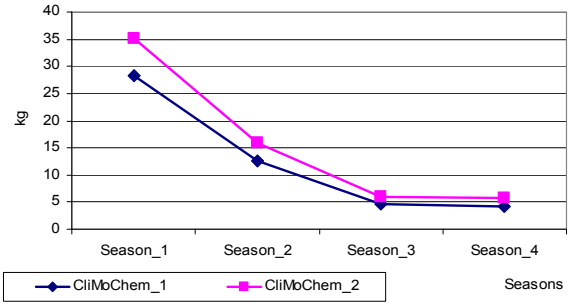


Fig. B.66. *PCB-28 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "own or alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.43.

Table B.43. *The percentage difference between calculation results on PCB-28 mass deposited into deep sea obtained by CliMoChem model on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_1_3	CliMoChem_2_3
Season_1	-76%	-75%
Season_2	-82%	-80%
Season_3	-90%	-89%
Season_4	-93%	-92%
Annual	**-83%**	**-82%**

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

B.3. Mass flows transported in/out the specified domain: inflow and outflow

Mass flows of PCB-28 transported in/out the specified domain (inflow and outflow) are calculated by the participating models on the basis of atmospheric emission estimates presented by [*Breivik et al*. 2002a] (see also www.nilu.no/projects/globalpcb/). The higher (or worst-case) emission estimates for 1981-2000 are applied.

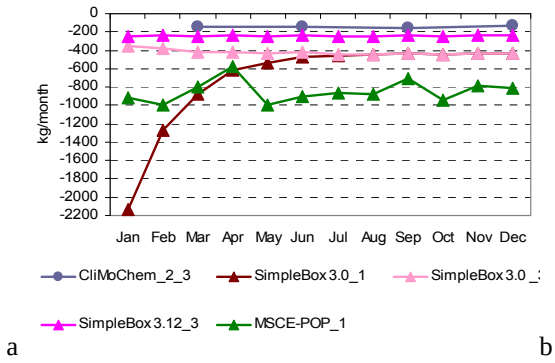
All amount of emissions is released into the atmosphere and is uniformly distributed throughout a year. In calculations of SimpleBox and MSCE-POP models, a value of PCB-28 total annual emissions in 2000 totals on average 17057 kg. In CliMoChem model the global emission data were summarized to zone-specific emissions (10 zones) and for the specified domain emission data for the model zones 2 and 3 (of 10) are used. At that emission value in 2000 used by CliMoChem for PCB-28 totals to 43697 kg.

It should be noted that transport into the calculation domain is supposed to be positive.

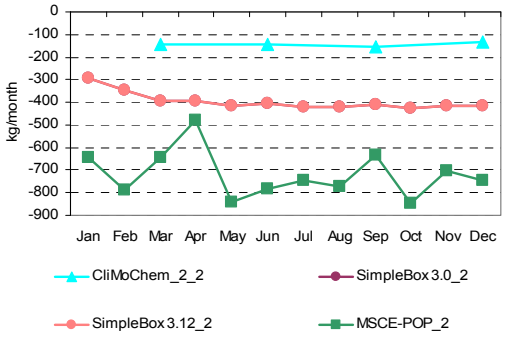
B.3.1. Comparison of calculated values of PCB-28 mass flows transported in/out the calculation domain through the atmosphere.

Reference data set. Calculation results on PCB-28 mass flows transported in/out the calculation domain through the atmosphere calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.44.

Monthly values of PCB-28 mass flows transported in/out the calculation domain through the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.67 a and b, respectively.



a



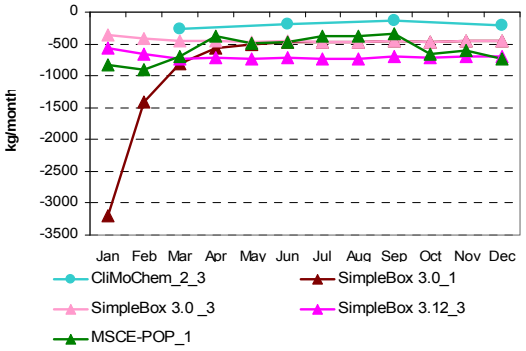
b

Fig. B.67a. *PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. B.67b. *PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported in/out the calculation domain through the atmosphere calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.45.

Monthly values of PCB-28 mass flows transported in/out of the calculation domain through atmosphere calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.68 a and b, respectively.



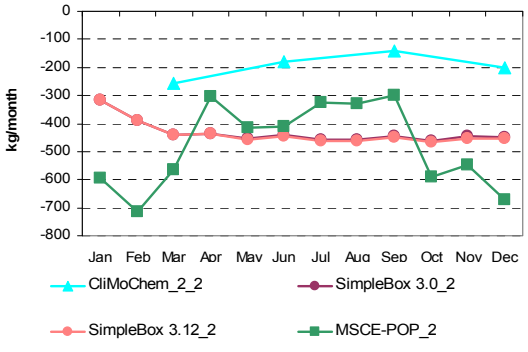


Fig. B.68a. *PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

Fig. B.68b. *PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.46.

Table B.44. *Calculation results: PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-2135.2	-913.9		-357.4	-245.9	*-913.1*	*865.5*	Jan		-293.2	-293.2	-642.3	*-409.6*	*201.5*
Feb	-1276.4	-1001.3		-381.3	-230.0	*-722.2*	*497.8*	Feb		-346.6	-346.7	-789.6	*-494.3*	*255.7*
Mar	-871.2	-796.3		-423.1	-245.9	*-584.1*	*298.8*	Mar		-393.7	-394.0	-643.7	*-477.1*	*144.2*
Seas_1	**-4282.8**	**-2711.5**	**-424.6**	**-1161.7**	**-721.8**	***-1860.5***	***1615.4***	**Seas_1**	**-424.3**	**-1033.6**	**-1034.0**	**-2075.5**	***-1141.8***	***685.6***
Apr	-618.4	-579.8		-417.5	-238.0	*-463.4*	*173.7*	Apr		-393.0	-393.4	-480.7	*-422.3*	*50.5*
May	-532.9	-992.3		-436.0	-245.9	*-551.8*	*317.0*	May		-413.0	-413.5	-842.4	*-556.3*	*247.8*
Jun	-468.0	-904.3		-424.8	-238.0	*-508.8*	*282.0*	Jun		-403.7	-404.4	-782.4	*-530.2*	*218.4*
Seas_2	**-1619.2**	**-2476.4**	**-448.9**	**-1278.3**	**-721.8**	***-1308.9***	***797.6***	**Seas_2**	**-435.9**	**-1209.7**	**-1211.3**	**-2105.5**	***-1240.6***	***682.5***
Jul	-460.7	-860.4		-440.9	-245.9	*-502.0*	*257.9*	Jul		-420.1	-420.9	-747.0	*-529.3*	*188.5*
Aug	-449.9	-875.8		-442.4	-245.9	*-503.5*	*265.5*	Aug		-422.2	-423.3	-773.6	*-539.7*	*202.6*
Sep	-430.4	-710.2		-429.3	-238.0	*-452.0*	*194.5*	Sep		-410.3	-411.4	-633.0	*-484.9*	*128.3*
Seas_3	**-1341.1**	**-2446.3**	**-478.9**	**-1312.5**	**-729.8**	***-1261.7***	***759.6***	**Seas_3**	**-471.2**	**-1252.5**	**-1255.6**	**-2153.5**	***-1283.2***	***687.6***
Oct	-442.3	-948.7		-444.6	-245.9	*-520.4*	*300.4*	Oct		-425.4	-426.8	-844.4	*-565.5*	*241.5*
Nov	-426.9	-781.7		-431.0	-238.0	*-469.4*	*226.8*	Nov		-412.9	-414.4	-703.4	*-510.2*	*167.3*
Dec	-427.4	-818.1		-431.7	-238.0	*-478.8*	*243.6*	Dec		-413.9	-415.6	-743.8	*-524.4*	*190.0*
Seas_4	**-1296.6**	**-2548.5**	**-388.9**	**-1307.3**	**-721.8**	***-1252.6***	***823.4***	**Seas_4**	**-391.7**	**-1252.2**	**-1256.7**	**-2291.7**	***-1298.1***	***777.3***
Annual	**-8539.7**	**-10182.7**	**-1741.4**	**-5059.8**	**-2895.2**	***-5683.8***	***3609.2***	**Annual**	**-1723.1**	**-4748.0**	**-4757.6**	**-8626.2**	***-4963.7***	***2828.7***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data are presented for moderate scale.

Table B.45. *Calculation results: PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMo Chem_ 2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-3205.7	-836.2		-355.4	-571.7	*-1242.2*	*1323.6*	Jan		-317.3	-317.4	-594.8	*-409.8*	*160.2*
Feb	-1413.7	-908.5		-404.8	-663.2	*-847.5*	*429.9*	Feb		-390.2	-390.7	-715.3	*-498.7*	*187.6*
Mar	-804.7	-703.1		-452.6	-736.7	*-674.3*	*153.7*	Mar		-440.8	-441.9	-565.8	*-482.8*	*71.9*
Seas_1	**-5424.1**	**-2447.7**	**-781.7**	**-1212.7**	**-1971.6**	***-2367.6***	***1827.2***	**Seas_1**	**-772.4**	**-1148.2**	**-1150.0**	**-1876.0**	***-1236.6***	***461.7***
Apr	-559.7	-370.3		-445.3	-718.2	*-523.4*	*151.5*	Apr		-435.3	-437.0	-303.4	*-391.9*	*76.6*
May	-508.4	-491.1		-463.5	-740.3	*-550.8*	*127.7*	May		-453.8	-456.2	-416.9	*-442.3*	*22.0*
Jun	-470.1	-470.9		-450.4	-712.8	*-526.1*	*124.9*	Jun		-441.3	-444.3	-411.3	*-432.3*	*18.3*
Seas_2	**-1538.3**	**-1332.2**	**-543.9**	**-1359.2**	**-2171.3**	***-1389.0***	***581.5***	**Seasl_2**	**-541.7**	**-1330.4**	**-1337.5**	**-1131.6**	***-1085.3***	***374.8***
Jul	-478.1	-374.8		-466.7	-732.4	*-513.0*	*153.4*	Jul		-457.6	-461.4	-326.9	*-415.3*	*76.6*
Aug	-475.0	-370.5		-467.7	-728.2	*-510.4*	*152.8*	Aug		-458.9	-463.3	-329.4	*-417.2*	*76.1*
Sep	-458.4	-337.6		-453.5	-700.8	*-487.6*	*152.7*	Sep		-445.1	-449.9	-301.5	*-398.8*	*84.3*
Seas_3	**-1411.5**	**-1082.8**	**-422.2**	**-1387.9**	**-2161.3**	***-1293.2***	***628.4***	**Seas_3**	**-420.6**	**-1361.6**	**-1374.6**	**-957.8**	***-1028.6***	***449.2***
Oct	-472.8	-662.4		-469.3	-720.3	*-581.2*	*129.4*	Oct		-460.8	-466.4	-589.2	*-505.5*	*72.6*
Nov	-457.1	-607.0		-454.7	-693.6	*-553.1*	*117.7*	Nov		-446.6	-452.7	-547.7	*-482.3*	*56.7*
Dec	-456.7	-733.6		-455.2	-690.3	*-584.0*	*148.9*	Dec		-447.3	-453.8	-670.4	*-523.9*	*127.0*
Seas_4	**-1386.6**	**-2003.0**	**-606.0**	**-1379.2**	**-2104.2**	***-1495.8***	***601.0***	**Seas_4**	**-605.5**	**-1354.7**	**-1372.9**	**-1807.3**	***-1285.1***	***499.0***
Annual	**-9760.4**	**-6865.8**	**-2353.8**	**-5339.0**	**-8408.5**	***-6545.5***	***2869.5***	**Annual**	**-2340.2**	**-5194.9**	**-5235.0**	**-5772.7**	***-4635.7***	***1552.8***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table B.46. *Comparison of the calculation results on PCB-28 mass flows transported in/out the calculation domain through the atmosphere (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative"*

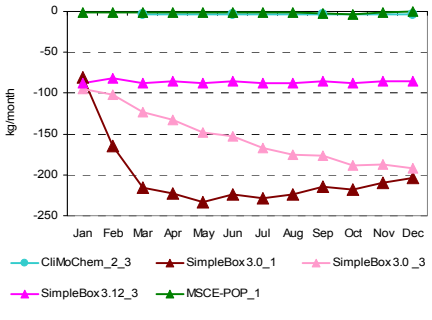
Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	own	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-2135.2	-3205.7	-293.2	-317.3	-293.2	-317.4	-357.4	-355.4	-245.9	-571.7	-913.9	-836.2	-203.3	-594.8		
Feb			-1276.4	-1413.7	-346.6	-390.2	-346.7	-390.7	-381.3	-404.8	-230.0	-663.2	-1001.3	-908.5	-199.8	-715.3		
Mar			-871.2	-804.7	-393.7	-440.8	-394.0	-441.9	-423.1	-452.6	-245.9	-736.7	-796.3	-703.1	-159.6	-565.8		
Seas_1	**-424.6**	**-781.7**	**-4282.8**	**-5424.1**	**-1033.6**	**-1148.2**	**-1034.0**	**-1150.0**	**-1161.7**	**-1212.7**	**-721.8**	**-1971.6**	**-2711.5**	**-2447.7**	**-562.7**	**-1876.0**	**-424.3**	**-772.4**
Apr			-618.4	-559.7	-393.0	-435.3	-393.4	-437.0	-417.5	-445.3	-238.0	-718.2	-579.8	-370.3	-134.2	-303.4		
May			-532.9	-508.4	-413.0	-453.8	-413.5	-456.2	-436.0	-463.5	-245.9	-740.3	-992.3	-491.1	-153.7	-416.9		
Jun			-468.0	-470.1	-403.7	-441.3	-404.4	-444.3	-424.8	-450.4	-238.0	-712.8	-904.3	-470.9	-145.1	-411.3		
Seas_2	**-448.9**	**-543.9**	**-1619.2**	**-1538.3**	**-1209.7**	**-1330.4**	**-1211.3**	**-1337.5**	**-1278.3**	**-1359.2**	**-721.8**	**-2171.3**	**-2476.4**	**-1332.2**	**-433.0**	**-1131.6**	**-435.9**	**-541.7**
Jul			-460.7	-478.1	-420.1	-457.6	-420.9	-461.4	-440.9	-466.7	-245.9	-732.4	-860.4	-374.8	-159.0	-326.9		
Aug			-449.9	-475.0	-422.2	-458.9	-423.3	-463.3	-442.4	-467.7	-245.9	-728.2	-875.8	-370.5	-143.6	-329.4		
Sep			-430.4	-458.4	-410.3	-445.1	-411.4	-449.9	-429.3	-453.5	-238.0	-700.8	-710.2	-337.6	-139.9	-301.5		
Seas_3	**-478.9**	**-422.2**	**-1341.1**	**-1411.5**	**-1252.5**	**-1361.6**	**-1255.6**	**-1374.6**	**-1312.5**	**-1387.9**	**-729.8**	**-2161.3**	**-2446.3**	**-1082.8**	**-442.5**	**-957.8**	**-471.2**	**-420.6**
Oct			-442.3	-472.8	-425.4	-460.8	-426.8	-466.4	-444.6	-469.3	-245.9	-720.3	-948.7	-662.4	-189.7	-589.2		
Nov			-426.9	-457.1	-412.9	-446.6	-414.4	-452.7	-431.0	-454.7	-238.0	-693.6	-781.7	-607.0	-169.6	-547.7		
Dec			-427.4	-456.7	-413.9	-447.3	-415.6	-453.8	-431.7	-455.2	-238.0	-690.3	-818.1	-733.6	-206.4	-670.4		
Seas_4	**-388.9**	**-606.0**	**-1296.6**	**-1386.6**	**-1252.2**	**-1354.7**	**-1256.7**	**-1372.9**	**-1307.3**	**-1379.2**	**-721.8**	**-2104.2**	**-2548.5**	**-2003.0**	**-565.7**	**-1807.3**	**-391.7**	**-605.5**
Annual	**-1741.4**	**-2353.8**	**-8539.7**	**-9760.4**	**-4748.0**	**-5194.9**	**-4757.6**	**-5235.0**	**-5059.8**	**-5339.0**	**-2895.2**	**-8408.5**	**-10182.7**	**-6865.8**	**-2003.9**	**-5772.7**	**-1723.1**	**-2340.2**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.3.2. Comparison of calculated values of PCB-28 mass flows transported in/out the calculation domain through ocean

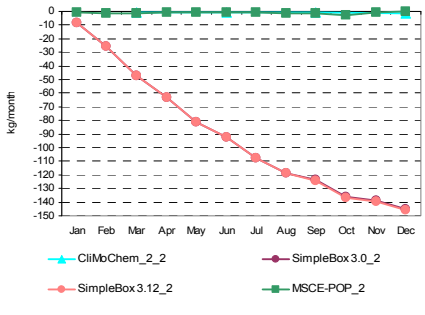
Reference data set. Calculation results on PCB-28 mass flows transported in/out the calculation domain through ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.47.

Monthly values of PCB-28 mass flows transported in/out the calculation domain through ocean calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.69 a and b, respectively.



a

Fig. B.69a. *PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

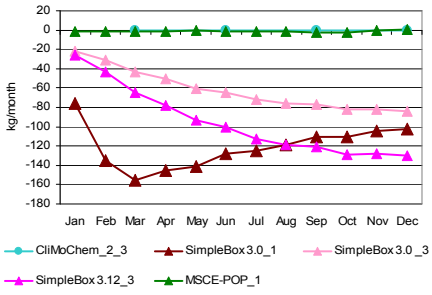


b

Fig. B.69b. *PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

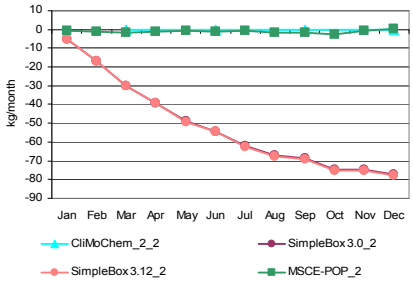
Own/alternative data set. Calculation results on PCB-28 mass flows transported in/out the calculation domain through ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.48.

Monthly values of PCB-28 mass flows transported in/out the calculation domain through ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.70 a and b, respectively.



a

Fig. B.70a. *PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*



b

Fig. B.70b. *PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.49.

Table B.47. *Calculation results: PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-0.9	-80.1		-94.3	-87.9	*-65.8*	*43.7*	Jan		-8.0	-8.0	-0.7	*-5.6*	*4.2*
Feb	-1.4	-164.3		-102.1	-82.3	*-87.5*	*67.2*	Feb		-26.0	-25.9	-1.1	*-17.7*	*14.3*
Mar	-1.5	-215.9		-123.4	-87.9	*-107.2*	*88.7*	Mar		-47.1	-47.1	-1.3	*-31.8*	*26.4*
Seas_1	**-3.8**	**-460.3**	**-9.2**	**-319.7**	**-258.2**	***-210.2***	***199.9***	**Seas_1**	**-1.5**	**-81.1**	**-81.0**	**-3.1**	***-41.7***	***45.5***
Apr	-1.1	-222.9		-132.1	-85.1	*-110.3*	*92.6*	Apr		-62.9	-62.9	-0.9	*-42.3*	*35.8*
May	-0.6	-233.2		-148.2	-87.9	*-117.5*	*98.1*	May		-81.0	-81.0	-0.6	*-54.2*	*46.4*
Jun	-1.1	-224.0		-153.3	-85.1	*-115.9*	*95.2*	Jun		-92.1	-92.1	-1.0	*-61.7*	*52.6*
Seas_2	**-2.8**	**-680.1**	**-10.4**	**-433.6**	**-258.2**	***-277.0***	***288.8***	**Seas_2**	**-2.2**	**-236.0**	**-236.0**	**-2.5**	***-119.2***	***134.9***
Jul	-0.9	-228.1		-167.4	-87.9	*-121.1*	*98.6*	Jul		-107.5	-107.5	-0.7	*-71.9*	*61.7*
Aug	-1.6	-224.5		-175.3	-87.9	*-122.4*	*98.3*	Aug		-118.5	-118.6	-1.4	*-79.5*	*67.7*
Sep	-2.0	-214.1		-176.3	-85.1	*-119.4*	*95.2*	Sep		-123.9	-124.0	-1.6	*-83.2*	*70.6*
Seas_3	**-4.5**	**-666.8**	**-10.2**	**-519.0**	**-261.0**	***-292.3***	***297.9***	**Seas_3**	**-2.7**	**-349.9**	**-350.1**	**-3.7**	***-176.6***	***200.2***
Oct	-3.0	-218.5		-188.1	-87.9	*-124.4*	*98.3*	Oct		-136.4	-136.5	-2.5	*-91.8*	*77.3*
Nov	-1.1	-209.2		-187.1	-85.1	*-120.6*	*96.3*	Nov		-139.1	-139.3	-0.9	*-93.1*	*79.9*
Dec	0.0	-204.0		-191.6	-85.1	*-120.2*	*96.3*	Dec		-145.4	-145.6	0.0	*-97.0*	*84.0*
Seas_4	**-4.1**	**-631.7**	**-9.0**	**-566.9**	**-258.2**	***-294.0***	***297.9***	**Seas_4**	**-3.3**	**-420.9**	**-421.5**	**-3.4**	***-212.3***	***241.2***
Annual	**-15.2**	**-2438.8**	**-38.8**	**-1839.2**	**-1035.5**	***-1073.5***	***1077.3***	**Annual**	**-9.7**	**-1087.9**	**-1088.7**	**-12.7**	***-549.7***	***621.8***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - SimpleBox data are presented for moderate scale.

Table B.48. *Calculation results: PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-75.4	-1.0		-22.0	-25.8	*-31.0*	*31.5*	Jan		-5.1	-5.1	-0.8	*-3.7*	*2.5*
Feb	-134.9	-1.5		-31.0	-43.1	*-52.6*	*57.6*	Feb		-16.7	-16.7	-1.2	*-11.5*	*8.9*
Mar	-155.6	-1.7		-43.6	-64.8	*-66.4*	*65.0*	Mar		-29.9	-29.9	-1.4	*-20.4*	*16.4*
Seas_1	**-365.9**	**-4.1**	**-1.2**	**-96.5**	**-133.8**	***-120.3***	***149.0***	**Seas_1**	**-1.2**	**-51.6**	**-51.6**	**-3.4**	***-27.0***	***28.5***
Apr	-145.3	-1.0		-50.9	-78.2	*-68.9*	*60.1*	Apr		-39.0	-39.1	-0.9	*-26.3*	*22.0*
May	-141.1	-0.8		-60.1	-93.7	*-74.0*	*59.0*	May		-49.0	-49.1	-0.8	*-33.0*	*27.9*
Jun	-128.2	-1.3		-64.2	-100.8	*-73.6*	*54.9*	Jun		-54.4	-54.6	-1.2	*-36.7*	*30.8*
Seas_2	**-414.7**	**-3.2**	**-1.6**	**-175.2**	**-272.7**	***-173.5***	***177.9***	**Seas_2**	**-1.2**	**-142.5**	**-142.8**	**-2.9**	***-72.3***	***81.2***
Jul	-125.2	-0.9		-71.4	-112.4	*-77.5*	*56.0*	Jul		-62.1	-62.4	-0.8	*-41.8*	*35.5*
Aug	-119.2	-1.8		-75.7	-119.2	*-79.0*	*55.4*	Aug		-67.1	-67.5	-1.6	*-45.4*	*37.9*
Sep	-110.8	-2.0		-76.7	-120.4	*-77.5*	*53.7*	Sep		-68.9	-69.3	-1.7	*-46.6*	*38.9*
Seas_3	**-355.2**	**-4.7**	**-0.7**	**-223.8**	**-352.0**	***-187.3***	***176.6***	**Seas_3**	**-0.7**	**-198.2**	**-199.2**	**-4.0**	***-100.5***	***113.4***
Oct	-110.7	-2.9		-82.1	-128.6	*-81.1*	*55.5*	Oct		-74.6	-75.1	-2.4	*-50.7*	*41.8*
Nov	-104.3	-0.8		-81.8	-127.7	*-78.6*	*55.2*	Nov		-74.9	-75.5	-0.6	*-50.3*	*43.1*
Dec	-102.1	0.6		-83.8	-130.2	*-78.9*	*56.3*	Dec		-77.2	-77.9	0.5	*-51.5*	*45.1*
Seas_4	**-317.0**	**-3.0**	**-0.6**	**-247.7**	**-386.5**	***-191.0***	***179.5***	**Seas_4**	**-0.9**	**-226.6**	**-228.5**	**-2.5**	***-114.7***	***130.4***
Annual	**-1452.8**	**-15.1**	**-4.0**	**-743.2**	**-1145.0**	***-672.0***	***655.0***	**Annual**	**-4.0**	**-618.9**	**-622.2**	**-12.9**	***-314.5***	***353.4***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table B.49. *Comparison of the calculation results on PCB-28 mass flows transported in/out the calculation domain through ocean (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-80.1	-75.4	-8.0	-5.1	-8.0	-5.1	-94.3	-22.0	-87.9	-25.8	-0.9	-1.0	-0.7	-0.8		
Feb			-164.3	-134.9	-26.0	-16.7	-25.9	-16.7	-102.1	-31.0	-82.3	-43.1	-1.4	-1.5	-1.1	-1.2		
Mar			-215.9	-155.6	-47.1	-29.9	-47.1	-29.9	-123.4	-43.6	-87.9	-64.8	-1.5	-1.7	-1.3	-1.4		
Seas_1	**-9.2**	**-1.2**	**-460.3**	**-365.9**	**-81.1**	**-51.6**	**-81.0**	**-51.6**	**-319.7**	**-96.5**	**-258.2**	**-133.8**	**-3.8**	**-4.1**	**-3.1**	**-3.4**	**-1.5**	**-1.2**
Apr			-222.9	-145.3	-62.9	-39.0	-62.9	-39.1	-132.1	-50.9	-85.1	-78.2	-1.1	-1.0	-0.9	-0.9		
May			-233.2	-141.1	-81.0	-49.0	-81.0	-49.1	-148.2	-60.1	-87.9	-93.7	-0.6	-0.8	-0.6	-0.8		
Jun			-224.0	-128.2	-92.1	-54.4	-92.1	-54.6	-153.3	-64.2	-85.1	-100.8	-1.1	-1.3	-1.0	-1.2		
Seas_2	**-10.4**	**-1.6**	**-680.1**	**-414.7**	**-236.0**	**-142.5**	**-236.0**	**-142.8**	**-433.6**	**-175.2**	**-258.2**	**-272.7**	**-2.8**	**-3.2**	**-2.5**	**-2.9**	**-2.2**	**-1.2**
Jul			-228.1	-125.2	-107.5	-62.1	-107.5	-62.4	-167.4	-71.4	-87.9	-112.4	-0.9	-0.9	-0.7	-0.8		
Aug			-224.5	-119.2	-118.5	-67.1	-118.6	-67.5	-175.3	-75.7	-87.9	-119.2	-1.6	-1.8	-1.4	-1.6		
Sep			-214.1	-110.8	-123.9	-68.9	-124.0	-69.3	-176.3	-76.7	-85.1	-120.4	-2.0	-2.0	-1.6	-1.7		
Seas_3	**-10.2**	**-0.7**	**-666.8**	**-355.2**	**-349.9**	**-198.2**	**-350.1**	**-199.2**	**-519.0**	**-223.8**	**-261.0**	**-352.0**	**-4.5**	**-4.7**	**-3.7**	**-4.0**	**-2.7**	**-0.7**
Oct			-218.5	-110.7	-136.4	-74.6	-136.5	-75.1	-188.1	-82.1	-87.9	-128.6	-3.0	-2.9	-2.5	-2.4		
Nov			-209.2	-104.3	-139.1	-74.9	-139.3	-75.5	-187.1	-81.8	-85.1	-127.7	-1.1	-0.8	-0.9	-0.6		
Dec			-204.0	-102.1	-145.4	-77.2	-145.6	-77.9	-191.6	-83.8	-85.1	-130.2	0.0	0.6	0.0	0.5		
Seas_4	**-9.0**	**-0.6**	**-631.7**	**-317.0**	**-420.9**	**-226.6**	**-421.5**	**-228.5**	**-566.9**	**-247.7**	**-258.2**	**-386.5**	**-4.1**	**-3.0**	**-3.4**	**-2.5**	**-3.3**	**-0.9**
Annual	**-38.8**	**-4.0**	**-2438.8**	**-1452.8**	**-1087.9**	**-618.9**	**-1088.7**	**-622.2**	**-1839.2**	**-743.2**	**-1035.5**	**-1145.0**	**-15.2**	**-15.1**	**-12.7**	**-12.9**	**-9.7**	**-4.0**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.3.3. Calculated values of PCB-28 mass flows transported in/out the calculation domain through other compartments

Reference data set. Calculation results on PCB-28 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.50.

Monthly values of PCB-28 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "reference" data set are presented in Fig. B.71.

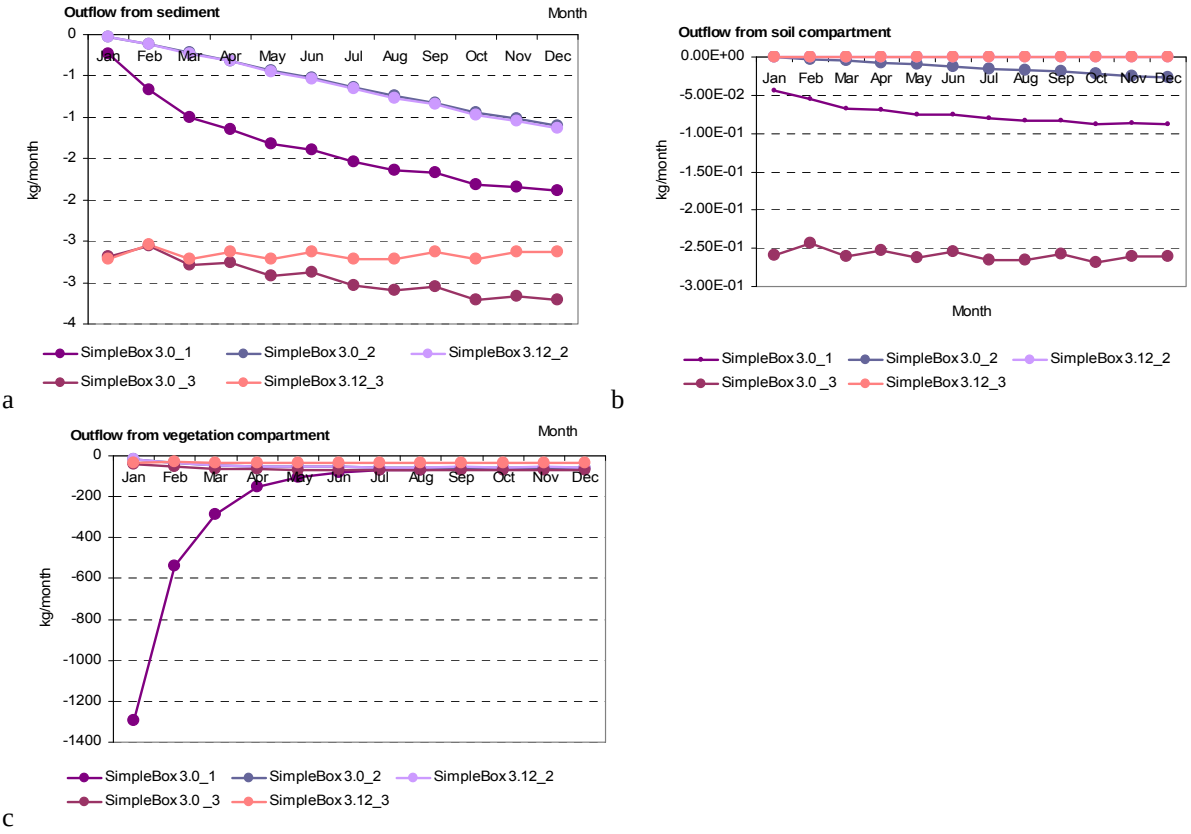


Fig. B.71. *PCB-28 mass flows transported in/out the calculation domain through sediment (a), soil (b) and vegetation(c) calculated by SimpleBox on the basis of "reference" data set*

Own/alternative data set. Calculation results on PCB-28 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "alternative" data sets together with statistical parameters used for evaluation are presented in Table B.51.

Monthly values of PCB-28 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "alternative" data set are compared in Fig. B.72.

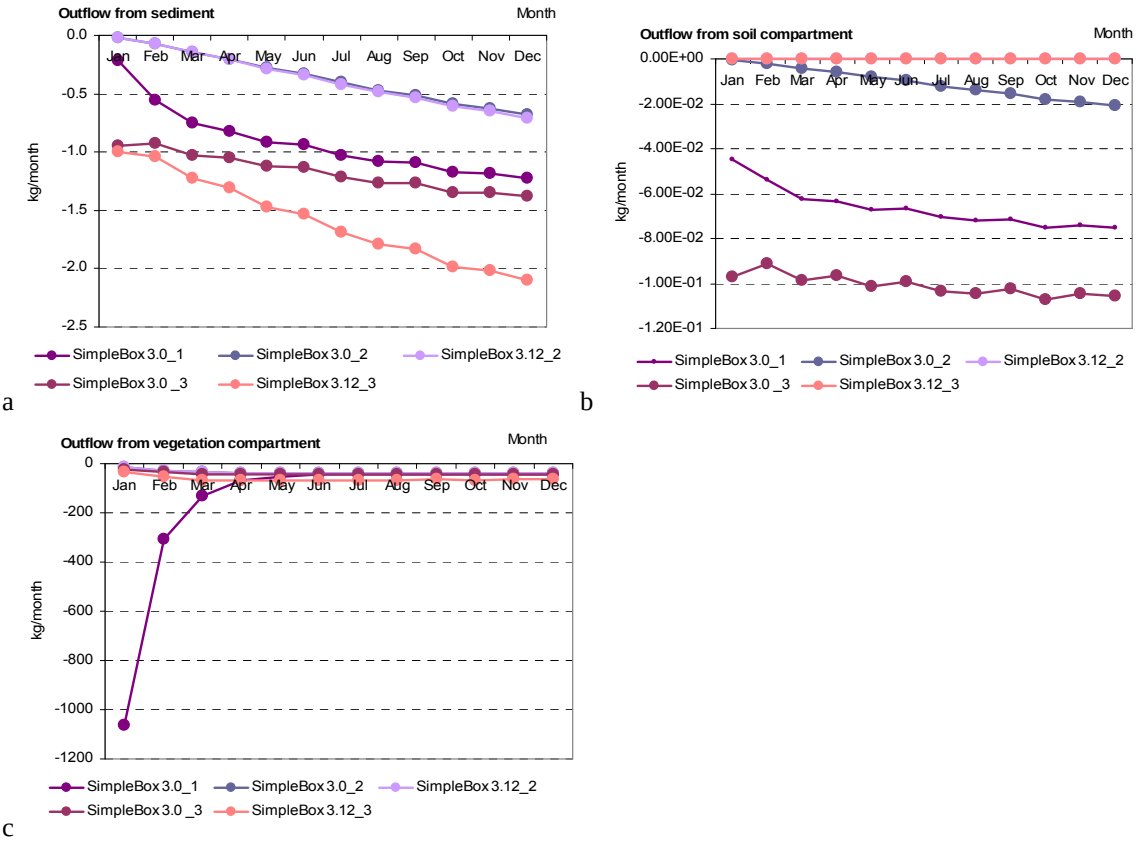


Fig. B.72. *PCB-28 mass flows transported in/out the calculation domain through sediment (a), soil (b) and vegetation(c) calculated by SimpleBox on the basis of "alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two different data sets of physical-chemical properties (for SimpleBox model) is shown in Table B.52.

Table B.50. *Calculation results: PCB-28 mass flows transported in/out the calculation domain through sediments, soil and vegetation (kg/month) calculated by SimpleBox on the basis of "reference" data set*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	-0.24	-0.03	-0.03	-2.69	-2.71	-4.43E-02	-7.29E-04	-1.26E-07	-2.59E-01	-4.17E-04	-1296.36	-14.83	-14.80	-43.57	-33.90
Feb	-0.67	-0.11	-0.12	-2.56	-2.54	-5.52E-02	-2.53E-03	-3.98E-07	-2.43E-01	-3.90E-04	-539.18	-34.59	-34.49	-54.43	-31.71
Mar	-1.00	-0.22	-0.23	-2.79	-2.71	-6.70E-02	-4.99E-03	-7.44E-07	-2.61E-01	-4.17E-04	-284.68	-47.20	-47.00	-64.92	-33.90
Apr	-1.15	-0.32	-0.32	-2.76	-2.63	-6.97E-02	-7.21E-03	-1.04E-06	-2.53E-01	-4.03E-04	-153.90	-50.41	-50.14	-65.95	-32.80
May	-1.32	-0.43	-0.44	-2.91	-2.71	-7.55E-02	-9.96E-03	-1.41E-06	-2.63E-01	-4.17E-04	-105.91	-54.50	-54.13	-69.74	-33.90
Jun	-1.39	-0.52	-0.54	-2.88	-2.63	-7.58E-02	-1.21E-02	-1.68E-06	-2.55E-01	-4.03E-04	-80.18	-54.01	-53.56	-68.31	-32.80
Jul	-1.54	-0.64	-0.66	-3.04	-2.71	-8.08E-02	-1.50E-02	-2.07E-06	-2.65E-01	-4.17E-04	-72.82	-56.61	-56.06	-71.10	-33.90
Aug	-1.64	-0.75	-0.77	-3.10	-2.71	-8.32E-02	-1.76E-02	-2.40E-06	-2.66E-01	-4.17E-04	-68.34	-57.17	-56.53	-71.46	-33.90
Sep	-1.67	-0.82	-0.84	-3.05	-2.63	-8.28E-02	-1.95E-02	-2.64E-06	-2.58E-01	-4.03E-04	-64.28	-55.74	-55.03	-69.42	-32.80
Oct	-1.81	-0.95	-0.97	-3.21	-2.71	-8.77E-02	-2.27E-02	-3.05E-06	-2.68E-01	-4.17E-04	-65.61	-57.96	-57.14	-71.96	-33.90
Nov	-1.84	-1.01	-1.04	-3.16	-2.63	-8.70E-02	-2.44E-02	-3.26E-06	-2.60E-01	-4.03E-04	-63.18	-56.41	-55.53	-69.82	-32.80
Dec	-1.89	-1.10	-1.13	-3.22	-2.63	-8.86E-02	-2.68E-02	-3.56E-06	-2.61E-01	-4.03E-04	-62.47	-56.69	-55.72	-70.00	-32.80
Annual	**-16.17**	**-6.91**	**-7.09**	**-35.37**	**-31.96**	**-8.98E-01**	**-1.63E-01**	**-2.24E-05**	**-3.11E+00**	**-4.91E-03**	**-2856.90**	**-596.13**	**-590.13**	**-790.67**	**-399.11**

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

* - SimpleBox data are presented for moderate scale

Table B.51. *Calculation results: PCB-28 mass flows transported in/out the calculation domain through sediment, soil and vegetation (kg/month) calculated by SimpleBox on the basis of "alternative" data set*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox x 3.12_3
Jan	-0.22	-0.02	-0.02	-0.95	-0.99	-4.49E-02	-5.80E-04	-3.55E-08	-9.68E-02	-5.96E-05	-1061.47	-13.58	-13.56	-22.82	-32.16
Feb	-0.55	-0.07	-0.07	-0.92	-1.04	-5.39E-02	-2.08E-03	-1.14E-07	-9.14E-02	-5.51E-05	-309.36	-28.74	-28.68	-34.92	-54.51
Mar	-0.76	-0.14	-0.15	-1.03	-1.23	-6.27E-02	-4.10E-03	-2.15E-07	-9.88E-02	-5.83E-05	-130.94	-36.36	-36.26	-42.04	-66.15
Apr	-0.82	-0.20	-0.21	-1.04	-1.31	-6.33E-02	-5.89E-03	-3.00E-07	-9.68E-02	-5.57E-05	-68.57	-37.10	-36.98	-42.27	-66.06
May	-0.91	-0.28	-0.28	-1.13	-1.47	-6.73E-02	-8.07E-03	-4.04E-07	-1.01E-01	-5.69E-05	-53.22	-39.11	-38.96	-44.31	-68.54
Jun	-0.94	-0.33	-0.34	-1.13	-1.53	-6.67E-02	-9.74E-03	-4.82E-07	-9.90E-02	-5.44E-05	-46.32	-38.23	-38.07	-43.19	-66.09
Jul	-1.03	-0.41	-0.42	-1.22	-1.69	-7.05E-02	-1.20E-02	-5.90E-07	-1.04E-01	-5.56E-05	-46.24	-39.78	-39.58	-44.83	-67.89
Aug	-1.08	-0.47	-0.48	-1.26	-1.79	-7.21E-02	-1.40E-02	-6.83E-07	-1.05E-01	-5.50E-05	-45.73	-40.00	-39.77	-45.00	-67.44
Sep	-1.09	-0.51	-0.53	-1.26	-1.83	-7.12E-02	-1.55E-02	-7.49E-07	-1.02E-01	-5.26E-05	-44.11	-38.90	-38.65	-43.68	-64.86
Oct	-1.18	-0.59	-0.61	-1.35	-1.99	-7.51E-02	-1.79E-02	-8.63E-07	-1.07E-01	-5.37E-05	-45.55	-40.37	-40.09	-45.26	-66.60
Nov	-1.18	-0.63	-0.65	-1.34	-2.01	-7.41E-02	-1.92E-02	-9.21E-07	-1.05E-01	-5.14E-05	-44.10	-39.23	-38.93	-43.92	-64.06
Dec	-1.23	-0.68	-0.71	-1.38	-2.10	-7.55E-02	-2.10E-02	-1.00E-06	-1.06E-01	-5.08E-05	-44.13	-39.38	-39.05	-44.02	-63.70
Annual	**-10.98**	**-4.33**	**-4.47**	**-14.03**	**-18.97**	**-7.97E-01**	**-1.30E-01**	**-6.36E-06**	**-1.21E+00**	**-6.59E-04**	**-1939.74**	**-430.77**	**-428.58**	**-496.26**	**-748.06**

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

* - SimpleBox data are presented for moderate scale.

Table B.52. *The percentage difference between calculation results on PCB-28 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of two data sets: "reference" and "alternative"*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	-8.1%	-38.2%	-38.2%	-64.7%	-63.4%	1%	-20%	-72%	-63%	-86%	-18%	-8%	-8%	-48%	-5%
Feb	-17.4%	-36.6%	-36.6%	-63.9%	-59.2%	-2%	-18%	-71%	-62%	-86%	-43%	-17%	-17%	-36%	72%
Mar	-24.4%	-36.1%	-36.0%	-63.1%	-54.7%	-6%	-18%	-71%	-62%	-86%	-54%	-23%	-23%	-35%	95%
Apr	-28.6%	-36.1%	-36.0%	-62.2%	-50.3%	-9%	-18%	-71%	-62%	-86%	-55%	-26%	-26%	-36%	101%
May	-31.0%	-36.4%	-36.2%	-61.4%	-45.9%	-11%	-19%	-71%	-61%	-86%	-50%	-28%	-28%	-36%	102%
Jun	-32.4%	-36.6%	-36.4%	-60.6%	-41.8%	-12%	-19%	-71%	-61%	-86%	-42%	-29%	-29%	-37%	101%
Jul	-33.4%	-36.9%	-36.6%	-59.9%	-37.8%	-13%	-20%	-71%	-61%	-87%	-37%	-30%	-29%	-37%	100%
Aug	-34.1%	-37.2%	-36.9%	-59.2%	-33.9%	-13%	-20%	-72%	-61%	-87%	-33%	-30%	-30%	-37%	99%
Sep	-34.7%	-37.4%	-37.1%	-58.6%	-30.3%	-14%	-21%	-72%	-60%	-87%	-31%	-30%	-30%	-37%	98%
Oct	-35.2%	-37.6%	-37.2%	-58.0%	-26.8%	-14%	-21%	-72%	-60%	-87%	-31%	-30%	-30%	-37%	96%
Nov	-35.6%	-37.9%	-37.4%	-57.5%	-23.4%	-15%	-21%	-72%	-60%	-87%	-30%	-30%	-30%	-37%	95%
Dec	-35.2%	-38.1%	-37.6%	-57.0%	-20.2%	-15%	-21%	-72%	-59%	-87%	-29%	-31%	-30%	-37%	94%
Annual	-32.1%	-37.3%	-37.0%	-60.3%	-40.6%	-11%	-20%	-72%	-61%	-87%	-32%	-28%	-27%	-37%	87%

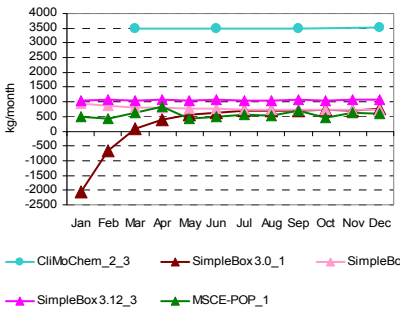
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

B.3.4. Comparison of calculated values of PCB-28 total mass flows transported in/out the specified domain

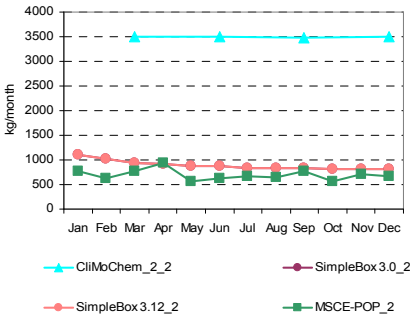
Values of total mass flow transported in/out the calculation domain are calculated as sum of inflow (emissions) and all outflows through the main transport media.

Reference data set. Calculation results on PCB-28 total mass flows transported in/out the specified domain calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.53.

Monthly values of PCB-28 total mass flows transported in/out the specified domain calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.73 a and b, respectively.



a



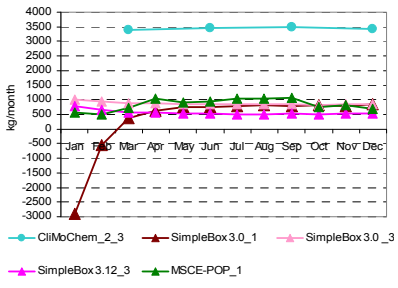
b

Fig. B.73a. *PCB-28 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

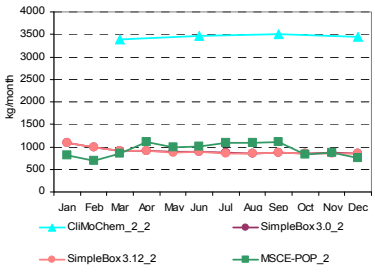
Fig. B.73b. *PCB-28 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-28 total mass flows transported in/out the specified domain calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.54.

Monthly values of PCB-28 mass flows transported in/out the specified domain calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.74 a and b, respectively.



a



b

Fig. B.74a. *PCB-28 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

Fig. B.74b. *PCB-28 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.55.

Table B.53. *Calculation results: PCB-28 total mass flows transported in/out the specified domain (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-2060.4	499.8		926.0	1053.7	*104.8*	*1462.8*	Jan		1108.1	1108.1	771.6	*995.9*	*194.3*
Feb	-669.6	411.9		883.6	1077.6	*425.9*	*782.0*	Feb		1016.9	1016.9	623.9	*885.9*	*226.9*
Mar	78.7	616.8		809.7	1053.7	*639.7*	*414.6*	Mar		935.9	935.9	769.7	*880.5*	*96.0*
Seas_1	**-2651.4**	**1528.5**	**10490.6**	**2619.3**	**3185.0**	***3034.4***	***4753.6***	**Seas_1**	**10498.6**	**3060.8**	**3060.8**	**2165.2**	***4696.4***	***3891.1***
Apr	408.2	833.8		805.6	1065.7	*778.3*	*272.9*	Apr		917.5	917.4	933.0	*922.6*	*9.0*
May	578.1	421.6		767.0	1053.7	*705.1*	*271.9*	May		875.2	875.1	571.6	*774.0*	*175.2*
Jun	631.0	509.2		774.6	1065.7	*745.1*	*239.6*	Jun		873.8	873.6	631.2	*792.9*	*140.0*
Seas_2	**1617.4**	**1764.6**	**10465.1**	**2347.3**	**3185.0**	***3875.9***	***3734.6***	**Seas_2**	**10486.2**	**2666.5**	**2666.0**	**2135.8**	***4488.7***	***4006.2***
Jul	688.2	553.3		741.5	1053.7	*759.2*	*211.7*	Jul		839.3	839.0	666.9	*781.7*	*99.4*
Aug	707.0	537.2		731.6	1053.7	*757.4*	*215.6*	Aug		825.5	825.0	639.7	*763.4*	*107.1*
Sep	694.0	702.4		745.9	1065.7	*802.0*	*177.2*	Sep		833.4	832.9	780.0	*815.4*	*30.7*
Seas_3	**2089.2**	**1793.0**	**10435.2**	**2219.0**	**3173.1**	***3941.9***	***3666.5***	**Seas_3**	**10450.5**	**2498.3**	**2496.8**	**2086.6**	***4383.0***	***4049.6***
Oct	723.1	462.9		716.0	1053.7	*738.9*	*242.2*	Oct		803.5	802.7	567.7	*724.6*	*135.9*
Nov	703.4	631.8		732.7	1065.7	*783.4*	*192.9*	Nov		814.7	813.9	710.3	*779.6*	*60.1*
Dec	755.6	596.5		727.4	1065.7	*786.3*	*198.7*	Dec		807.1	806.1	670.8	*761.3*	*78.4*
Seas_4	**2182.2**	**1691.2**	**10526.4**	**2176.1**	**3185.0**	***3952.2***	***3715.1***	**Seas_4**	**10529.3**	**2425.2**	**2422.8**	**1948.7**	***4331.5***	***4137.9***
Annual	**3237.4**	**6777.3**	**41917.2**	**9361.8**	**12728.1**	***14804.4***	***15550.5***	**Annual**	**41964.6**	**10650.9**	**10646.5**	**8336.3**	***17899.6***	***16080.3***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table B.54. *Calculation results: PCB-28 total mass flows transported in/out the specified domain (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-2891.3	577.5		1022.9	793.5	*-124.4*	*1853.6*	Jan		1088.2	1088.1	819.0	*998.4*	*155.3*
Feb	-547.6	504.6		952.5	662.3	*392.9*	*653.9*	Feb		988.5	988.0	698.0	*891.5*	*167.6*
Mar	359.4	709.8		884.9	555.2	*627.3*	*223.7*	Mar		917.0	916.0	847.3	*893.5*	*39.9*
Seas_1	**-3079.5**	**1791.9**	**10141.5**	**2860.2**	**2011.0**	***2745.0***	***4745.9***	**Seas_1**	**10150.8**	**2993.7**	**2992.1**	**2364.4**	***4625.2***	***3695.6***
Apr	630.2	1043.3		884.6	560.4	*779.6*	*224.3*	Apr		912.6	910.9	1110.2	*977.9*	*114.6*
May	747.7	922.7		855.0	520.1	*761.4*	*176.3*	May		882.0	879.6	996.9	*919.5*	*67.1*
Jun	758.9	942.4		865.2	543.0	*777.4*	*173.4*	Jun		889.9	886.8	1002.1	*926.3*	*65.7*
Seas_2	**2136.9**	**2908.4**	**10378.8**	**2604.7**	**1623.4**	***3930.4***	***3637.4***	**Seas_2**	**10381.5**	**2684.4**	**2677.3**	**3109.3**	***4713.1***	***3784.3***
Jul	800.8	1038.9		839.9	509.8	*797.3*	*218.2*	Jul		864.2	860.4	1086.9	*937.2*	*129.7*
Aug	810.4	1042.3		834.3	507.6	*798.7*	*220.2*	Aug		857.7	853.1	1083.6	*931.5*	*131.8*
Sep	790.3	1075.0		849.0	536.3	*812.6*	*221.4*	Sep		870.8	865.7	1111.5	*949.3*	*140.4*
Seas_3	**2401.5**	**3156.2**	**10501.4**	**2523.2**	**1553.7**	***4027.2***	***3663.9***	**Seas_3**	**10503.1**	**2592.6**	**2579.3**	**3282.0**	***4739.2***	***3856.5***
Oct	821.1	749.4		826.1	506.6	*725.8*	*150.3*	Oct		847.8	842.0	823.0	*837.6*	*13.0*
Nov	798.0	806.8		842.3	536.8	*746.0*	*140.8*	Nov		862.7	856.4	866.3	*861.8*	*5.0*
Dec	847.2	681.6		839.7	537.9	*726.6*	*147.2*	Dec		859.6	852.7	744.7	*819.0*	*64.4*
Seas_4	**2466.4**	**2237.7**	**10317.8**	**2508.0**	**1581.3**	***3822.2***	***3650.0***	**Seas_4**	**10317.9**	**2570.2**	**2551.0**	**2433.9**	***4468.3***	***3900.2***
Annual	**3925.2**	**10094.3**	**41339.6**	**10496.2**	**6769.4**	***14524.9***	***15226.5***	**Annual**	**41353.2**	**10840.9**	**10799.7**	**11189.6**	***18545.9***	***15205.9***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table B.55. *Comparison of the calculation results on PCB-28 mass flows transported in/out the specified domain (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative"*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0_3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-2060.4	-2891.3	1108.1	1088.2	1108.1	1088.1	926.0	1022.9	1053.7	793.5	499.8	577.5	771.6	819.0		
Feb			-669.6	-547.6	1016.9	988.5	1016.9	988.0	883.6	952.5	1077.6	662.3	411.9	504.6	623.9	698.0		
Mar			78.7	359.4	935.9	917.0	935.9	916.0	809.7	884.9	1053.7	555.2	616.8	709.8	769.7	847.3		
Seas_1	**10490.6**	**10141.5**	**-2651.4**	**-3079.5**	**3060.8**	**2993.7**	**3060.8**	**2992.1**	**2619.3**	**2860.2**	**3185.0**	**2011.0**	**1528.5**	**1791.9**	**2165.2**	**2364.4**	**10498.6**	**10150.8**
Apr			408.2	630.2	917.5	912.6	917.4	910.9	805.6	884.6	1065.7	560.4	833.8	1043.3	933.0	1110.2		
May			578.1	747.7	875.2	882.0	875.1	879.6	767.0	855.0	1053.7	520.1	421.6	922.7	571.6	996.9		
Jun			631.0	758.9	873.8	889.9	873.6	886.8	774.6	865.2	1065.7	543.0	509.2	942.4	631.2	1002.1		
Seas_2	**10465.1**	**10378.8**	**1617.4**	**2136.9**	**2666.5**	**2684.4**	**2666.0**	**2677.3**	**2347.3**	**2604.7**	**3185.0**	**1623.4**	**1764.6**	**2908.4**	**2135.8**	**3109.3**	**10486.2**	**10381.5**
Jul			688.2	800.8	839.3	864.2	839.0	860.4	741.5	839.9	1053.7	509.8	553.3	1038.9	666.9	1086.9		
Aug			707.0	810.4	825.5	857.7	825.0	853.1	731.6	834.3	1053.7	507.6	537.2	1042.3	639.7	1083.6		
Sep			694.0	790.3	833.4	870.8	832.9	865.7	745.9	849.0	1065.7	536.3	702.4	1075.0	780.0	1111.5		
Seas_3	**10435.2**	**10501.4**	**2089.2**	**2401.5**	**2498.3**	**2592.6**	**2496.8**	**2579.3**	**2219.0**	**2523.2**	**3173.1**	**1553.7**	**1793.0**	**3156.2**	**2086.6**	**3282.0**	**10450.5**	**10503.1**
Oct			723.1	821.1	803.5	847.8	802.7	842.0	716.0	826.1	1053.7	506.6	462.9	749.4	567.7	823.0		
Nov			703.4	798.0	814.7	862.7	813.9	856.4	732.7	842.3	1065.7	536.8	631.8	806.8	710.3	866.3		
Dec			755.6	847.2	807.1	859.6	806.1	852.7	727.4	839.7	1065.7	537.9	596.5	681.6	670.8	744.7		
Seas_4	**10526.4**	**10317.8**	**2182.2**	**2466.4**	**2425.2**	**2570.2**	**2422.8**	**2551.0**	**2176.1**	**2508.0**	**3185.0**	**1581.3**	**1691.2**	**2237.7**	**1948.7**	**2433.9**	**10529.3**	**10317.9**
Annual	**41917.2**	**41339.6**	**3237.4**	**3925.2**	**10650.9**	**10840.9**	**10646.5**	**10799.7**	**9361.8**	**10496.2**	**12728.1**	**6769.4**	**6777.3**	**10094.3**	**8336.3**	**11189.6**	**41964.6**	**41353.2**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

B.3.5. Comparison of PCB-28 mass flows transported in/out the specified domain

The calculation results on PCB-28 transport inside and outside the calculation domain through main transport media such as atmosphere and seawater are discussed in this subsection. Transport of this pollutant from sediment, soil and vegetation compartments due to such processes as burial, leaching and harvest of agricultural vegetation, respectively, is considered in SimpleBox model.

The results considered in Sections B.3.1-B.3.4 above are obtained with one-year calculations with zero initial concentrations (CliMoChem, MSCE-POP, SimpleBox) and with initial concentrations in media (MSCE-POP, SimpleBox); and with long-term calculations with historical emissions (CliMoChem, SimpleBox). CliMoChem, MSCE-POP, and SimpleBox models presented results obtained on the basis of two different physical-chemical data sets. Of note, the calculated values compared below are negative in the case if a model predicted PCB-28 transport out the calculation domain through the considered media.

A preliminary analysis of the comparison of absolute values PCB-28 transport mass flows inside and outside the calculation domain through main transport media is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions and for results based on zero initial conditions.

Transport through the atmosphere. Comparison of annual values of PCB-28 mass flows transported out the calculation domain through the atmosphere calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. B.75a together with the averaged value given as the blue line. Fig. B.75b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

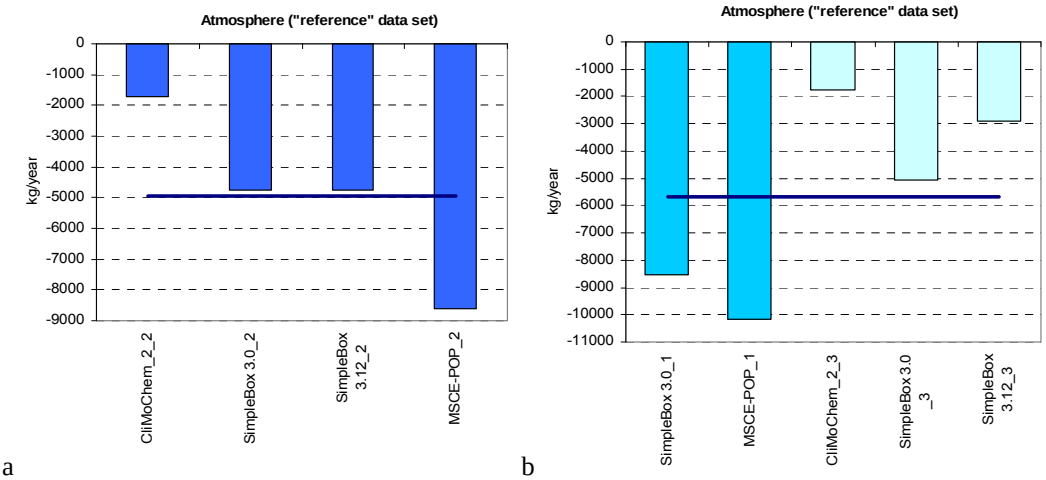
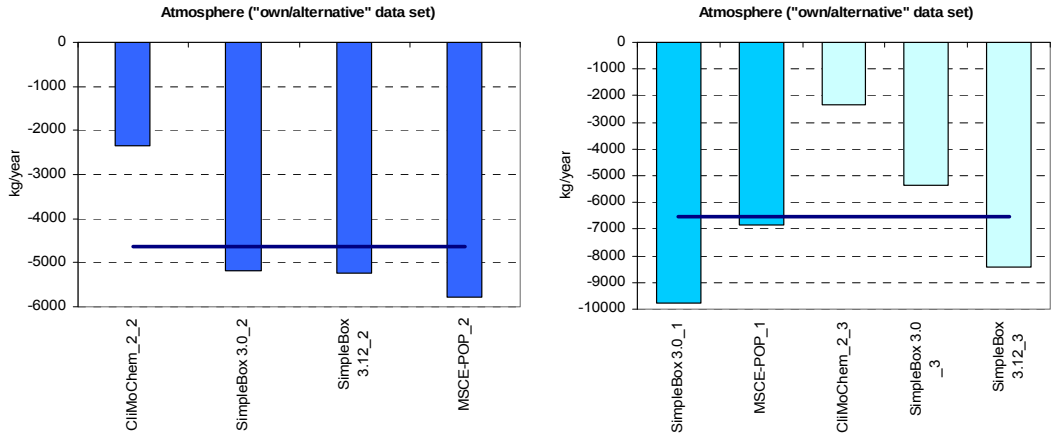


Fig. B.75. *Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fig. B.76a demonstrates the comparison of the annual values of PCB-28 mass flows transported out the calculation domain through the atmosphere calculated on the basis of zero initial concentrations and with the use of "***own or alternative*****"** data sets. Fig. B.76b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial

data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig. B.76. *Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-28 mass flows transported out the calculation domain through the atmosphere obtained with "reference" and "own/alternative" data sets is presented in and in Fig. B.77 (see also Table B.46 given in Section B.3.1).

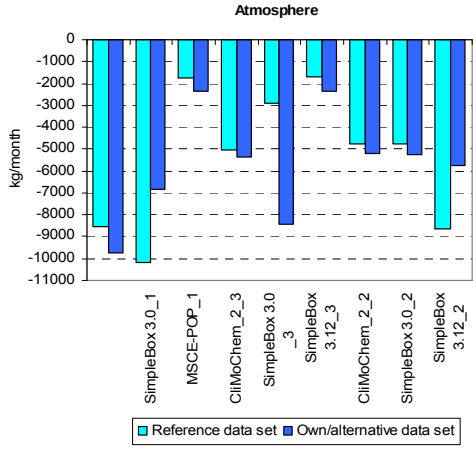


Fig. B.77. *Comparison of PCB-28 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of two physical-chemical data sets*

Transport through ocean. Comparison of annual values of PCB-28 mass flows transported out the calculation domain through ocean calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. B.78a. Fig. B.78b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

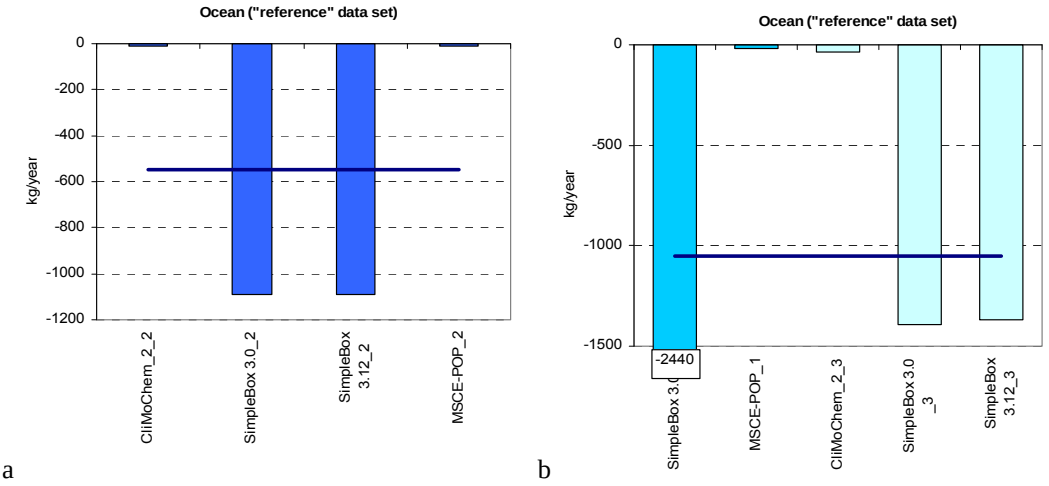


Fig. B.78. *Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-28 mass flows transported out the calculation domain through ocean calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative***" data sets is presented in Fig. B.79a. Fig. B.79b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

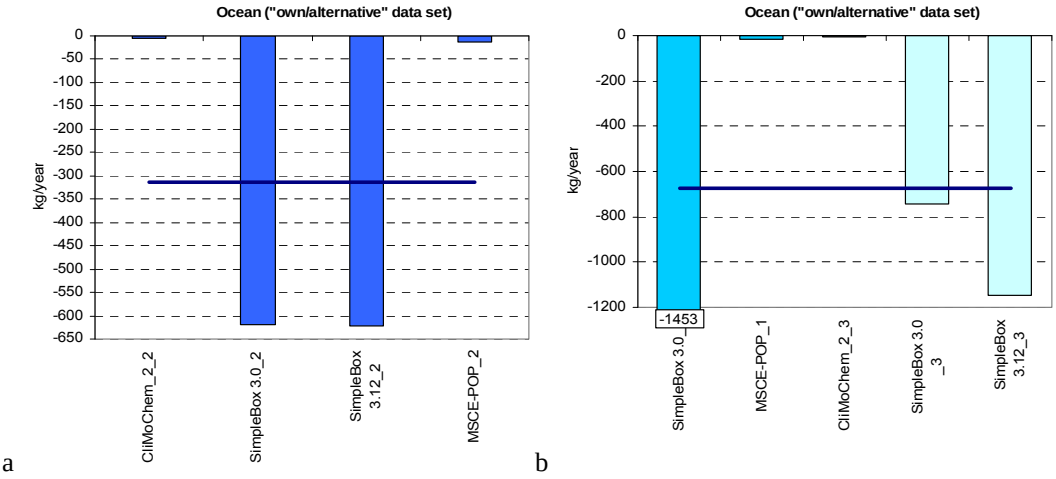


Fig. B.79. *Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-28 mass flows transported out the calculation domain through ocean obtained with "reference" and "own/alternative" data sets is presented in Table B.49 given in Section B.3.2 and in Fig. B.80a below. The same data for models with low values of mass flows transported out the calculation domain through ocean are also shown in Fig. B.80b in more detail.

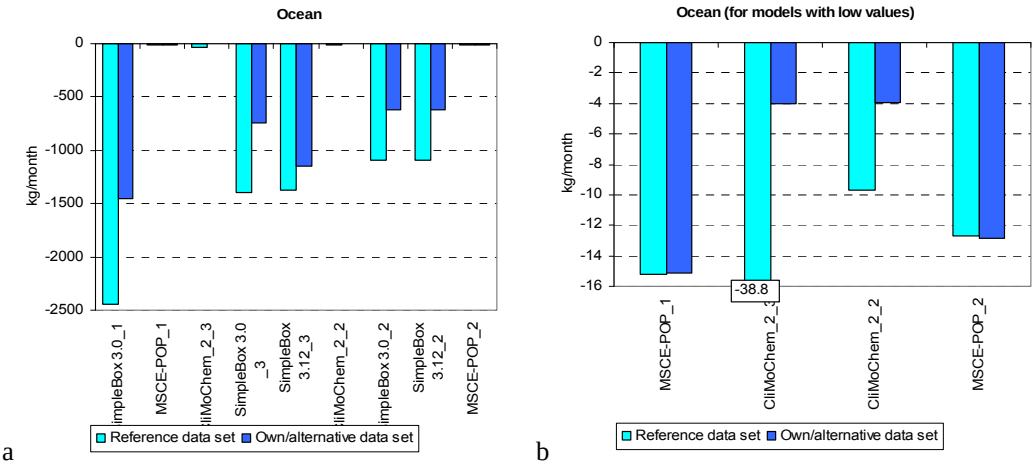


Fig. B.80. *Comparison of PCB-28 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of two data sets (a - all models; b – models with low values of PCB-28 mass flows transported in/out of ocean).*

Transport through other media. In addition to the results on mass flows of PCB-28 transported out the calculation domain via the atmosphere and ocean, Simple Box model presented calculated values of outflows from sediments, soil and vegetation. Transport of this pollutant from these compartments is considered to be due to such processes as burial, leaching and harvest of agricultural vegetation, respectively.

Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. B.81a. Fig. B.81b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between calculations of different types.

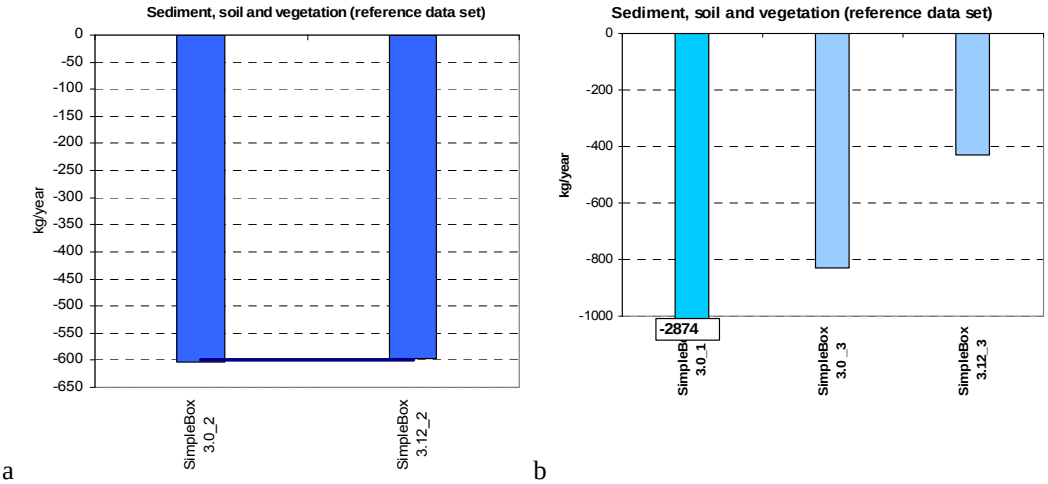
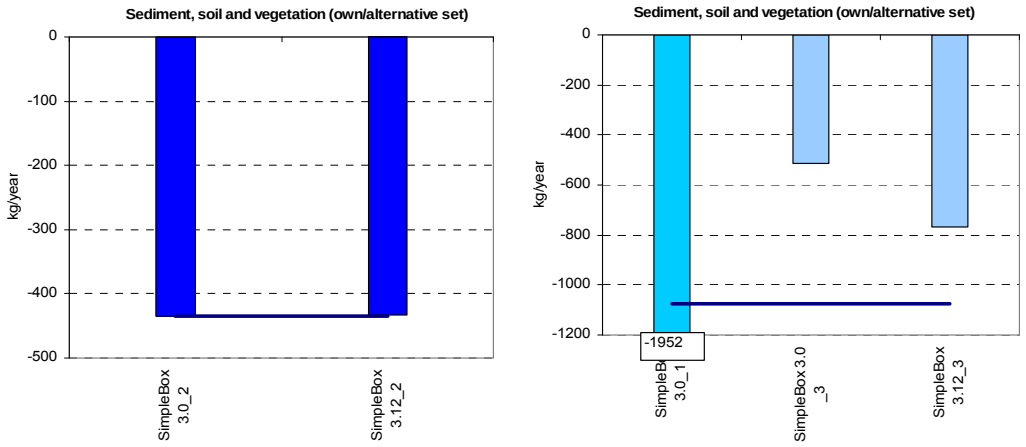


Fig. B.81. *Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions).*

The annual values of PCB-28 mass flows transported out the calculation domain through three considered media calculated by SimpleBox model on the basis of zero initial concentrations and "**alternative**" data set are compared in Fig. B.82a. Fig. B.82b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between different versions of this model.



a b

Fig. B.82. *Comparison of annual values of PCB-28 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Annual values of PCB-28 mass flows transported out the calculation domain through such media as sediment, soil and vegetation obtained with "reference" and "own/alternative" data sets are compared in Fig. B.83.

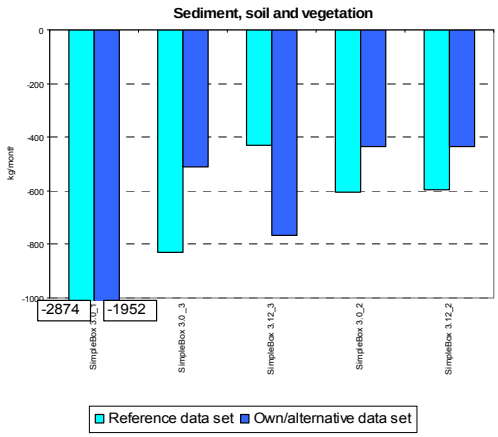


Fig. B.83. *Comparison of PCB-28 mass flows transported in/out the calculation domain through the atmosphere (a), other media (sediment, soil and vegetation)(b) and seawater(c, d) calculated by different models on the basis of two data sets*

Total mass flow. Comparison of annual values of PCB-28 total mass flows transported in/out the calculation domain calculated by different models on the basis of zero initial concentrations and with the use of "***reference*****"** data set is presented in Fig. B.84a. Fig. B.84b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis

of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

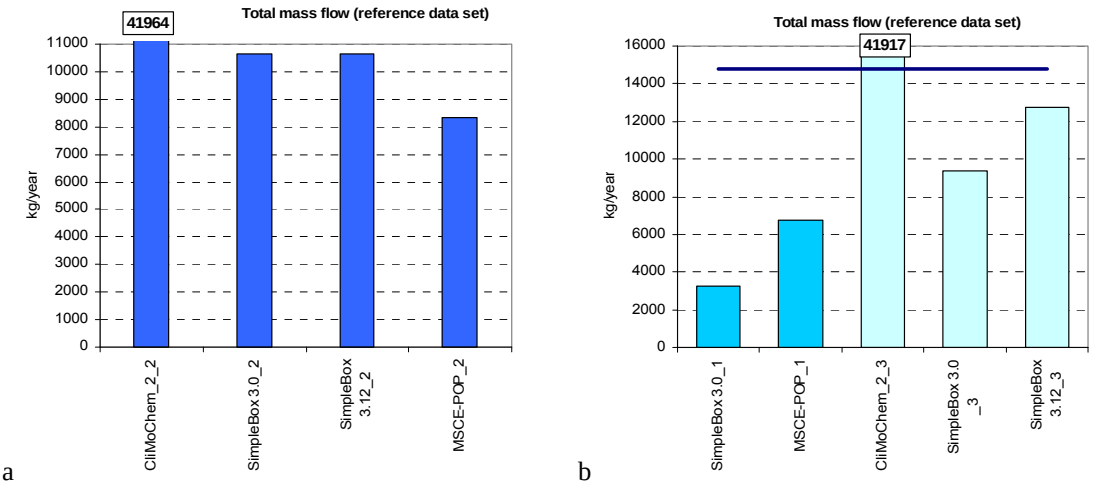


Fig. B.84. *Comparison of annual values of PCB-28 total mass flows transported in/out the calculation domain calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-28 total mass flows transported in/out the calculation domain calculated by different models on the basis of zero initial concentrations and "***own or alternative***" data sets is presented in Fig. B.85a. Fig. B.85b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

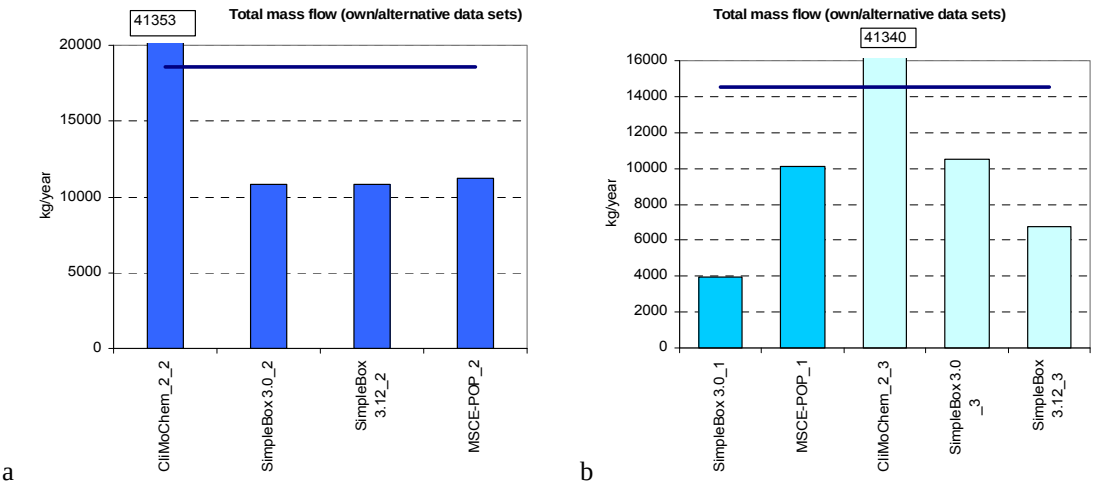


Fig. B.85. *Comparison of annual values of PCB-28 total mass flows transported in/out the calculation domain calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

For models performed calculations on two data sets, the annual values of PCB-28 mass flow transported inside and outside the calculation domain (taking into account emissions) obtained with

"reference" and "own/alternative" data sets are compared in Fig. B.86a. Fig. B.86b presents also the comparison of absolute values of overall mass flow transported outside the calculation domain (not taking into account emission value).

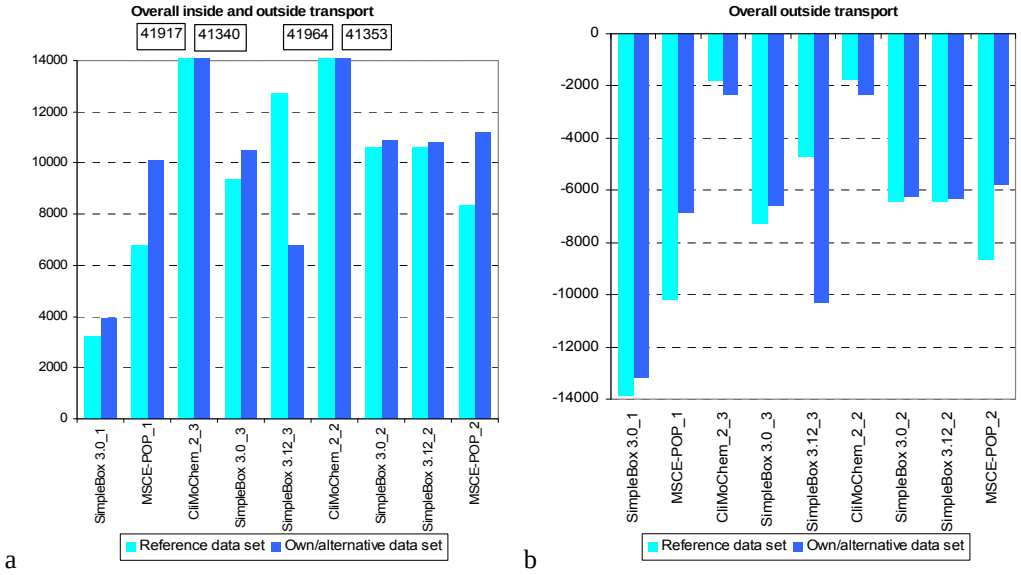
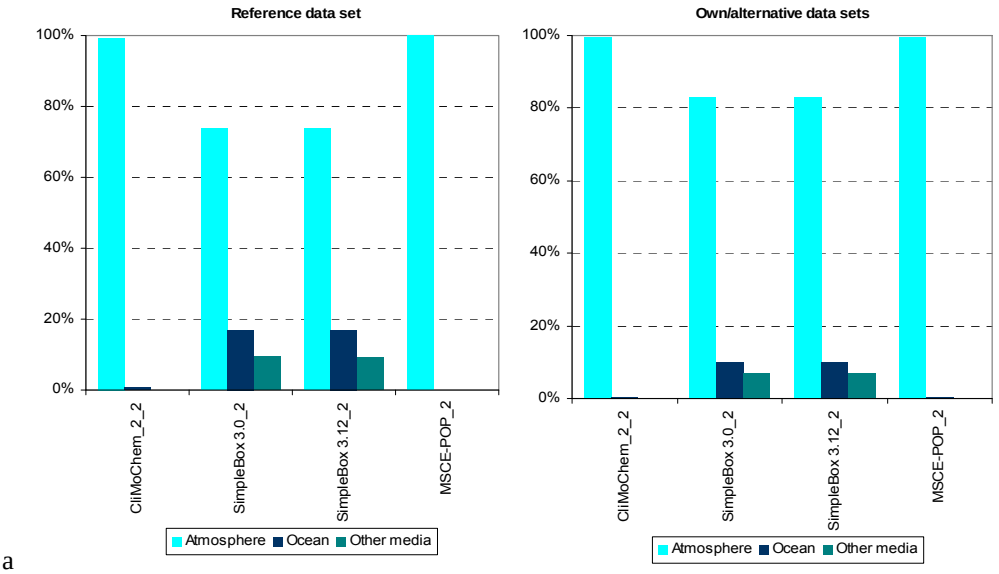
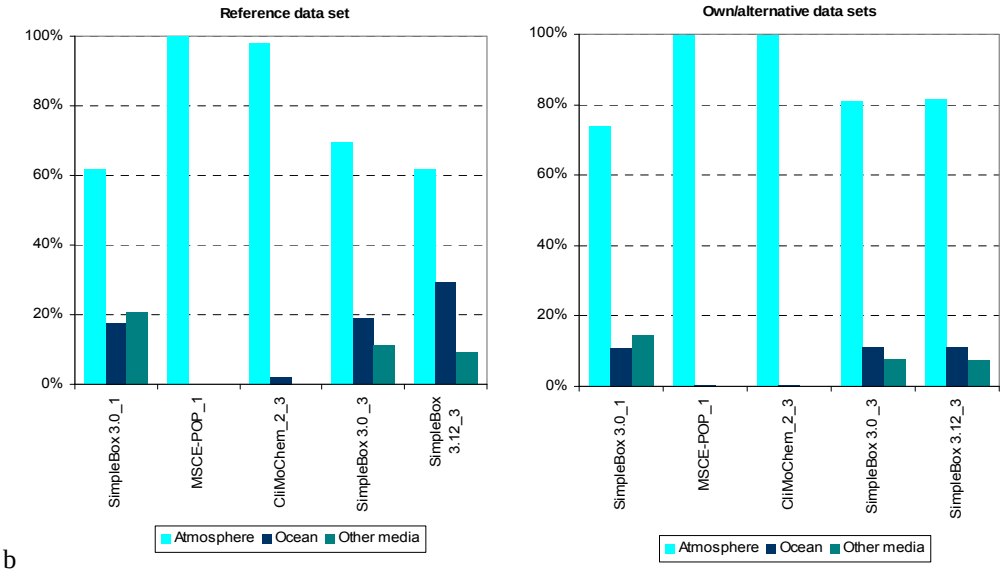


Fig. B.86. *Comparison of PCB-28 overall transport inside and outside the calculation domain (taking into account emissions) (a) and overall transport outside the calculation domain (b) calculated by different models on the basis of two data sets*

Fractions of overall outside transport through atmosphere, ocean and other media (sediment, soil and vegetation) calculated on the basis of zero and non-zero initial conditions are presented in Figs. B.87a and b, respectively. In these figures fractions of PCB-28 mass in soil calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.



a



b

Fig. B.87. *Comparison of PCB-28 fractions of overall outside transport through atmosphere, ocean and other media (sediment, soil and vegetation) calculated by different models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

B.4. Mass flows transported from one compartment to another in both directions

B.4.1. Comparison of calculated values of PCB-28 mass flows transported from the atmosphere to soil

Dry deposition

Reference data set. Calculation results on PCB-28 mass flows transported from the atmosphere to soil: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.56.

Monthly values of PCB-28 mass flows transported from the atmosphere to soil: dry deposition calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.88 a and b, respectively.

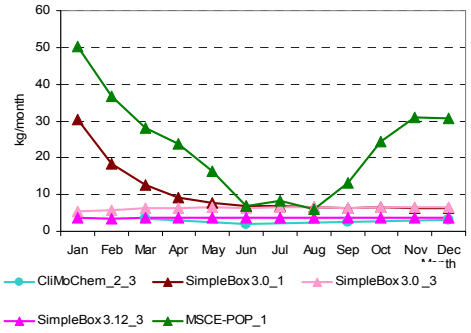


Fig. B.88a. *PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

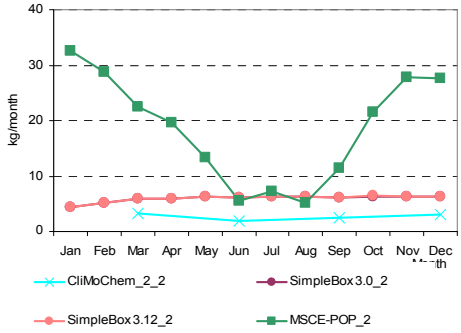


Fig. B.88b. *PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported from the atmosphere to soil: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.57.

Monthly values of PCB-28 mass flows transported from the atmosphere to soil: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.89a and b, respectively.

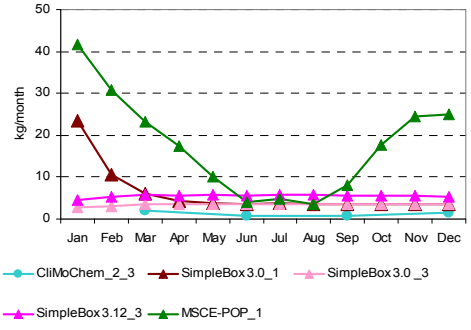


Fig. B.89a. *PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

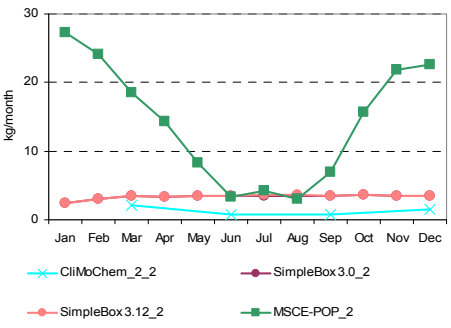


Fig. B.89b. *PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.56. *Calculation results: PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	30.56	50.30		5.39	3.73	*22.50*	*22.23*	Jan		4.43	4.43	32.50	*13.79*	*16.21*
Feb	18.50	36.70		5.75	3.48	*16.11*	*15.24*	Feb		5.23	5.23	28.80	*13.09*	*13.61*
Mar	12.70	28.20		6.37	3.73	*12.75*	*10.97*	Mar		5.93	5.93	22.50	*11.45*	*9.57*
Seas_1	**61.76**	**115.20**	**10.04**	**17.51**	**10.94**	***43.09***	***45.63***	**Seas_1**	**9.49**	**15.59**	**15.60**	**83.80**	***31.12***	***35.24***
Apr	9.09	23.90		6.28	3.60	*10.72*	*9.07*	Apr		5.91	5.91	19.70	*10.51*	*7.96*
May	7.89	16.30		6.56	3.73	*8.62*	*5.41*	May		6.20	6.21	13.40	*8.60*	*4.15*
Jun	6.96	6.75		6.38	3.60	*5.93*	*1.57*	Jun		6.06	6.07	5.55	*5.89*	*0.30*
Seas_2	**23.94**	**46.95**	**6.15**	**19.22**	**10.94**	***21.44***	***15.86***	**Seas_2**	**5.81**	**18.17**	**18.19**	**38.65**	***20.20***	***13.61***
Jul	6.88	8.46		6.62	3.73	*6.42*	*1.97*	Jul		6.30	6.32	7.26	*6.63*	*0.55*
Aug	6.73	6.02		6.65	3.73	*5.78*	*1.41*	Aug		6.33	6.35	5.18	*5.95*	*0.67*
Sep	6.44	13.10		6.45	3.60	*7.40*	*4.03*	Sep		6.15	6.17	11.40	*7.91*	*3.02*
Seas_3	**20.04**	**27.58**	**7.83**	**19.72**	**11.06**	***17.25***	***7.87***	**Seas_3**	**7.46**	**18.79**	**18.83**	**23.84**	***17.23***	***6.93***
Oct	6.62	24.50		6.68	3.73	*10.38*	*9.51*	Oct		6.38	6.40	21.60	*11.46*	*8.78*
Nov	6.40	31.10		6.48	3.60	*11.89*	*12.87*	Nov		6.19	6.21	27.80	*13.40*	*12.47*
Dec	6.40	30.60		6.49	3.60	*11.77*	*12.62*	Dec		6.21	6.23	27.60	*13.35*	*12.34*
Seas_4	**19.42**	**86.20**	**9.44**	**19.64**	**10.94**	***29.13***	***32.25***	**Seas_4**	**9.24**	**18.78**	**18.84**	**77.00**	***30.96***	***31.02***
Annual	**125.17**	**275.93**	**33.45**	**76.09**	**43.86**	***110.90***	***98.92***	**Annual**	**31.99**	**71.33**	**71.47**	**223.29**	*99.52*	*84.58*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.57. *Calculation results: PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			***m***	**σ**	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	23.55	41.70		2.75	4.52	*18.13*	*18.32*	Jan		2.46	2.46	27.30	*10.74*	*14.34*
Feb	10.58	30.70		3.13	5.25	*12.41*	*12.59*	Feb		3.02	3.02	24.10	*10.05*	*12.17*
Mar	6.08	23.30		3.50	5.82	*9.67*	*9.16*	Mar		3.40	3.41	18.60	*8.47*	*8.77*
Seas_1	**40.21**	**95.70**	**6.31**	**9.38**	**15.59**	***33.4***	***37.3***	**Seas_1**	**6.15**	**8.88**	**8.90**	**70.00**	***23.5***	***31.0***
Apr	4.27	17.50		3.44	5.66	*7.72*	*6.59*	Apr		3.36	3.37	14.30	*7.01*	*6.31*
May	3.90	10.10		3.58	5.83	*5.85*	*3.00*	May		3.50	3.52	8.22	*5.08*	*2.72*
Jun	3.61	4.05		3.47	5.61	*4.19*	*0.98*	Jun		3.40	3.43	3.31	*3.38*	*0.06*
Seas_2	**11.78**	**31.65**	**2.48**	**10.49**	**17.11**	***14.7***	***10.8***	**Seas_2**	**2.45**	**10.26**	**10.32**	**25.83**	***12.2***	***9.8***
Jul	3.68	4.92		3.60	5.77	*4.49*	*1.04*	Jul		3.53	3.56	4.20	*3.76*	*0.38*
Aug	3.66	3.47		3.61	5.73	*4.12*	*1.08*	Aug		3.54	3.57	2.98	*3.36*	*0.33*
Sep	3.53	8.11		3.50	5.51	*5.16*	*2.18*	Sep		3.43	3.47	7.00	*4.63*	*2.05*
Seas_3	**10.87**	**16.50**	**2.16**	**10.70**	**17.01**	***11.4***	***6.0***	**Seas_3**	**2.13**	**10.50**	**10.60**	**14.18**	***9.4***	***5.1***
Oct	3.64	17.70		3.62	5.66	*7.66*	*6.76*	Oct		3.55	3.60	15.70	*7.62*	*7.00*
Nov	3.52	24.40		3.51	5.45	*9.22*	*10.16*	Nov		3.44	3.49	21.90	*9.61*	*10.64*
Dec	3.52	24.90		3.51	5.42	*9.34*	*10.41*	Dec		3.45	3.50	22.60	*9.85*	*11.04*
Seas_4	**10.68**	**67.00**	**4.67**	**10.64**	**16.54**	***21.9***	***25.6***	**Seas_4**	**4.64**	**10.44**	**10.58**	**60.20**	***21.5***	***26.0***
Annual	**73.54**	**210.85**	**15.61**	**41.21**	**66.25**	***81.49***	***75.82***	**Annual**	**15.37**	**40.08**	**40.39**	**170.21**	***66.51***	***70.12***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.58.

Table B.58. *The percentage difference between calculation results on PCB-28 mass flows transported from the atmosphere to soil: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-23.0%	-44.5%	-44.5%	-48.9%	21.4%	-17.1%	-16.0%
Feb			-42.8%	-42.3%	-42.2%	-45.5%	50.6%	-16.3%	-16.3%
Mar			-52.1%	-42.6%	-42.5%	-45.1%	56.1%	-17.4%	-17.3%
Seas_1	**-35.2%**	**-37.1%**	**-34.9%**	**-43.0%**	**-43.0%**	**-46.4%**	**42.5%**	**-16.9%**	**-16.5%**
Apr			-53.0%	-43.2%	-43.0%	-45.3%	57.1%	-26.8%	-27.4%
May			-50.6%	-43.6%	-43.3%	-45.5%	56.6%	-38.0%	-38.7%
Jun			-48.1%	-43.8%	-43.6%	-45.6%	55.7%	-40.0%	-40.4%
Seas_2	**-57.9%**	**-59.7%**	**-50.8%**	**-43.5%**	**-43.3%**	**-45.4%**	**56.5%**	**-32.6%**	**-33.2%**
Jul			-46.5%	-44.0%	-43.7%	-45.7%	54.8%	-41.8%	-42.1%
Aug			-45.6%	-44.1%	-43.7%	-45.7%	53.8%	-42.4%	-42.5%
Sep			-45.2%	-44.2%	-43.8%	-45.8%	52.9%	-38.1%	-38.6%
Seas_3	**-71.5%**	**-72.5%**	**-45.8%**	**-44.1%**	**-43.7%**	**-45.7%**	**53.9%**	**-40.2%**	**-40.5%**
Oct			-45.0%	-44.3%	-43.8%	-45.8%	52.1%	-27.8%	-27.3%
Nov			-44.9%	-44.4%	-43.8%	-45.8%	51.2%	-21.5%	-21.2%
Dec			-45.0%	-44.5%	-43.9%	-45.9%	50.5%	-18.6%	-18.1%
Seas_4	**-49.7%**	**-50.5%**	**-45.0%**	**-44.4%**	**-43.8%**	**-45.8%**	**51.3%**	**-22.3%**	**-21.8%**
Annual	**-52.0%**	**-53.3%**	**-41.2%**	**-43.8%**	**-43.5%**	**-45.8%**	**51.0%**	**-23.6%**	**-23.8%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations; SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data; SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations; SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Wet deposition

Reference data set. Calculation results on PCB-28 mass flows transported from the atmosphere to soil: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.59.

Monthly values of PCB-28 mass flows transported from the atmosphere to soil: wet deposition calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.90 a and b, respectively.

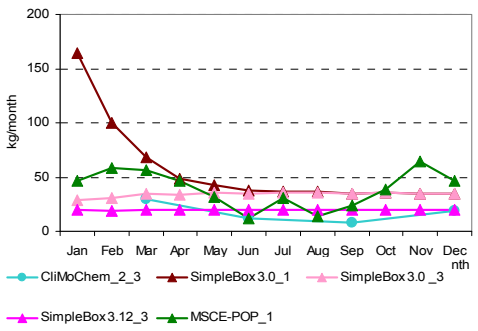


Fig. B.90a. *PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

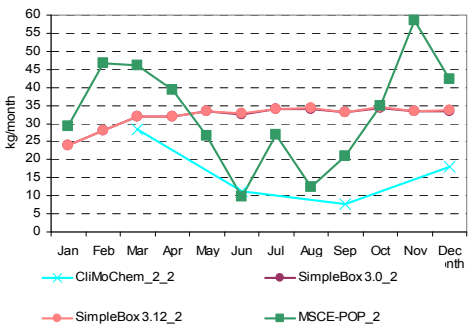


Fig. B.90b. *PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported from the atmosphere to soil: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.60.

Monthly values of PCB-28 mass flows transported from the atmosphere to soil: wet deposition calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.91 a and b, respectively. Seasonal variations of low values of wet deposition flows calculated by the participating models on the basis of "own or alternative" data set are also shown in Figs. B.91c and B.91d in more detail.

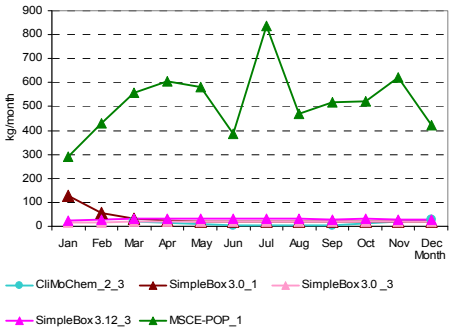


Fig. B.91a. *PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

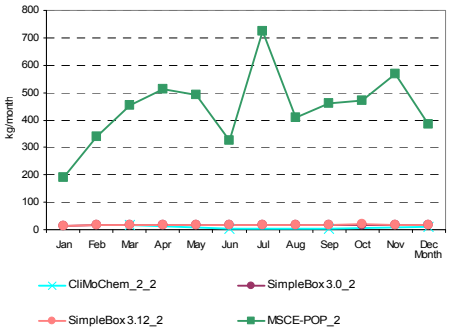


Fig. B.91b. *PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions (all models)*

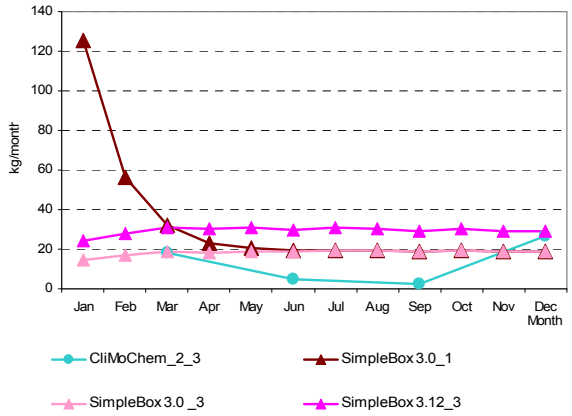


Fig. B.91c. *PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (low values)*

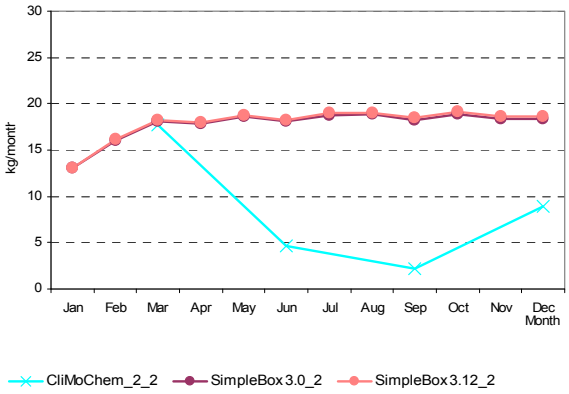


Fig. B.91d. *PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions (low values)*

Table B.59. *Calculation results: PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by models on the basis of "reference" data set" and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	MSCE-POP_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	164.73	46.10		29.05	20.07	*64.99*	*67.36*	Jan		29.20	23.87	23.87	*25.65*	*3.08*
Feb	99.70	58.90		30.98	18.78	*52.09*	*35.91*	Feb		46.80	28.19	28.19	*34.39*	*10.74*
Mar	68.44	56.50		34.33	20.07	*44.83*	*21.73*	Mar		46.10	31.94	31.96	*36.67*	*8.17*
Seas_1	**332.87**	**161.50**	**90.14**	**94.36**	**58.92**	***147.56***	***110.13***	**Seas_1**	**85.25**	**122.10**	**84.00**	**84.03**	***93.84***	***18.85***
Apr	48.97	46.70		33.84	19.42	*37.23*	*13.61*	Apr		39.20	31.83	31.86	*34.30*	*4.25*
May	42.50	31.80		35.32	20.07	*32.42*	*9.36*	May		26.60	33.41	33.46	*31.16*	*3.95*
Jun	37.52	11.70		34.40	19.42	*25.76*	*12.26*	Jun		9.66	32.65	32.70	*25.00*	*13.29*
Seas_2	**128.99**	**90.20**	**35.89**	**103.56**	**58.92**	***83.51***	***36.70***	**Seas_2**	**33.88**	**75.46**	**97.89**	**98.02**	***76.31***	***30.21***
Jul	37.05	31.10		35.70	20.07	*30.98*	*7.71*	Jul		27.00	33.96	34.03	*31.66*	*4.04*
Aug	36.24	14.30		35.81	20.07	*26.61*	*11.13*	Aug		12.30	34.13	34.21	*26.88*	*12.63*
Sep	34.71	24.00		34.75	19.42	*28.22*	*7.75*	Sep		21.10	33.16	33.25	*29.17*	*6.99*
Seas_3	**108.01**	**69.40**	**24.59**	**106.26**	**59.56**	***73.56***	***34.88***	**Seas_3**	**23.43**	**60.40**	**101.24**	**101.48**	***71.64***	***37.50***
Oct	35.69	38.90		35.99	20.07	*32.66*	*8.52*	Oct		34.90	34.37	34.48	*34.59*	*0.28*
Nov	34.46	64.50		34.89	19.42	*38.32*	*18.88*	Nov		58.50	33.36	33.48	*41.78*	*14.48*
Dec	34.51	46.40		34.95	19.42	*33.82*	*11.06*	Dec		42.20	33.45	33.58	*36.41*	*5.02*
Seas_4	**104.66**	**149.80**	**55.68**	**105.82**	**58.92**	***94.98***	***38.93***	**Seas_4**	**54.50**	**135.60**	**101.18**	**101.54**	***98.20***	***33.31***
Annual	**674.53**	**470.90**	**206.29**	**410.01**	**236.31**	***399.61***	***190.27***	**Annual**	**197.06**	**393.56**	**384.31**	**385.07**	***340.00***	***95.39***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.60. *Calculation results: PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	125.51	291.00		14.68	24.09	*113.82*	*128.34*	Jan		13.11	13.11	189.00	*71.74*	*101.55*
Feb	56.38	429.00		16.68	27.98	*132.51*	*198.36*	Feb		16.09	16.11	338.00	*123.40*	*185.85*
Mar	32.39	558.00		18.62	30.99	*160.00*	*265.40*	Mar		18.14	18.18	453.00	*163.11*	*251.06*
Seas_1	**214.29**	**1278.00**	**54.77**	**49.99**	**83.06**	***336.0***	***530.8***	**Seas_1**	**53.34**	**47.33**	**47.40**	**980.00**	***282.0***	***465.3***
Apr	22.75	606.00		18.31	30.18	*169.31*	*291.17*	Apr		17.89	17.96	511.00	*182.29*	*284.67*
May	20.78	581.00		19.05	31.09	*162.98*	*278.73*	May		18.65	18.75	493.00	*176.80*	*273.84*
Jun	19.26	387.00		18.51	29.92	*113.67*	*182.29*	Jun		18.13	18.26	326.00	*120.80*	*177.71*
Seas_2	**62.79**	**1574.00**	**14.13**	**55.88**	**91.18**	***359.6***	***679.4***	**Seas_2**	**13.95**	**54.67**	**54.97**	**1330.00**	***363.4***	***644.7***
Jul	19.61	835.00		19.18	30.73	*226.13*	*405.95*	Jul		18.80	18.95	723.00	*253.58*	*406.53*
Aug	19.49	468.00		19.22	30.54	*134.31*	*222.52*	Aug		18.85	19.03	408.00	*148.63*	*224.62*
Sep	18.81	519.00		18.63	29.38	*146.46*	*248.41*	Sep		18.28	18.48	461.00	*165.92*	*255.55*
Seas_3	**57.91**	**1822.00**	**6.64**	**57.04**	**90.65**	***406.8***	***791.7***	**Seas_3**	**6.56**	**55.93**	**56.47**	**1592.00**	***427.7***	***776.5***
Oct	19.41	520.00		19.28	30.19	*147.22*	*248.57*	Oct		18.93	19.16	472.00	*170.03*	*261.52*
Nov	18.77	622.00		18.69	29.06	*172.13*	*299.95*	Nov		18.35	18.59	569.00	*201.98*	*317.85*
Dec	18.75	421.00		18.71	28.91	*121.84*	*199.50*	Dec		18.37	18.64	386.00	*141.00*	*212.17*
Seas_4	**56.93**	**1563.00**	**26.73**	**56.68**	**88.15**	***358.3***	***673.8***	**Seas_4**	**26.61**	**55.64**	**56.39**	**1427.00**	***391.4***	***690.5***
Annual	**391.91**	**6237.00**	**102.27**	**219.57**	**353.05**	***1460.8***	***2672.5***	**Annual**	**100.45**	**213.57**	**215.23**	**5329.00**	***1464.56***	***2576.85***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.61.

Table B.61. *The percentage difference between calculation results on PCB-28 mass flows transported from the atmosphere to soil: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-23.8%	-45.1%	-45.1%	-49.5%	20.0%	531.2%	547.3%
Feb			-43.4%	-42.9%	-42.9%	-46.2%	49.0%	628.4%	622.2%
Mar			-52.7%	-43.2%	-43.1%	-45.7%	54.4%	887.6%	882.6%
Seas_1	**-37.4%**	**-39.2%**	**-35.6%**	**-43.7%**	**-43.6%**	**-47.0%**	**41.0%**	**691.3%**	**702.6%**
Apr			-53.5%	-43.8%	-43.6%	-45.9%	55.4%	1197.6%	1203.6%
May			-51.1%	-44.2%	-44.0%	-46.1%	54.9%	1727.0%	1753.4%
Jun			-48.7%	-44.5%	-44.2%	-46.2%	54.0%	3207.7%	3274.7%
Seas_2	**-58.8%**	**-60.6%**	**-51.3%**	**-44.2%**	**-43.9%**	**-46.0%**	**54.8%**	**1645.0%**	**1662.5%**
Jul			-47.1%	-44.6%	-44.3%	-46.3%	53.1%	2584.9%	2577.8%
Aug			-46.2%	-44.8%	-44.4%	-46.3%	52.2%	3172.7%	3217.1%
Sep			-45.8%	-44.9%	-44.4%	-46.4%	51.3%	2062.5%	2084.8%
Seas_3	**-72.0%**	**-73.0%**	**-46.4%**	**-44.8%**	**-44.4%**	**-46.3%**	**52.2%**	**2525.4%**	**2535.8%**
Oct			-45.6%	-44.9%	-44.4%	-46.4%	50.4%	1236.8%	1252.4%
Nov			-45.5%	-45.0%	-44.5%	-46.4%	49.6%	864.3%	872.6%
Dec			-45.6%	-45.1%	-44.5%	-46.5%	48.8%	807.3%	814.7%
Seas_4	**-51.2%**	**-52.0%**	**-45.6%**	**-45.0%**	**-44.5%**	**-46.4%**	**49.6%**	**943.4%**	**952.4%**
Annual	**-49.0%**	**-50.4%**	**-41.9%**	**-44.4%**	**-44.1%**	**-46.4%**	**49.4%**	**1224.5%**	**1254.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Gaseous exchange

Reference data set. Calculation results on PCB-28 mass flows between the atmosphere and soil: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.62.

Monthly values of PCB-28 mass flows between the atmosphere and soil: gaseous exchange calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.92 a and b, respectively.

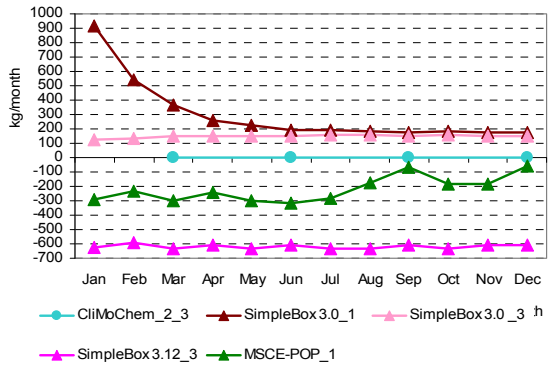


Fig. B.92a. *PCB-28 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

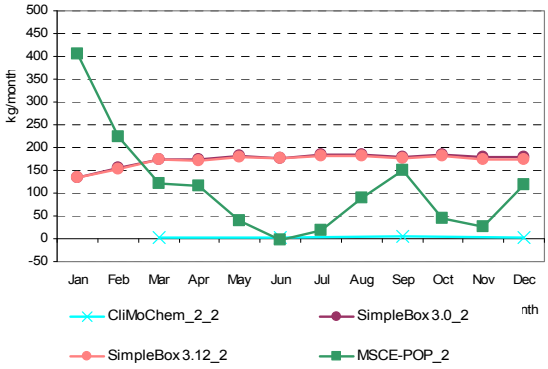


Fig. B.92b. *PCB-28 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows between the atmosphere and soil: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.63.

Monthly values of PCB-28 mass flows between the atmosphere and soil: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.93 a and b, respectively.

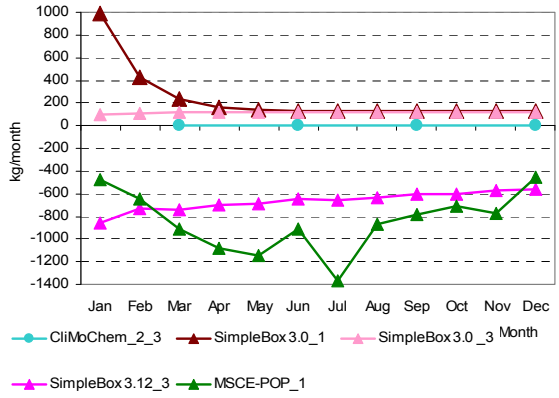


Fig. B.93a. *PCB-28 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

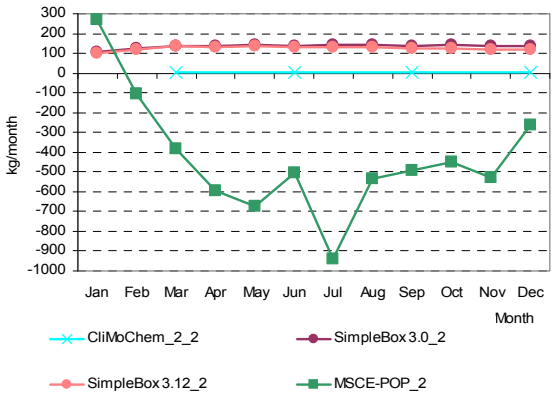


Fig. B.93b. *PCB-28 mass between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.64.

Table B.62. *Calculation results: PCB-28 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMoChem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE- POP_2		
Jan	920.40	-289.00		122.05	-626.50	*31.74*	*666.84*	Jan		133.83	133.76	406.00	*224.53*	*157.16*
Feb	541.96	-234.00		131.70	-588.59	*-37.23*	*485.36*	Feb		154.36	153.93	224.00	*177.43*	*40.33*
Mar	367.06	-298.00		147.33	-629.19	*-103.20*	*446.66*	Mar		174.64	173.73	121.00	*156.46*	*30.71*
Seas_1	**1829.42**	**-821.00**	**9.55**	**401.08**	**-1844.28**	***-85.0***	***1373.6***	**Seas_1**	**6.06**	**462.84**	**461.42**	**751.00**	***420.3***	***307.9***
Apr	258.88	-240.00		145.85	-608.89	*-111.04*	*394.68*	Apr		173.73	172.37	115.00	*153.70*	*33.52*
May	222.08	-299.00		152.54	-629.19	*-138.39*	*400.52*	May		182.02	180.13	40.40	*134.18*	*81.22*
Jun	194.46	-320.00		148.65	-608.89	*-146.45*	*386.12*	Jun		177.49	175.18	-2.72	*116.65*	*103.38*
Seas_2	**675.42**	**-859.00**	**8.41**	**447.04**	**-1846.97**	***-315.0***	***1037.9***	**Seas_2**	**9.94**	**533.24**	**527.67**	**152.68**	***305.9***	***265.8***
Jul	191.00	-281.00		154.28	-629.19	*-141.23*	*389.59*	Jul		184.23	181.33	18.20	*127.92*	*95.03*
Aug	186.11	-171.00		154.77	-629.19	*-114.83*	*379.02*	Aug		184.74	181.35	88.40	*151.50*	*54.67*
Sep	177.75	-70.50		150.11	-608.89	*-87.88*	*364.67*	Sep		179.12	175.35	150.00	*168.16*	*15.84*
Seas_3	**554.87**	**-522.50**	**7.67**	**459.17**	**-1867.26**	***-273.6***	***987.9***	**Seas_3**	**19.00**	**548.09**	**538.04**	**256.60**	***340.4***	***253.3***
Oct	182.34	-183.00		155.39	-629.19	*-118.61*	*378.81*	Oct		185.31	180.94	46.00	*137.42*	*79.20*
Nov	175.68	-180.00		150.58	-608.89	*-115.66*	*366.60*	Nov		179.48	174.78	26.80	*127.02*	*86.82*
Dec	175.67	-62.20		150.75	-608.89	*-86.17*	*364.46*	Dec		179.56	174.41	119.00	*157.66*	*33.58*
Seas_4	**533.69**	**-425.20**	**10.21**	**456.72**	**-1846.97**	***-254.3***	***969.8***	**Seas_4**	**8.90**	**544.36**	**530.14**	**191.80**	***318.8***	***263.1***
Annual	**3593.39**	**-2627.70**	**35.84**	**1764.01**	**-7405.48**	***-927.99***	***4285.60***	**Annual**	**43.91**	**2088.52**	**2057.26**	**1352.08**	***1385.44***	***956.82***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.63. *Calculation results: PCB-28 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	986.42	-478.00		93.32	-860.86	*-64.78*	*803.02*	Jan		103.76	103.22	270.00	*158.99*	*96.13*
Feb	423.38	-650.00		106.77	-734.57	*-213.61*	*568.69*	Feb		123.43	121.37	-106.00	*46.27*	*131.87*
Mar	235.38	-916.00		119.99	-746.12	*-326.69*	*588.40*	Mar		138.78	134.69	-383.00	*-36.51*	*300.08*
Seas_1	**1645.17**	**-2044.00**	**9.55**	**320.08**	**-2341.56**	***-482.2***	***1681.3***	**Seas_1**	**9.57**	**365.97**	**359.28**	**-219.00**	***129.0***	***285.5***
Apr	160.52	-1080.00		118.07	-693.86	*-373.82*	*613.35*	Apr		136.50	130.66	-592.00	*-108.28*	*418.92*
May	144.23	-1140.00		122.75	-692.97	*-391.50*	*633.14*	May		141.78	133.83	-675.00	*-133.13*	*469.29*
Jun	132.62	-908.00		119.08	-650.30	*-326.65*	*533.02*	Jun		137.42	127.90	-505.00	*-79.89*	*368.18*
Seas_2	**437.37**	**-3128.00**	**8.41**	**359.90**	**-2037.13**	***-871.9***	***1616.6***	**Seas_2**	**9.95**	**415.70**	**392.39**	**-1772.00**	***-238.5***	***1039.1***
Jul	134.36	-1370.00		123.17	-653.17	*-441.41*	*720.50*	Jul		142.01	130.34	-938.00	*-221.88*	*620.20*
Aug	133.10	-874.00		123.20	-635.80	*-313.38*	*519.04*	Aug		141.92	128.43	-534.00	*-87.88*	*386.41*
Sep	128.06	-782.00		119.21	-600.15	*-283.72*	*476.21*	Sep		137.20	122.45	-493.00	*-77.78*	*359.66*
Seas_3	**395.52**	**-3026.00**	**7.67**	**365.57**	**-1889.12**	***-829.3***	***1547.3***	**Seas_3**	**12.65**	**421.13**	**381.22**	**-1965.00**	***-287.5***	***1133.4***
Oct	131.75	-715.00		123.13	-605.71	*-266.46*	*457.03*	Oct		141.58	124.63	-452.00	*-61.93*	*337.92*
Nov	127.02	-770.00		119.07	-573.11	*-274.25*	*465.76*	Nov		136.80	118.78	-526.00	*-90.14*	*377.57*
Dec	126.60	-460.00		118.98	-561.22	*-193.91*	*368.03*	Dec		136.57	116.99	-260.00	*-2.15*	*223.52*
Seas_4	**385.37**	**-1945.00**	**10.21**	**361.18**	**-1740.04**	***-585.7***	***1159.2***	**Seas_4**	**10.82**	**414.95**	**360.40**	**-1238.00**	***-113.0***	***771.1***
Annual	**2863.44**	**-10143.00**	**35.84**	**1406.73**	**-8007.85**	***-2768.97***	***5891.72***	**Annual**	**42.99**	**1617.75**	**1493.29**	**-5194.00**	***-509.99***	***3203.44***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.64. *Comparison of the calculation results on PCB-28 mass flows between the atmosphere and soil: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets.*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			920.40	986.42	133.83	103.76	133.76	103.22	122.05	93.32	-626.50	-860.86	-289.00	-478.00	406.00	270.00		
Feb			541.96	423.38	154.36	123.43	153.93	121.37	131.70	106.77	-588.59	-734.57	-234.00	-650.00	224.00	-106.00		
Mar			367.06	235.38	174.64	138.78	173.73	134.69	147.33	119.99	-629.19	-746.12	-298.00	-916.00	121.00	-383.00		
Seas_1	**9.55**	**9.55**	**1829.42**	**1645.17**	**462.84**	**365.97**	**461.42**	**359.28**	**401.08**	**320.08**	**-1844.28**	**-2341.56**	**-821.00**	**-2044.00**	**751.00**	**-219.00**	**6.06**	**9.57**
Apr			258.88	160.52	173.73	136.50	172.37	130.66	145.85	118.07	-608.89	-693.86	-240.00	-1080.00	115.00	-592.00		
May			222.08	144.23	182.02	141.78	180.13	133.83	152.54	122.75	-629.19	-692.97	-299.00	-1140.00	40.40	-675.00		
Jun			194.46	132.62	177.49	137.42	175.18	127.90	148.65	119.08	-608.89	-650.30	-320.00	-908.00	-2.72	-505.00		
Seas_2	**8.41**	**8.41**	**675.42**	**437.37**	**533.24**	**415.70**	**527.67**	**392.39**	**447.04**	**359.90**	**-1846.97**	**-2037.13**	**-859.00**	**-3128.00**	**152.68**	**-1772.00**	**9.94**	**9.95**
Jul			191.00	134.36	184.23	142.01	181.33	130.34	154.28	123.17	-629.19	-653.17	-281.00	-1370.00	18.20	-938.00		
Aug			186.11	133.10	184.74	141.92	181.35	128.43	154.77	123.20	-629.19	-635.80	-171.00	-874.00	88.40	-534.00		
Sep			177.75	128.06	179.12	137.20	175.35	122.45	150.11	119.21	-608.89	-600.15	-70.50	-782.00	150.00	-493.00		
Seas_3	**7.67**	**7.67**	**554.87**	**395.52**	**548.09**	**421.13**	**538.04**	**381.22**	**459.17**	**365.57**	**-1867.26**	**-1889.12**	**-522.50**	**-3026.00**	**256.60**	**-1965.00**	**19.00**	**12.65**
Oct			182.34	131.75	185.31	141.58	180.94	124.63	155.39	123.13	-629.19	-605.71	-183.00	-715.00	46.00	-452.00		
Nov			175.68	127.02	179.48	136.80	174.78	118.78	150.58	119.07	-608.89	-573.11	-180.00	-770.00	26.80	-526.00		
Dec			175.67	126.60	179.56	136.57	174.41	116.99	150.75	118.98	-608.89	-561.22	-62.20	-460.00	119.00	-260.00		
Seas_4	**10.21**	**10.21**	**533.69**	**385.37**	**544.36**	**414.95**	**530.14**	**360.40**	**456.72**	**361.18**	**-1846.97**	**-1740.04**	**-425.20**	**-1945.00**	**191.80**	**-1238.00**	**8.90**	**10.82**
Annual	**35.84**	**35.84**	**3593.39**	**2863.44**	**2088.52**	**1617.75**	**2057.26**	**1493.29**	**1764.01**	**1406.73**	**-7405.48**	**-8007.85**	**-2627.70**	**-10143.00**	**1352.08**	**-5194.00**	**43.91**	**42.99**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

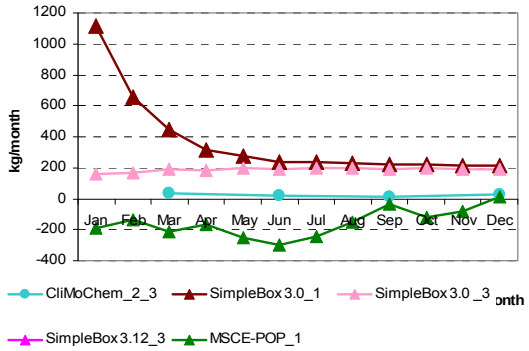
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Net mass flows between the atmosphere and soil

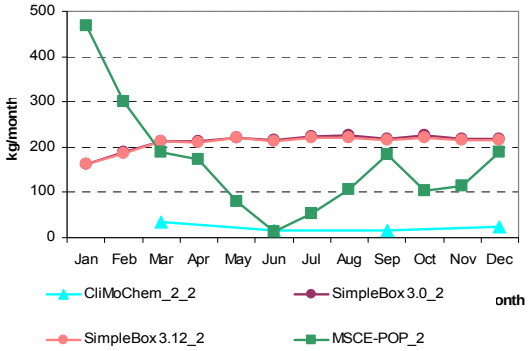
Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-28 net mass flows between the atmosphere and soil calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.65.

Monthly values of PCB-28 net mass flows between the atmosphere and soil calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.94 a and b, respectively.



a



b

Fig. B.94a. *PCB-28 net mass flows between the atmosphere and soil (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

Fig. B.94b. *PCB-28 net mass flows between the atmosphere and soil (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table B.65. *Calculation results: PCB-28 net mass flows between the atmosphere and soil (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1115.69	-192.60		156.48	-602.70	*119.22*	*733.20*	Jan		162.14	162.06	-192.60	*43.87*	*204.79*
Feb	660.17	-138.40		168.44	-566.33	*30.97*	*516.48*	Feb		187.78	187.36	-138.40	*78.91*	*188.20*
Mar	448.19	-213.30		188.03	-605.39	*-45.62*	*461.84*	Mar		212.51	211.62	-213.30	*70.28*	*245.58*
Seas_1	**2224.05**	**-544.30**	**109.72**	**512.95**	**-1774.43**	***105.60***	***1467.19***	**Seas_1**	**100.81**	**562.43**	**561.04**	**-544.30**	***169.99***	***523.43***
Apr	316.93	-169.40		185.97	-585.86	*-63.09*	*404.57*	Apr		211.46	210.14	-169.40	*84.07*	*219.51*
May	272.48	-250.90		194.42	-605.39	*-97.35*	*409.71*	May		221.64	219.79	-250.90	*63.51*	*272.29*
Jun	238.94	-301.55		189.43	-585.86	*-114.76*	*397.69*	Jun		216.20	213.95	-301.55	*42.87*	*298.28*
Seas_2	**828.35**	**-721.85**	**50.45**	**569.82**	**-1777.12**	***-210.07***	***1057.35***	**Seas_2**	**49.63**	**649.30**	**643.89**	**-721.85**	***155.24***	***648.93***
Jul	234.93	-241.44		196.61	-605.39	*-103.82*	*398.13*	Jul		224.49	221.68	-241.44	*68.24*	*268.20*
Aug	229.08	-150.68		197.23	-605.39	*-82.44*	*388.76*	Aug		225.20	221.91	-150.68	*98.81*	*216.07*
Sep	218.91	-33.40		191.31	-585.86	*-52.26*	*373.25*	Sep		218.42	214.77	-33.40	*133.26*	*144.35*
Seas_3	**682.92**	**-425.52**	**40.09**	**585.15**	**-1796.65**	***-182.80***	***1006.52***	**Seas_3**	**49.89**	**668.12**	**658.36**	**-425.52**	***237.71***	***528.31***
Oct	224.66	-119.60		198.05	-605.39	*-75.57*	*386.29*	Oct		226.07	221.82	-119.60	*109.43*	*198.36*
Nov	216.53	-84.40		191.95	-585.86	*-65.44*	*372.81*	Nov		219.03	214.47	-84.40	*116.37*	*173.89*
Dec	216.58	14.80		192.18	-585.86	*-40.58*	*374.48*	Dec		219.22	214.22	14.80	*149.41*	*116.60*
Seas_4	**657.77**	**-189.20**	**75.32**	**582.19**	**-1777.12**	***-130.21***	***985.70***	**Seas_4**	**72.64**	**664.31**	**650.52**	**-189.20**	***299.57***	***426.85***
Annual	**4393.09**	**-1880.87**	**275.58**	**2250.11**	**-7125.30**	*-417.48*	*4412.32*	**Annual**	**272.96**	**2544.16**	**2513.80**	**-1880.87**	*862.51*	*2115.69*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates;

B.4.2. Comparison of calculated values of PCB-28 mass flows transported from vegetation to soil: Litterfall

Reference data set. Calculation results on PCB-28 mass flows transported from the vegetation to soil: litterfall calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.66.

Monthly values of PCB-28 mass flows transported from vegetation to soil: litterfall calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.95 a and b, respectively. Seasonal variations of low values of mass flows transported from vegetation to soil calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. B.95c in more detail.

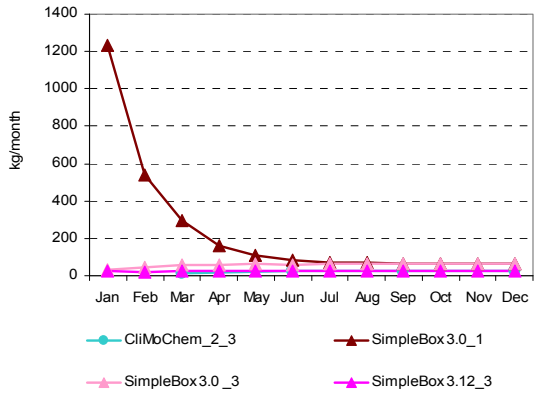


Fig. B.95a. *PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

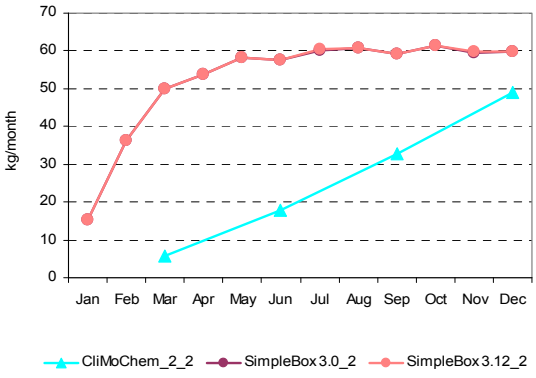


Fig. B.95b. *PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

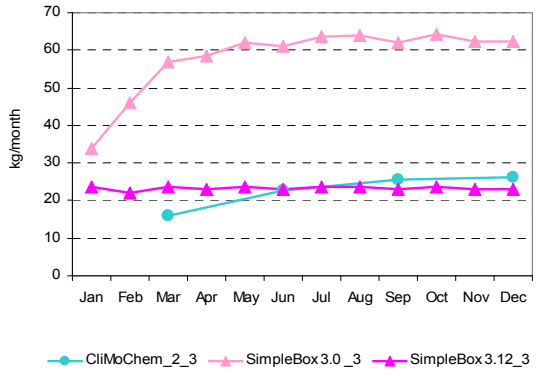
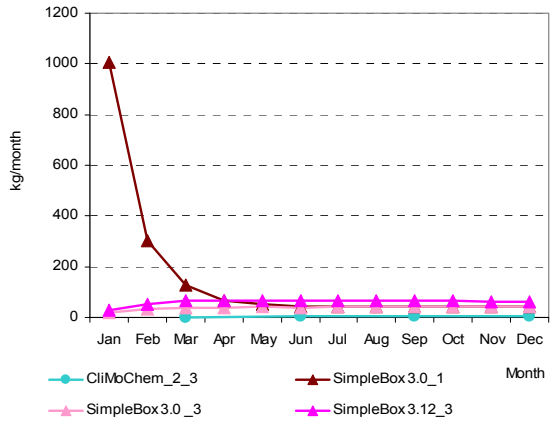


Fig. B.95c. *PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

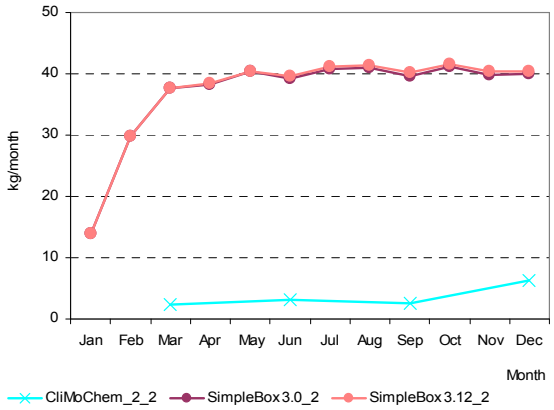
Own/alternative data set. Calculation results on PCB-28 mass flows transported from vegetation to soil: litterfall calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.67.

Monthly values of PCB-28 mass flows transported from vegetation to soil: litterfall calculated by all participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.96 a and b, respectively. Seasonal variations of low values of mass flows from vegetation to soil calculated by the participating models on the basis of “reference” data set and non-zero initial conditions are also shown in Fig. B.96c in more detail.



a

Fig. B.96a. *PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (all models)*



b

Fig. B.96b. *PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and zero-initial conditions*

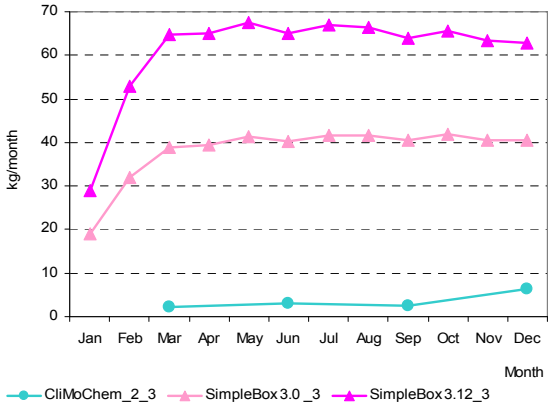


Fig. B.96c. *PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (models with low values)*

Table B.66. *Calculation results: PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	CliMoChem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	1235.01		33.79	23.72	*430.84*	*696.45*	Jan		15.41	15.41	*15.41*	*0.00*
Feb	540.63		46.18	22.19	*203.00*	*292.64*	Feb		36.42	36.43	*36.42*	*0.00*
Mar	295.64		56.76	23.72	*125.37*	*148.38*	Mar		50.09	50.11	*50.10*	*0.01*
Seas_1	**2071.28**	**47.83**	**136.73**	**69.62**	***581.37***	***993.99***	**Seas_1**	**17.49**	**101.92**	**101.95**	***73.79***	***48.76***
Apr	162.11		58.41	22.95	*81.16*	*72.31*	Apr		53.71	53.75	*53.73*	*0.02*
May	110.76		62.12	23.72	*65.53*	*43.62*	May		58.14	58.19	*58.17*	*0.04*
Jun	82.37		61.00	22.95	*55.44*	*30.10*	Jun		57.59	57.66	*57.63*	*0.05*
Seas_2	**355.24**	**68.22**	**181.53**	**69.62**	***168.65***	***135.24***	**Seas_2**	**53.79**	**169.44**	**169.61**	***130.95***	***66.82***
Jul	73.53		63.56	23.72	*53.60*	*26.36*	Jul		60.28	60.38	*60.33*	*0.07*
Aug	68.17		63.89	23.72	*51.93*	*24.52*	Aug		60.77	60.89	*60.83*	*0.09*
Sep	63.63		62.06	22.95	*49.55*	*23.04*	Sep		59.13	59.27	*59.20*	*0.10*
Seas_3	**205.33**	**76.26**	**189.51**	**70.39**	***135.37***	***71.98***	**Seas_3**	**98.16**	**180.18**	**180.55**	***152.96***	***47.46***
Oct	64.63		64.30	23.72	*50.88*	*23.53*	Oct		61.36	61.53	*61.45*	*0.12*
Nov	62.04		62.37	22.95	*49.12*	*22.66*	Nov		59.58	59.77	*59.68*	*0.13*
Dec	61.11		62.49	22.95	*48.85*	*22.44*	Dec		59.76	59.97	*59.86*	*0.15*
Seas_4	**187.78**	**78.20**	**189.16**	**69.62**	***131.19***	***66.23***	**Seas_4**	**147.45**	**180.70**	**181.27**	***169.81***	***19.37***
Annual	**2819.62**	**270.52**	**696.93**	**279.25**	***1016.58***	***1218.38***	**Annual**	**316.88**	**632.24**	**633.37**	*527.50*	*182.40*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.67. *Calculation results: PCB-28 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1a	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a		
Jan	1004.27		18.98	28.92	*350.72*	*566.01*	Jan		14.00	14.00	*14.00*	*0.00*
Feb	304.17		31.87	52.78	*129.60*	*151.54*	Feb		29.73	29.75	*29.74*	*0.02*
Mar	129.78		38.95	64.80	*77.84*	*46.80*	Mar		37.60	37.67	*37.63*	*0.05*
Seas_1	**1438.21**	**7.02**	**89.80**	**146.49**	***420.38***	***680.97***	**Seas_1**	**7.02**	**81.33**	**81.42**	***56.59***	***42.93***
Apr	66.72		39.31	64.94	*56.99*	*15.34*	Apr		38.30	38.42	*38.36*	*0.09*
May	50.65		41.22	67.46	*53.11*	*13.30*	May		40.30	40.48	*40.39*	*0.13*
Jun	43.52		40.15	65.09	*49.59*	*13.53*	Jun		39.31	39.54	*39.42*	*0.17*
Seas_2	**160.89**	**9.14**	**120.67**	**197.50**	***122.05***	***81.55***	**Seas_2**	**9.14**	**117.90**	**118.44**	***81.83***	***62.95***
Jul	43.18		41.64	66.90	*50.57*	*14.16*	Jul		40.80	41.10	*40.95*	*0.21*
Aug	42.57		41.74	66.50	*50.27*	*14.06*	Aug		40.93	41.29	*41.11*	*0.25*
Sep	40.98		40.48	63.97	*48.47*	*13.42*	Sep		39.70	40.11	*39.90*	*0.28*
Seas_3	**126.73**	**7.36**	**123.86**	**197.37**	***113.83***	***78.70***	**Seas_3**	**7.36**	**121.43**	**122.49**	***83.76***	***66.17***
Oct	42.24		41.89	65.72	*49.95*	*13.66*	Oct		41.11	41.58	*41.35*	*0.33*
Nov	40.82		40.60	63.25	*48.22*	*13.01*	Nov		39.86	40.36	*40.11*	*0.36*
Dec	40.79		40.65	62.92	*48.12*	*12.82*	Dec		39.92	40.47	*40.19*	*0.39*
Seas_4	**123.85**	**18.99**	**123.14**	**191.89**	***114.47***	***71.35***	**Seas_4**	**18.99**	**120.88**	**122.42**	***87.43***	***59.27***
Annual	**1849.68**	**42.51**	**457.47**	**733.25**	***770.73***	***773.30***	**Annual**	**42.51**	**441.54**	**444.77**	*309.61*	*231.32*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.68.

Table B.68. *The percentage difference between calculation results on PCB-28 mass flows transported from vegetation to soil: litterfall obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan			-18.7%	-9.1%	-9.1%	-43.8%	21.9%
Feb			-43.7%	-18.4%	-18.3%	-31.0%	137.9%
Mar			-56.1%	-24.9%	-24.8%	-31.4%	173.2%
Seas_1	**-59.9%**	**-85.3%**	**-30.6%**	**-20.2%**	**-20.1%**	**-34.3%**	**110.4%**
Apr			-58.8%	-28.7%	-28.5%	-32.7%	182.9%
May			-54.3%	-30.7%	-30.4%	-33.6%	184.5%
Jun			-47.2%	-31.7%	-31.4%	-34.2%	183.6%
Seas_2	**-83.0%**	**-86.6%**	**-54.7%**	**-30.4%**	**-30.2%**	**-33.5%**	**183.7%**
Jul			-41.3%	-32.3%	-31.9%	-34.5%	182.1%
Aug			-37.6%	-32.7%	-32.2%	-34.7%	180.4%
Sep			-35.6%	-32.9%	-32.3%	-34.8%	178.7%
Seas_3	**-92.5%**	**-90.3%**	**-38.3%**	**-32.6%**	**-32.2%**	**-34.6%**	**180.4%**
Oct			-34.6%	-33.0%	-32.4%	-34.8%	177.1%
Nov			-34.2%	-33.1%	-32.5%	-34.9%	175.6%
Dec			-33.2%	-33.2%	-32.5%	-35.0%	174.1%
Seas_4	**-87.1%**	**-75.7%**	**-34.0%**	**-33.1%**	**-32.5%**	**-34.9%**	**175.6%**
Annual	**-86.6%**	**-84.3%**	**-34.4%**	**-30.2%**	**-29.8%**	**-34.4%**	**162.6%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.4.3. Comparison of calculated values of PCB-28 mass flows transported from the atmosphere to water

Dry deposition

Reference data set. Calculation results on PCB-28 mass flows transported from the atmosphere to water: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.69.

Monthly values of PCB-28 mass flows transported from the atmosphere to water: dry deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.97 a and b, respectively.

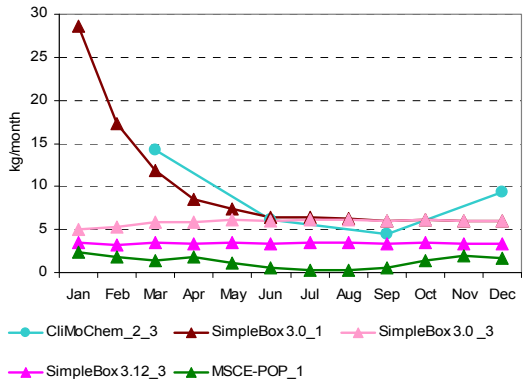


Fig. B.97a. *PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

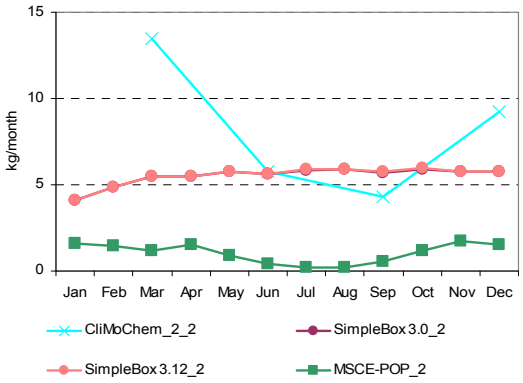


Fig. B.97b. *PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported from the atmosphere to water: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.70.

Monthly values of PCB-28 mass flows transported from the atmosphere to water: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.98 a and b, respectively.

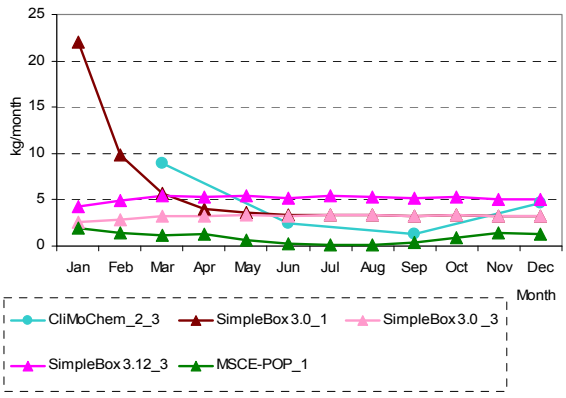


Fig. B.98a. *PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

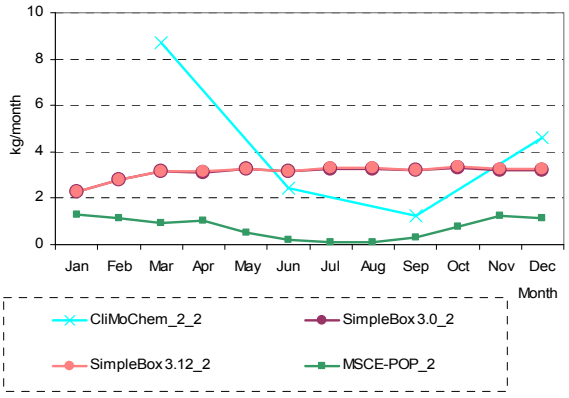


Fig. B.98b. *PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table B.69. *Calculation results: PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	28.54	2.39		5.00	3.46	*9.85*	*12.51*	Jan		4.11	4.11	1.60	*3.27*	*1.45*
Feb	17.28	1.77		5.34	3.23	*6.91*	*7.07*	Feb		4.86	4.86	1.44	*3.72*	*1.97*
Mar	11.85	1.45		5.92	3.46	*5.67*	*4.51*	Mar		5.51	5.51	1.20	*4.07*	*2.49*
Seas_1	**57.68**	**5.61**	**42.66**	**16.27**	**10.15**	***26.47***	***22.59***	**Seas_1**	**40.35**	**14.47**	**14.47**	**4.24**	***18.38***	***15.42***
Apr	8.47	1.81		5.84	3.35	*4.87*	*2.92*	Apr		5.49	5.49	1.55	*4.18*	*2.27*
May	7.35	1.06		6.09	3.46	*4.49*	*2.80*	May		5.76	5.77	0.90	*4.14*	*2.81*
Jun	6.48	0.50		5.93	3.35	*4.07*	*2.74*	Jun		5.63	5.64	0.43	*3.90*	*3.01*
Seas_2	**22.30**	**3.37**	**18.39**	**17.86**	**10.15**	***14.41***	***7.58***	**Seas_2**	**17.36**	**16.88**	**16.90**	**2.88**	***13.51***	***7.09***
Jul	6.40	0.28		6.16	3.46	*4.07*	*2.86*	Jul		5.86	5.87	0.24	*3.99*	*3.25*
Aug	6.25	0.24		6.18	3.46	*4.03*	*2.84*	Aug		5.89	5.90	0.21	*4.00*	*3.28*
Sep	5.99	0.63		6.00	3.35	*3.99*	*2.57*	Sep		5.72	5.73	0.55	*4.00*	*2.99*
Seas_3	**18.64**	**1.15**	**13.51**	**18.33**	**10.26**	***12.38***	***7.19***	**Seas_3**	**12.87**	**17.46**	**17.50**	**1.00**	***12.21***	***7.78***
Oct	6.16	1.36		6.21	3.46	*4.30*	*2.34*	Oct		5.93	5.95	1.21	*4.36*	*2.73*
Nov	5.95	1.89		6.02	3.35	*4.30*	*2.03*	Nov		5.75	5.78	1.71	*4.41*	*2.34*
Dec	5.95	1.62		6.03	3.35	*4.24*	*2.15*	Dec		5.77	5.79	1.50	*4.35*	*2.47*
Seas_4	**18.06**	**4.87**	**28.21**	**18.26**	**10.15**	***15.91***	***8.89***	**Seas_4**	**27.61**	**17.45**	**17.51**	**4.42**	***16.75***	***9.51***
Annual	**116.67**	**15.00**	**102.76**	**70.72**	**40.71**	***69.17***	***42.22***	**Annual**	**98.19**	**66.26**	**66.40**	**12.54**	*60.85*	*35.53*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.70. *Calculation results: PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	22.01	1.96		2.56	4.21	*7.68*	*9.60*	Jan		2.28	2.28	1.32	*1.96*	*0.56*
Feb	9.89	1.42		2.91	4.90	*4.78*	*3.69*	Feb		2.81	2.81	1.16	*2.26*	*0.95*
Mar	5.67	1.11		3.25	5.42	*3.86*	*2.13*	Mar		3.16	3.17	0.93	*2.42*	*1.30*
Seas_1	**37.57**	**4.49**	**26.83**	**8.72**	**14.53**	***18.43***	***13.61***	**Seas_1**	**26.13**	**8.25**	**8.26**	**3.41**	***11.51***	***10.01***
Apr	3.98	1.24		3.20	5.28	*3.42*	*1.69*	Apr		3.12	3.13	1.06	*2.44*	*1.19*
May	3.63	0.59		3.33	5.44	*3.25*	*2.00*	May		3.25	3.27	0.50	*2.34*	*1.59*
Jun	3.36	0.27		3.23	5.24	*3.02*	*2.05*	Jun		3.16	3.19	0.23	*2.19*	*1.70*
Seas_2	**10.97**	**2.10**	**7.41**	**9.75**	**15.96**	***9.24***	***5.07***	**Seas_2**	**7.32**	**9.54**	**9.59**	**1.79**	***7.06***	***3.67***
Jul	3.42	0.13		3.35	5.38	*3.07*	*2.17*	Jul		3.28	3.31	0.12	*2.23*	*1.84*
Aug	3.40	0.12		3.35	5.35	*3.05*	*2.17*	Aug		3.29	3.32	0.10	*2.24*	*1.85*
Sep	3.28	0.34		3.25	5.14	*3.00*	*1.98*	Sep		3.19	3.23	0.30	*2.24*	*1.68*
Seas_3	**10.11**	**0.59**	**3.72**	**9.95**	**15.87**	***8.05***	***5.99***	**Seas_3**	**3.67**	**9.76**	**9.86**	**0.52**	***5.95***	***4.63***
Oct	3.39	0.88		3.37	5.28	*3.23*	*1.80*	Oct		3.30	3.34	0.79	*2.48*	*1.47*
Nov	3.28	1.39		3.26	5.09	*3.25*	*1.51*	Nov		3.20	3.25	1.26	*2.57*	*1.13*
Dec	3.27	1.24		3.27	5.06	*3.21*	*1.56*	Dec		3.21	3.25	1.15	*2.54*	*1.20*
Seas_4	**9.94**	**3.51**	**13.95**	**9.89**	**15.43**	***10.54***	***4.63***	**Seas_4**	**13.89**	**9.71**	**9.84**	**3.20**	***9.16***	***4.42***
Annual	**68.59**	**10.69**	**51.91**	**38.32**	**61.79**	***46.26***	***22.91***	**Annual**	**51.01**	**37.26**	**37.55**	**8.91**	***33.68***	***17.72***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.71.

Table B.71. *The percentage difference between calculation results on PCB-28 mass flows transported from the atmosphere to water: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-22.9%	-44.5%	-44.4%	-48.9%	21.8%	-18.0%	-17.5%
Feb			-42.8%	-42.2%	-42.2%	-45.5%	51.4%	-19.8%	-19.4%
Mar			-52.1%	-42.5%	-42.4%	-45.1%	56.9%	-23.4%	-22.9%
Seas_1	**-35.2%**	**-37.1%**	**-34.9%**	**-43.0%**	**-42.9%**	**-46.4%**	**43.2%**	**-20.0%**	**-19.7%**
Apr			-53.0%	-43.1%	-42.9%	-45.3%	57.9%	-31.5%	-31.6%
May			-50.6%	-43.5%	-43.3%	-45.4%	57.4%	-44.1%	-44.2%
Jun			-48.1%	-43.8%	-43.5%	-45.6%	56.5%	-47.1%	-47.1%
Seas_2	**-57.9%**	**-59.7%**	**-50.8%**	**-43.5%**	**-43.2%**	**-45.4%**	**57.3%**	**-37.8%**	**-37.9%**
Jul			-46.5%	-44.0%	-43.6%	-45.6%	55.6%	-52.3%	-52.1%
Aug			-45.6%	-44.1%	-43.7%	-45.7%	54.6%	-51.9%	-51.2%
Sep			-45.2%	-44.2%	-43.8%	-45.8%	53.7%	-45.8%	-45.6%
Seas_3	**-71.5%**	**-72.5%**	**-45.8%**	**-44.1%**	**-43.7%**	**-45.7%**	**54.6%**	**-48.7%**	**-48.3%**
Oct			-45.0%	-44.3%	-43.8%	-45.8%	52.8%	-35.1%	-35.0%
Nov			-44.9%	-44.4%	-43.8%	-45.8%	52.0%	-26.5%	-26.3%
Dec			-45.0%	-44.4%	-43.8%	-45.9%	51.2%	-23.5%	-23.3%
Seas_4	**-49.7%**	**-50.5%**	**-45.0%**	**-44.4%**	**-43.8%**	**-45.8%**	**52.0%**	**-27.9%**	**-27.7%**
Annual	**-48.1%**	**-49.5%**	**-41.2%**	**-43.8%**	**-43.4%**	**-45.8%**	**51.8%**	**-28.7%**	**-29.0%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Wet deposition

Reference data set. Calculation results on PCB-28 mass flows transported from the atmosphere to water: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.72.

Monthly values of PCB-28 mass flows transported from the atmosphere to water: wet deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.99 a and b, respectively.

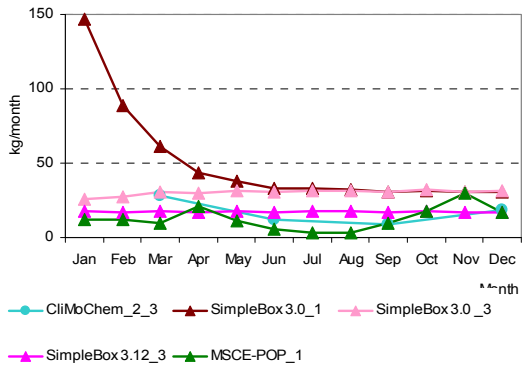


Fig. B.99a. *PCB-28 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

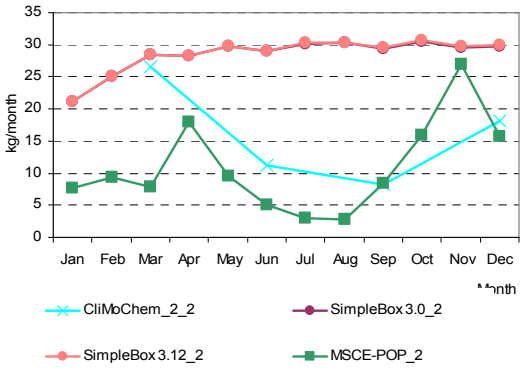


Fig. B.99b. *PCB-28 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported from the atmosphere to water: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.73.

Monthly values of PCB-28 mass flows transported from the atmosphere to water: wet deposition calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.100 a and b, respectively.

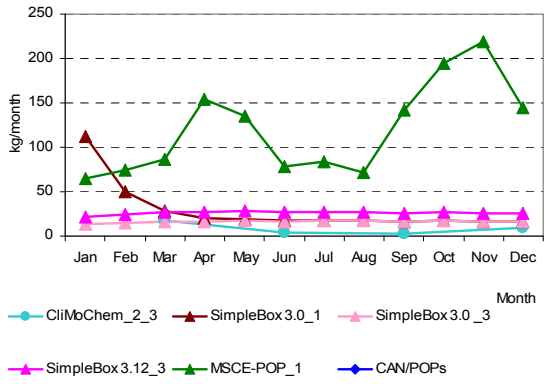


Fig. B.100a. *PCB-28 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

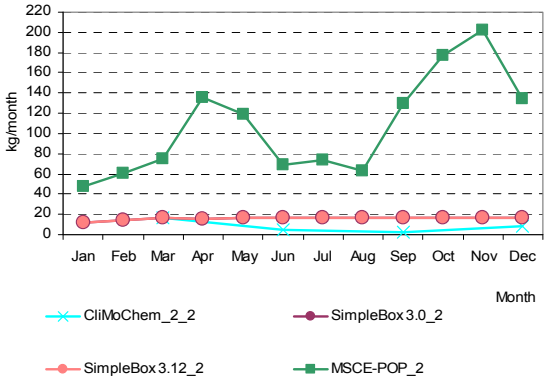


Fig. B.100b. *PCB-28 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.74.

Gaseous exchange

Reference data set. Calculation results on PCB-28 mass flows between the atmosphere and water: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.75.

Monthly values of PCB-28 mass flows between the atmosphere and water: gaseous exchange calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.101 a and b, respectively.

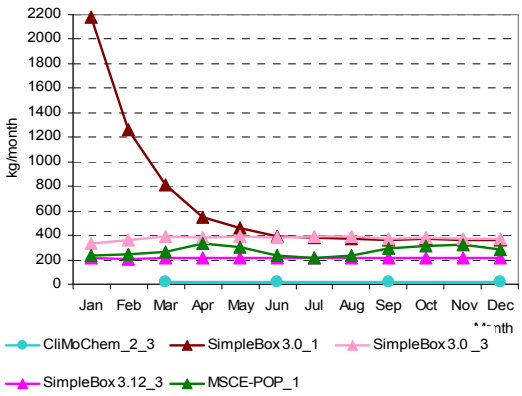


Fig. B.101a. *PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

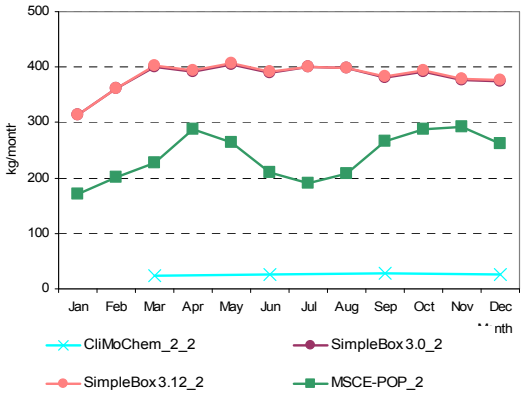


Fig. B.101b. *PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table B.72. *Calculation results: PCB-28 mass flows between the atmosphere and water: wet deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	147.13	12.00		25.79	17.82	*50.69*	*64.54*	Jan		21.17	21.17	7.76	*16.70*	*7.74*
Feb	89.08	11.70		27.54	16.67	*36.25*	*35.84*	Feb		25.03	25.04	9.33	*19.80*	*9.07*
Mar	61.10	9.28		30.52	17.82	*29.68*	*22.69*	Mar		28.38	28.39	7.81	*21.53*	*11.88*
Seas_1	**297.30**	**32.98**	**84.57**	**83.85**	**52.31**	***110.20***	***106.86***	**Seas_1**	**79.98**	**74.58**	**74.61**	**24.90**	***63.52***	***25.87***
Apr	43.66	20.80		30.09	17.25	*27.95*	*11.79*	Apr		28.29	28.31	17.90	*24.83*	*6.00*
May	37.86	11.30		31.41	17.82	*24.60*	*12.18*	May		29.70	29.74	9.62	*23.02*	*11.60*
Jun	33.40	5.94		30.59	17.25	*21.79*	*12.70*	Jun		29.02	29.07	4.97	*21.02*	*13.90*
Seas_2	**114.92**	**38.04**	**35.73**	**92.08**	**52.31**	***66.62***	***35.20***	**Seas_2**	**33.73**	**87.01**	**87.13**	**32.49**	***60.09***	***31.16***
Jul	32.97	3.52		31.74	17.82	*21.51*	*13.82*	Jul		30.19	30.25	3.00	*21.15*	*15.72*
Aug	32.24	3.46		31.85	17.82	*21.34*	*13.68*	Aug		30.34	30.41	2.90	*21.22*	*15.86*
Sep	30.88	9.55		30.90	17.25	*22.14*	*10.58*	Sep		29.48	29.56	8.46	*22.50*	*12.16*
Seas_3	**96.09**	**16.53**	**26.08**	**94.50**	**52.89**	***57.22***	***37.23***	**Seas_3**	**24.84**	**90.01**	**90.22**	**14.36**	***54.86***	***40.94***
Oct	31.75	17.80		32.00	17.82	*24.84*	*8.12*	Oct		30.56	30.66	15.90	*25.71*	*8.49*
Nov	30.65	29.70		31.03	17.25	*27.16*	*6.63*	Nov		29.66	29.77	27.00	*28.81*	*1.57*
Dec	30.69	17.20		31.08	17.25	*24.05*	*7.89*	Dec		29.74	29.85	15.70	*25.10*	*8.14*
Seas_4	**93.09**	**64.70**	**55.43**	**94.12**	**52.31**	***71.93***	***20.30***	**Seas_4**	**54.26**	**89.96**	**90.28**	**58.60**	***73.28***	***19.53***
Annual	**601.40**	**152.25**	**201.81**	**364.54**	**209.83**	***305.97***	***183.33***	**Annual**	**192.82**	**341.56**	**342.24**	**130.35**	***251.74***	***107.19***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.73. *Calculation results: PCB-28 mass flows between the atmosphere and water: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	112.23	64.40		13.04	21.48	*52.79*	*45.56*	Jan		11.63	11.64	48.00	*23.76*	*21.00*
Feb	50.43	74.20		14.84	24.96	*41.11*	*26.66*	Feb		14.30	14.32	61.10	*29.91*	*27.01*
Mar	28.93	86.00		16.57	27.66	*39.79*	*31.30*	Mar		16.13	16.18	74.50	*35.60*	*33.69*
Seas_1	**191.59**	**224.60**	**51.39**	**44.45**	**74.10**	***117.22***	***84.48***	**Seas_1**	**50.04**	**42.07**	**42.13**	**183.60**	***79.46***	***69.53***
Apr	20.28	154.00		16.29	26.93	*54.38*	*66.56*	Apr		15.92	15.98	136.00	*55.97*	*69.31*
May	18.51	135.00		16.96	27.75	*49.55*	*57.16*	May		16.59	16.68	119.00	*50.76*	*59.10*
Jun	17.15	78.60		16.47	26.70	*34.73*	*29.62*	Jun		16.13	16.25	69.40	*33.93*	*30.72*
Seas_2	**55.93**	**367.60**	**14.06**	**49.72**	**81.38**	***113.74***	***143.93***	**Seas_2**	**13.89**	**48.65**	**48.91**	**324.40**	***108.96***	***144.56***
Jul	17.45	84.10		17.07	27.42	*36.51*	*32.09*	Jul		16.73	16.87	74.10	*35.90*	*33.08*
Aug	17.35	71.60		17.11	27.26	*33.33*	*25.95*	Aug		16.77	16.94	63.00	*32.24*	*26.64*
Sep	16.74	142.00		16.58	26.22	*50.39*	*61.24*	Sep		16.27	16.45	130.00	*54.24*	*65.61*
Seas_3	**51.55**	**297.70**	**7.04**	**50.76**	**80.90**	***97.59***	***114.93***	**Seas_3**	**6.95**	**49.77**	**50.25**	**267.10**	***93.52***	***117.49***
Oct	17.28	194.00		17.16	26.94	*63.84*	*86.89*	Oct		16.84	17.05	177.00	*70.30*	*92.41*
Nov	16.70	219.00		16.63	25.93	*69.57*	*99.72*	Nov		16.33	16.55	202.00	*78.29*	*107.13*
Dec	16.69	144.00		16.65	25.79	*50.78*	*62.29*	Dec		16.35	16.59	134.00	*55.65*	*67.86*
Seas_4	**50.67**	**557.00**	**26.62**	**50.44**	**78.66**	***152.68***	***226.77***	**Seas_4**	**26.49**	**49.52**	**50.19**	**513.00**	***159.80***	***235.72***
Annual	**349.74**	**1446.90**	**99.11**	**195.37**	**315.05**	***481.23***	***548.90***	**Annual**	**97.37**	**190.01**	**191.49**	**1288.10**	***441.74***	***565.95***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.74. *The percentage difference between calculation results on PCB-28 mass flows between the atmosphere and water: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-23.7%	-45.1%	-45.0%	-49.5%	20.5%	436.7%	518.6%
Feb			-43.4%	-42.9%	-42.8%	-46.1%	49.7%	534.2%	554.9%
Mar			-52.7%	-43.1%	-43.0%	-45.7%	55.2%	826.7%	853.9%
Seas_1	**-37.4%**	**-39.2%**	**-35.6%**	**-43.6%**	**-43.5%**	**-47.0%**	**41.6%**	**581.0%**	**637.3%**
Apr			-53.6%	-43.7%	-43.5%	-45.8%	56.2%	640.4%	659.8%
May			-51.1%	-44.1%	-43.9%	-46.0%	55.7%	1094.7%	1137.0%
Jun			-48.7%	-44.4%	-44.1%	-46.1%	54.8%	1223.2%	1296.4%
Seas_2	**-58.8%**	**-60.6%**	**-51.3%**	**-44.1%**	**-43.9%**	**-46.0%**	**55.6%**	**866.4%**	**898.5%**
Jul			-47.1%	-44.6%	-44.2%	-46.2%	53.9%	2289.2%	2370.0%
Aug			-46.2%	-44.7%	-44.3%	-46.3%	52.9%	1969.4%	2072.4%
Sep			-45.8%	-44.8%	-44.4%	-46.3%	52.0%	1386.9%	1436.6%
Seas_3	**-72.0%**	**-73.0%**	**-46.4%**	**-44.7%**	**-44.3%**	**-46.3%**	**53.0%**	**1701.0%**	**1760.0%**
Oct			-45.6%	-44.9%	-44.4%	-46.4%	51.2%	989.9%	1013.2%
Nov			-45.5%	-45.0%	-44.4%	-46.4%	50.3%	637.4%	648.1%
Dec			-45.6%	-45.0%	-44.4%	-46.4%	49.6%	737.2%	753.5%
Seas_4	**-51.2%**	**-52.0%**	**-45.6%**	**-45.0%**	**-44.4%**	**-46.4%**	**50.4%**	**760.9%**	**775.4%**
Annual	**-49.5%**	**-50.9%**	**-41.8%**	**-44.4%**	**-44.0%**	**-46.4%**	**50.1%**	**850.3%**	**888.2%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-28 mass flows between the atmosphere and water: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.76.

Monthly values of PCB-28 mass flows between the atmosphere and water: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.102 a and b, respectively. Seasonal variations of gaseous exchange flows between the atmosphere and water calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions are also shown in Fig. B.102c in more detail.

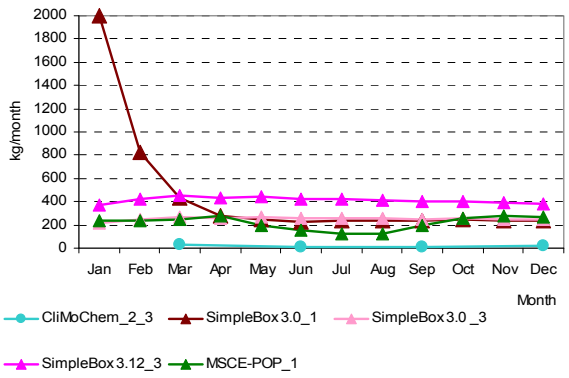


Fig. B.102a. *PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

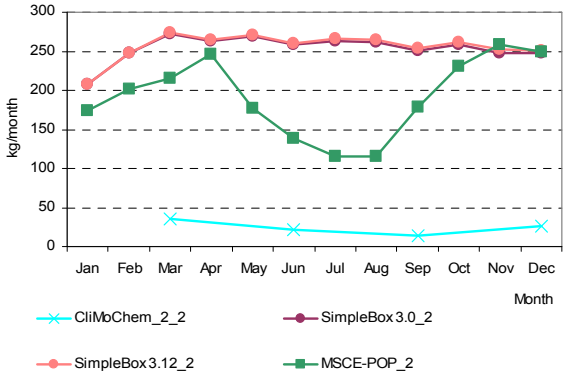


Fig. B.102b. *PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

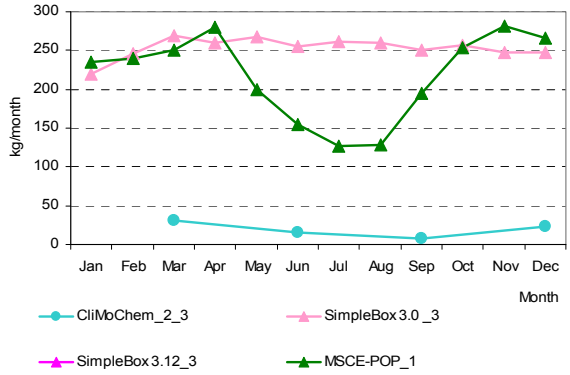


Fig. B.102c. *PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (models with low values)*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.77.

Table B.75. *Calculation results: PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[1]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2180.81	233.00		335.01	218.81	*741.91*	*960.66*	Jan		314.10	314.10	171.00	*266.40*	*82.62*
Feb	1256.60	241.00		357.00	204.70	*514.82*	*498.76*	Feb		361.41	361.50	202.00	*308.30*	*92.06*
Mar	814.13	262.00		391.14	218.81	*421.52*	*271.79*	Mar		401.47	401.70	227.00	*343.39*	*100.80*
Seas_1	**4251.54**	**736.00**	**63.87**	**1083.16**	**642.32**	***1355.38***	***1659.96***	**Seas_1**	**73.94**	**1076.98**	**1077.31**	**600.00**	***707.06***	***478.27***
Apr	549.93	328.00		380.95	211.75	*367.66*	*140.57*	Apr		392.83	393.20	288.00	*358.01*	*60.63*
May	457.83	301.00		393.04	218.81	*342.67*	*104.69*	May		405.55	406.10	265.00	*358.88*	*81.30*
Jun	394.81	237.00		378.63	211.75	*305.55*	*94.52*	Jun		390.28	390.98	210.00	*330.42*	*104.29*
Seas_2	**1402.57**	**866.00**	**58.61**	**1152.63**	**642.32**	***824.43***	***515.59***	**Seas_2**	**79.52**	**1188.66**	**1190.28**	**763.00**	***805.36***	***524.00***
Jul	385.85	215.00		389.08	218.81	*302.19*	*98.49*	Jul		400.43	401.30	191.00	*330.91*	*121.17*
Aug	376.09	231.00		386.88	218.81	*303.20*	*90.64*	Aug		397.44	398.48	207.00	*334.31*	*110.25*
Sep	360.08	294.00		372.44	211.75	*309.57*	*73.74*	Sep		381.95	383.09	266.00	*343.68*	*67.27*
Seas_3	**1122.01**	**740.00**	**48.51**	**1148.40**	**649.38**	***741.66***	***446.96***	**Seas_3**	**83.08**	**1179.83**	**1182.88**	**664.00**	***777.44***	***523.23***
Oct	370.55	317.00		383.00	218.81	*322.34*	*74.72*	Oct		392.14	393.48	288.00	*357.87*	*60.52*
Nov	358.13	318.00		369.05	211.75	*314.23*	*71.76*	Nov		377.27	378.72	292.00	*349.33*	*49.65*
Dec	361.01	279.00		367.61	211.75	*304.84*	*74.00*	Dec		375.31	376.90	261.00	*337.73*	*66.46*
Seas_4	**1089.69**	**914.00**	**61.18**	**1119.65**	**642.32**	***765.37***	***436.98***	**Seas_4**	**74.69**	**1144.73**	**1149.09**	**841.00**	***802.38***	***506.11***
Annual	**7865.80**	**3256.00**	**232.16**	**4503.83**	**2576.34**	***3686.83***	***2805.57***	**Annual**	**311.23**	**4590.19**	**4599.56**	**2868.00**	***3092.24***	***2024.86***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.76. *Calculation results: PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE- POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1997.44	235.00		219.69	370.72	*705.71*	*863.82*	Jan		207.66	207.73	174.00	*196.46*	*19.45*
Feb	828.61	240.00		246.29	422.09	*434.25*	*276.12*	Feb		247.48	247.81	202.00	*232.43*	*26.35*
Mar	428.93	250.00		269.80	457.42	*351.54*	*106.76*	Mar		272.51	273.24	216.00	*253.92*	*32.84*
Seas_1	**3254.98**	**725.00**	**94.57**	**735.79**	**1250.23**	***1212.11***	***1213.24***	**Seas_1**	**105.22**	**727.66**	**728.77**	**592.00**	***538.41***	***295.85***
Apr	278.91	280.00		260.55	436.28	*313.94*	*82.05*	Apr		263.22	264.32	246.00	*257.84*	*10.27*
May	248.87	200.00		266.88	441.39	*289.28*	*105.27*	May		269.30	270.84	177.00	*239.05*	*53.74*
Jun	231.60	154.00		255.82	418.27	*264.92*	*111.07*	Jun		257.79	259.66	138.00	*218.48*	*69.71*
Seas_2	**759.38**	**634.00**	**46.17**	**783.25**	**1295.94**	***703.75***	***446.48***	**Seas_2**	**64.32**	**790.30**	**794.82**	**561.00**	***552.61***	***343.35***
Jul	238.45	127.00		262.08	423.97	*262.87*	*122.49*	Jul		263.76	266.08	115.00	*214.95*	*86.56*
Aug	239.80	128.00		260.11	416.64	*261.14*	*118.83*	Aug		261.48	264.18	116.00	*213.89*	*84.78*
Sep	233.67	195.00		250.14	397.08	*268.97*	*88.48*	Sep		251.22	254.16	178.00	*227.79*	*43.15*
Seas_3	**711.92**	**450.00**	**24.54**	**772.32**	**1237.69**	***639.29***	***445.76***	**Seas_3**	**42.12**	**776.46**	**784.41**	**409.00**	***503.00***	***353.66***
Oct	242.94	253.00		257.11	404.74	*289.45*	*77.09*	Oct		258.00	261.39	231.00	*250.13*	*16.65*
Nov	236.29	281.00		247.69	386.91	*287.97*	*68.63*	Nov		248.37	251.97	259.00	*253.11*	*5.41*
Dec	237.20	266.00		246.75	382.70	*283.16*	*67.43*	Dec		247.28	251.19	250.00	*249.49*	*2.01*
Seas_4	**716.43**	**800.00**	**69.33**	**751.54**	**1174.34**	***702.33***	***398.64***	**Seas_4**	**78.72**	**753.64**	**764.55**	**740.00**	***584.23***	***337.16***
Annual	**5442.71**	**2609.00**	**234.60**	**3042.90**	**4958.20**	***3257.48***	***2077.98***	**Annual**	**290.38**	**3048.06**	**3072.55**	**2302.00**	***2178.25***	***1308.40***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.77. *Comparison of the calculation results on PCB-28 mass flows between the atmosphere and water: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			2180.81	1997.44	314.10	207.66	314.10	207.73	335.01	219.69	218.81	370.72	233.00	235.00	171.00	174.00		
Feb			1256.60	828.61	361.41	247.48	361.50	247.81	357.00	246.29	204.70	422.09	241.00	240.00	202.00	202.00		
Mar			814.13	428.93	401.47	272.51	401.70	273.24	391.14	269.80	218.81	457.42	262.00	250.00	227.00	216.00		
Seas_1	**63.87**	**94.57**	**4251.54**	**3254.98**	**1076.98**	**727.66**	**1077.31**	**728.77**	**1083.16**	**735.79**	**642.32**	**1250.23**	**736.00**	**725.00**	**600.00**	**592.00**	**73.94**	**105.22**
Apr			549.93	278.91	392.83	263.22	393.20	264.32	380.95	260.55	211.75	436.28	328.00	280.00	288.00	246.00		
May			457.83	248.87	405.55	269.30	406.10	270.84	393.04	266.88	218.81	441.39	301.00	200.00	265.00	177.00		
Jun			394.81	231.60	390.28	257.79	390.98	259.66	378.63	255.82	211.75	418.27	237.00	154.00	210.00	138.00		
Seas_2	**58.61**	**46.17**	**1402.57**	**759.38**	**1188.66**	**790.30**	**1190.28**	**794.82**	**1152.63**	**783.25**	**642.32**	**1295.94**	**866.00**	**634.00**	**763.00**	**561.00**	**79.52**	**64.32**
Jul			385.85	238.45	400.43	263.76	401.30	266.08	389.08	262.08	218.81	423.97	215.00	127.00	191.00	115.00		
Aug			376.09	239.80	397.44	261.48	398.48	264.18	386.88	260.11	218.81	416.64	231.00	128.00	207.00	116.00		
Sep			360.08	233.67	381.95	251.22	383.09	254.16	372.44	250.14	211.75	397.08	294.00	195.00	266.00	178.00		
Seas_3	**48.51**	**24.54**	**1122.01**	**711.92**	**1179.83**	**776.46**	**1182.88**	**784.41**	**1148.40**	**772.32**	**649.38**	**1237.69**	**740.00**	**450.00**	**664.00**	**409.00**	**83.08**	**42.12**
Oct			370.55	242.94	392.14	258.00	393.48	261.39	383.00	257.11	218.81	404.74	317.00	253.00	288.00	231.00		
Nov			358.13	236.29	377.27	248.37	378.72	251.97	369.05	247.69	211.75	386.91	318.00	281.00	292.00	259.00		
Dec			361.01	237.20	375.31	247.28	376.90	251.19	367.61	246.75	211.75	382.70	279.00	266.00	261.00	250.00		
Seas_4	**61.18**	**69.33**	**1089.69**	**716.43**	**1144.73**	**753.64**	**1149.09**	**764.55**	**1119.65**	**751.54**	**642.32**	**1174.34**	**914.00**	**800.00**	**841.00**	**740.00**	**74.69**	**78.72**
Annual	**232.16**	**234.60**	**7865.80**	**5442.71**	**4590.19**	**3048.06**	**4599.56**	**3072.55**	**4503.83**	**3042.90**	**2576.34**	**4958.20**	**3256.00**	**2609.00**	**2868.00**	**2302.00**	**311.23**	**290.38**

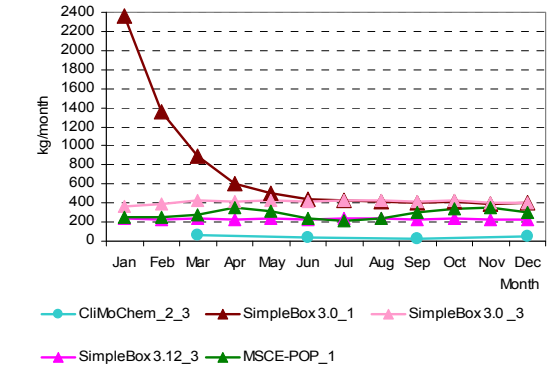
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Net mass flows between the atmosphere and water

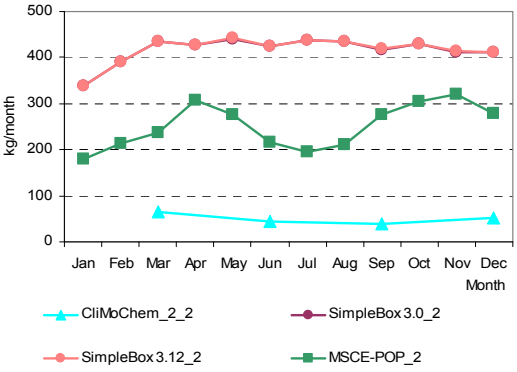
Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-28 net mass flows PCB-28 between the atmosphere and water calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.78.

Monthly values of PCB-28 net mass flows PCB-28 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.103 a and b, respectively.



a



b

Fig. B.103a. *PCB-28 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. B.103b. *PCB-28 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table B.78. *Calculation results: PCB-28 net mass flows between the atmosphere and water (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2356.48	247.39		365.81	240.09	*802.44*	*1037.62*	Jan		339.38	339.39	180.36	*286.37*	*91.81*
Feb	1362.96	254.47		389.88	224.60	*557.98*	*541.45*	Feb		391.30	391.40	212.77	*331.82*	*103.10*
Mar	887.08	272.73		427.58	240.09	*456.87*	*298.24*	Mar		435.36	435.61	236.01	*368.99*	*115.17*
Seas_1	**4606.52**	**774.59**	**191.10**	**1183.27**	**704.78**	***1492.05***	***1776.39***	**Seas_1**	**194.27**	**1166.03**	**1166.39**	**629.14**	***788.96***	***470.40***
Apr	602.06	350.61		416.87	232.35	*400.47*	*154.55*	Apr		426.60	427.01	307.45	*387.02*	*68.91*
May	503.04	313.36		430.55	240.09	*371.76*	*117.53*	May		441.01	441.61	275.52	*386.05*	*95.72*
Jun	434.69	243.44		415.15	232.35	*331.41*	*108.37*	Jun		424.94	425.69	215.40	*355.34*	*121.20*
Seas_2	**1539.79**	**907.41**	**112.73**	**1262.57**	**704.78**	***905.46***	***547.40***	**Seas_2**	**130.61**	**1292.55**	**1294.31**	**798.37**	***878.96***	***550.78***
Jul	425.22	218.80		426.98	240.09	*327.77*	*113.87*	Jul		436.48	437.42	194.24	*356.05*	*140.13*
Aug	414.58	234.70		424.91	240.09	*328.57*	*105.39*	Aug		433.67	434.80	210.11	*359.53*	*129.40*
Sep	396.94	304.18		409.33	232.35	*335.70*	*83.36*	Sep		417.14	418.38	275.01	*370.18*	*82.42*
Seas_3	**1236.74**	**757.68**	**88.09**	**1261.22**	**712.53**	***811.25***	***479.35***	**Seas_3**	**120.79**	**1287.29**	**1290.60**	**679.36**	***844.51***	***561.57***
Oct	408.45	336.16		421.21	240.09	*351.48*	*83.17*	Oct		428.63	430.09	305.11	*387.94*	*71.74*
Nov	394.73	349.59		406.10	232.35	*345.69*	*79.41*	Nov		412.69	414.26	320.71	*382.55*	*53.56*
Dec	397.65	297.82		404.72	232.35	*333.13*	*83.05*	Dec		410.81	412.54	278.20	*367.19*	*77.07*
Seas_4	**1200.83**	**983.57**	**144.82**	**1232.03**	**704.78**	***853.21***	***448.66***	**Seas_4**	**156.55**	**1252.14**	**1256.89**	**904.02**	***892.40***	***517.65***
Annual	**8583.88**	**3423.25**	**536.73**	**4939.10**	**2826.88**	***4061.97***	***2982.35***	**Annual**	**602.23**	**4998.01**	**5008.20**	**3010.89**	***3404.83***	***2091.16***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates;

B.4.4. Comparison of calculated values of PCB-28 mass flows transported from the atmosphere to vegetation

Dry deposition

Reference data set. Calculation results on PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.79.

Monthly values of PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.104 a and b, respectively.

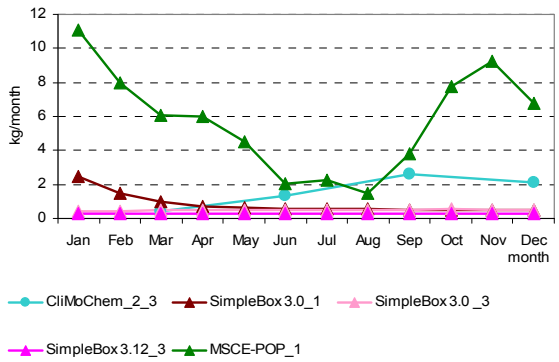


Fig. B.104a. *PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

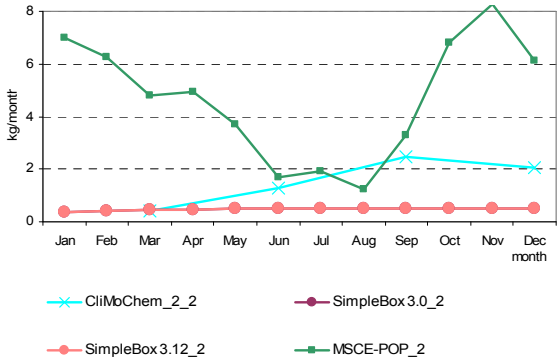


Fig. B.104b. *PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.80.

Monthly values of PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.105 a and b, respectively.

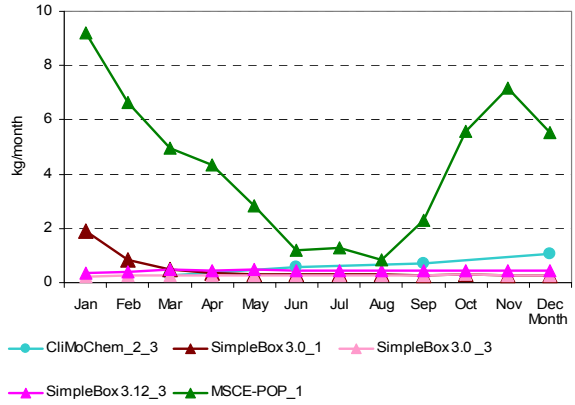


Fig. B.105a. *PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

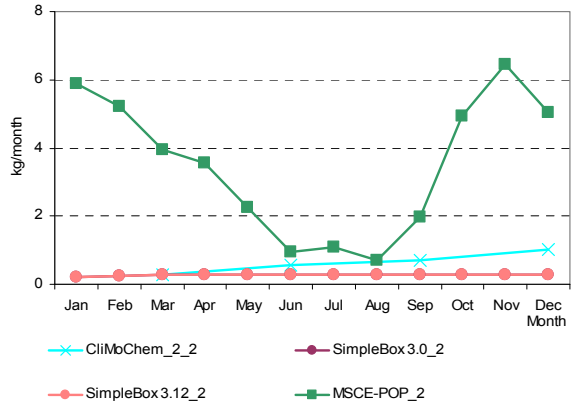


Fig. B.105b. *PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.79 *Calculation results: PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.45	11.10		0.43	0.30	*3.57*	*5.12*	Jan		0.35	0.35	6.99	*2.56*	*3.83*
Feb	1.48	7.96		0.46	0.28	*2.54*	*3.65*	Feb		0.42	0.42	6.25	*2.36*	*3.37*
Mar	1.02	6.04		0.51	0.30	*1.96*	*2.73*	Mar		0.47	0.47	4.81	*1.92*	*2.50*
Seas_1	**4.94**	**25.10**	**1.32**	**1.39**	**0.87**	***6.72***	***10.40***	**Seas_1**	**1.25**	**1.24**	**1.24**	**18.05**	***5.44***	***8.40***
Apr	0.73	5.99		0.50	0.29	*1.88*	*2.75*	Apr		0.47	0.47	4.95	*1.96*	*2.59*
May	0.63	4.54		0.52	0.30	*1.50*	*2.03*	May		0.49	0.49	3.71	*1.57*	*1.86*
Jun	0.56	2.05		0.51	0.29	*0.85*	*0.81*	Jun		0.48	0.48	1.67	*0.88*	*0.69*
Seas_2	**1.91**	**12.58**	**4.13**	**1.53**	**0.87**	***4.20***	***4.84***	**Seas_2**	**3.90**	**1.45**	**1.45**	**10.33**	***4.28***	***4.20***
Jul	0.55	2.26		0.53	0.30	*0.91*	*0.91*	Jul		0.50	0.50	1.94	*0.98*	*0.83*
Aug	0.54	1.47		0.53	0.30	*0.71*	*0.52*	Aug		0.50	0.51	1.25	*0.75*	*0.43*
Sep	0.51	3.79		0.51	0.29	*1.28*	*1.68*	Sep		0.49	0.49	3.27	*1.42*	*1.60*
Seas_3	**1.60**	**7.52**	**7.84**	**1.57**	**0.88**	***3.88***	***3.48***	**Seas_3**	**7.47**	**1.50**	**1.50**	**6.46**	***4.23***	***3.18***
Oct	0.53	7.74		0.53	0.30	*2.27*	*3.65*	Oct		0.51	0.51	6.82	*2.61*	*3.64*
Nov	0.51	9.24		0.52	0.29	*2.64*	*4.40*	Nov		0.49	0.49	8.28	*3.09*	*4.50*
Dec	0.51	6.79		0.52	0.29	*2.03*	*3.18*	Dec		0.49	0.50	6.14	*2.38*	*3.26*
Seas_4	**1.55**	**23.77**	**6.33**	**1.56**	**0.87**	***6.82***	***9.73***	**Seas_4**	**6.20**	**1.49**	**1.50**	**21.24**	***7.61***	***9.35***
Annual	**10.00**	**68.97**	**19.61**	**6.06**	**3.49**	***21.62***	***27.17***	**Annual**	**18.81**	**5.68**	**5.69**	**56.08**	***21.56***	***23.83***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.80. *Calculation results: PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.89	9.22		0.22	0.36	*2.92*	*4.27*	Jan		0.20	0.20	5.88	*2.09*	*3.28*
Feb	0.85	6.64		0.25	0.42	*2.04*	*3.08*	Feb		0.24	0.24	5.23	*1.90*	*2.88*
Mar	0.49	4.96		0.28	0.46	*1.55*	*2.28*	Mar		0.27	0.27	3.95	*1.50*	*2.12*
Seas_1	**3.22**	**20.82**	**0.83**	**0.75**	**1.25**	***5.37***	***8.69***	**Seas_1**	**0.81**	**0.71**	**0.71**	**15.06**	***4.32***	***7.16***
Apr	0.34	4.33		0.27	0.45	*1.35*	*1.99*	Apr		0.27	0.27	3.55	*1.36*	*1.89*
May	0.31	2.81		0.28	0.47	*0.97*	*1.23*	May		0.28	0.28	2.26	*0.94*	*1.14*
Jun	0.29	1.20		0.28	0.45	*0.55*	*0.44*	Jun		0.27	0.27	0.97	*0.50*	*0.40*
Seas_2	**0.94**	**8.34**	**1.66**	**0.84**	**1.37**	***2.63***	***3.21***	**Seas_2**	**1.64**	**0.82**	**0.82**	**6.78**	***2.51***	***2.87***
Jul	0.29	1.30		0.29	0.46	*0.59*	*0.48*	Jul		0.28	0.28	1.10	*0.55*	*0.47*
Aug	0.29	0.83		0.29	0.46	*0.47*	*0.25*	Aug		0.28	0.28	0.71	*0.42*	*0.24*
Sep	0.28	2.30		0.28	0.44	*0.83*	*0.99*	Sep		0.27	0.28	1.97	*0.84*	*0.98*
Seas_3	**0.87**	**4.43**	**2.16**	**0.85**	**1.36**	***1.93***	***1.49***	**Seas_3**	**2.13**	**0.84**	**0.84**	**3.78**	***1.90***	***1.39***
Oct	0.29	5.58		0.29	0.45	*1.65*	*2.62*	Oct		0.28	0.29	4.92	*1.83*	*2.68*
Nov	0.28	7.17		0.28	0.44	*2.04*	*3.42*	Nov		0.27	0.28	6.46	*2.34*	*3.57*
Dec	0.28	5.52		0.28	0.43	*1.63*	*2.60*	Dec		0.27	0.28	5.03	*1.86*	*2.74*
Seas_4	**0.85**	**18.27**	**3.13**	**0.85**	**1.32**	***4.88***	***7.54***	**Seas_4**	**3.12**	**0.83**	**0.84**	**16.41**	***5.30***	***7.48***
Annual	**5.88**	**51.86**	**7.78**	**3.28**	**5.29**	***14.82***	***20.77***	**Annual**	**7.70**	**3.19**	**3.22**	**42.02**	***14.03***	***18.78***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.81.

Table B.81. *The percentage difference between calculation results on PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-22.9%	-44.5%	-44.4%	-48.9%	21.9%	-16.9%	-15.9%
Feb			-42.8%	-42.2%	-42.2%	-45.5%	51.5%	-16.6%	-16.3%
Mar			-52.1%	-42.5%	-42.4%	-45.1%	57.0%	-17.9%	-17.9%
Seas_1	**-35.2%**	**-37.1%**	**-34.9%**	**-43.0%**	**-42.9%**	**-46.4%**	**43.3%**	**-17.1%**	**-16.6%**
Apr			-53.0%	-43.1%	-42.9%	-45.2%	58.0%	-27.7%	-28.3%
May			-50.6%	-43.5%	-43.3%	-45.4%	57.5%	-38.1%	-39.1%
Jun			-48.1%	-43.8%	-43.5%	-45.6%	56.6%	-41.5%	-42.0%
Seas_2	**-57.9%**	**-59.7%**	**-50.8%**	**-43.5%**	**-43.2%**	**-45.4%**	**57.3%**	**-33.7%**	**-34.4%**
Jul			-46.5%	-44.0%	-43.6%	-45.6%	55.7%	-42.5%	-43.3%
Aug			-45.6%	-44.1%	-43.7%	-45.7%	54.7%	-43.6%	-43.5%
Sep			-45.2%	-44.2%	-43.7%	-45.7%	53.8%	-39.3%	-39.8%
Seas_3	**-71.5%**	**-72.5%**	**-45.8%**	**-44.1%**	**-43.7%**	**-45.7%**	**54.7%**	**-41.1%**	**-41.5%**
Oct			-45.0%	-44.3%	-43.8%	-45.8%	52.9%	-27.9%	-27.9%
Nov			-44.9%	-44.4%	-43.8%	-45.8%	52.1%	-22.4%	-22.0%
Dec			-45.0%	-44.4%	-43.8%	-45.8%	51.3%	-18.7%	-18.1%
Seas_4	**-49.7%**	**-50.5%**	**-45.0%**	**-44.4%**	**-43.8%**	**-45.8%**	**52.1%**	**-23.1%**	**-22.7%**
Annual	**-59.1%**	**-60.3%**	**-41.2%**	**-43.8%**	**-43.4%**	**-45.8%**	**51.9%**	**-24.8%**	**-25.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Wet deposition

Reference data set. Calculation results on PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.82.

Monthly values of PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.105 a and b, respectively.

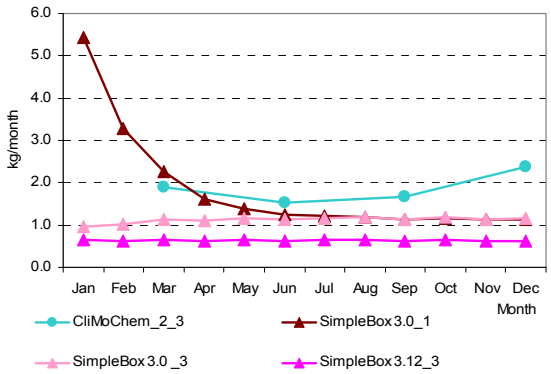


Fig. B.105a. *PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

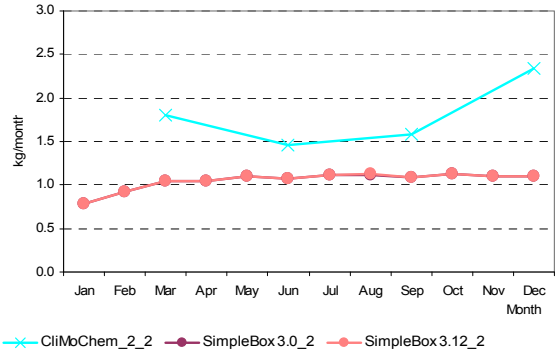


Fig. B.105b. *PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.83.

Monthly values of PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.107 a and b, respectively.

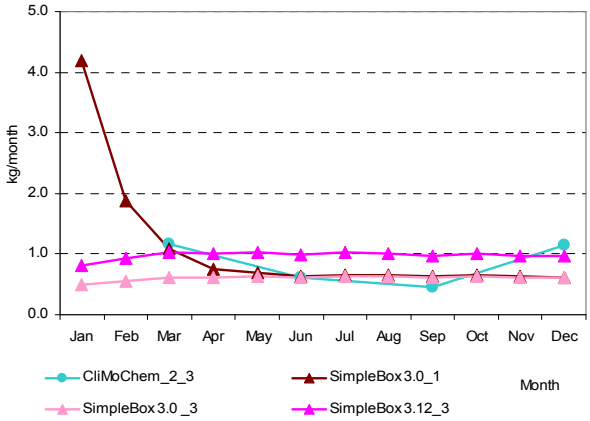


Fig. B.107a. *PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

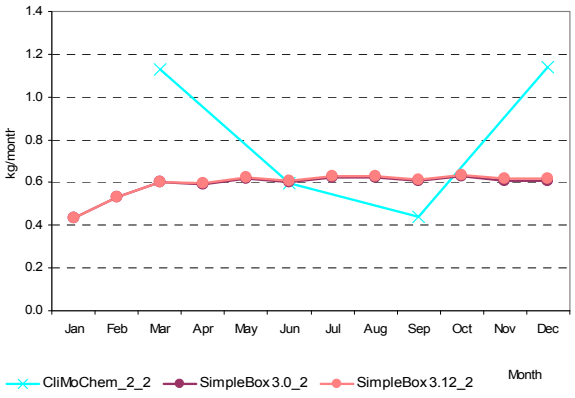


Fig. B.107b. *PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.82. *Calculation results: PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	5.43		0.95	0.66	*2.35*	*2.67*	Jan		0.78	0.78	*0.78*	*0.00*
Feb	3.29		1.02	0.61	*1.64*	*1.44*	Feb		0.92	0.92	*0.92*	*0.00*
Mar	2.25		1.13	0.66	*1.35*	*0.82*	Mar		1.05	1.05	*1.05*	*0.00*
Seas_1	**10.97**	**5.72**	**3.09**	**1.93**	***5.43***	***4.02***	**Seas_1**	**5.41**	**2.75**	**2.75**	***3.64***	***1.54***
Apr	1.61		1.11	0.64	*1.12*	*0.49*	Apr		1.04	1.04	*1.04*	*0.00*
May	1.40		1.16	0.66	*1.07*	*0.38*	May		1.10	1.10	*1.10*	*0.00*
Jun	1.23		1.13	0.64	*1.00*	*0.32*	Jun		1.07	1.07	*1.07*	*0.00*
Seas_2	**4.24**	**4.61**	**3.40**	**1.93**	***3.54***	***1.19***	**Seas_2**	**4.36**	**3.21**	**3.21**	***3.59***	***0.66***
Jul	1.22		1.17	0.66	*1.01*	*0.31*	Jul		1.11	1.12	*1.11*	*0.00*
Aug	1.19		1.17	0.66	*1.01*	*0.30*	Aug		1.12	1.12	*1.12*	*0.00*
Sep	1.14		1.14	0.64	*0.97*	*0.29*	Sep		1.09	1.09	*1.09*	*0.00*
Seas_3	**3.54**	**4.97**	**3.49**	**1.95**	***3.49***	***1.23***	**Seas_3**	**4.74**	**3.32**	**3.33**	***3.79***	***0.82***
Oct	1.17		1.18	0.66	*1.00*	*0.30*	Oct		1.13	1.13	*1.13*	*0.00*
Nov	1.13		1.14	0.64	*0.97*	*0.29*	Nov		1.09	1.10	*1.10*	*0.00*
Dec	1.13		1.15	0.64	*0.97*	*0.29*	Dec		1.10	1.10	*1.10*	*0.00*
Seas_4	**3.43**	**7.16**	**3.47**	**1.93**	***4.00***	***2.23***	**Seas_4**	**7.01**	**3.32**	**3.33**	***4.55***	***2.13***
Annual	**22.19**	**22.46**	**13.45**	**7.74**	***16.46***	***7.17***	**Annual**	**21.51**	**12.60**	**12.62**	***15.58***	***5.14***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.
* - In MSCE-POP model wet deposition on vegetation is not taken into account since it is considered as a part of deposition directly to soil.

Table B.83. *Calculation results: PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	4.19		0.49	0.80	*1.82*	*2.05*	Jan		0.43	0.43	*0.43*	*0.00*
Feb	1.88		0.55	0.93	*1.12*	*0.68*	Feb		0.53	0.53	*0.53*	*0.00*
Mar	1.08		0.62	1.03	*0.91*	*0.25*	Mar		0.60	0.60	*0.60*	*0.00*
Seas_1	**7.15**	**3.48**	**1.66**	**2.76**	***3.76***	***2.38***	**Seas_1**	**3.39**	**1.57**	**1.57**	***2.18***	***1.05***
Apr	0.76		0.61	1.00	*0.79*	*0.20*	Apr		0.59	0.60	*0.59*	*0.00*
May	0.69		0.63	1.03	*0.79*	*0.22*	May		0.62	0.62	*0.62*	*0.00*
Jun	0.64		0.61	1.00	*0.75*	*0.21*	Jun		0.60	0.61	*0.60*	*0.00*
Seas_2	**2.09**	**1.82**	**1.85**	**3.04**	***2.20***	***0.57***	**Seas_2**	**1.79**	**1.81**	**1.82**	***1.81***	***0.02***
Jul	0.65		0.64	1.02	*0.77*	*0.22*	Jul		0.62	0.63	*0.63*	*0.00*
Aug	0.65		0.64	1.02	*0.77*	*0.22*	Aug		0.63	0.63	*0.63*	*0.00*
Sep	0.62		0.62	0.98	*0.74*	*0.21*	Sep		0.61	0.61	*0.61*	*0.00*
Seas_3	**1.92**	**1.34**	**1.89**	**3.02**	***2.04***	***0.70***	**Seas_3**	**1.33**	**1.86**	**1.87**	***1.69***	***0.31***
Oct	0.64		0.64	1.00	*0.76*	*0.21*	Oct		0.63	0.64	*0.63*	*0.01*
Nov	0.62		0.62	0.97	*0.74*	*0.20*	Nov		0.61	0.62	*0.61*	*0.01*
Dec	0.62		0.62	0.96	*0.74*	*0.20*	Dec		0.61	0.62	*0.61*	*0.01*
Seas_4	**1.89**	**3.44**	**1.88**	**2.93**	***2.54***	***0.78***	**Seas_4**	**3.42**	**1.85**	**1.87**	***2.38***	***0.90***
Annual	**13.05**	**10.07**	**7.29**	**11.75**	***10.54***	***2.49***	**Annual**	**9.93**	**7.08**	**7.14**	***8.05***	***1.62***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.
* - In MSCE-POP model wet deposition on vegetation is not taken into account since it is considered as a part of deposition directly to soil.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.84.

Table B.84. *The percentage difference between calculation results on PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_ 2_2	CliMoChem_ 2_3	Simple Box 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan			-22.9%	-44.5%	-44.4%	-48.9%	21.9%
Feb			-42.8%	-42.2%	-42.2%	-45.5%	51.5%
Mar			-52.1%	-42.5%	-42.4%	-45.1%	57.0%
Seas_1	**-37.4%**	**-39.2%**	**-34.9%**	**-43.0%**	**-42.9%**	**-46.4%**	**43.3%**
Apr			-53.0%	-43.1%	-42.9%	-45.2%	58.0%
May			-50.6%	-43.5%	-43.3%	-45.4%	57.5%
Jun			-48.1%	-43.8%	-43.5%	-45.6%	56.6%
Seas_2	**-58.8%**	**-60.6%**	**-50.8%**	**-43.5%**	**-43.2%**	**-45.4%**	**57.3%**
Jul			-46.5%	-44.0%	-43.6%	-45.6%	55.7%
Aug			-45.6%	-44.1%	-43.7%	-45.7%	54.7%
Sep			-45.2%	-44.2%	-43.7%	-45.7%	53.8%
Seas_3	**-72.0%**	**-73.0%**	**-45.8%**	**-44.1%**	**-43.7%**	**-45.7%**	**54.7%**
Oct			-45.0%	-44.3%	-43.8%	-45.8%	52.9%
Nov			-44.9%	-44.4%	-43.8%	-45.8%	52.1%
Dec			-45.0%	-44.4%	-43.8%	-45.8%	51.3%
Seas_4	**-51.2%**	**-52.0%**	**-45.0%**	**-44.4%**	**-43.8%**	**-45.8%**	**52.1%**
Annual	**-53.9%**	**-55.2%**	**-41.2%**	**-43.8%**	**-43.4%**	**-45.8%**	**51.9%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Gaseous exchange

Reference data set. Calculation results on PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.85.

Monthly values of PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.108a and b, respectively. Seasonal variations for models with positive values of gaseous exchange flows between the atmosphere and vegetation calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. B.108c in more detail.

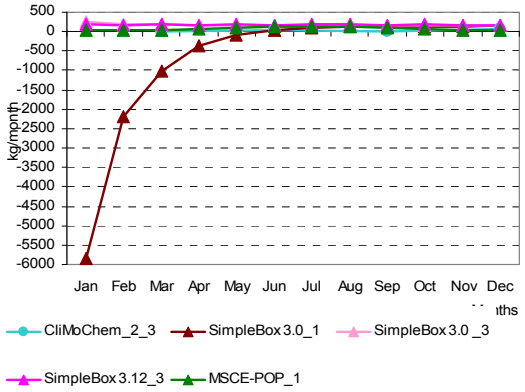


Fig. B.108a. *PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

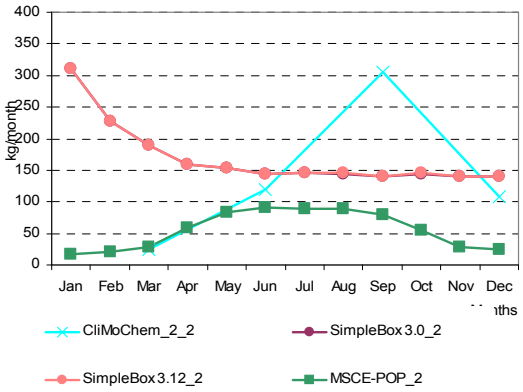


Fig. B.108b. *PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

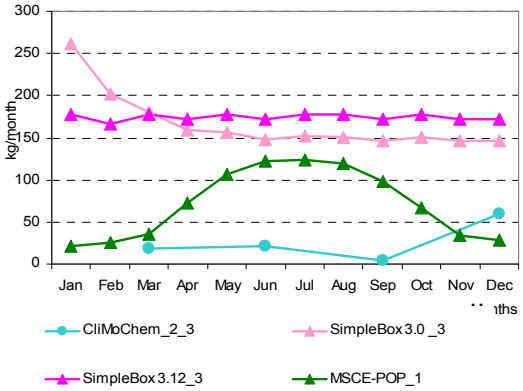


Fig. B.108c. *PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with positive values)*

Own/alternative data set. Calculation results on PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.86.

Monthly values of PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.109a and b, respectively. Seasonal variations for models with positive values of gaseous exchange flows between the atmosphere and vegetation calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions are also shown in Fig. B.109c in more detail.

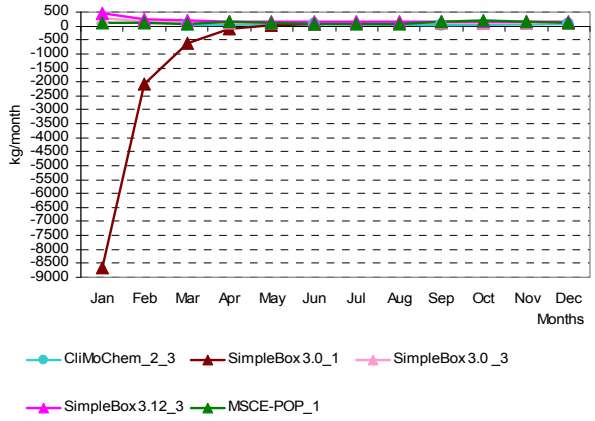


Fig. B.109a. *PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

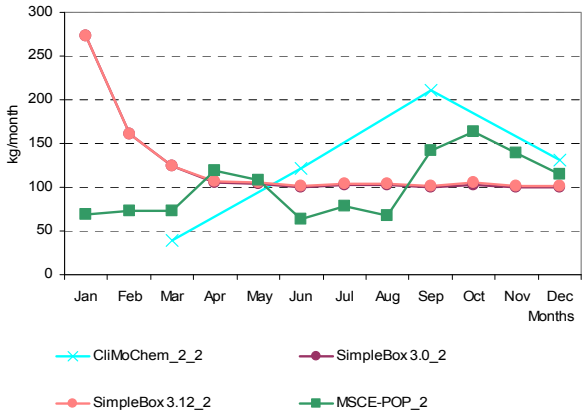


Fig. B.109b. *PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

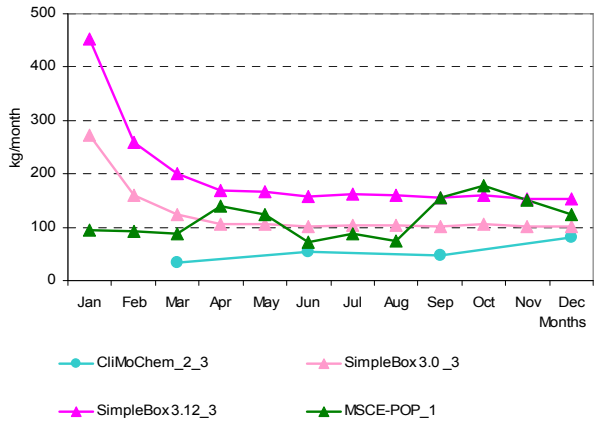


Fig. B.109c. *PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions (models with positive values)*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.87.

Table B.85. *Calculation results: PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-5839.10	20.70		262.24	177.58	*-1344.65*	*2997.98*	Jan		311.58	311.60	18.00	*213.73*	*169.51*
Feb	-2194.25	26.00		202.39	166.12	*-449.94*	*1165.36*	Feb		228.33	228.43	21.50	*159.42*	*119.44*
Mar	-1005.79	35.30		180.67	177.58	*-153.06*	*572.52*	Mar		190.00	190.18	29.10	*136.43*	*92.95*
Seas_1	**-9039.15**	**82.00**	**56.25**	**645.31**	**521.27**	***-1546.86***	***4196.44***	**Seas_1**	**73.98**	**729.91**	**730.20**	**68.60**	***400.67***	***380.35***
Apr	-366.78	72.60		158.63	171.85	*9.07*	*254.40*	Apr		159.29	159.54	57.90	*125.58*	*58.61*
May	-94.47	107.00		156.35	177.58	*86.61*	*124.29*	May		153.16	153.51	84.00	*130.22*	*40.03*
Jun	35.23	122.00		148.08	171.85	*119.29*	*59.62*	Jun		143.27	143.68	90.20	*125.72*	*30.76*
Seas_2	**-426.03**	**301.60**	**62.13**	**463.06**	**521.27**	***184.41***	***384.85***	**Seas_2**	**359.63**	**455.72**	**456.73**	**232.10**	***376.04***	***106.22***
Jul	96.24	123.00		151.57	177.58	*137.10*	*35.19*	Jul		145.89	146.34	89.00	*127.08*	*32.98*
Aug	124.16	120.00		151.02	177.58	*143.19*	*26.73*	Aug		145.01	145.53	89.80	*126.78*	*32.03*
Sep	132.39	98.30		145.99	171.85	*137.13*	*30.63*	Sep		140.11	140.63	79.80	*120.18*	*34.97*
Seas_3	**352.79**	**341.30**	**12.11**	**448.57**	**527.00**	***336.35***	***196.45***	**Seas_3**	**912.97**	**431.01**	**432.50**	**258.60**	***508.77***	***281.56***
Oct	142.62	67.50		150.85	177.58	*134.64*	*47.18*	Oct		144.80	145.39	55.00	*115.06*	*52.02*
Nov	140.68	33.70		146.07	171.85	*123.08*	*61.12*	Nov		140.25	140.88	29.10	*103.41*	*64.35*
Dec	148.92	28.00		146.18	171.85	*123.74*	*64.85*	Dec		140.40	141.10	25.50	*102.33*	*66.54*
Seas_4	**432.23**	**129.20**	**180.21**	**443.10**	**521.27**	***341.20***	***174.61***	**Seas_4**	**321.50**	**425.45**	**427.37**	**109.60**	***320.98***	***149.35***
Annual	**-8680.16**	**854.10**	**310.71**	**2000.04**	**2090.82**	***-684.90***	***4533.14***	**Annual**	**1668.08**	**2042.09**	**2046.80**	**668.90**	***1606.47***	***649.74***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.86. *Calculation results: PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-8650.78	95.70		259.11	453.22	*-1960.69*	*4462.46*	Jan		272.38	272.49	69.40	*204.75*	*117.22*
Feb	-2084.62	91.70		151.73	259.91	*-395.32*	*1128.35*	Feb		160.24	160.63	72.70	*131.19*	*50.66*
Mar	-624.39	87.10		122.44	200.15	*-53.67*	*383.40*	Mar		123.96	124.60	73.40	*107.32*	*29.38*
Seas_1	**-11359.79**	**274.50**	**102.38**	**533.29**	**913.29**	***-1907.27***	***5292.94***	**Seas_1**	**117.16**	**556.58**	**557.72**	**215.50**	***361.74***	***229.18***
Apr	-112.91	140.00		106.34	169.26	*75.67*	*128.32*	Apr		105.48	106.34	119.00	*110.27*	*7.57*
May	36.94	125.00		106.19	166.60	*108.68*	*54.08*	May		104.60	105.59	108.00	*106.06*	*1.75*
Jun	81.35	71.60		101.73	158.13	*103.20*	*38.71*	Jun		99.97	101.09	63.70	*88.25*	*21.27*
Seas_2	**5.38**	**336.60**	**163.07**	**314.26**	**493.99**	***262.66***	***185.58***	**Seas_2**	**365.38**	**310.05**	**313.01**	**290.70**	***319.79***	***31.97***
Jul	98.32	88.60		104.85	161.84	*113.40*	*32.98*	Jul		103.01	104.28	79.00	*95.43*	*14.24*
Aug	102.73	74.60		104.82	160.80	*110.74*	*36.11*	Aug		102.99	104.40	67.00	*91.46*	*21.20*
Sep	100.72	156.00		101.48	154.77	*128.24*	*31.35*	Sep		99.74	101.20	142.00	*114.31*	*23.99*
Seas_3	**301.77**	**319.20**	**142.54**	**311.14**	**477.41**	***310.41***	***118.56***	**Seas_3**	**633.58**	**305.73**	**309.88**	**288.00**	***384.30***	***166.46***
Oct	104.47	178.00		104.91	159.10	*136.62*	*37.67*	Oct		103.13	104.78	163.00	*123.64*	*34.10*
Nov	101.24	150.00		101.59	153.26	*126.52*	*29.02*	Nov		99.87	101.60	139.00	*113.49*	*22.11*
Dec	101.33	123.00		101.65	152.58	*119.64*	*24.19*	Dec		99.96	101.80	115.00	*105.59*	*8.21*
Seas_4	**307.04**	**451.00**	**244.67**	**308.15**	**464.94**	***355.16***	***97.43***	**Seas_4**	**393.29**	**302.97**	**308.17**	**417.00**	***355.36***	***58.34***
Annual	**-10745.60**	**1381.30**	**652.66**	**1466.84**	**2349.64**	***-979.03***	***5492.76***	**Annual**	**1509.41**	**1475.33**	**1488.79**	**1211.20**	***1421.18***	***140.69***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table B.87. *Comparison of the calculation results on PCB-28 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0_3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-5839.10	-8650.78	311.58	272.38	311.60	272.49	262.24	259.11	177.58	453.22	20.70	95.70	18.00	69.40		
Feb			-2194.25	-2084.62	228.33	160.24	228.43	160.63	202.39	151.73	166.12	259.91	26.00	91.70	21.50	72.70		
Mar			-1005.79	-624.39	190.00	123.96	190.18	124.60	180.67	122.44	177.58	200.15	35.30	87.10	29.10	73.40		
Seas_1	**56.25**	**102.38**	**-9039.15**	**-11359.79**	**729.91**	**556.58**	**730.20**	**557.72**	**645.31**	**533.29**	**521.27**	**913.29**	**82.00**	**274.50**	**68.60**	**215.50**	**73.98**	**117.16**
Apr			-366.78	-112.91	159.29	105.48	159.54	106.34	158.63	106.34	171.85	169.26	72.60	140.00	57.90	119.00		
May			-94.47	36.94	153.16	104.60	153.51	105.59	156.35	106.19	177.58	166.60	107.00	125.00	84.00	108.00		
Jun			35.23	81.35	143.27	99.97	143.68	101.09	148.08	101.73	171.85	158.13	122.00	71.60	90.20	63.70		
Seas_2	**62.13**	**163.07**	**-426.03**	**5.38**	**455.72**	**310.05**	**456.73**	**313.01**	**463.06**	**314.26**	**521.27**	**493.99**	**301.60**	**336.60**	**232.10**	**290.70**	**359.63**	**365.38**
Jul			96.24	98.32	145.89	103.01	146.34	104.28	151.57	104.85	177.58	161.84	123.00	88.60	89.00	79.00		
Aug			124.16	102.73	145.01	102.99	145.53	104.40	151.02	104.82	177.58	160.80	120.00	74.60	89.80	67.00		
Sep			132.39	100.72	140.11	99.74	140.63	101.20	145.99	101.48	171.85	154.77	98.30	156.00	79.80	142.00		
Seas_3	**12.11**	**142.54**	**352.79**	**301.77**	**431.01**	**305.73**	**432.50**	**309.88**	**448.57**	**311.14**	**527.00**	**477.41**	**341.30**	**319.20**	**258.60**	**288.00**	**912.97**	**633.58**
Oct			142.62	104.47	144.80	103.13	145.39	104.78	150.85	104.91	177.58	159.10	67.50	178.00	55.00	163.00		
Nov			140.68	101.24	140.25	99.87	140.88	101.60	146.07	101.59	171.85	153.26	33.70	150.00	29.10	139.00		
Dec			148.92	101.33	140.40	99.96	141.10	101.80	146.18	101.65	171.85	152.58	28.00	123.00	25.50	115.00		
Seas_4	**180.21**	**244.67**	**432.23**	**307.04**	**425.45**	**302.97**	**427.37**	**308.17**	**443.10**	**308.15**	**521.27**	**464.94**	**129.20**	**451.00**	**109.60**	**417.00**	**321.50**	**393.29**
Annual	**310.71**	**652.66**	**-8680.16**	**-10745.60**	**2042.09**	**1475.33**	**2046.80**	**1488.79**	**2000.04**	**1466.84**	**2090.82**	**2349.64**	**854.10**	**1381.30**	**668.90**	**1211.20**	**1668.08**	**1509.41**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Net mass flows between the atmosphere and vegetation

Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-28 net mass flows between the atmosphere and vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.88.

Monthly values of PCB-28 net mass flows between the atmosphere and vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.110 a and b, respectively. Seasonal variations for models with low positive values of net mass flows between the atmosphere and vegetation calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. B.110c in more detail.

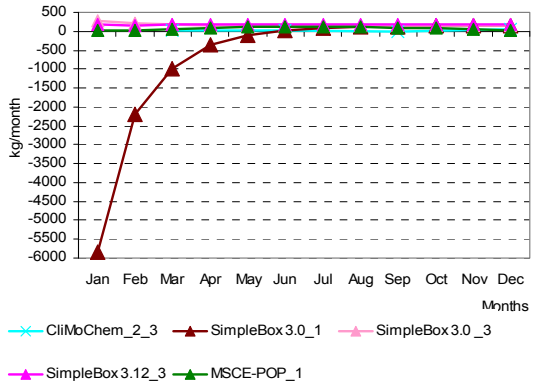


Fig. B.110a. *PCB-28 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

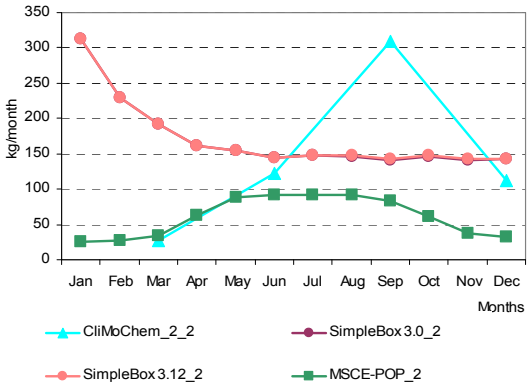


Fig. B.110b. *PCB-28 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

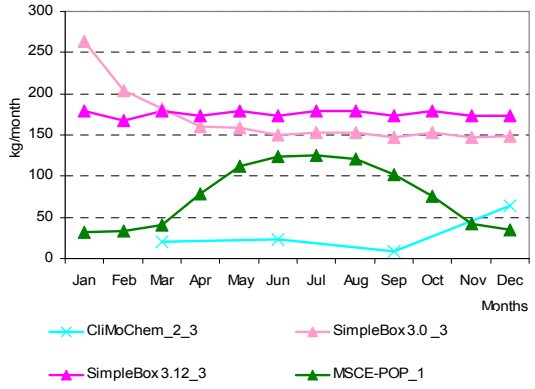


Fig. B.110c. *PCB-28 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Table B.88. *Calculation results: PCB-28 net mass flows between the atmosphere and vegetation (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-5831.23	31.80		263.62	178.53	*-1339.32*	*2996.14*	Jan		312.72	312.73	24.99	*216.81*	*166.12*
Feb	-2189.49	33.96		203.87	167.01	*-446.16*	*1164.50*	Feb		229.66	229.77	27.75	*162.39*	*116.60*
Mar	-1002.52	41.34		182.31	178.53	*-150.09*	*572.06*	Mar		191.52	191.70	33.91	*139.04*	*91.05*
Seas_1	**-9023.23**	**107.10**	**63.29**	**649.80**	**524.07**	***-1535.80***	***4193.38***	**Seas_1**	**80.64**	**733.90**	**734.20**	**86.65**	***408.84***	***375.52***
Apr	-364.44	78.59		160.23	172.77	*11.79*	*254.27*	Apr		160.80	161.06	62.85	*128.24*	*56.63*
May	-92.45	111.54		158.03	178.53	*88.91*	*124.11*	May		154.75	155.10	87.71	*132.52*	*38.81*
Jun	37.02	124.05		149.72	172.77	*120.89*	*59.35*	Jun		144.83	145.23	91.87	*127.31*	*30.69*
Seas_2	**-419.88**	**314.18**	**70.87**	**467.98**	**524.07**	***191.45***	***384.20***	**Seas_2**	**367.88**	**460.38**	**461.39**	**242.43**	***383.02***	***103.47***
Jul	98.01	125.26		153.26	178.53	*138.77*	*34.81*	Jul		147.51	147.95	90.94	*128.80*	*32.79*
Aug	125.88	121.47		152.72	178.53	*144.65*	*26.47*	Aug		146.64	147.16	91.05	*128.28*	*32.25*
Sep	134.04	102.09		147.64	172.77	*139.13*	*29.45*	Sep		141.69	142.21	83.07	*122.32*	*34.00*
Seas_3	**357.93**	**348.82**	**24.92**	**453.62**	**529.83**	***343.03***	***192.73***	**Seas_3**	**925.18**	**435.83**	**437.33**	**265.06**	***515.85***	***284.61***
Oct	144.32	75.24		152.57	178.53	*137.66*	*44.10*	Oct		146.43	147.03	61.82	*118.43*	*49.02*
Nov	142.32	42.94		147.73	172.77	*126.44*	*57.23*	Nov		141.83	142.47	37.38	*107.23*	*60.49*
Dec	150.56	34.79		147.84	172.77	*126.49*	*62.15*	Dec		141.99	142.69	31.64	*105.44*	*63.92*
Seas_4	**437.21**	**152.97**	**193.70**	**448.14**	**524.07**	***351.22***	***166.42***	**Seas_4**	**334.70**	**430.26**	**432.20**	**130.84**	***332.00***	***141.62***
Annual	**-8647.97**	**923.07**	**352.78**	**2019.54**	**2102.04**	***-650.11***	***4531.77***	**Annual**	**1708.40**	**2060.36**	**2065.11**	**724.98**	***1639.71***	***632.29***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

B.5. Concentrations at each interface

B.5.1. Comparison of calculated values of PCB-28 concentration in the atmosphere at its interface with soil

Reference data set. Calculation results on PCB-28 concentration in the atmosphere at its interface with soil calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.90.

Monthly values of PCB-28 concentration in the atmosphere at its interface with soil calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.111 a and b, respectively.

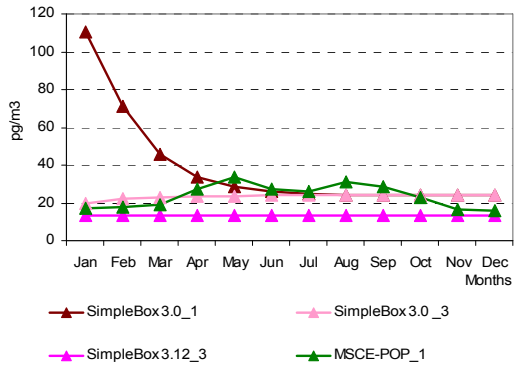


Fig. B.111a. *PCB-28 concentration in the atmosphere at its interface with soil (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

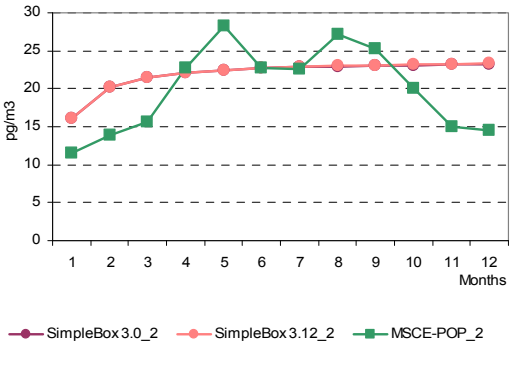


Fig. B.111b. *PCB-28 concentration in the atmosphere at its interface with soil (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 concentration in the atmosphere at its interface with soil calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.91.

Monthly values of PCB-28 concentration in the atmosphere at its interface with soil calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.112 a and b, respectively.

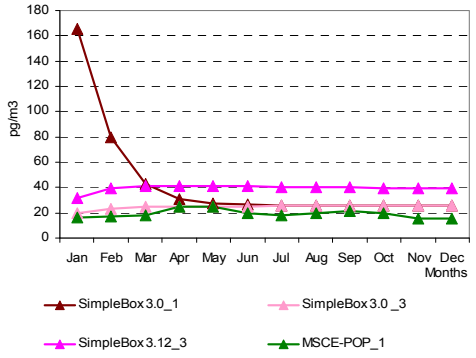


Fig. B.112a. *PCB-28 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

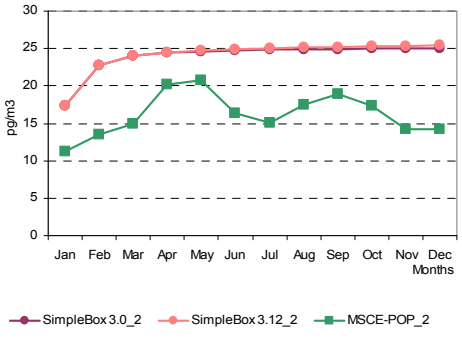


Fig. B.112b. *PCB-28 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.90. *Calculation results: PCB-28 concentration in the atmosphere at interface with soil (pg/m3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1	MSCE-POP_1	SimpleBox 3.0_3	SimpleBox 3.12_3				SimpleBox 3.0_2	SimpleBox 3.12_2	MSCE-POP_2		
Jan	110.38	17.20	19.54	13.50	*40.16*	*46.88*	Jan	16.07	16.08	11.60	*14.58*	*2.58*
Feb	71.40	17.70	22.27	13.50	*31.22*	*27.03*	Feb	20.27	20.27	13.90	*18.15*	*3.68*
Mar	45.87	19.10	23.08	13.50	*25.39*	*14.21*	Mar	21.48	21.49	15.60	*19.52*	*3.40*
Apr	33.94	27.60	23.50	13.50	*24.64*	*8.58*	Apr	22.11	22.13	22.80	*22.35*	*0.39*
May	28.53	33.50	23.74	13.50	*24.82*	*8.53*	May	22.47	22.49	28.20	*24.39*	*3.30*
Jun	26.04	27.00	23.89	13.50	*22.61*	*6.21*	Jun	22.68	22.72	22.80	*22.73*	*0.06*
Jul	24.89	26.20	23.99	13.50	*22.15*	*5.83*	Jul	22.83	22.87	22.60	*22.77*	*0.15*
Aug	24.35	31.20	24.07	13.50	*23.28*	*7.31*	Aug	22.94	23.00	27.10	*24.34*	*2.39*
Sep	24.10	28.50	24.13	13.50	*22.56*	*6.38*	Sep	23.03	23.09	25.30	*23.81*	*1.29*
Oct	23.99	22.60	24.18	13.50	*21.07*	*5.09*	Oct	23.11	23.18	20.10	*22.13*	*1.76*
Nov	23.93	16.80	24.23	13.50	*19.62*	*5.33*	Nov	23.17	23.25	15.00	*20.47*	*4.74*
Dec	23.96	16.10	24.27	13.50	*19.46*	*5.48*	Dec	23.23	23.32	14.60	*20.38*	*5.01*
Annual	**38.45**	**25.06**	**23.41**	**13.50**	***25.11***	***10.26***	**Annual**	**21.95**	**21.99**	**21.00**	***21.65***	***0.56***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table B.91. *Calculation results: PCB-28 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	165.23	16.30	19.41	31.78	*58.18*	*71.68*	Jan	17.34	17.34	11.20	*15.29*	*3.55*
Feb	79.33	17.30	23.57	39.42	*39.90*	*27.88*	Feb	22.72	22.75	13.50	*19.66*	*5.33*
Mar	42.68	18.40	24.60	40.85	*31.63*	*11.99*	Mar	23.96	24.02	15.00	*20.99*	*5.19*
Apr	31.01	24.50	24.99	41.10	*30.40*	*7.72*	Apr	24.43	24.52	20.20	*23.05*	*2.47*
May	27.43	24.60	25.17	40.98	*29.54*	*7.72*	May	24.63	24.76	20.70	*23.36*	*2.31*
Jun	26.28	19.40	25.26	40.75	*27.92*	*9.07*	Jun	24.75	24.92	16.40	*22.02*	*4.87*
Jul	25.89	17.60	25.33	40.51	*27.33*	*9.56*	Jul	24.83	25.03	15.10	*21.65*	*5.68*
Aug	25.74	20.10	25.39	40.26	*27.87*	*8.65*	Aug	24.90	25.13	17.50	*22.51*	*4.34*
Sep	25.67	21.30	25.43	40.02	*28.11*	*8.19*	Sep	24.95	25.22	18.90	*23.02*	*3.57*
Oct	25.63	19.50	25.47	39.80	*27.60*	*8.62*	Oct	25.00	25.30	17.40	*22.57*	*4.48*
Nov	25.61	15.80	25.50	39.58	*26.62*	*9.79*	Nov	25.04	25.37	14.20	*21.54*	*6.36*
Dec	25.59	15.60	25.53	39.38	*26.52*	*9.77*	Dec	25.07	25.44	14.20	*21.57*	*6.39*
Annual	**43.84**	**19.90**	**24.64**	**39.54**	***31.98***	***11.51***	**Annual**	**23.97**	**24.15**	**16.59**	***21.57***	***4.31***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.92.

Table B.92. *The percentage difference between calculation results on PCB-28 concentration in the atmosphere at its interface with soil obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	49.7%	7.9%	7.9%	-0.7%	135.3%	-5.2%	-3.4%
Feb	11.1%	12.1%	12.2%	5.8%	192.0%	-2.3%	-2.9%
Mar	-7.0%	11.6%	11.8%	6.6%	202.5%	-3.7%	-3.8%
Apr	-8.6%	10.4%	10.8%	6.3%	204.4%	-11.2%	-11.4%
May	-3.9%	9.6%	10.1%	6.0%	203.5%	-26.6%	-26.6%
Jun	0.9%	9.1%	9.7%	5.7%	201.8%	-28.1%	-28.1%
Jul	4.0%	8.8%	9.4%	5.6%	200.0%	-32.8%	-33.2%
Aug	5.7%	8.5%	9.3%	5.5%	198.2%	-35.6%	-35.4%
Sep	6.5%	8.3%	9.2%	5.4%	196.4%	-25.3%	-25.3%
Oct	6.9%	8.2%	9.2%	5.3%	194.7%	-13.7%	-13.4%
Nov	7.0%	8.1%	9.1%	5.2%	193.1%	-6.0%	-5.3%
Dec	6.8%	7.9%	9.1%	5.2%	191.6%	-3.1%	-2.7%
Annual	**14.0%**	**9.2%**	**9.8%**	**5.2%**	**192.8%**	**-20.6%**	**-21.0%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.5.2. Comparison of calculated values of PCB-28 concentration in the atmosphere at its interface with ocean

Reference data set. Calculation results on PCB-28 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.93.

Monthly values of PCB-28 concentration in the atmosphere at its interface with ocean calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.113 a and b, respectively.

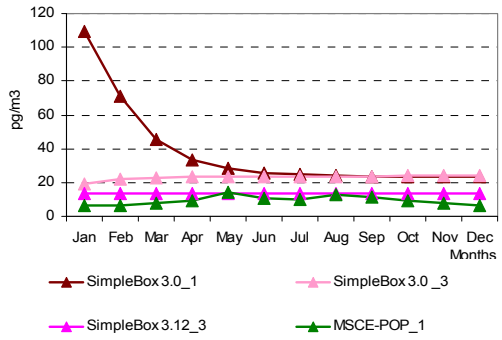


Fig. B.113a. *PCB-28 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

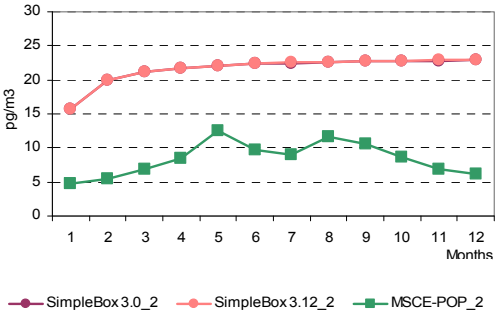


Fig. B.113b. *PCB-28 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 concentration in the atmosphere at its interface with ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.94.

Monthly values of PCB-28 concentration in the atmosphere at its interface with ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.114 a and b, respectively.

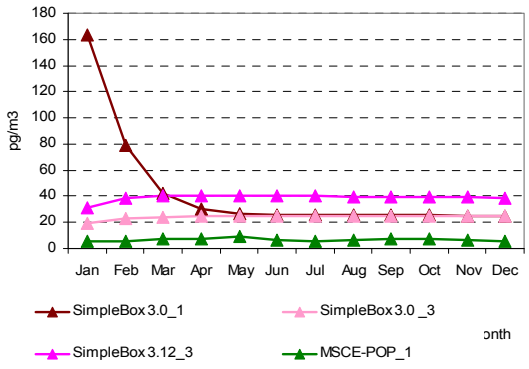


Fig. B.114a. *PCB-28 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

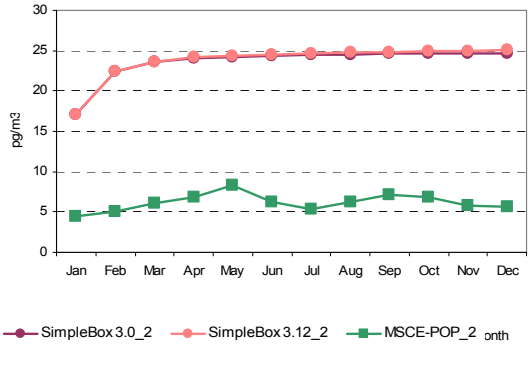


Fig. B.114b. *PCB-28 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.93. *Calculation results: PCB-28 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	109.39	6.04	19.21	13.28	*36.98*	*48.57*	Jan	15.78	15.78	4.68	*12.08*	*6.41*
Feb	70.79	6.39	21.92	13.28	*28.09*	*29.17*	Feb	19.93	19.94	5.50	*15.12*	*8.33*
Mar	45.43	7.79	22.72	13.28	*22.30*	*16.61*	Mar	21.13	21.15	6.89	*16.39*	*8.23*
Apr	33.56	9.58	23.15	13.28	*19.89*	*10.76*	Apr	21.77	21.79	8.41	*17.32*	*7.72*
May	28.17	14.10	23.39	13.28	*19.73*	*7.26*	May	22.12	22.15	12.60	*18.95*	*5.50*
Jun	25.69	10.80	23.53	13.28	*18.32*	*7.38*	Jun	22.33	22.37	9.68	*18.13*	*7.32*
Jul	24.54	10.10	23.63	13.28	*17.89*	*7.29*	Jul	22.48	22.53	9.00	*18.00*	*7.80*
Aug	24.00	12.90	23.71	13.28	*18.47*	*6.22*	Aug	22.59	22.65	11.60	*18.95*	*6.36*
Sep	23.75	11.60	23.77	13.28	*18.10*	*6.57*	Sep	22.68	22.74	10.60	*18.67*	*6.99*
Oct	23.64	9.43	23.83	13.28	*17.54*	*7.32*	Oct	22.76	22.83	8.61	*18.06*	*8.19*
Nov	23.58	7.48	23.87	13.28	*17.05*	*8.06*	Nov	22.82	22.90	6.85	*17.53*	*9.24*
Dec	23.61	6.56	23.91	13.28	*16.84*	*8.45*	Dec	22.88	22.97	6.14	*17.33*	*9.69*
Annual	**38.01**	**9.87**	**23.06**	**13.28**	***21.05***	***12.61***	**Annual**	**21.61**	**21.65**	**8.76**	***17.34***	***7.43***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table B.94. *Calculation results: PCB-28 concentration in the atmosphere at its interface with ocean (pg/m3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	163.92	5.62	19.08	31.40	*55.01*	*73.37*	Jan	17.03	17.04	4.39	*12.82*	*7.30*
Feb	78.74	5.87	23.21	39.00	*36.70*	*31.12*	Feb	22.37	22.40	5.08	*16.62*	*9.99*
Mar	42.27	6.91	24.24	40.42	*28.46*	*16.49*	Mar	23.60	23.66	6.13	*17.80*	*10.11*
Apr	30.64	7.72	24.63	40.67	*25.92*	*13.82*	Apr	24.07	24.16	6.79	*18.34*	*10.00*
May	27.06	9.32	24.80	40.55	*25.43*	*12.80*	May	24.27	24.40	8.39	*19.02*	*9.21*
Jun	25.92	6.87	24.90	40.33	*24.50*	*13.70*	Jun	24.39	24.56	6.23	*18.39*	*10.53*
Jul	25.53	5.90	24.97	40.08	*24.12*	*14.02*	Jul	24.47	24.67	5.36	*18.17*	*11.09*
Aug	25.38	6.84	25.02	39.83	*24.27*	*13.51*	Aug	24.54	24.77	6.29	*18.53*	*10.60*
Sep	25.31	7.69	25.07	39.60	*24.42*	*13.06*	Sep	24.59	24.86	7.11	*18.85*	*10.17*
Oct	25.27	7.39	25.11	39.37	*24.28*	*13.10*	Oct	24.64	24.94	6.79	*18.79*	*10.39*
Nov	25.25	6.34	25.14	39.16	*23.97*	*13.47*	Nov	24.68	25.01	5.83	*18.51*	*10.98*
Dec	25.23	5.96	25.17	38.96	*23.83*	*13.56*	Dec	24.71	25.08	5.60	*18.46*	*11.14*
Annual	**43.37**	**7.01**	**24.28**	**39.11**	***28.45***	***16.47***	**Annual**	**23.61**	**23.80**	**6.26**	***17.89***	***10.08***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.95.

Table B.95. *The percentage difference between calculation results on PCB-28 concentration in the atmosphere at its interface with ocean obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	49.8%	7.9%	8.0%	-0.7%	136.5%	-7.0%	-6.2%
Feb	11.2%	12.2%	12.4%	5.9%	193.8%	-8.1%	-7.6%
Mar	-7.0%	11.7%	11.9%	6.7%	204.5%	-11.3%	-11.0%
Apr	-8.7%	10.6%	10.9%	6.4%	206.4%	-19.4%	-19.3%
May	-3.9%	9.7%	10.2%	6.1%	205.4%	-33.9%	-33.4%
Jun	0.9%	9.2%	9.8%	5.8%	203.8%	-36.4%	-35.6%
Jul	4.0%	8.9%	9.5%	5.6%	201.9%	-41.6%	-40.4%
Aug	5.7%	8.6%	9.4%	5.5%	200.1%	-47.0%	-45.8%
Sep	6.6%	8.4%	9.3%	5.4%	198.3%	-33.7%	-32.9%
Oct	6.9%	8.3%	9.3%	5.4%	196.6%	-21.6%	-21.1%
Nov	7.1%	8.1%	9.2%	5.3%	195.0%	-15.2%	-14.9%
Dec	6.9%	8.0%	9.2%	5.2%	193.5%	-9.1%	-8.8%
Annual	14.1%	9.3%	9.9%	5.3%	194.6%	-29.0%	-28.6%

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.5.3. Comparison of calculated values of PCB-28 concentration in the atmosphere at its interface with vegetation

Reference data set. Calculation results on PCB-28 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.96.

Monthly values of PCB-28 concentration in the atmosphere at its interface with vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.115 a and b, respectively.

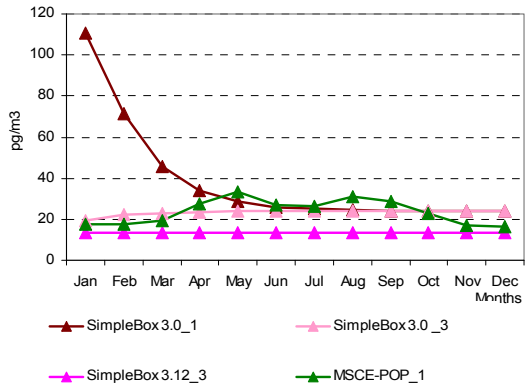


Fig. 3.115a. *PCB-28 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

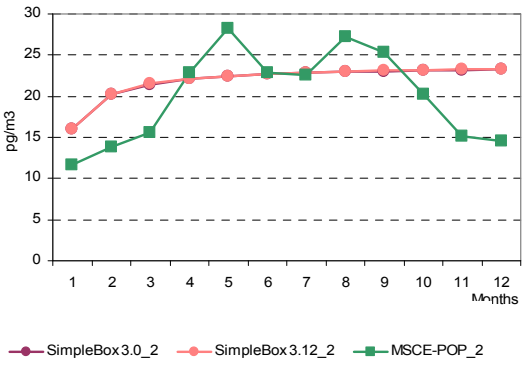


Fig. 3.115b. *PCB-28 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 concentration in the atmosphere at its interface with vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.97.

Monthly values of PCB-28 concentration in the atmosphere at its interface with vegetation calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.116 a and b, respectively.

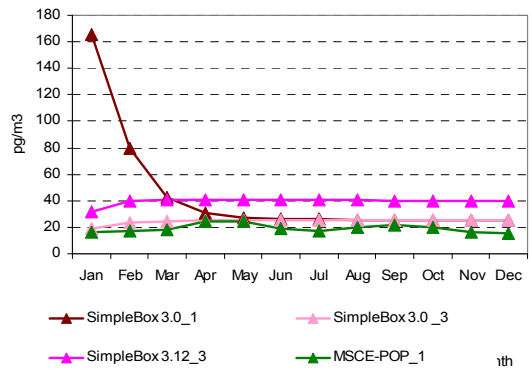


Fig. B.116a. *PCB-28 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

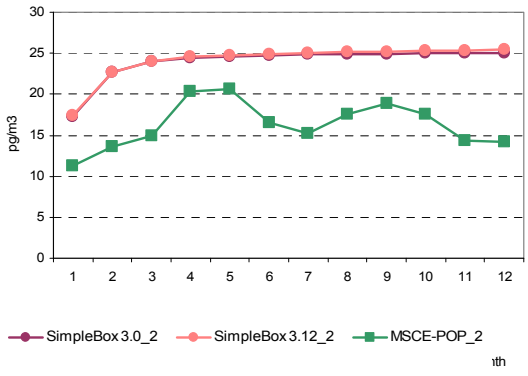


Fig. B.116b. *PCB-28 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.96. *Calculation results: PCB-28 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE- POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	110.38	17.30	19.54	13.50	*40.18*	*46.86*	Jan	16.07	16.08	11.60	*14.58*	*2.58*
Feb	71.40	17.80	22.27	13.50	*31.24*	*27.01*	Feb	20.27	20.27	13.90	*18.15*	*3.68*
Mar	45.87	19.10	23.08	13.50	*25.39*	*14.21*	Mar	21.48	21.49	15.60	*19.52*	*3.40*
Apr	33.94	27.70	23.50	13.50	*24.66*	*8.59*	Apr	22.11	22.13	22.90	*22.38*	*0.45*
May	28.53	33.60	23.74	13.50	*24.84*	*8.57*	May	22.47	22.49	28.20	*24.39*	*3.30*
Jun	26.04	27.00	23.89	13.50	*22.61*	*6.21*	Jun	22.68	22.72	22.80	*22.73*	*0.06*
Jul	24.89	26.30	23.99	13.50	*22.17*	*5.86*	Jul	22.83	22.87	22.60	*22.77*	*0.15*
Aug	24.35	31.30	24.07	13.50	*23.31*	*7.34*	Aug	22.94	23.00	27.20	*24.38*	*2.44*
Sep	24.10	28.60	24.13	13.50	*22.58*	*6.41*	Sep	23.03	23.09	25.40	*23.84*	*1.35*
Oct	23.99	22.70	24.18	13.50	*21.09*	*5.10*	Oct	23.11	23.18	20.20	*22.16*	*1.70*
Nov	23.93	16.90	24.23	13.50	*19.64*	*5.31*	Nov	23.17	23.25	15.10	*20.51*	*4.68*
Dec	23.96	16.20	24.27	13.50	*19.48*	*5.46*	Dec	23.23	23.32	14.60	*20.38*	*5.01*
Annual	**38.45**	**25.14**	**23.41**	**13.50**	***25.13***	***10.26***	**Annual**	**21.95**	**21.99**	**21.04**	***21.66***	***0.54***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table B.97. *Calculation results: PCB-28 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	165.23	16.30	19.41	31.78	*58.18*	*71.68*	Jan	17.34	17.34	11.20	*15.29*	*3.55*
Feb	79.33	17.40	23.57	39.42	*39.93*	*27.86*	Feb	22.72	22.75	13.60	*19.69*	*5.28*
Mar	42.68	18.40	24.60	40.85	*31.63*	*11.99*	Mar	23.96	24.02	15.00	*20.99*	*5.19*
Apr	31.01	24.60	24.99	41.10	*30.43*	*7.70*	Apr	24.43	24.52	20.30	*23.08*	*2.41*
May	27.43	24.70	25.17	40.98	*29.57*	*7.70*	May	24.63	24.76	20.70	*23.36*	*2.31*
Jun	26.28	19.40	25.26	40.75	*27.92*	*9.07*	Jun	24.75	24.92	16.50	*22.05*	*4.81*
Jul	25.89	17.60	25.33	40.51	*27.33*	*9.56*	Jul	24.83	25.03	15.20	*21.69*	*5.62*
Aug	25.74	20.20	25.39	40.26	*27.90*	*8.62*	Aug	24.90	25.13	17.50	*22.51*	*4.34*
Sep	25.67	21.30	25.43	40.02	*28.11*	*8.19*	Sep	24.95	25.22	18.90	*23.02*	*3.57*
Oct	25.63	19.60	25.47	39.80	*27.62*	*8.59*	Oct	25.00	25.30	17.50	*22.60*	*4.42*
Nov	25.61	15.90	25.50	39.58	*26.65*	*9.75*	Nov	25.04	25.37	14.30	*21.57*	*6.30*
Dec	25.59	15.60	25.53	39.38	*26.52*	*9.77*	Dec	25.07	25.44	14.20	*21.57*	*6.39*
Annual	**43.84**	**19.95**	**24.64**	**39.54**	***31.99***	***11.49***	**Annual**	**23.97**	**24.15**	**16.64**	***21.59***	***4.28***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.98.

Table B.98. *The percentage difference between calculation results on PCB-28 concentration in the atmosphere at interface with vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	49.7%	7.9%	7.9%	-0.7%	135.3%	-5.8%	-3.4%
Feb	11.1%	12.1%	12.2%	5.8%	192.0%	-2.2%	-2.2%
Mar	-7.0%	11.6%	11.8%	6.6%	202.5%	-3.7%	-3.8%
Apr	-8.6%	10.4%	10.8%	6.3%	204.4%	-11.2%	-11.4%
May	-3.9%	9.6%	10.1%	6.0%	203.5%	-26.5%	-26.6%
Jun	0.9%	9.1%	9.7%	5.7%	201.8%	-28.1%	-27.6%
Jul	4.0%	8.8%	9.4%	5.6%	200.0%	-33.1%	-32.7%
Aug	5.7%	8.5%	9.3%	5.5%	198.2%	-35.5%	-35.7%
Sep	6.5%	8.3%	9.2%	5.4%	196.4%	-25.5%	-25.6%
Oct	6.9%	8.2%	9.2%	5.3%	194.7%	-13.7%	-13.4%
Nov	7.0%	8.1%	9.1%	5.2%	193.1%	-5.9%	-5.3%
Dec	6.8%	7.9%	9.1%	5.2%	191.6%	-3.7%	-2.7%
Annual	14.0%	9.2%	9.8%	5.2%	192.8%	-20.6%	-20.9%

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.5.4. Comparison of calculated values of PCB-28 concentration in surface ocean layer

Reference data set. Calculation results on PCB-28 concentration in surface ocean layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.99.

Monthly values of PCB-28 concentration in surface ocean layer calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.117 a and b, respectively.

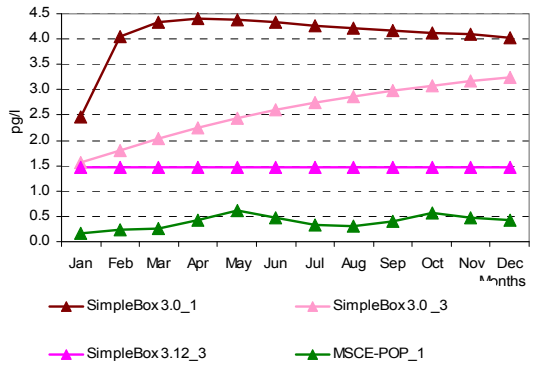


Fig. B.117a. *PCB-28 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

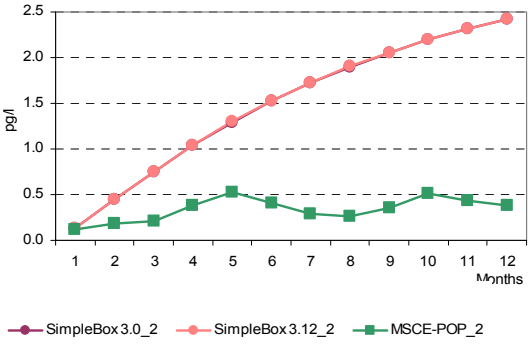


Fig. B.117b. *PCB-28 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 concentration in surface ocean layer calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.100.

Monthly values of PCB-28 concentration in surface ocean layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.118 a and b, respectively.

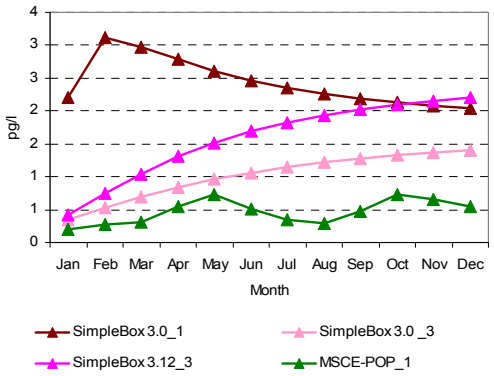


Fig. B.118a. *PCB-28 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

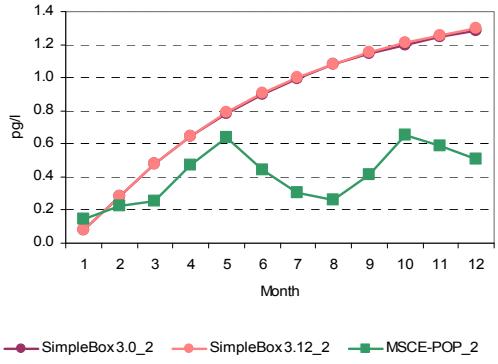


Fig. B.118b. *PCB-28 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.99. *Calculation results: PCB-28 concentration in surface ocean layer (pg/l) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.46	0.17	1.56	1.46	*1.41*	*0.94*	Jan	0.13	0.13	0.12	*0.13*	*0.00*
Feb	4.06	0.23	1.80	1.46	*1.89*	*1.60*	Feb	0.44	0.44	0.19	*0.36*	*0.15*
Mar	4.34	0.25	2.03	1.46	*2.02*	*1.71*	Mar	0.75	0.75	0.21	*0.57*	*0.31*
Apr	4.40	0.44	2.24	1.46	*2.14*	*1.68*	Apr	1.04	1.04	0.38	*0.82*	*0.38*
May	4.38	0.61	2.43	1.46	*2.22*	*1.62*	May	1.30	1.30	0.53	*1.04*	*0.44*
Jun	4.33	0.47	2.60	1.46	*2.21*	*1.66*	Jun	1.52	1.52	0.40	*1.15*	*0.65*
Jul	4.27	0.33	2.75	1.46	*2.20*	*1.69*	Jul	1.72	1.72	0.29	*1.25*	*0.83*
Aug	4.21	0.31	2.88	1.46	*2.21*	*1.70*	Aug	1.90	1.90	0.27	*1.36*	*0.94*
Sep	4.17	0.40	2.99	1.46	*2.26*	*1.66*	Sep	2.06	2.06	0.36	*1.49*	*0.98*
Oct	4.13	0.57	3.09	1.46	*2.31*	*1.60*	Oct	2.19	2.20	0.52	*1.63*	*0.97*
Nov	4.10	0.48	3.18	1.46	*2.31*	*1.64*	Nov	2.31	2.32	0.43	*1.69*	*1.09*
Dec	4.02	0.42	3.26	1.46	*2.29*	*1.64*	Dec	2.42	2.43	0.38	*1.74*	*1.18*
Annual	**4.07**	**0.38**	**2.57**	**1.46**	***2.12***	***1.58***	**Annual**	**1.48**	**1.48**	**0.33**	***1.10***	***0.67***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table B.100. *Calculation results: PCB-28 concentration in surface ocean layer (pg/l) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.20	0.21	0.35	0.42	*0.79*	*0.94*	Jan	0.08	0.08	0.15	*0.10*	*0.04*
Feb	3.12	0.28	0.53	0.74	*1.17*	*1.32*	Feb	0.29	0.29	0.23	*0.27*	*0.03*
Mar	2.98	0.30	0.70	1.05	*1.26*	*1.19*	Mar	0.48	0.48	0.26	*0.40*	*0.13*
Apr	2.79	0.54	0.84	1.31	*1.37*	*1.00*	Apr	0.65	0.65	0.47	*0.59*	*0.10*
May	2.61	0.73	0.96	1.52	*1.46*	*0.84*	May	0.79	0.79	0.64	*0.74*	*0.08*
Jun	2.47	0.51	1.06	1.69	*1.43*	*0.84*	Jun	0.90	0.90	0.44	*0.75*	*0.27*
Jul	2.35	0.35	1.15	1.83	*1.42*	*0.87*	Jul	1.00	1.00	0.31	*0.77*	*0.40*
Aug	2.26	0.30	1.22	1.94	*1.43*	*0.87*	Aug	1.08	1.08	0.26	*0.81*	*0.47*
Sep	2.18	0.47	1.28	2.03	*1.49*	*0.79*	Sep	1.14	1.15	0.42	*0.90*	*0.42*
Oct	2.13	0.72	1.32	2.10	*1.57*	*0.67*	Oct	1.20	1.21	0.65	*1.02*	*0.32*
Nov	2.08	0.65	1.36	2.16	*1.56*	*0.71*	Nov	1.25	1.26	0.59	*1.03*	*0.38*
Dec	2.05	0.55	1.40	2.20	*1.55*	*0.75*	Dec	1.29	1.30	0.51	*1.03*	*0.45*
Annual	**2.43**	**0.44**	**1.02**	**1.58**	***1.37***	***0.85***	**Annual**	**0.84**	**0.85**	**0.38**	***0.69***	***0.27***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.101.

Table B.101. *The percentage difference between calculation results on PCB-28 concentration in surface ocean layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-10.4%	-36.0%	-36.0%	-77.5%	-71.6%	19.2%	20.3%
Feb	-23.1%	-35.6%	-35.5%	-70.5%	-49.1%	20.0%	20.2%
Mar	-31.4%	-36.5%	-36.4%	-65.6%	-28.4%	20.8%	21.8%
Apr	-36.6%	-37.9%	-37.8%	-62.4%	-10.6%	23.8%	24.5%
May	-40.3%	-39.4%	-39.3%	-60.4%	3.8%	20.3%	21.2%
Jun	-42.9%	-40.8%	-40.6%	-59.0%	15.5%	9.2%	9.7%
Jul	-44.9%	-42.1%	-41.9%	-58.2%	24.9%	4.8%	5.1%
Aug	-46.4%	-43.3%	-43.0%	-57.7%	32.5%	-3.6%	-3.3%
Sep	-47.6%	-44.3%	-44.0%	-57.3%	38.6%	16.0%	17.1%
Oct	-48.6%	-45.3%	-44.9%	-57.2%	43.5%	26.1%	27.0%
Nov	-49.3%	-46.1%	-45.8%	-57.1%	47.4%	35.0%	36.0%
Dec	-49.1%	-46.9%	-46.5%	-57.1%	50.5%	31.8%	32.6%
Annual	**-40.2%**	**-43.1%**	**-42.8%**	**-60.5%**	**8.1%**	**16.4%**	**17.1%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.5.5. Comparison of calculated values of PCB-28 concentration in vegetation

Reference data set. Calculation results on PCB-28 concentration in vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.102.

Monthly values of PCB-28 concentration in vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.119 a and b, respectively.

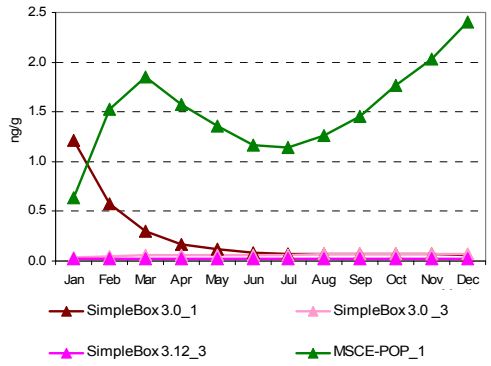


Fig. B.119a. *PCB-28 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

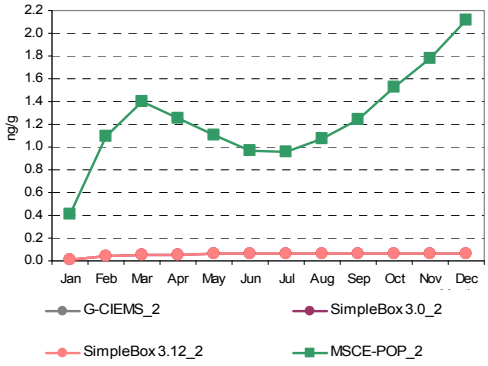


Fig. B.119b. *PCB-28 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 concentration in vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.103.

Monthly values of PCB-28 concentration in vegetation calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.121 a and b, respectively.

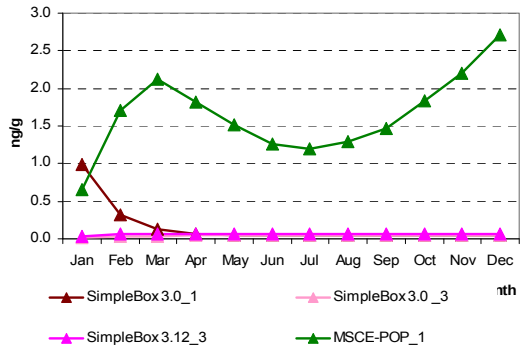


Fig. B.120a. *PCB-28 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

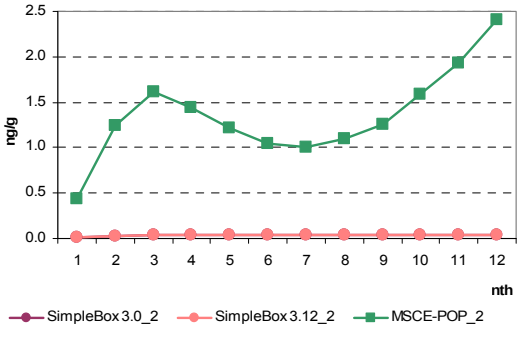


Fig. B.120b. *PCB-28 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.102. *Calculation results: PCB-28 concentration in vegetation (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.21	0.64	0.03	0.02	*0.48*	*0.57*	Jan	0.02	0.02	0.41	*0.15*	*0.23*
Feb	0.58	1.53	0.05	0.02	*0.55*	*0.70*	Feb	0.04	0.04	1.10	*0.39*	*0.61*
Mar	0.30	1.85	0.06	0.02	*0.56*	*0.87*	Mar	0.05	0.05	1.40	*0.50*	*0.78*
Apr	0.17	1.58	0.06	0.02	*0.46*	*0.75*	Apr	0.06	0.06	1.25	*0.45*	*0.69*
May	0.12	1.36	0.06	0.02	*0.39*	*0.65*	May	0.06	0.06	1.11	*0.41*	*0.61*
Jun	0.09	1.17	0.07	0.02	*0.34*	*0.56*	Jun	0.06	0.06	0.97	*0.36*	*0.52*
Jul	0.08	1.14	0.07	0.02	*0.33*	*0.54*	Jul	0.06	0.06	0.96	*0.36*	*0.52*
Aug	0.07	1.26	0.07	0.02	*0.36*	*0.60*	Aug	0.06	0.06	1.07	*0.40*	*0.58*
Sep	0.07	1.45	0.07	0.02	*0.40*	*0.70*	Sep	0.06	0.06	1.24	*0.46*	*0.68*
Oct	0.07	1.77	0.07	0.02	*0.48*	*0.86*	Oct	0.06	0.06	1.53	*0.55*	*0.85*
Nov	0.07	2.03	0.07	0.02	*0.55*	*0.99*	Nov	0.06	0.06	1.78	*0.64*	*0.99*
Dec	0.07	2.40	0.07	0.02	*0.64*	*1.17*	Dec	0.06	0.06	2.12	*0.75*	*1.19*
Annual	**0.24**	**1.37**	**0.06**	**0.02**	***0.43***	***0.64***	**Annual**	**0.06**	**0.06**	**1.10**	***0.41***	***0.60***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table B.103. *Calculation results: PCB-28 concentration in vegetation (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.98	0.66	0.02	0.03	*0.42*	*0.48*	Jan	0.01	0.01	0.43	*0.15*	*0.24*
Feb	0.33	1.71	0.03	0.06	*0.53*	*0.80*	Feb	0.03	0.03	1.24	*0.43*	*0.70*
Mar	0.13	2.12	0.04	0.07	*0.59*	*1.02*	Mar	0.04	0.04	1.61	*0.56*	*0.91*
Apr	0.07	1.82	0.04	0.07	*0.50*	*0.88*	Apr	0.04	0.04	1.44	*0.51*	*0.81*
May	0.05	1.51	0.04	0.07	*0.42*	*0.73*	May	0.04	0.04	1.22	*0.43*	*0.68*
Jun	0.05	1.26	0.04	0.07	*0.35*	*0.60*	Jun	0.04	0.04	1.04	*0.37*	*0.58*
Jul	0.04	1.20	0.04	0.07	*0.34*	*0.57*	Jul	0.04	0.04	1.01	*0.36*	*0.56*
Aug	0.04	1.29	0.04	0.07	*0.36*	*0.62*	Aug	0.04	0.04	1.10	*0.39*	*0.61*
Sep	0.04	1.47	0.04	0.07	*0.41*	*0.71*	Sep	0.04	0.04	1.26	*0.45*	*0.70*
Oct	0.04	1.83	0.04	0.07	*0.50*	*0.89*	Oct	0.04	0.04	1.59	*0.56*	*0.89*
Nov	0.04	2.20	0.04	0.07	*0.59*	*1.07*	Nov	0.04	0.04	1.93	*0.67*	*1.09*
Dec	0.04	2.71	0.04	0.07	*0.72*	*1.33*	Dec	0.04	0.04	2.41	*0.83*	*1.37*
Annual	**0.16**	**1.49**	**0.04**	**0.07**	***0.44***	***0.70***	**Annual**	**0.04**	**0.04**	**1.19**	***0.43***	***0.67***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.104.

Table B.104. *The percentage difference between calculation results on PCB-28 concentration in vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-18.9%	-9.5%	-9.5%	-44.6%	20.2%	3.6%	5.6%
Feb	-44.1%	-19.0%	-19.0%	-31.8%	134.7%	11.8%	12.7%
Mar	-56.7%	-25.8%	-25.7%	-32.3%	169.7%	14.6%	15.0%
Apr	-59.6%	-29.6%	-29.4%	-33.7%	179.3%	15.2%	15.2%
May	-55.3%	-31.7%	-31.4%	-34.6%	180.8%	11.0%	9.9%
Jun	-48.3%	-32.8%	-32.4%	-35.2%	180.0%	7.7%	7.4%
Jul	-42.4%	-33.3%	-33.0%	-35.5%	178.5%	5.3%	5.2%
Aug	-38.7%	-33.7%	-33.2%	-35.7%	176.8%	2.4%	2.8%
Sep	-36.7%	-33.9%	-33.4%	-35.8%	175.1%	1.4%	1.6%
Oct	-35.7%	-34.0%	-33.5%	-35.9%	173.5%	3.4%	3.9%
Nov	-35.3%	-34.1%	-33.5%	-35.9%	172.0%	8.4%	8.4%
Dec	-34.3%	-34.2%	-33.6%	-36.0%	170.6%	12.9%	13.7%
Annual	**-35.4%**	**-31.6%**	**-31.3%**	**-34.9%**	**171.9%**	**8.2%**	**8.2%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.5.6. Comparison of calculated values of PCB-28 concentration in surface soil layer

Reference data set. Calculation results on PCB-28 concentration in surface soil layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.105.

Monthly values of PCB-28 concentration in surface soil layer calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.121 a and b, respectively.

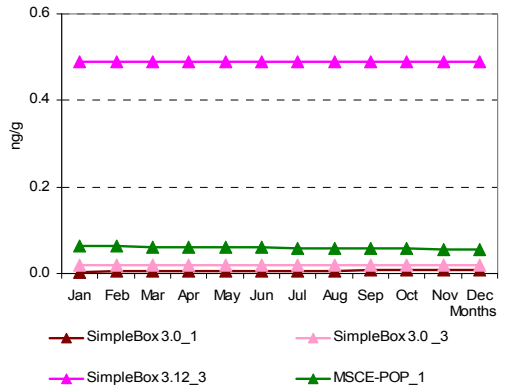


Fig.B.121a. *PCB-28 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

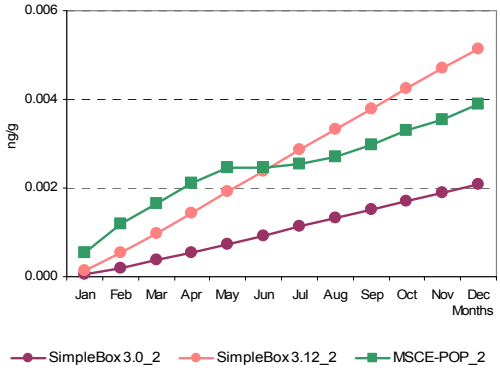


Fig.B.121b. *PCB-28 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-28 concentration in surface soil layer calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table B.106.

Monthly values of PCB-28 concentration in surface soil layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. B.122a and b, respectively.

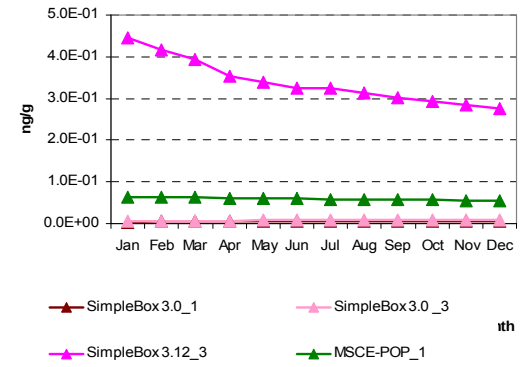


Fig. B.122a. *PCB-28 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

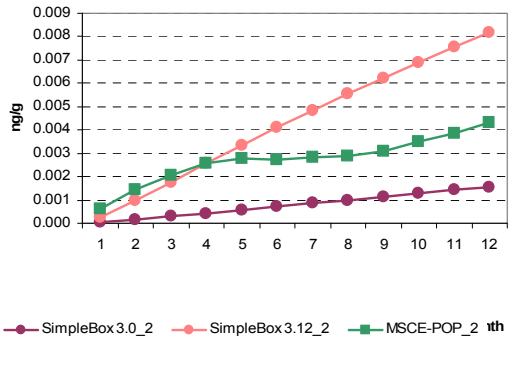


Fig. B.122b. *PCB-28 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table B.105. *Calculation results: PCB-28 concentration in surface soil layer (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	3.88E-03	6.37E-02	1.90E-02	4.88E-01	*1.44E-01*	*2.31E-01*	Jan	5.33E-05	1.44E-04	5.44E-04	*2.47E-04*	*2.61E-04*
Feb	5.06E-03	6.28E-02	1.90E-02	4.88E-01	*1.44E-01*	*2.31E-01*	Feb	2.00E-04	5.32E-04	1.18E-03	*6.37E-04*	*4.98E-04*
Mar	5.69E-03	6.20E-02	1.91E-02	4.88E-01	*1.44E-01*	*2.31E-01*	Mar	3.70E-04	9.73E-04	1.65E-03	*9.98E-04*	*6.40E-04*
Apr	6.07E-03	6.14E-02	1.92E-02	4.88E-01	*1.44E-01*	*2.31E-01*	Apr	5.54E-04	1.44E-03	2.12E-03	*1.37E-03*	*7.85E-04*
May	6.33E-03	6.07E-02	1.92E-02	4.88E-01	*1.44E-01*	*2.31E-01*	May	7.42E-04	1.91E-03	2.46E-03	*1.71E-03*	*8.78E-04*
Jun	6.55E-03	5.97E-02	1.93E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Jun	9.32E-04	2.39E-03	2.47E-03	*1.93E-03*	*8.65E-04*
Jul	6.73E-03	5.87E-02	1.94E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Jul	1.12E-03	2.86E-03	2.54E-03	*2.17E-03*	*9.24E-04*
Aug	6.91E-03	5.79E-02	1.95E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Aug	1.32E-03	3.33E-03	2.69E-03	*2.45E-03*	*1.03E-03*
Sep	7.08E-03	5.74E-02	1.96E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Sep	1.51E-03	3.79E-03	2.96E-03	*2.75E-03*	*1.16E-03*
Oct	7.24E-03	5.69E-02	1.97E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Oct	1.70E-03	4.25E-03	3.31E-03	*3.08E-03*	*1.29E-03*
Nov	7.40E-03	5.64E-02	1.98E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Nov	1.89E-03	4.70E-03	3.54E-03	*3.37E-03*	*1.41E-03*
Dec	7.52E-03	5.61E-02	1.98E-02	4.88E-01	*1.43E-01*	*2.31E-01*	Dec	2.07E-03	5.14E-03	3.89E-03	*3.70E-03*	*1.54E-03*
Annual	**6.37E-03**	**6.01E-02**	**1.94E-02**	**4.88E-01**	***1.44E-01***	***2.31E-01***	**Annual**	**1.13E-03**	**2.62E-03**	**2.19E-03**	***1.98E-03***	***7.70E-04***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table B.106. *Calculation results: PCB-28 concentration in surface soil layer (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	3.87E-03	6.37E-02	6.87E-03	4.47E-01	*1.30E-01*	*2.13E-01*	Jan	4.06E-05	2.59E-04	6.22E-04	*3.07E-04*	*2.94E-04*
Feb	4.83E-03	6.29E-02	6.93E-03	4.18E-01	*1.23E-01*	*1.98E-01*	Feb	1.57E-04	9.72E-04	1.43E-03	*8.53E-04*	*6.45E-04*
Mar	5.21E-03	6.22E-02	7.02E-03	3.93E-01	*1.17E-01*	*1.86E-01*	Mar	2.91E-04	1.76E-03	2.04E-03	*1.36E-03*	*9.40E-04*
Apr	5.40E-03	6.15E-02	7.10E-03	3.54E-01	*1.07E-01*	*1.67E-01*	Apr	4.32E-04	2.56E-03	2.59E-03	*1.86E-03*	*1.24E-03*
May	5.54E-03	6.05E-02	7.19E-03	3.38E-01	*1.03E-01*	*1.59E-01*	May	5.75E-04	3.34E-03	2.79E-03	*2.23E-03*	*1.46E-03*
Jun	5.65E-03	5.92E-02	7.28E-03	3.24E-01	*9.91E-02*	*1.52E-01*	Jun	7.18E-04	4.09E-03	2.71E-03	*2.51E-03*	*1.70E-03*
Jul	5.76E-03	5.82E-02	7.37E-03	3.24E-01	*9.89E-02*	*1.52E-01*	Jul	8.59E-04	4.82E-03	2.81E-03	*2.83E-03*	*1.98E-03*
Aug	5.87E-03	5.72E-02	7.46E-03	3.12E-01	*9.57E-02*	*1.46E-01*	Aug	1.00E-03	5.54E-03	2.87E-03	*3.14E-03*	*2.28E-03*
Sep	5.97E-03	5.66E-02	7.54E-03	3.02E-01	*9.30E-02*	*1.41E-01*	Sep	1.14E-03	6.22E-03	3.11E-03	*3.49E-03*	*2.56E-03*
Oct	6.08E-03	5.61E-02	7.63E-03	2.93E-01	*9.06E-02*	*1.37E-01*	Oct	1.28E-03	6.89E-03	3.49E-03	*3.89E-03*	*2.83E-03*
Nov	6.18E-03	5.57E-02	7.72E-03	2.84E-01	*8.85E-02*	*1.33E-01*	Nov	1.42E-03	7.54E-03	3.88E-03	*4.28E-03*	*3.08E-03*
Dec	6.28E-03	5.54E-02	7.80E-03	2.77E-01	*8.67E-02*	*1.29E-01*	Dec	1.56E-03	8.16E-03	4.33E-03	*4.68E-03*	*3.32E-03*
Annual	**5.55E-03**	**5.98E-02**	**7.37E-03**	**3.43E-01**	***1.04E-01***	***1.61E-01***	**Annual**	**8.58E-04**	**4.35E-03**	**2.45E-03**	***2.55E-03***	***1.75E-03***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table B.107.

Table B.107. *The percentage difference between calculation results on PCB-28 concentration in surface soil layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-0.4%	-24.0%	79.7%	-63.8%	-8.5%	0.0%	14.3%
Feb	-4.5%	-21.7%	82.7%	-63.5%	-14.4%	0.2%	21.2%
Mar	-8.5%	-21.4%	81.0%	-63.2%	-19.4%	0.3%	23.6%
Apr	-11.0%	-21.9%	77.8%	-62.9%	-27.5%	0.2%	22.2%
May	-12.6%	-22.5%	74.5%	-62.6%	-30.8%	-0.3%	13.4%
Jun	-13.7%	-23.0%	71.4%	-62.3%	-33.6%	-0.8%	9.7%
Jul	-14.4%	-23.4%	68.7%	-62.0%	-33.6%	-0.9%	10.6%
Aug	-15.1%	-23.8%	66.3%	-61.8%	-36.1%	-1.2%	6.7%
Sep	-15.6%	-24.1%	64.1%	-61.5%	-38.2%	-1.4%	5.1%
Oct	-16.1%	-24.4%	62.2%	-61.2%	-40.1%	-1.4%	5.4%
Nov	-16.6%	-24.7%	60.4%	-60.9%	-41.8%	-1.2%	9.6%
Dec	-16.5%	-24.9%	58.9%	-60.7%	-43.2%	-1.2%	11.3%
Annual	-12.9%	-23.9%	65.8%	-62.1%	-29.8%	-0.5%	11.6%

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.5.7. Comparison of PCB-28 intermedia mass flows and concentrations at the interfaces of main environmental media

A preliminary analysis of model results on intermedia mass flows and on concentrations in the main environmental media formed at their interfaces is presented in this section. In the comparison the calculated values of PCB-28 mass flows from the atmosphere to soil, to water, to vegetation and from vegetation to soil (see Sections B.4.1-B.4.4 above) and values of PCB-28 concentrations in the atmosphere at its interface with underlying surfaces (soil, ocean and vegetation); in the surface layer of soil, ocean and vegetation (see Sections B.5.1–B.5.6 above) are considered.

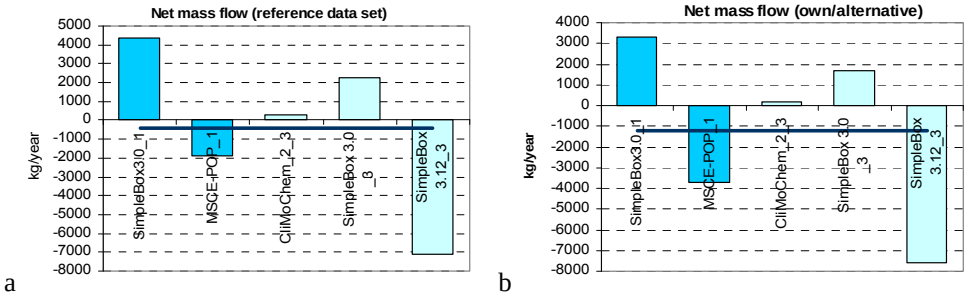
The comparison of PCB-28 mass flows transported from one compartment to another presented in Sections B.4.1-B.4.4 includes results of one-year calculation with zero initial concentrations obtained by CliMoChem, MSCE-POP, SimpleBox models and with initial concentrations in media given as input data calculated by MSCE-POP and SimpleBox models; as well as results of long-term calculations for 20-year period with zero initial data with historical emissions carried out by CliMoChem and SimpleBox models. Results of CliMoChem, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of the estimates on intermedia mass flows to the variations in the input data.

The comparison of calculated concentrations presented in Sections B.5.1–B.5.6 includes results of one-year calculations made on the basis of initial conditions (MSCE-POP, SimpleBox) and zero initial

concentrations (MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (SimpleBox B.0 and B.12). The results on concentrations in the main environmental media are obtained with the use of two different physical-chemical data sets by MSCE-POP and SimpleBox models.

In the section below the analysis of mass flows and concentrations in the media is presented for model results obtained on the basis of initial conditions and historical emissions. Calculated values of PCB intermedia mass flows and concentrations in the main media are presented in this section for four following interfaces: atmosphere-soil; vegetation – soil; atmosphere - seawater and atmosphere – vegetation.

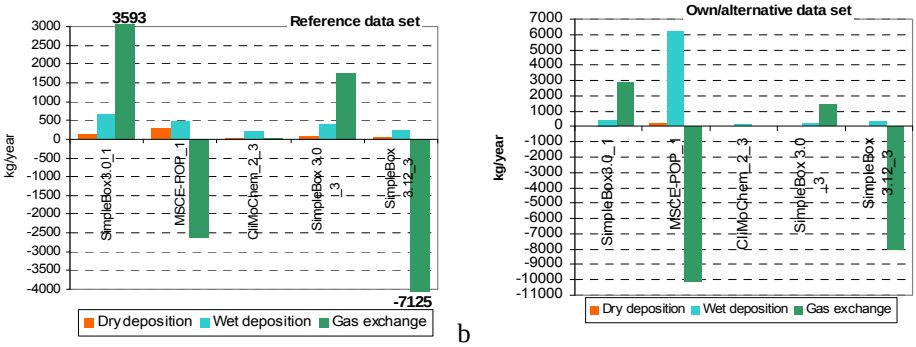
Atmosphere-soil. Annual values of net exchange flow between atmosphere and soil calculated on the basis of two data sets of physical-chemical properties are compared between different models in Fig. B.123. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig.B.123. *Comparison of PCB-28 annual values of net exchange flow between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Since the net exchange flow is a sum of different types of exchange flows, below the latter are considered separately. Comparison of annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by models on the basis of two physical-chemical data sets is presented in Fig. B.124.

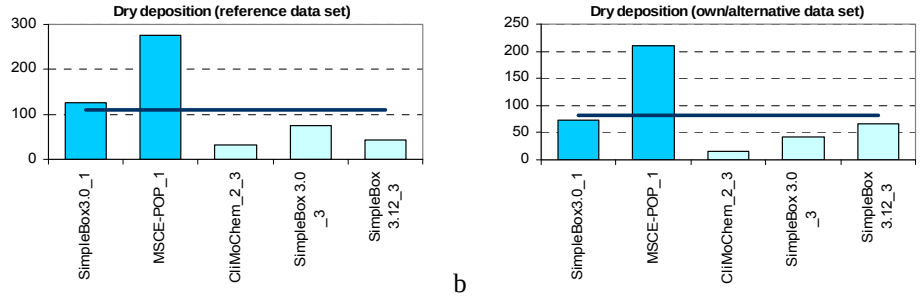


a b

Fig.B.124. *Comparison of PCB-28 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

To reveal differences in calculated values obtained on “reference” and “own/alternative” data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

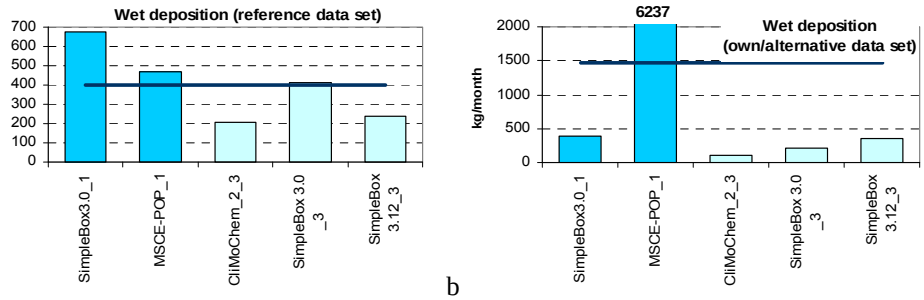
Comparison of annual values of PCB-28 dry deposition from the atmosphere to soil calculated by the models on the basis of “**reference”** and “**own or alternative”** data sets is presented in Fig. B.125. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.125. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to soil: dry deposition (kg/year) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

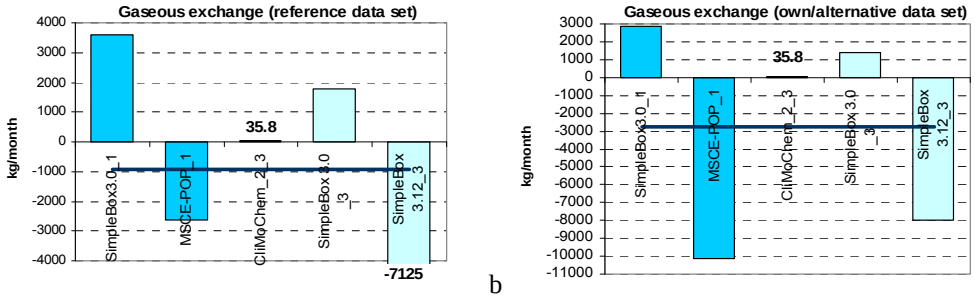
Comparison of annual values of PCB-28 wet deposition mass flows from the atmosphere to soil calculated by the models on the basis of “**reference**” and “**own or alternative**” data sets is presented in Fig.B.126. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.126. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to soil: wet deposition (kg/year) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

A comparison of annual values of PCB-28 gaseous exchange between the atmosphere and soil calculated by the models on the basis of “**reference**” and “**own or alternative”** data sets is presented in Fig.B.127. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

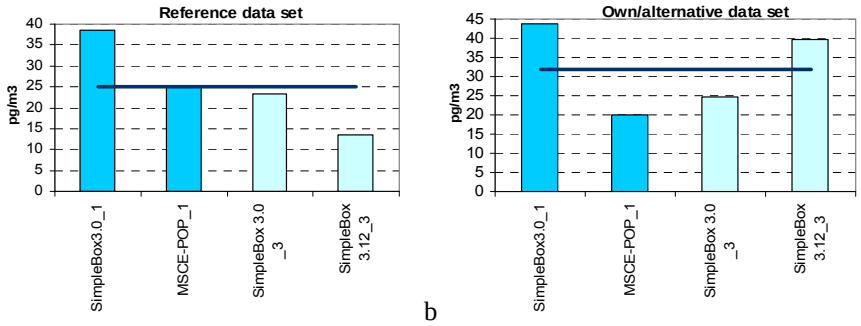


a b

Fig.B.127. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to soil: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

Model results on concentrations of PCB-28 in the atmosphere at its interface with soil and in the surface soil layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

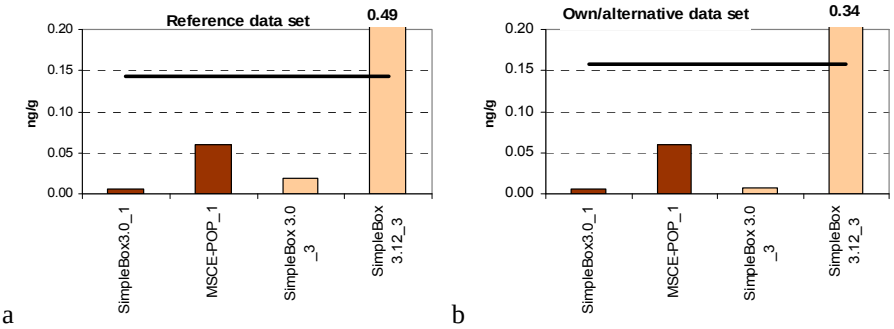
Comparison of annual values of PCB-28 concentration in the atmosphere at its interface with soil calculated by the models on the basis of "reference" and "own or alternative" data set is presented in Fig.B.128. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.128. *Comparison of annual values of PCB-28 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

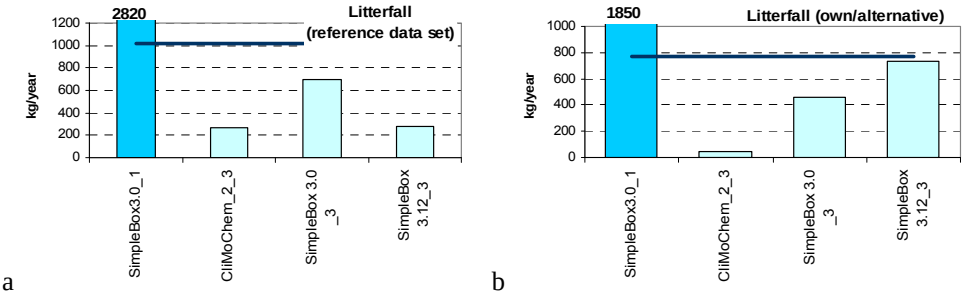
Comparison of annual values of PCB-28 concentration in surface soil layer calculated by the models on the basis of "reference" and "own/alternative" data sets is presented in Fig.B.129. The black line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.129. *Comparison of annual values of PCB-28 concentration in surface soil layer (ng/g) calculated by different models on the basis of "reference" (a) and "own or alternative" (b) data sets.*

Vegetation – soil. Comparison of annual values of PCB-28 mass flows from vegetation to soil calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.130. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).



a b

Fig.B.130. *Comparison of annual values of PCB-28 mass flows transported from vegetation to soil (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" data sets (b)*

Comparison of annual values of litterfall mass flows calculated by models on the basis of two physical-chemical data sets is presented in Fig. B.131 (see also Table B.70 given in Section B.4.2).

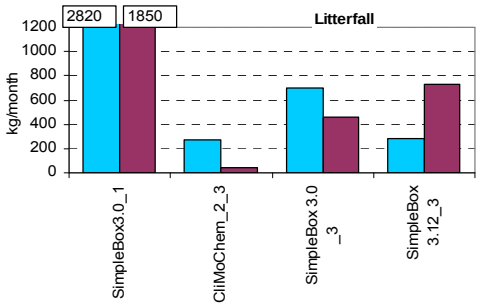
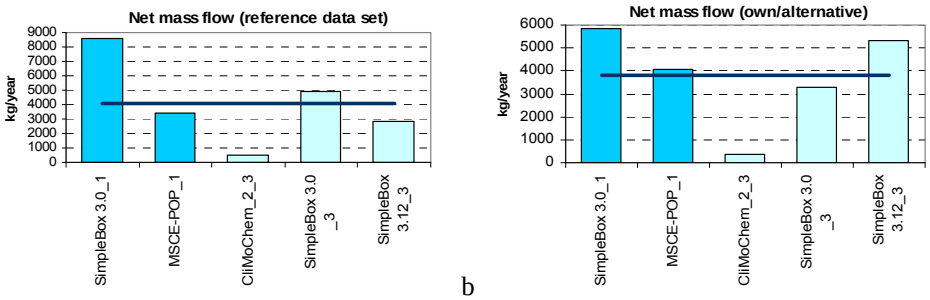


Fig.3.131. *Comparison of PCB-28 annual values of mass flows between vegetation and soil calculated by different models on the basis of two data sets*

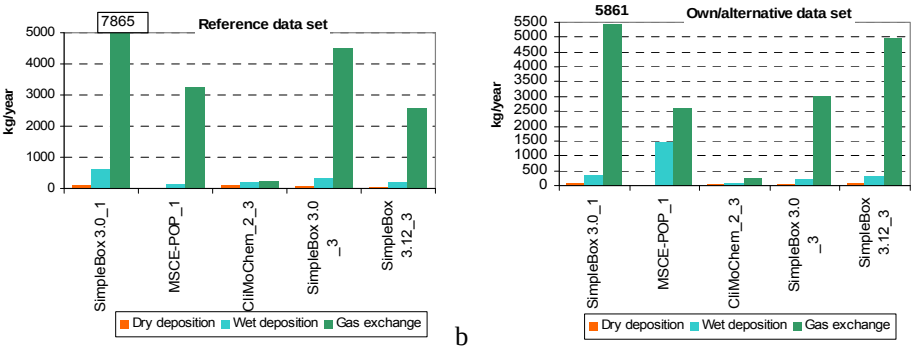
Atmosphere - seawater. Annual values of net exchange flow between atmosphere and seawater calculated on the basis of two data sets are compared between different models in Fig. B.132. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.132. *Comparison of PCB-28 annual values of net exchange flow between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Annual absolute values of dry and wet deposition and gaseous exchange flows, which formed the considered net exchange flows between the atmosphere and seawater, are compared below. Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and seawater calculated by models on the basis of two physical-chemical data sets is presented in Fig. B.133.

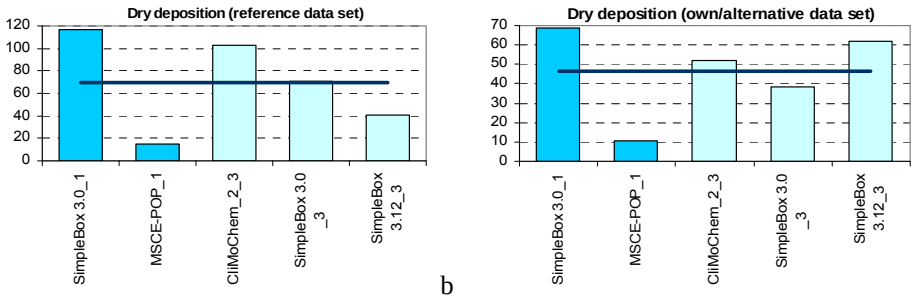


a b

Fig.B.133. *Comparison of PCB-28 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

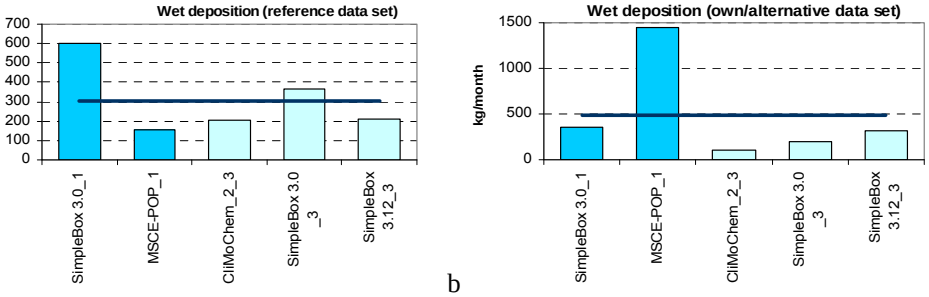
Comparison of annual values of PCB-28 dry deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.134. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.134. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to water: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

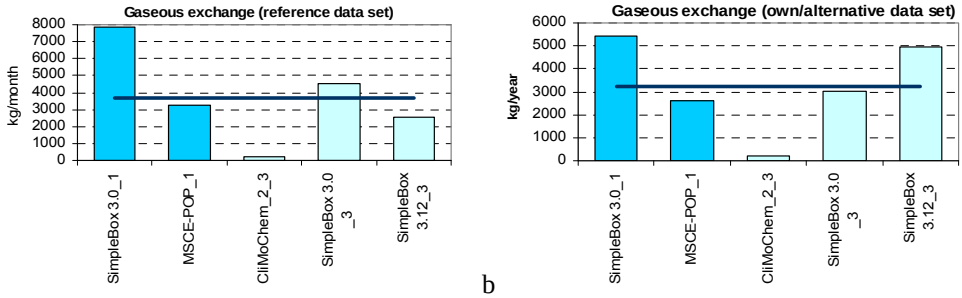
Comparison of annual values of PCB-28 wet deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.135. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.135. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to water: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Comparison of annual values of PCB-28 gaseous exchange mass flows between the atmosphere and water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.136. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

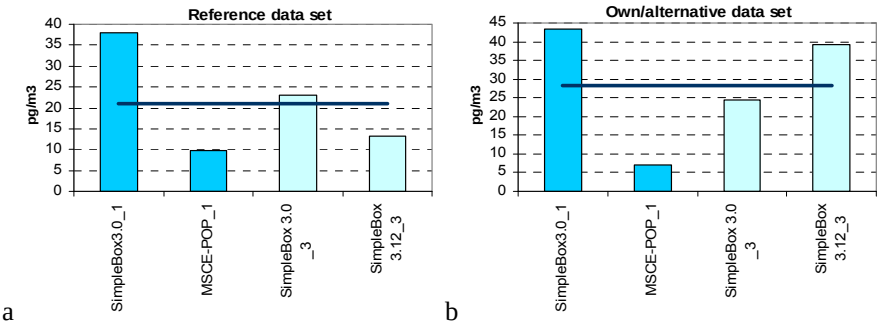


a b

Fig.B.136. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to water: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Model results on concentrations of PCB-28 in the atmosphere at its interface with ocean and in the surface water layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

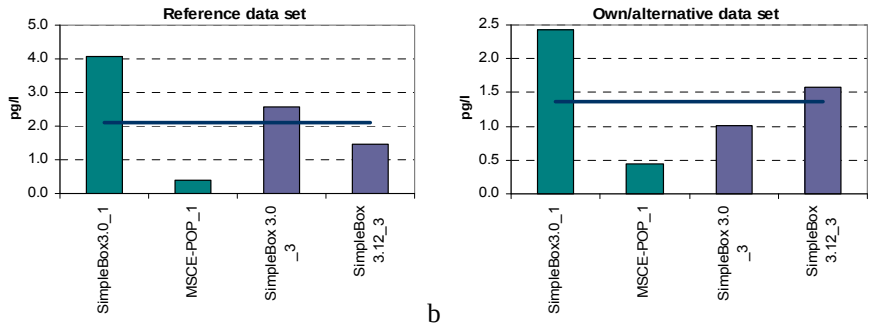
Comparison of annual values of PCB-28 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" and "own/alternative" data sets is presented in Fig.B.137. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.137. *Comparison of annual values of PCB-28 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

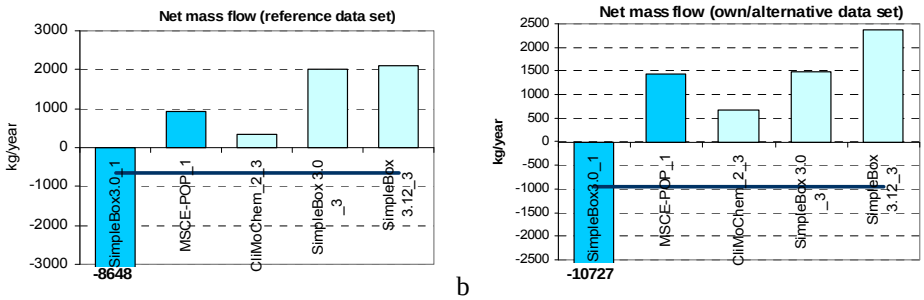
Comparison of annual values of PCB-28 concentration in surface ocean layer calculated by the models on the basis of "reference" and "own/alternative" data sets is presented in Fig.B.138. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.138. *Comparison of annual values of PCB-28 concentration in surface ocean layer (pg/l) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

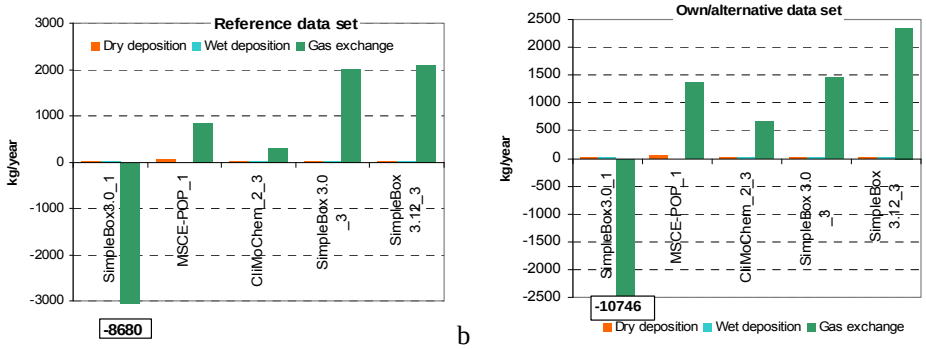
Atmosphere – vegetation. Annual values of net exchange flow between atmosphere and vegetation calculated on the basis of two data sets ("reference" and "own/alternative") are compared between different models in Fig. B.139. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.139. *Comparison of PCB-28 annual values of net exchange flow between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and vegetation calculated by models on the basis of two physical-chemical data sets is presented in Fig. B.140.

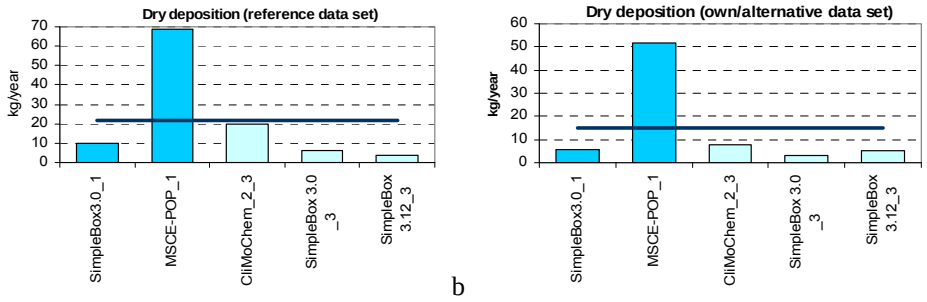


a b

Fig.B.140. *Comparison of PCB-28 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

To reveal differences in calculated values obtained on "reference" and "own/alternative" data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

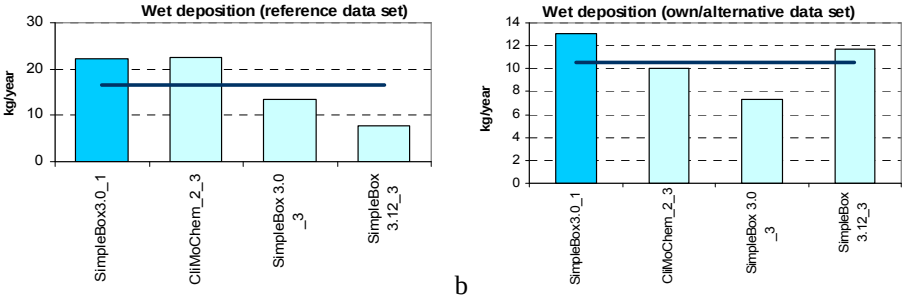
Comparison of annual values of PCB-28 dry deposition mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.142. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.141. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to vegetation: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

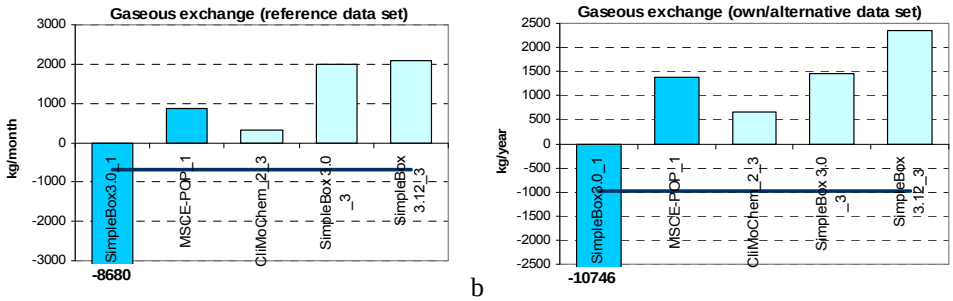
Comparison of annual values of PCB-28 wet deposition mass flows transported from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.142. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.142. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to vegetation: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Comparison of annual values of PCB-28 gaseous exchange mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.B.143. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

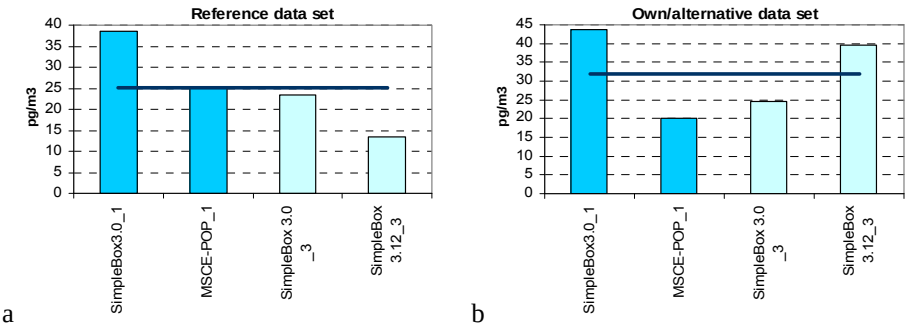


a b

Fig.B.143. *Comparison of annual values of PCB-28 mass flows transported from the atmosphere to vegetation: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Model results on concentrations of PCB-28 in the atmosphere at its interface with vegetation and in vegetation, which are conditioned by the considered above intermedia flows calculated with “reference” and “own/alternative” data sets are considered below.

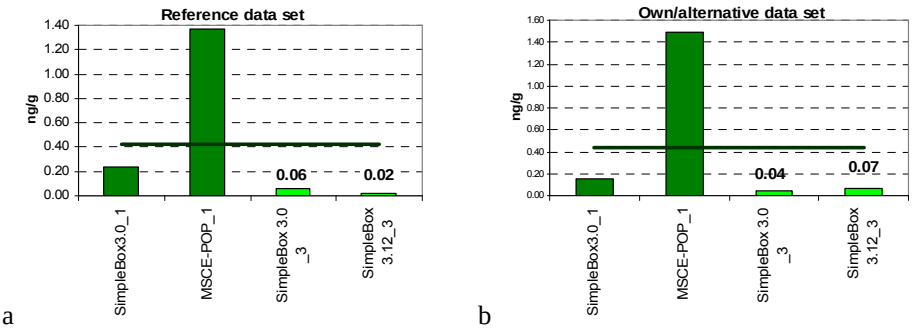
Comparison of annual values of PCB-28 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of “reference” and ‘own/alternative” data sets is presented in Fig.B.144. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.144. *Comparison of annual values of PCB-28 concentration in the atmosphere at its interface with vegetation (pg/m3) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

Comparison of annual values of PCB-28 concentration in vegetation calculated by the models on the basis of “reference” and ‘own/alternative” data sets is presented in Fig.B.145. The green line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.B.145. *Comparison of annual values of PCB-28 concentration in vegetation (ng/g) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

B.6. Spatial distribution of depositions and concentrations in different compartments (optional)

Four models present results on spatial distribution of depositions and concentrations of PCB-28 in different environmental compartments: DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox.

Calculated fields of PCB-28 concentrations in the atmosphere, soil, water and vegetation and net deposition fluxes in 2000 obtained by the participating models with the use of two different data sets ("reference" and "own or alternative") are compared below. The results on spatial distribution of PCB-28 deposition and concentrations in the main environmental media are obtained with the use of the two physical-chemical data sets by DEHM-POP, MSCE-POP and different versions of SimpleBox model.

The comparison of calculated deposition and concentration fields presented in Sections B.6.1 and 3.6.2 below includes results of one-year calculations made on the basis of initial conditions (DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP, SimpleBox), zero initial concentrations (DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (EVN-BETR and UK-MODEL, SimpleBox 3.0 and 3.12) (See Table B.109). The model results obtained taking into account initial concentrations of pollutants in media and historical emissions, and on the basis of zero initial concentrations in the environmental media are compared in two different groups.

Table B.109. *Results on spatial distribution of PCB-28 depositions and concentrations in different compartments presented by the models*

Maps	Data set used	DEHM-POP_1	DEHM-POP_2	EVN-BETR _1[a]	EVN-BETR _2[a]	EVN-BETR _3[a]	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Surface atmospheric concentrations, pg/m^3	ref	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt	+	+				+	+	+	+	+	+	+
Surface soil concentration, ng/g	ref	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt	+	+				+	+	+	+	+	+	+
Surface water concentration, pg/l	ref	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt	+	+				+	+	+	+	+	+	+
Concentration in vegetation, ng/g (optional)	ref			+	+	+	+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+
Net deposition flux, mg/m^2/hour	ref						+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+
Wet deposition of gaseous phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Wet deposition of particle phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Wet deposition total, mg/m^2/hour	ref						+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+
Dry deposition of gaseous phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Dry deposition of particle phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Dry deposition total, mg/m^2/hour	ref						+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data, the only exception was that the initial conditions for the vegetation were set to zero;

EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;

EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;

DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;

DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - EVN-BETR and UK-MODEL results were calculated with the help of a spatially resolved version of the model;

[b] – SimpleBox: results were calculated on the basis of initial concentrations given as input data. The concentrations calculated are the bulk concentrations in the compartments. Maps of concentrations are obtained on the basis of annual values of concentrations at regional and continental levels.

B.6.1. Comparison of results on spatial distribution of PCB-28 depositions and concentrations in different compartments obtained on the basis of "reference" data set

In this section a comparison of spatial distributions of PCB-28 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models with the use of "reference" data set on the basis of initial PCB-28 concentrations in the media, historical emissions and zero initial conditions is presented.

Concentration in the atmosphere. The calculated fields of PCB-28 annual concentrations in the atmosphere of the European calculation domain presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. B.147.

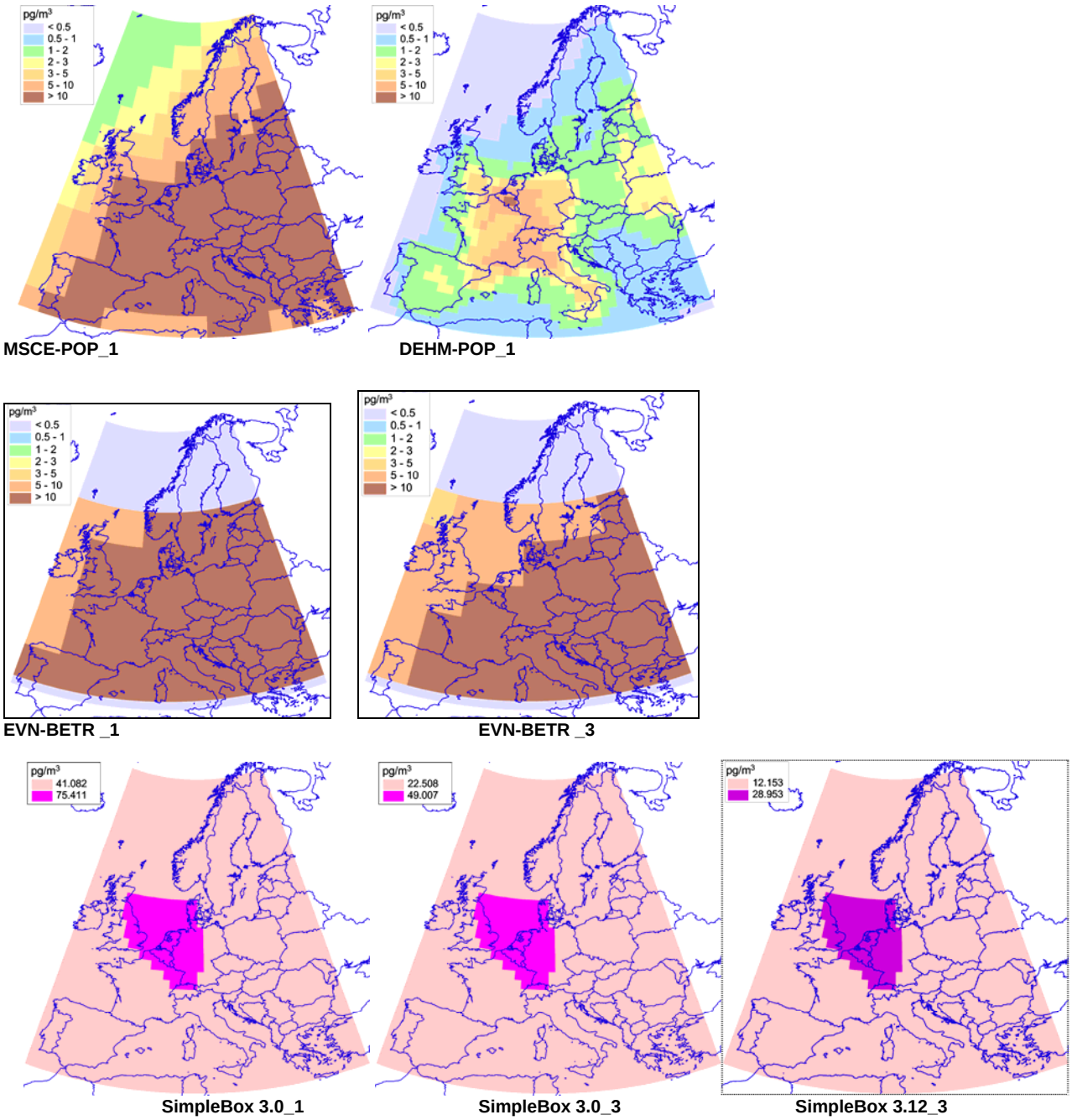


Fig. B.147. *Spatial distribution of PCB-28 concentrations in the atmosphere calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

Soil concentration. The spatial distributions of PCB-28 concentration in soil of the European region presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.B.148.

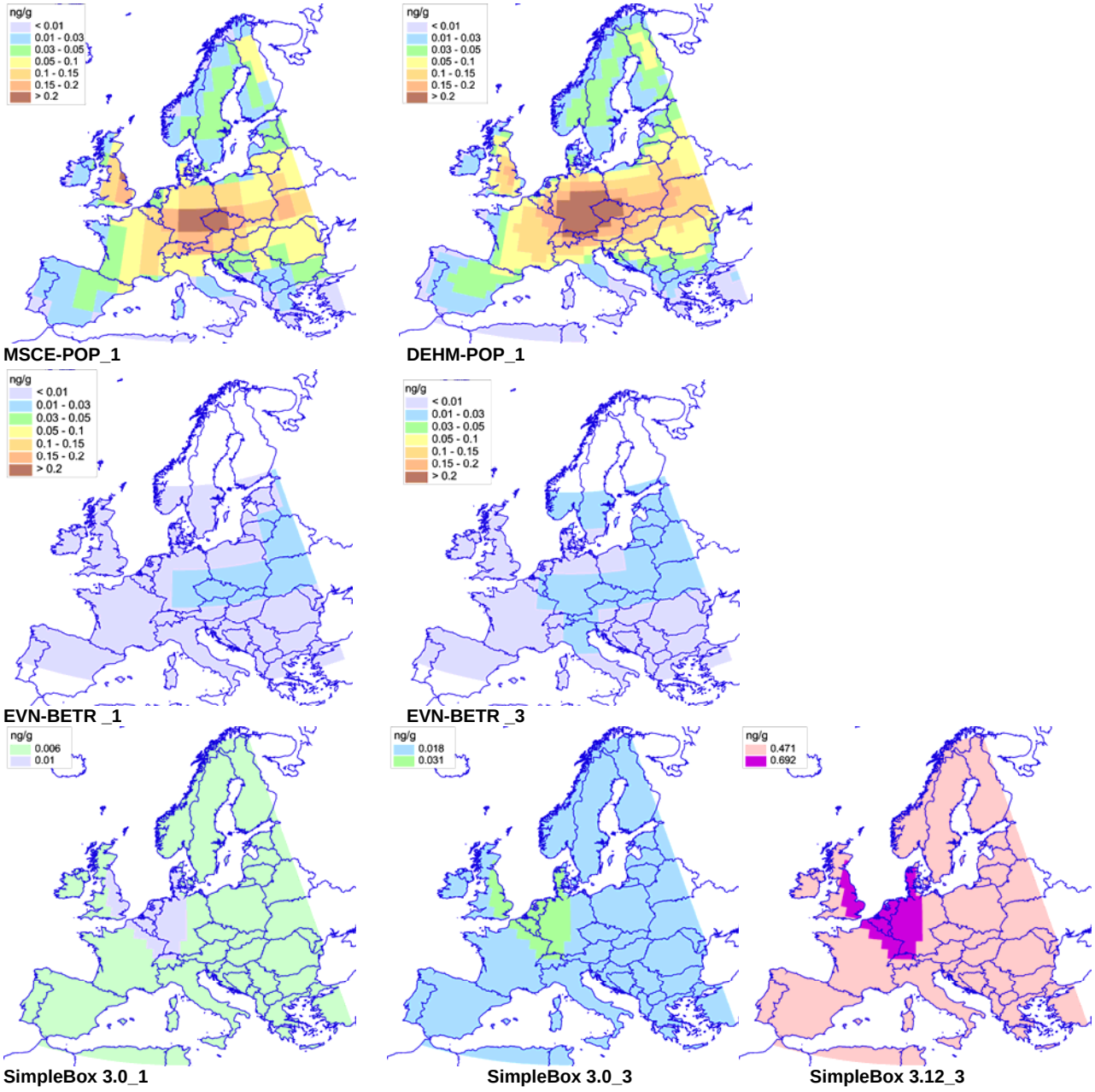


Fig. B.148. *Spatial distribution of PCB-28 concentrations in soil calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Water concentration. The calculated fields of PCB-28 annual concentrations in water of the European calculation domain in 2000 presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. B.149.

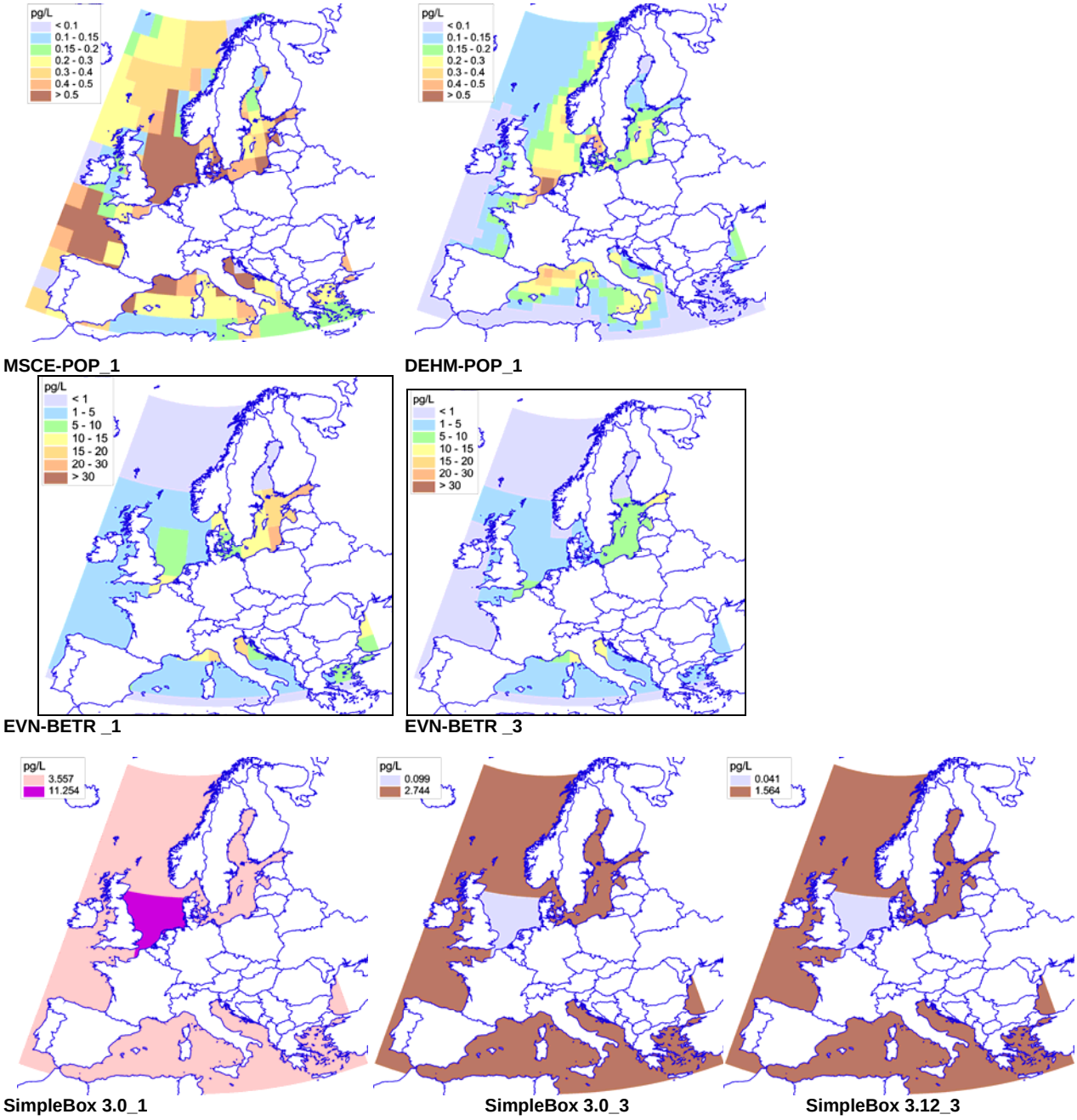


Fig. B.149. *Spatial distribution of PCB-28 concentrations in water calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Concentration in vegetation. The spatial distributions of PCB-28 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.B.150.

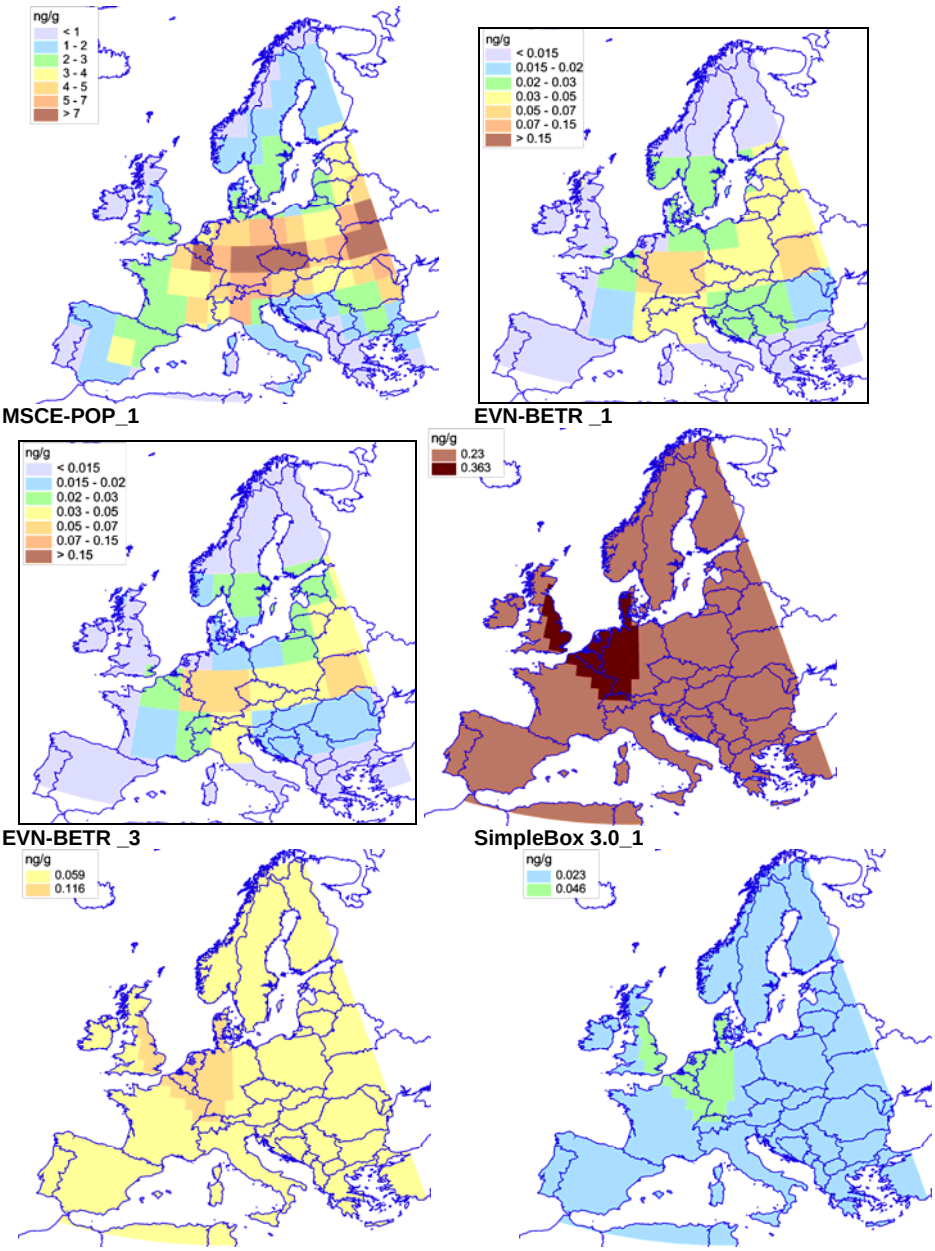


Fig. B.150. *Spatial distribution of PCB-28 concentrations in vegetation calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Net deposition flux. Spatial distributions of PCB-28 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.B.151. The values of net deposition flux include dry and wet depositions and gaseous exchange. Of note, the spatial variability of SimpleBox results in this case is higher than that in the presented above results on concentrations in the media since the deposition values in this model are dependent on the different types of underlying surfaces, which were taken into account in their calculations.

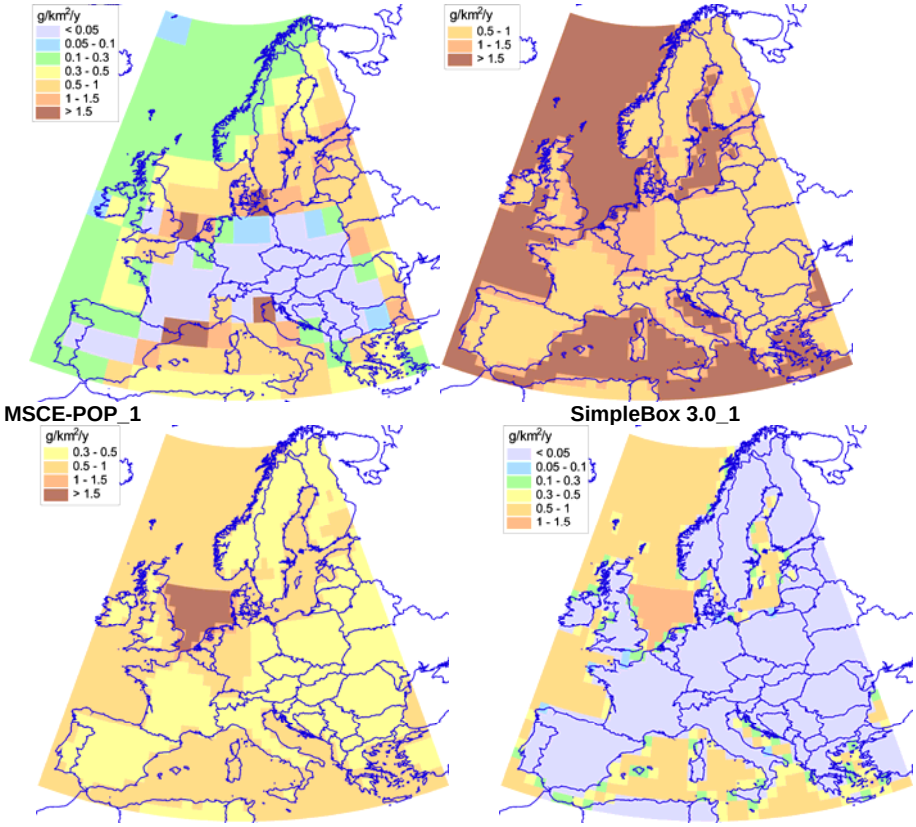


Fig. B.151. *Spatial distribution of PCB-28 net depositions calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

Below the comparison of model results obtained on the basis of zero initial concentrations in the environmental media is presented.

Concentration in the atmosphere. The calculated fields of PCB-28 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models for 2000 are compared in Fig. B.152.

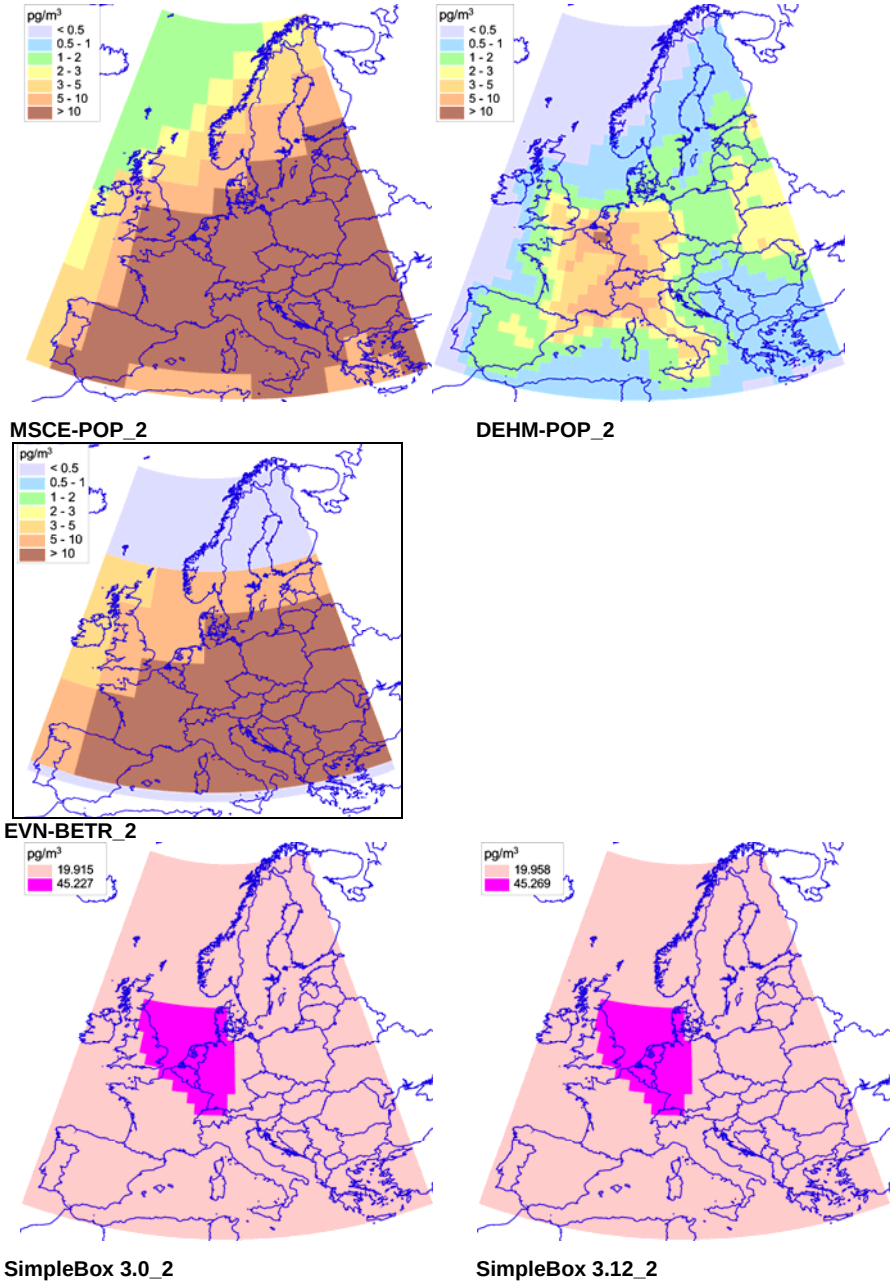
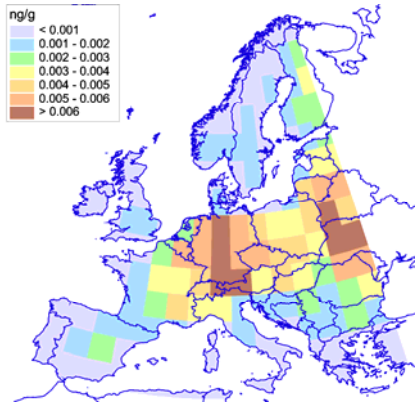
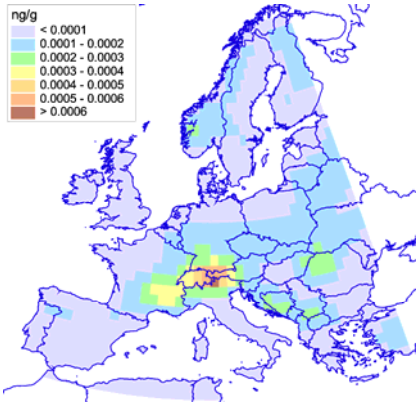


Fig. B.152. *Spatial distribution of PCB-28 concentrations in the atmosphere calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

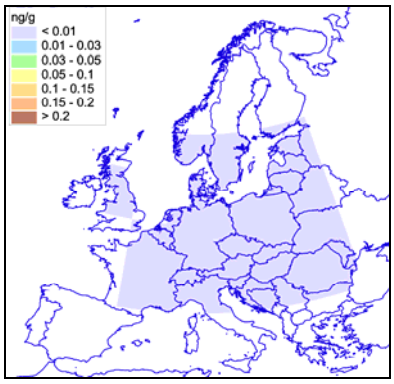
Soil concentration. The spatial distributions of PCB-28 concentration in soil of the European region presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are illustrated in Fig.B.153.



MSCE-POP_2



DEHM-POP_2



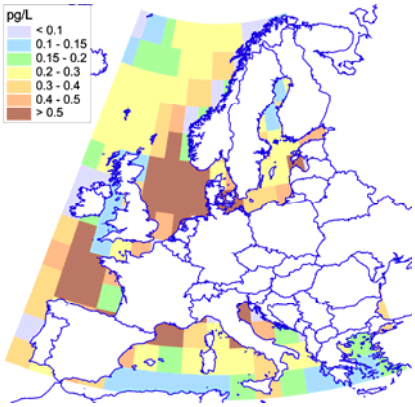
EVN-BETR_2

SimpleBox 3.0_2

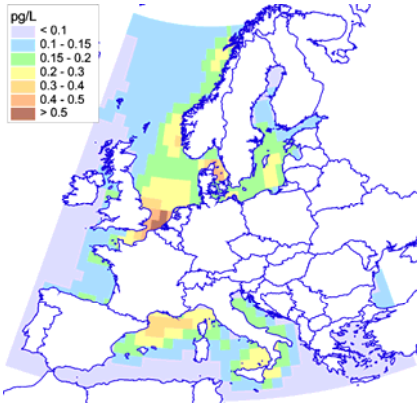
SimpleBox 3.12_2

Fig. B.153. *Spatial distribution of PCB-28 concentrations in soil calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

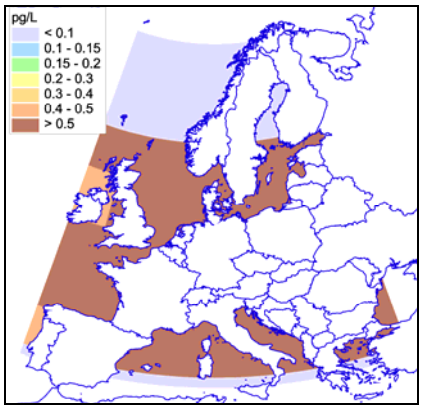
Water concentration. The calculated fields of PCB-28 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig. B.154.



MSCE-POP_2



DEHM-POP_2



EVN-BETR_2

SimpleBox 3.0_2

SimpleBox 3.12_2

Fig. B.154. *Spatial distribution of PCB-28 concentrations in water calculated by the participating models on the basis of "reference" data set and zero initial concentrations.*

Concentration in vegetation. The spatial distributions of PCB-28 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig. B.155.

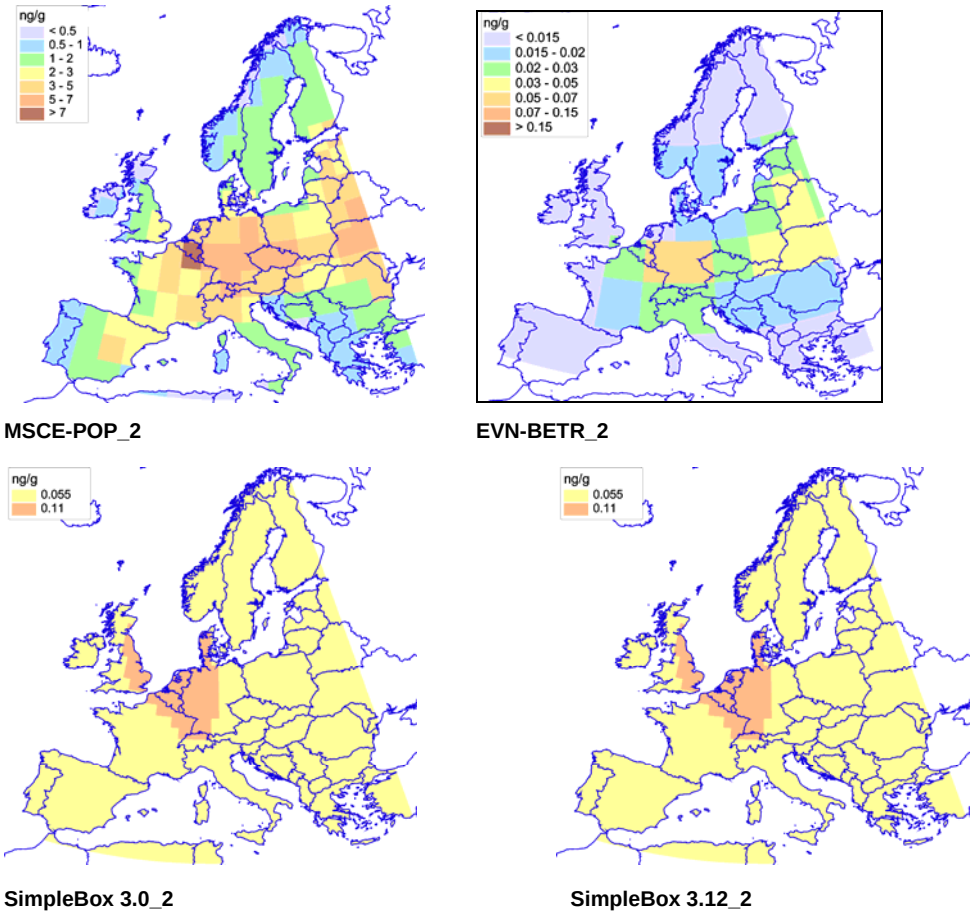


Fig. B.155. *Spatial distribution of PCB-28 concentrations in vegetation calculated by the participating models on the basis of "reference" data set and zero initial concentrations.*

Net deposition flux. Spatial distributions of PCB-28 net deposition flux in 2000 presented by ADEPT, MSCE-POP and SimpleBox models are shown in Fig. B.156. The values of net deposition flux include dry and wet depositions and gaseous exchange.

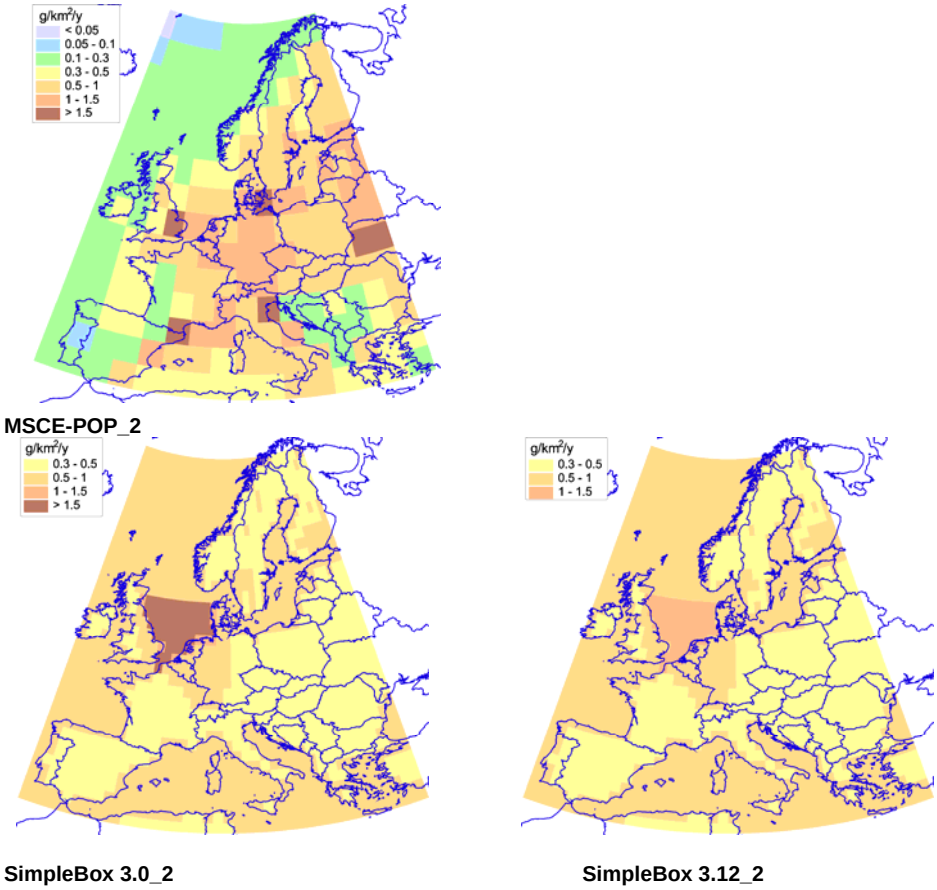


Fig. B.156. *Spatial distribution of PCB-28 net depositions calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

B.6.2. Comparison of results on spatial distribution of PCB-28 depositions and concentrations in different compartments obtained on the basis of "own or alternative" data sets

In this section a comparison of spatial distributions of PCB-28 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models "own or alternative" data sets on the basis of initial concentrations of pollutants in media, historical emissions and zero initial conditions is presented.

Concentration in the atmosphere. The calculated fields of PCB-28 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. B.157.

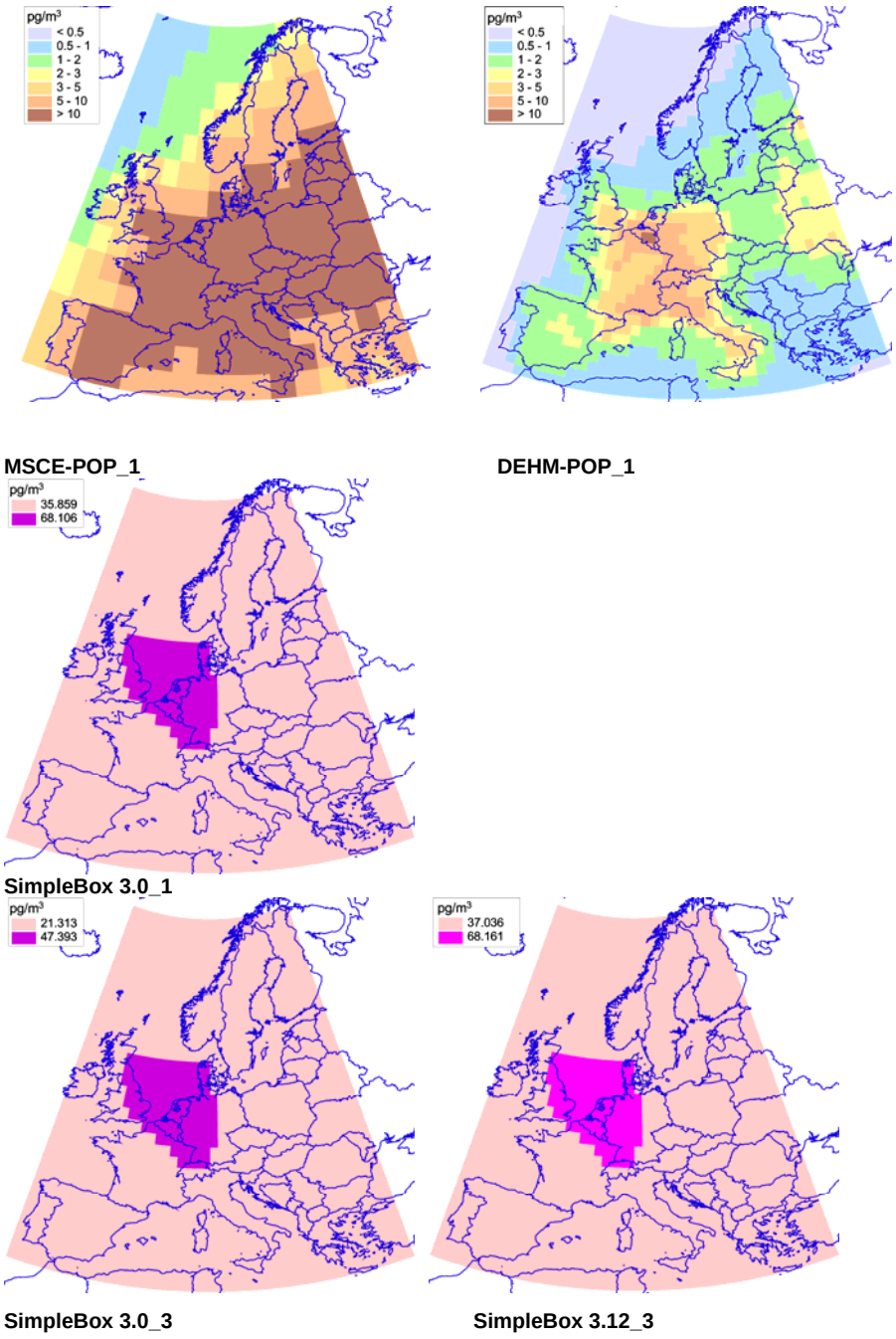
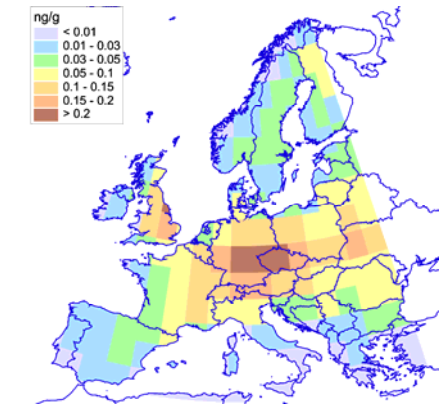
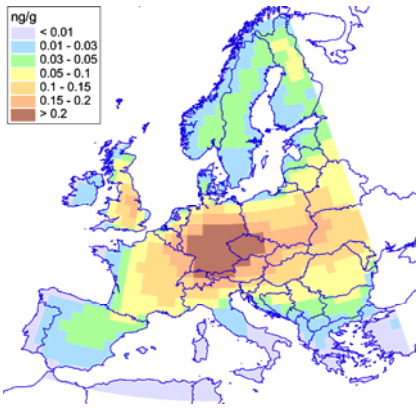


Fig. B.157. *Spatial distribution of PCB-28 concentrations in the atmosphere calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*

Soil concentration. The spatial distributions of PCB-28 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.B.158.



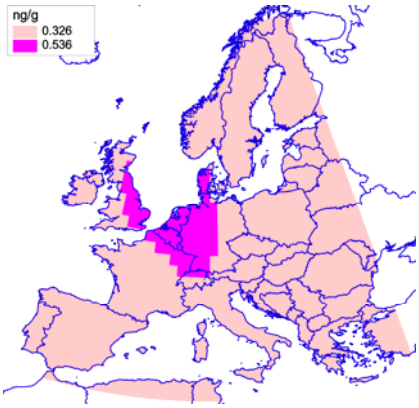
MSCE-POP_1



DEHM-POP_1

SimpleBox 3.0_1

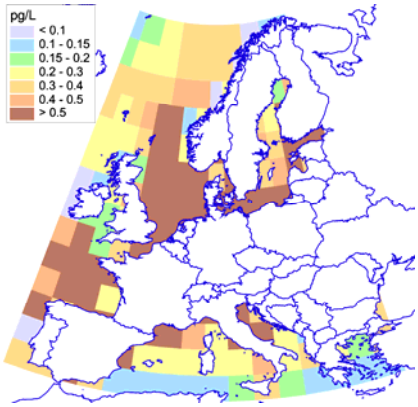
SimpleBox 3.0_3



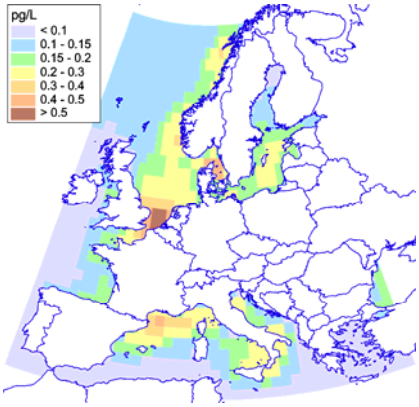
SimpleBox 3.12_3

Fig. B.158. *Spatial distribution of PCB-28 concentrations in soil calculated by the participating models on the basis of "own or alternative" data set taking into account initial concentrations of pollutants in media or historical emissions*

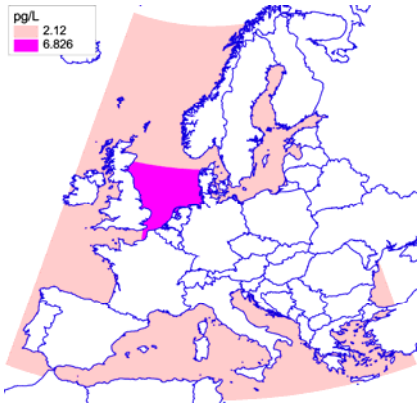
Water concentration. The calculated fields of PCB-28 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. B.159.



MSCE-POP_1



DEHM-POP_1



SimpleBox 3.0_1

SimpleBox 3.0_3

SimpleBox 3.12_3

Fig. B.159. *Spatial distribution of PCB-28 concentrations in water calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*

Concentration in vegetation. The spatial distributions of PCB-28 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig. B.160.

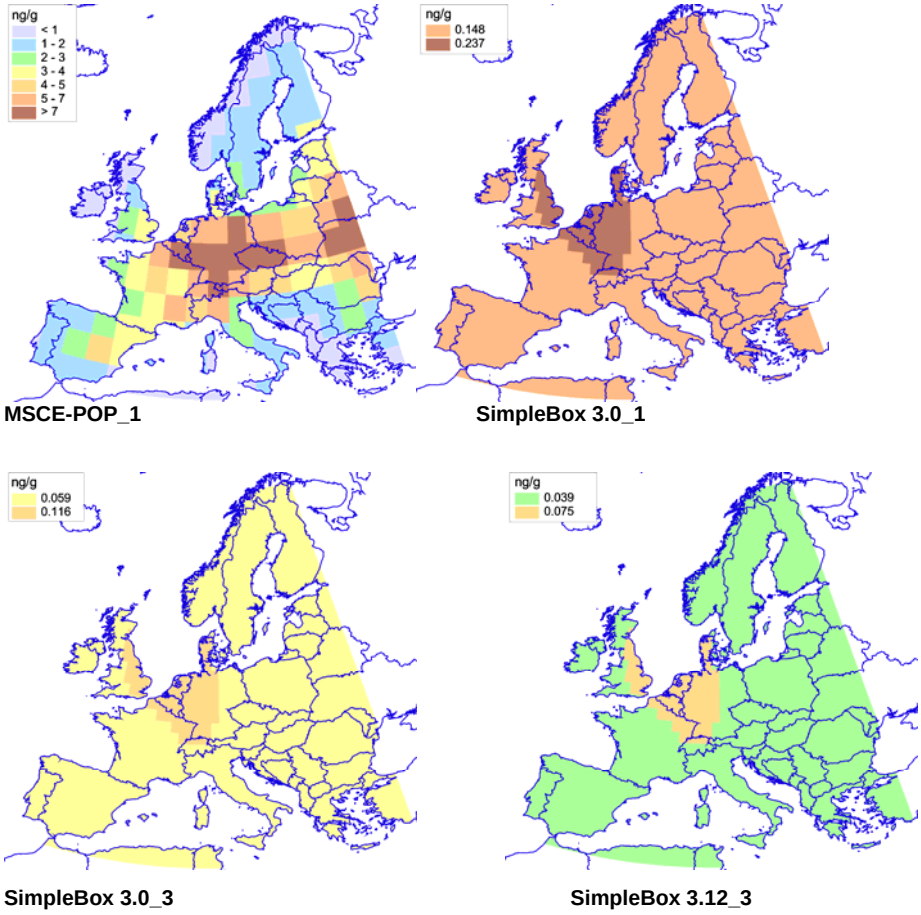


Fig. B.160. *Spatial distribution of PCB-28 concentrations in vegetation calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*.

Net deposition flux. Spatial distributions of PCB-28 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.B.161. The values of net deposition flux include dry and wet depositions and gaseous exchange.

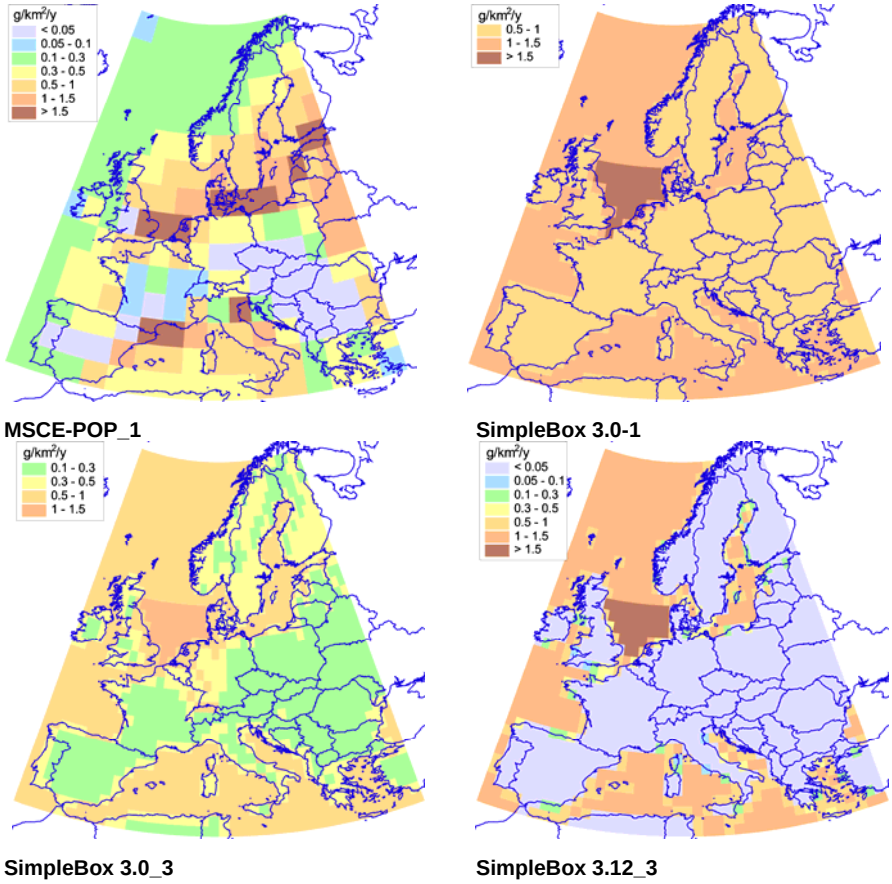


Fig. B.161. *Spatial distribution of PCB-28 net depositions calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*.

The model results obtained on the basis of zero initial concentrations in the environmental media are compared below.

Concentration in the atmosphere. The calculated fields of PCB-28 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. B.162.

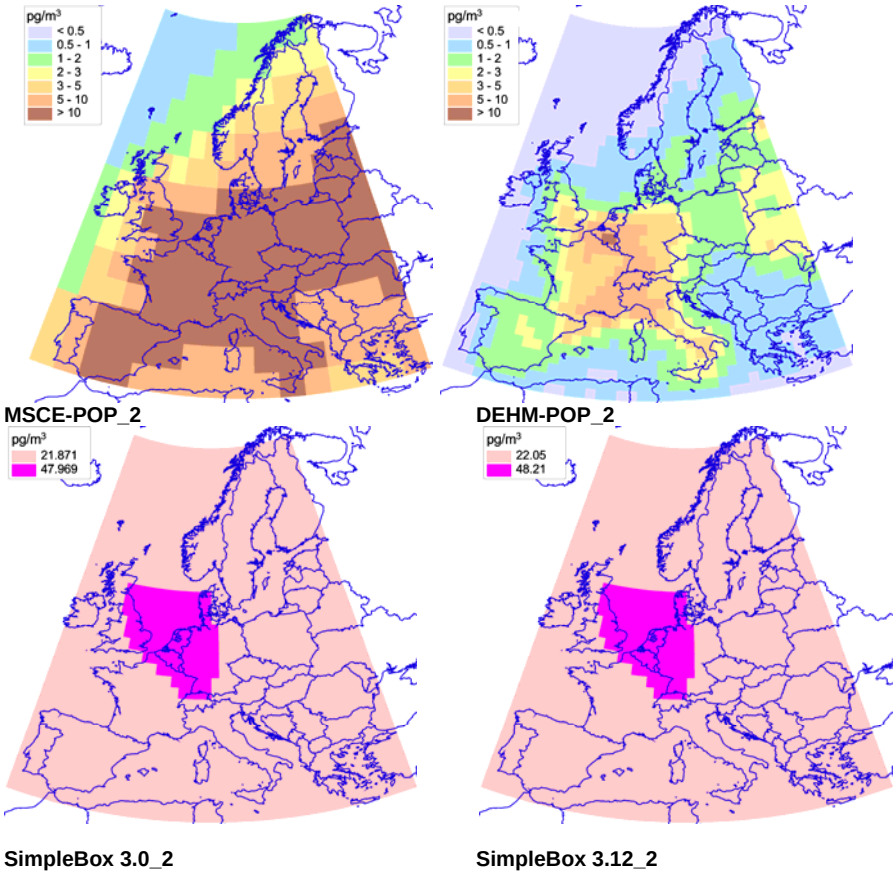


Fig. B.162. *Spatial distribution of PCB-28 concentrations in the atmosphere calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations.*

Soil concentration. The spatial distributions of PCB-28 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.B.163.

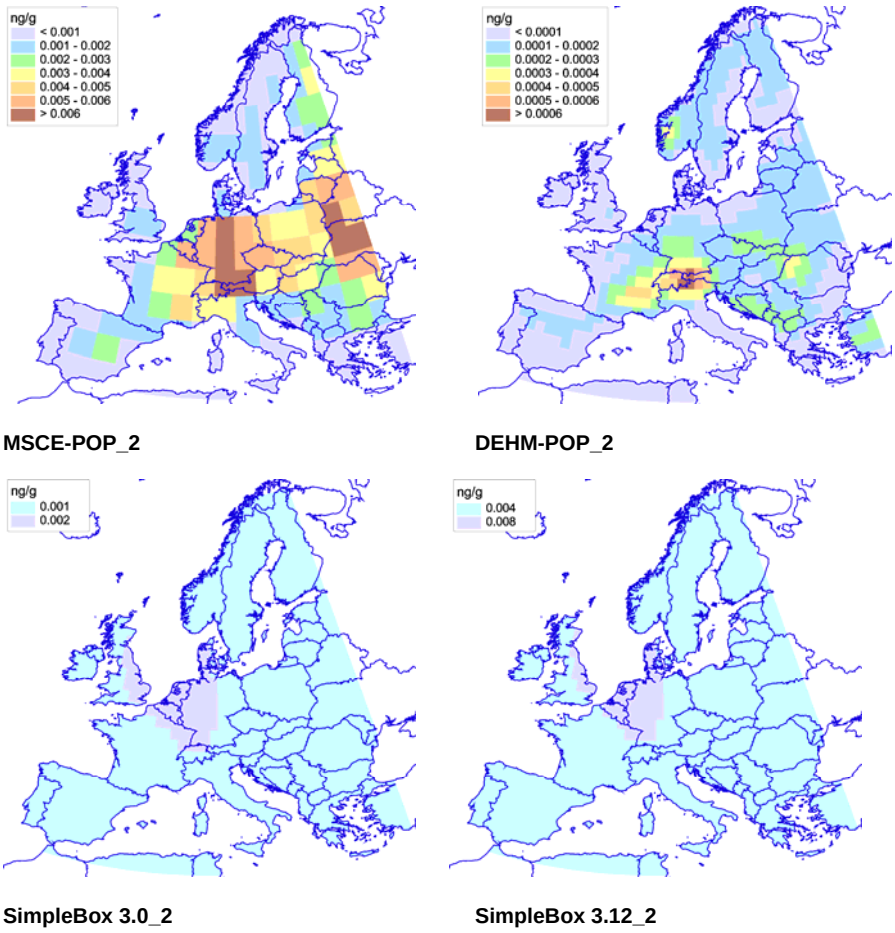


Fig. B.163. *Spatial distribution of PCB-28 concentrations in soil calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*.

Water concentration. The calculated fields of PCB-28 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. B.188.

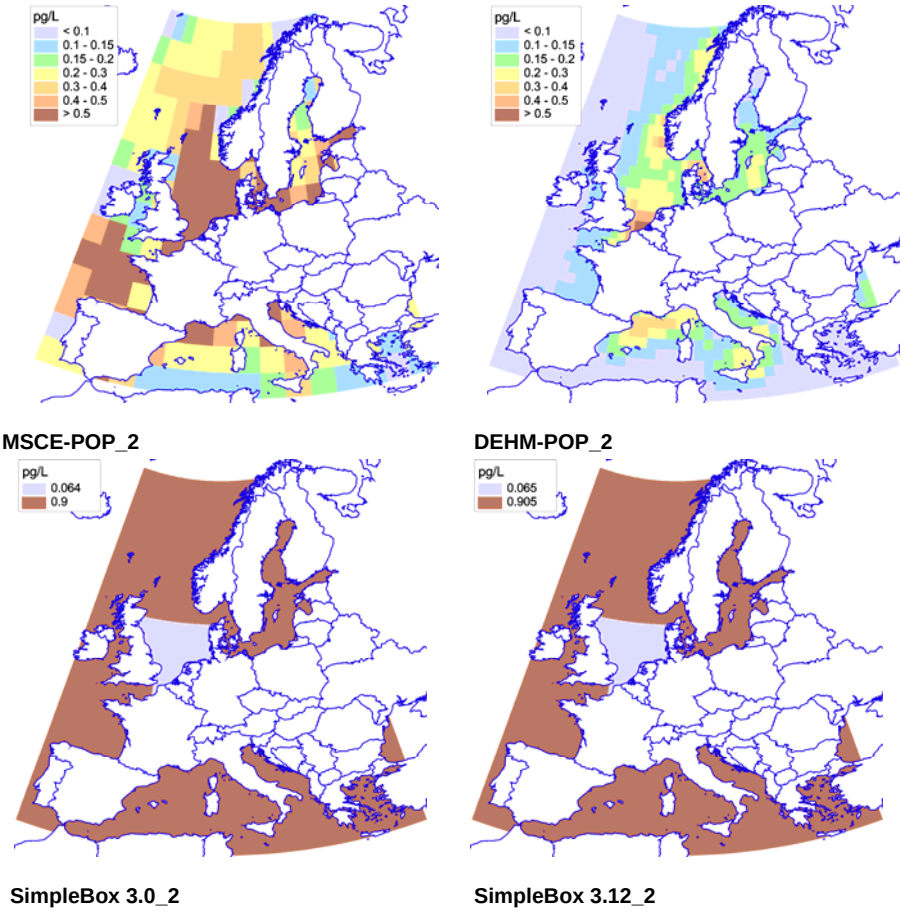
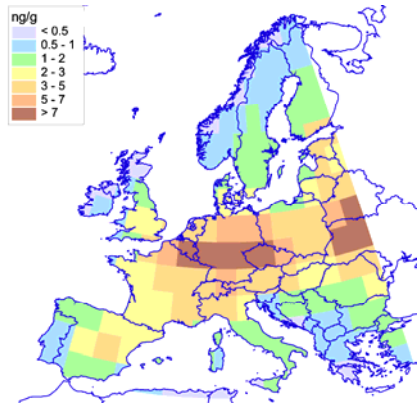
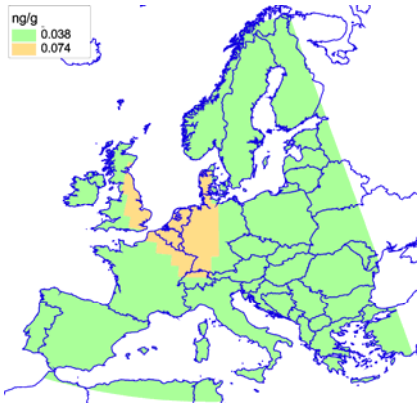


Fig. B.164. *Spatial distribution of PCB-28 concentrations in water calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

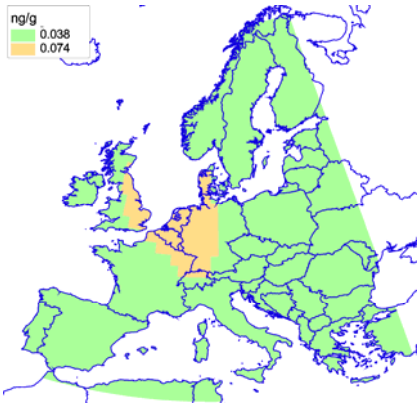
Concentration in vegetation. The spatial distributions of PCB-28 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.B.165.



MSCE-POP_2



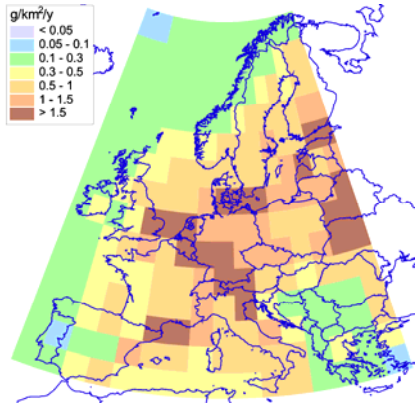
SimpleBox 3.0_2



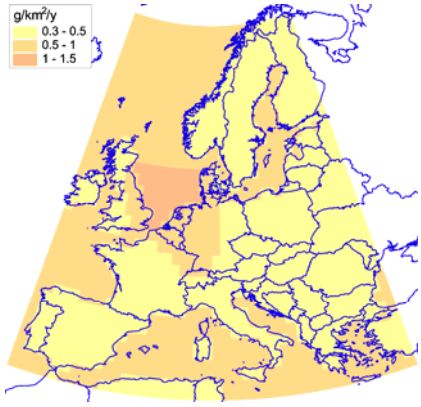
SimpleBox 3.12_2

Fig.B.165. *Spatial distribution of PCB-28 concentrations in vegetation calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

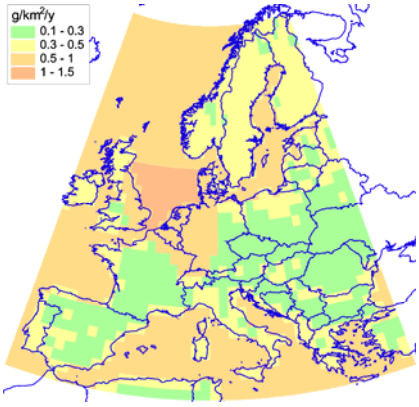
Net deposition flux. Spatial distributions of PCB-28 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.B.166. The values of net deposition flux include dry and wet depositions and gaseous exchange.



MSCE-POP_2



SimpleBox 3.0_2



SimpleBox 3.12_2

Fig. B.166. *Spatial distribution of PCB-28 net depositions calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

Annex C

COMPARISON OF RESULTS OF STAGE II COMPUTATIONAL EXPERIMENTS FOR PCB-180

A comparison of results on computational experiments of Stage II for PCB-180 obtained by the participating models is presented in this Annex. Six models participated in this comparison: CAN/POPs; CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, SimpleBox, and MSCE-POP.

C.1. Distribution of PCB-180 mass between environmental compartments

C.1.1. Comparison of calculated values of PCB-180 mass in the atmosphere

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-180 contained in the atmosphere within layers of 1 km, 5 km and 10 km height.

Reference data set. Calculation results on PCB-180 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.1.

Monthly values of PCB-180 mass contained in 1 km layer of the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.1 a and b, respectively.

Calculation results on PCB-180 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table B.2.

Monthly values of PCB-180 mass contained in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. C.2.

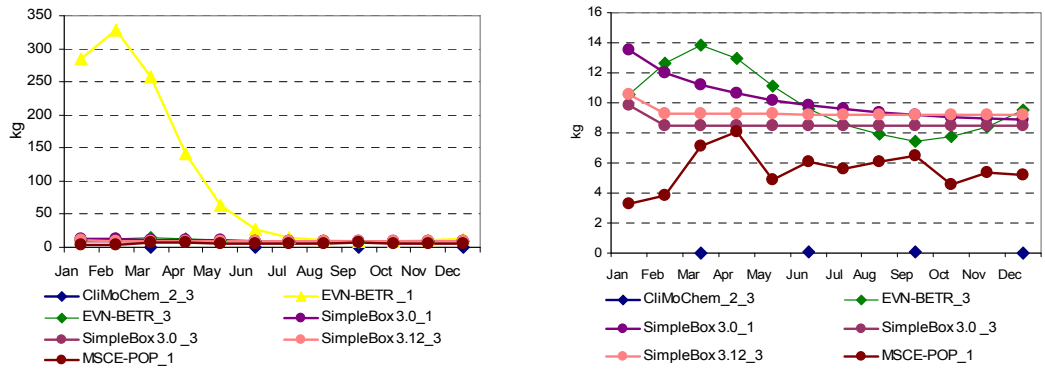


Fig. C.1a. *PCB-180 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

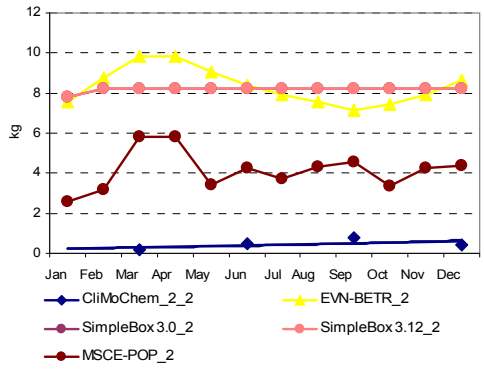


Fig. C.1b. *PCB-180 mass in the 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

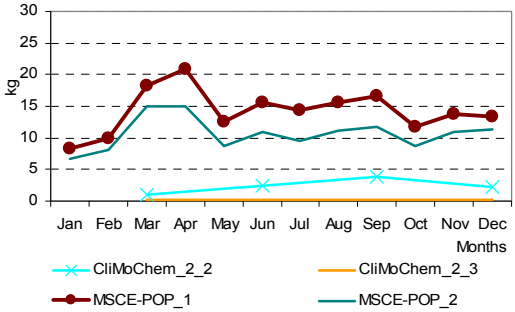


Fig. C.2. *PCB-180 mass in the 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

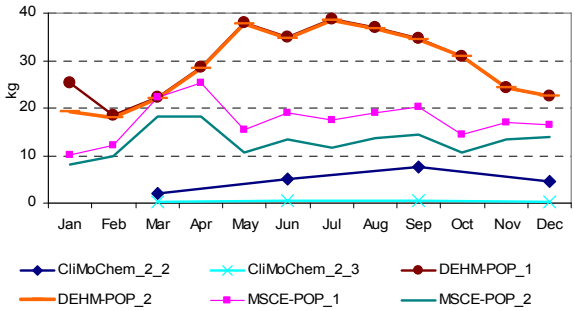


Fig. C.3. *PCB-180 mass in the 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference data set*

Table C.1. *Calculation results: PCB-180 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	EVN-BETR_1[a]	SimpleBox 3.0_1[b]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0_3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	283.93	13.50	3.24	10.57		9.814	10.55	*55.27*	*112.07*	Jan	7.56		7.80	7.80	2.60	*6.44*	*2.56*
Feb	327.42	12.04	3.83	12.66		8.498	9.27	*62.29*	*129.93*	Feb	8.74		8.21	8.21	3.18	*7.09*	*2.62*
Mar	257.02	11.23	7.13	13.83		8.490	9.26	*51.16*	*100.88*	Mar	9.87		8.21	8.21	5.83	*8.03*	*1.66*
Seas_1	**289.46**	**12.26**	**4.74**	**12.35**	**0.03**	**8.93**	**9.69**	***48.21***	***106.47***	**Seas_1**	**8.72**	**0.20**	**8.08**	**8.08**	**3.87**	***5.79***	***3.67***
Apr	141.41	10.63	8.09	12.99		8.485	9.25	*31.81*	*53.72*	Apr	9.85		8.22	8.22	5.84	*8.03*	*1.65*
May	62.92	10.18	4.89	11.10		8.480	9.24	*17.80*	*22.21*	May	9.06		8.22	8.22	3.42	*7.23*	*2.57*
Jun	27.81	9.84	6.06	9.59		8.476	9.23	*11.83*	*7.95*	Jun	8.42		8.22	8.22	4.28	*7.28*	*2.01*
Seas_2	**77.38**	**10.21**	**6.35**	**11.23**	**0.05**	**8.48**	**9.24**	***17.56***	***26.64***	**Seas_2**	**9.11**	**0.50**	**8.22**	**8.22**	**4.51**	***6.11***	***3.60***
Jul	14.83	9.57	5.58	8.58		8.472	9.23	*9.38*	*3.02*	Jul	7.95		8.22	8.22	3.70	*7.02*	*2.22*
Aug	10.47	9.37	6.07	7.92		8.469	9.22	*8.59*	*1.51*	Aug	7.54		8.22	8.22	4.33	*7.08*	*1.86*
Sep	8.89	9.20	6.46	7.41		8.467	9.22	*8.27*	*1.12*	Sep	7.11		8.22	8.22	4.58	*7.04*	*1.72*
Seas_3	**11.40**	**9.38**	**6.03**	**7.97**	**0.06**	**8.47**	**9.22**	***7.50***	***3.66***	**Seas_3**	**7.53**	**0.76**	**8.22**	**8.22**	**4.20**	***5.79***	***3.27***
Oct	9.24	9.07	4.57	7.79		8.464	9.21	*8.06*	*1.80*	Oct	7.46		8.22	8.22	3.37	*6.82*	*2.33*
Nov	10.50	8.96	5.37	8.44		8.462	9.20	*8.49*	*1.71*	Nov	7.95		8.23	8.23	4.26	*7.16*	*1.94*
Dec	13.08	8.87	5.22	9.49		8.460	9.20	*9.05*	*2.51*	Dec	8.66		8.23	8.23	4.41	*7.38*	*1.99*
Seas_4	**10.94**	**8.97**	**5.05**	**8.57**	**0.03**	**8.46**	**9.20**	***7.32***	***3.66***	**Seas_4**	**8.02**	**0.44**	**8.23**	**8.23**	**4.01**	***5.79***	***3.49***
Annual	**97.29**	**10.20**	**5.54**	**10.03**	**0.04**	**8.59**	**9.34**	***20.15***	***34.21***	**Annual**	**8.35**	**0.48**	**8.19**	**8.19**	**4.15**	***5.87***	***3.50***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.
[b] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.2. *Calculation results: PCB-180 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	8.34				Jan		6.68		
Feb	9.85				Feb		8.16		
Mar	18.31				Mar		14.97		
Seas_1	**12.17**	**0.14**	***6.16***	***8.50***	**Seas_1**	**1.02**	**9.94**	***5.48***	***6.31***
Apr	20.80				Apr		15.00		
May	12.56				May		8.78		
Jun	15.56				Jun		10.99		
Seas_2	**16.31**	**0.23**	***8.27***	***11.37***	**Seas_2**	**2.52**	**11.59**	***7.05***	***6.42***
Jul	14.33				Jul		9.50		
Aug	15.59				Aug		11.12		
Sep	16.59				Sep		11.77		
Seas_3	**15.50**	**0.28**	***7.89***	***10.77***	**Seas_3**	**3.79**	**10.80**	***7.29***	***4.96***
Oct	11.75				Oct		8.67		
Nov	13.79				Nov		10.94		
Dec	13.41				Dec		11.33		
Seas_4	**12.98**	**0.16**	***6.57***	***9.07***	**Seas_4**	**2.22**	**10.31**	***6.27***	***5.72***
Annual	14.24	**0.20**	***7.22***	***9.93***	**Annual**	**2.38**	**10.66**	***6.52***	***5.85***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Calculation results on PCB-180 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table C.3.

Monthly values of PCB-180 mass contained in 10 km layer of the atmosphere calculated by the participating models on the basis of “reference” data set are compared in Fig. C.3.

Own/alternative data set. Calculation results on PCB-180 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data sets together with statistical parameters used for evaluation are presented in Table C.4.

Monthly values of PCB-180 mass contained in 1 km layer of the atmosphere calculated by participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.4 a and b, respectively.

Calculation results on PCB-180 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data set together with statistical parameters used for evaluation are presented in Table C.5.

Monthly values of PCB-180 mass contained in 5 km layer of the atmosphere calculated by the models on the basis of “own or alternative” data sets are compared in Fig. C.5.

Calculation results on PCB-180 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of “own or alternative” data sets together with statistical parameters used for evaluation are presented in Table C.6.

Monthly values of PCB-180 mass contained in 10 km layer of the atmosphere calculated by the participating models on the basis of “own or alternative” data sets are compared in Fig. C.6.

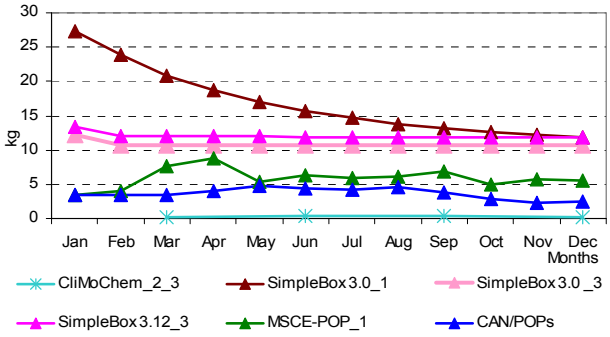


Fig. C.4a. *PCB-180 mass contained in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions*

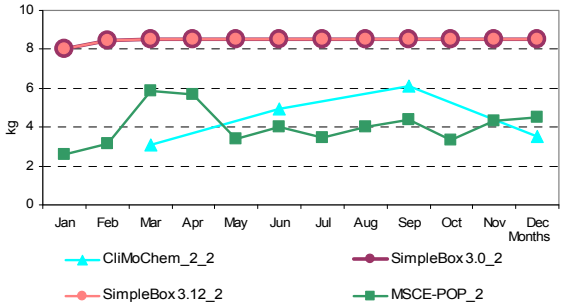


Fig. C.4b. *PCB-180 mass contained in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets and zero initial conditi*

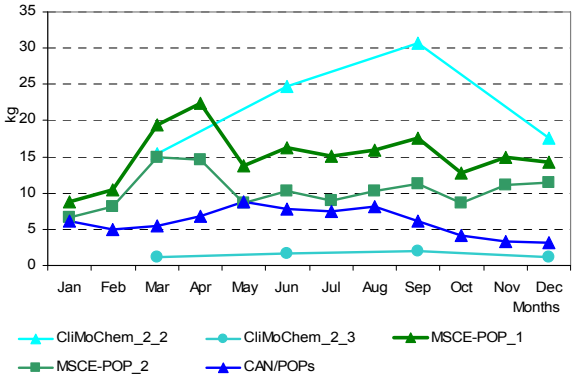


Fig. C.5. *PCB-180 mass in the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets*

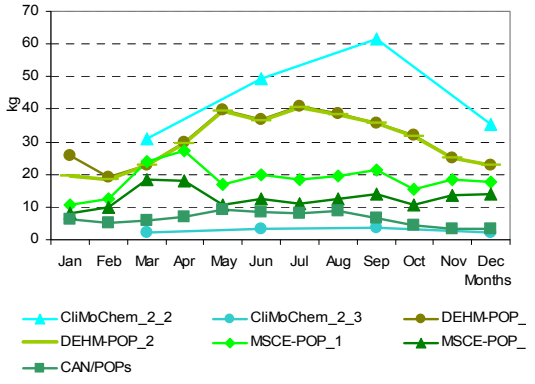


Fig. C.6. *PCB-180 mass contained in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of “own or alternative” data sets*

Table C.3. *Calculation results: PCB-180 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	25.33	10.20		*17.76*	*10.70*	Jan		19.20	8.17	*13.69*	*7.80*
Feb	18.40	12.05		*15.22*	*4.49*	Feb		18.01	9.98	*14.00*	*5.68*
Mar	22.21	22.39		*22.30*	*0.13*	Mar		21.98	18.31	*20.14*	*2.60*
Season_1	**21.98**	**14.88**	**0.29**	***12.38***	***11.06***	**Season_1**	**2.04**	**19.73**	**12.15**	***11.31***	***8.88***
Apr	28.67	25.44		*27.05*	*2.29*	Apr		28.43	18.34	*23.39*	*7.13*
May	38.03	15.37		*26.70*	*16.03*	May		37.77	10.74	*24.26*	*19.11*
Jun	34.98	19.03		*27.01*	*11.28*	Jun		34.71	13.44	*24.07*	*15.04*
Season_2	**33.89**	**19.94**	**0.45**	***18.10***	***16.80***	**Season_2**	**5.03**	**33.64**	**14.17**	***17.61***	***14.61***
Jul	38.68	17.53		*28.10*	*14.96*	Jul		38.41	11.61	*25.01*	*18.95*
Aug	36.86	19.07		*27.96*	*12.58*	Aug		36.63	13.60	*25.12*	*16.28*
Sep	34.57	20.29		*27.43*	*10.10*	Sep		34.42	14.39	*24.41*	*14.16*
Season_3	**36.70**	**18.96**	**0.55**	***18.74***	***18.08***	**Season_3**	**7.57**	**36.49**	**13.20**	***19.09***	***15.33***
Oct	31.01	14.37		*22.69*	*11.77*	Oct		30.93	10.60	*20.76*	*14.38*
Nov	24.35	16.86		*20.61*	*5.29*	Nov		24.30	13.38	*18.84*	*7.72*
Dec	22.47	16.40		*19.44*	*4.29*	Dec		22.44	13.86	*18.15*	*6.07*
Season_4	**25.94**	**15.88**	**0.31**	***14.04***	***12.91***	**Season_4**	**4.44**	**25.89**	**12.61**	***14.31***	***10.83***
Annual	**29.63**	**17.42**	**0.40**	***15.82***	***14.68***	**Annual**	**4.77**	**28.94**	**13.04**	***15.58***	***12.28***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
* - data of DEHM-POP are given for 15 km layer of the atmosphere.

Table C.4. *Calculation results: PCB-180 mass contained in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CAN/POPs	CliMo Chem_ 2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	27.26	3.45	3.53		12.21	13.37	*11.96*	*9.74*	Jan		8.03	8.03	2.59	*6.21*	*3.14*
Feb	23.83	4.04	3.47		10.78	12.01	*10.82*	*8.22*	Feb		8.48	8.48	3.17	*6.71*	*3.06*
Mar	20.92	7.58	3.42		10.76	11.98	*10.93*	*6.49*	Mar		8.49	8.49	5.84	*7.60*	*1.53*
Seas_1	**24.00**	**5.02**	**3.47**	**0.23**	**11.25**	**12.45**	***9.41***	***8.54***	**Seas_1**	**3.08**	**8.33**	**8.33**	**3.86**	***5.90***	***2.82***
Apr	18.69	8.73	4.05		10.74	11.97	*10.83*	*5.33*	Apr		8.50	8.50	5.70	*7.56*	*1.62*
May	16.99	5.34	4.84		10.73	11.95	*9.97*	*5.04*	May		8.51	8.51	3.37	*6.79*	*2.97*
Jun	15.68	6.33	4.34		10.71	11.94	*9.80*	*4.52*	Jun		8.51	8.51	4.02	*7.02*	*2.59*
Seas_2	**17.12**	**6.80**	**4.41**	**0.32**	**10.73**	**11.95**	***8.56***	***5.96***	**Seas_2**	**4.95**	**8.51**	**8.51**	**4.36**	***6.58***	***2.24***
Jul	14.65	5.87	4.22		10.70	11.93	*9.47*	*4.33*	Jul		8.52	8.52	3.46	*6.83*	*2.92*
Aug	13.82	6.20	4.62		10.69	11.92	*9.45*	*3.89*	Aug		8.52	8.52	4.03	*7.02*	*2.59*
Sep	13.15	6.84	3.86		10.68	11.91	*9.29*	*3.85*	Sep		8.53	8.53	4.40	*7.15*	*2.38*
Seas_3	**13.87**	**6.31**	**4.23**	**0.38**	**10.69**	**11.92**	***7.90***	***5.14***	**Seas_3**	**6.14**	**8.52**	**8.52**	**3.97**	***6.79***	***2.19***
Oct	12.61	4.94	2.85		10.67	11.90	*8.59*	*4.41*	Oct		8.53	8.53	3.35	*6.80*	*2.99*
Nov	12.15	5.82	2.37		10.67	11.89	*8.58*	*4.31*	Nov		8.53	8.53	4.32	*7.13*	*2.43*
Dec	11.77	5.57	2.49		10.66	11.88	*8.47*	*4.23*	Dec		8.54	8.54	4.48	*7.18*	*2.34*
Seas_4	**12.17**	**5.45**	**2.57**	**0.22**	**10.67**	**11.89**	***7.16***	***5.14***	**Seas_4**	**3.53**	**8.53**	**8.53**	**4.05**	***6.16***	***2.75***
Annual	**16.79**	**5.89**	**3.67**	**0.29**	**10.83**	**12.05**	***8.26***	***6.07***	**Annual**	**4.42**	**8.47**	**8.47**	**4.06**	***6.36***	***2.45***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.5. *Calculation results: PCB-180 mass contained in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CAN/POPs	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	8.86	6.14		*7.50*	*1.93*	Jan		6.65		
Feb	10.38	4.97		*7.68*	*3.83*	Feb		8.15		
Mar	19.48	5.48		*12.48*	*9.90*	Mar		14.99		
Seas_1	**12.91**	**5.53**	**1.15**	***6.53***	***5.94***	**Seas_1**	**15.39**	**9.93**	***12.66***	***3.86***
Apr	22.42	6.79		*14.61*	*11.05*	Apr		14.64		
May	13.73	8.77		*11.25*	*3.51*	May		8.65		
Jun	16.28	7.75		*12.01*	*6.03*	Jun		10.33		
Seas_2	**17.48**	**7.77**	**1.61**	***8.95***	***8.00***	**Seas_2**	**24.75**	**11.21**	***17.98***	***9.58***
Jul	15.09	7.41		*11.25*	*5.43*	Jul		8.90		
Aug	15.94	8.10		*12.02*	*5.54*	Aug		10.36		
Sep	17.58	6.15		*11.87*	*8.08*	Sep		11.31		
Seas_3	**16.20**	**7.22**	**1.92**	***7.22***	***7.22***	**Seas_3**	**30.71**	**10.19**	***20.45***	***14.51***
Oct	12.70	4.09		*8.40*	*6.09*	Oct		8.62		
Nov	14.96	3.30		*9.13*	*8.24*	Nov		11.11		
Dec	14.32	3.17		*8.74*	*7.89*	Dec		11.52		
Seas_4	**13.99**	**3.52**	**1.09**	***6.86***	***6.86***	**Seas_4**	**17.64**	**10.41**	***14.03***	***5.11***
Annual	**15.15**	**6.01**	**1.44**	***7.53***	***6.98***	**Annual**	**22.12**	**10.44**	***16.28***	***8.26***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table C.6. *Calculation results: PCB-180 mass contained in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	*σ*	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	CAN/POPs	CliMoChem_2_3				CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	25.68	10.84	6.43		*14.31*	*10.09*	Jan		19.37	8.13	*13.75*	*7.95*
Feb	19.00	12.70	5.26		*12.32*	*6.88*	Feb		18.48	9.96	*14.22*	*6.02*
Mar	22.97	23.83	5.80		*17.53*	*10.17*	Mar		22.69	18.34	*20.51*	*3.08*
Seas_1	**22.55**	**15.79**	**5.83**	**2.30**	***11.62***	***9.26***	**Seas_1**	**30.77**	**20.18**	**12.14**	***21.03***	***9.34***
Apr	29.83	27.42	7.11		*21.45*	*12.48*	Apr		29.56	17.90	*23.73*	*8.24*
May	39.76	16.79	9.29		*21.95*	*15.88*	May		39.48	10.58	*25.03*	*20.43*
Jun	36.82	19.91	8.37		*21.70*	*14.31*	Jun		36.56	12.64	*24.60*	*16.92*
Seas_2	**35.47**	**21.37**	**8.26**	**3.22**	***17.08***	***14.45***	**Seas_2**	**49.50**	**35.20**	**13.71**	***32.80***	***18.02***
Jul	40.73	18.45	8.10		*22.43*	*16.67*	Jul		40.46	10.89	*25.67*	*20.91*
Aug	38.69	19.49	8.85		*22.34*	*15.12*	Aug		38.47	12.67	*25.57*	*18.25*
Sep	35.87	21.50	6.75		*21.37*	*14.56*	Sep		35.73	13.84	*24.78*	*15.48*
Seas_3	**38.43**	**19.82**	**7.90**	**3.84**	***17.50***	***15.52***	**Seas_3**	**61.41**	**38.22**	**12.46**	***37.37***	***24.49***
Oct	31.89	15.54	4.37		*17.27*	*13.84*	Oct		31.81	10.54	*21.17*	*15.04*
Nov	25.01	18.29	3.48		*15.59*	*11.02*	Nov		24.97	13.59	*19.28*	*8.05*
Dec	22.98	17.51	3.28		*14.59*	*10.17*	Dec		22.96	14.08	*18.52*	*6.28*
Seas_4	**26.63**	**17.11**	**3.71**	**2.19**	***12.41***	***11.61***	**Seas_4**	**35.28**	**26.58**	**12.74**	***24.87***	***11.37***
Annual	**30.77**	**18.52**	**6.42**	**2.89**	***14.65***	***12.66***	**Annual**	**44.24**	**30.05**	**12.76**	***29.02***	***15.77***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - data of DEHM-POP are given for 15 km layer of the atmosphere.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-180 mass contained in 1, 5 and 10 km layers of the atmosphere obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables C.7-C.9.

Table C.7. *The percentage difference between calculation results on PCB-180 mass contained in 1 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			101.9%	2.9%	2.9%	24.4%	26.7%	6.3%	-0.5%
Feb			97.9%	3.2%	3.2%	26.9%	29.5%	5.4%	-0.2%
Mar			86.2%	3.3%	3.3%	26.7%	29.4%	6.4%	0.2%
Seas_1	**1411.5%**	**698.0%**	**95.8%**	**3.2%**	**3.2%**	**25.9%**	**28.5%**	**6.1%**	**-0.1%**
Apr			75.8%	3.4%	3.4%	26.6%	29.4%	7.8%	-2.4%
May			67.0%	3.5%	3.5%	26.5%	29.3%	9.3%	-1.5%
Jun			59.4%	3.6%	3.6%	26.4%	29.3%	4.6%	-6.0%
Seas_2	**883.8%**	**609.6%**	**67.6%**	**3.5%**	**3.5%**	**26.5%**	**29.3%**	**7.2%**	**-3.3%**
Jul			53.0%	3.6%	3.6%	26.3%	29.3%	5.3%	-6.3%
Aug			47.5%	3.6%	3.6%	26.2%	29.2%	2.2%	-6.9%
Sep			42.9%	3.7%	3.7%	26.2%	29.2%	6.0%	-3.9%
Seas_3	**711.2%**	**594.3%**	**47.9%**	**3.6%**	**3.6%**	**26.2%**	**29.2%**	**4.5%**	**-5.6%**
Oct			39.0%	3.7%	3.7%	26.1%	29.2%	8.1%	-0.6%
Nov			35.6%	3.7%	3.7%	26.0%	29.2%	8.5%	1.6%
Dec			32.7%	3.8%	3.8%	26.0%	29.2%	6.8%	1.6%
Seas_4	**694.9%**	**597.7%**	**35.8%**	**3.7%**	**3.7%**	**26.0%**	**29.2%**	**7.8%**	**1.0%**
Annual	**827.7%**	**617.9%**	**64.6%**	**3.5%**	**3.5%**	**26.2%**	**29.0%**	**6.4%**	**-2.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table C.8.*The percentage difference between calculation results on PCB-180 mass contained in 5 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			6.3%	-0.5%
Feb			5.4%	-0.2%
Mar			6.4%	0.2%
Seas_1	**1411.5%**	**698.0%**	**6.1%**	**-0.1%**
Apr			7.8%	-2.4%
May			9.3%	-1.5%
Jun			4.6%	-6.0%
Seas_2	**883.8%**	**609.6%**	**7.2%**	**-3.3%**
Jul			5.3%	-6.3%
Aug			2.2%	-6.9%
Sep			6.0%	-3.9%
Seas_3	**711.2%**	**594.3%**	**4.5%**	**-5.6%**
Oct			8.1%	-0.6%
Nov			8.5%	1.6%
Dec			6.8%	1.6%
Seas_4	**694.9%**	**597.7%**	**7.8%**	**1.0%**
Annual	**827.7%**	**617.9%**	**6.4%**	**-2.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table C.9. *The percentage difference between calculation results on PCB-180 mass contained in 10 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	DEHM-POP_1	DEHM-POP_2	MSCE-POP_1	MSCE-POP_2
Jan			1.4%	0.9%	6.3%	-0.5%
Feb			3.3%	2.6%	5.4%	-0.2%
Mar			3.4%	3.2%	6.4%	0.2%
Seas_1	**1411.5%**	**698.0%**	**2.6%**	**2.3%**	**6.1%**	**-0.1%**
Apr			4.0%	4.0%	7.8%	-2.4%
May			4.5%	4.5%	9.3%	-1.5%
Jun			5.3%	5.3%	4.6%	-6.0%
Seas_2	**883.8%**	**609.6%**	**4.7%**	**4.6%**	**7.2%**	**-3.3%**
Jul			5.3%	5.3%	5.3%	-6.3%
Aug			5.0%	5.0%	2.2%	-6.9%
Sep			3.8%	3.8%	6.0%	-3.9%
Seas_3	**711.2%**	**594.3%**	**4.7%**	**4.8%**	**4.5%**	**-5.6%**
Oct			2.8%	2.8%	8.1%	-0.6%
Nov			2.7%	2.8%	8.5%	1.6%
Dec			2.3%	2.3%	6.8%	1.6%
Seas_4	**694.9%**	**597.7%**	**2.6%**	**2.7%**	**7.8%**	**1.0%**
Annual	**827.7%**	**617.9%**	**3.8%**	**3.8%**	**6.4%**	**-2.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data; DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data. MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

C.1.2. Comparison of calculated values of PCB-180 mass in soil

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-180 contained in soil within 5 cm and 10 cm depth.

Reference data set. Calculation results on PCB-180 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.10.

Monthly values of PCB-180 mass contained in 5cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.7a and b, respectively.

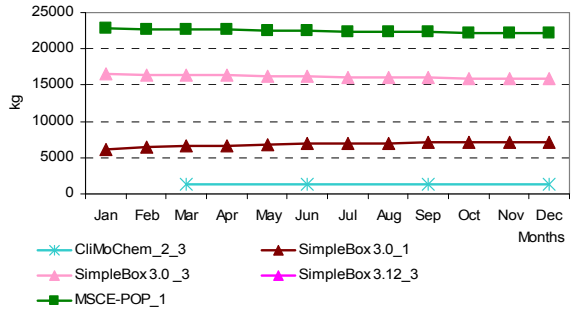


Fig. C.7a. *PCB-180 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

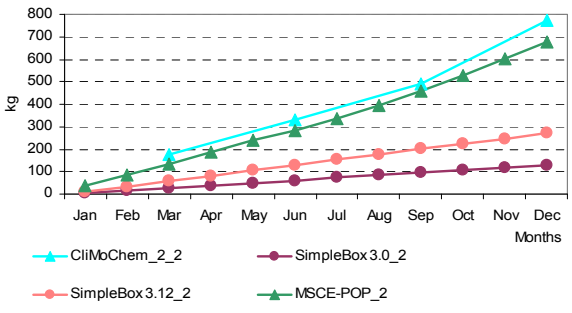


Fig. C.7b. *PCB-180 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Calculation results on PCB-180 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of “reference” data set together with statistical parameters used for evaluation are presented in Table C.11.

Monthly values of PCB-180 mass contained in 10 cm layer of soil calculated by the participating models on the basis of “reference” data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.8a and b, respectively.

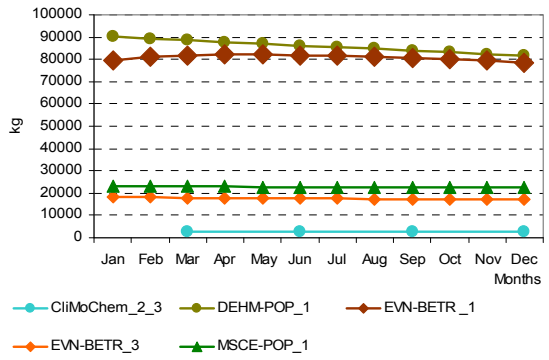


Fig. C.8a. *PCB-180 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and non-zero initial conditions*

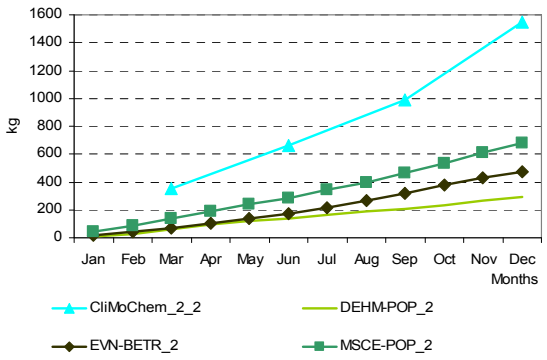


Fig. C.8b. *PCB-180 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of “reference” data set and zero initial conditions*

Table C.10. *Calculation results: PCB-180 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	Simple Box 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6160.7	22829.2		16493.9	271374.7	*79214.7*	*128290.8*	Jan		5.2	11.0	38.9	*18.4*	*18.0*
Feb	6379.7	22763.8		16433.3	270154.4	*78932.8*	*127659.5*	Feb		16.2	34.4	86.3	*45.6*	*36.4*
Mar	6552.3	22692.0		16373.6	268937.0	*78638.7*	*127039.2*	Mar		27.2	57.9	133.8	*73.0*	*54.8*
Seas_1	**6364.2**	**22761.7**	**1356.7**	**16433.6**	**270155.4**	***63414.3***	***115874.5***	**Seas_1**	**177.4**	**16.2**	**34.5**	**86.3**	***78.6***	***72.2***
Apr	6693.0	22626.8		16312.2	267934.9	*78391.7*	*126531.9*	Apr		38.5	80.6	185.9	*101.7*	*76.0*
May	6805.6	22558.1		16251.3	266480.4	*78023.9*	*125804.3*	May		49.7	105.7	237.8	*131.0*	*96.6*
Jun	6897.4	22477.4		16191.0	265262.1	*77707.0*	*125200.4*	Jun		60.9	129.5	283.1	*157.8*	*113.8*
Seas_2	**6798.7**	**22554.1**	**1328.4**	**16251.5**	**266559.1**	***62698.4***	***114257.5***	**Seas_2**	**330.4**	**49.7**	**105.2**	**235.6**	***180.2***	***126.9***
Jul	6971.0	22403.0		16130.9	264052.7	*77389.4*	*124603.4*	Jul		72.1	153.2	337.6	*187.6*	*136.0*
Aug	7032.5	22335.5		16070.0	260637.1	*76518.8*	*122906.2*	Aug		83.5	177.3	393.3	*218.0*	*158.9*
Sep	7081.3	22296.1		16010.1	261633.5	*76755.2*	*123410.1*	Sep		94.6	200.9	460.3	*251.9*	*188.1*
Seas_3	**7028.3**	**22344.9**	**1301.3**	**16070.3**	**262107.8**	***61770.5***	***112284.4***	**Seas_3**	**493.1**	**83.4**	**177.1**	**397.1**	***287.7***	***189.8***
Oct	7120.7	22253.4		15950.6	260443.0	*76441.9*	*122824.3*	Oct		105.7	224.4	526.1	*285.4*	*216.7*
Nov	7152.3	22234.7		15891.0	259254.6	*76133.2*	*122237.5*	Nov		116.8	247.9	603.4	*322.7*	*251.8*
Dec	7176.5	22208.6		15832.6	258095.0	*75828.2*	*121667.3*	Dec		127.7	271.3	675.1	*358.0*	*283.8*
Seas_4	**7149.8**	**22232.3**	**1282.1**	**15891.4**	**259264.2**	***61164.0***	***111031.9***	**Seas_4**	**775.2**	**116.8**	**247.9**	**601.5**	***435.3***	***305.4***
Annual	**6835.3**	**22473.2**	**1317.1**	**16161.7**	**264521.6**	***62261.8***	***113362.0***	**Annual**	**444.0**	**66.5**	**141.2**	**330.1**	***245.5***	***172.7***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-180 mass contained in 5cm layer of soil (kg) calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.12.

Monthly values of PCB-180 mass contained in 5cm layer of soil calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.9a and b, respectively.

Calculation results on PCB-180 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.13.

Monthly values of PCB-180 mass contained in 10 cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.10a and b, respectively.

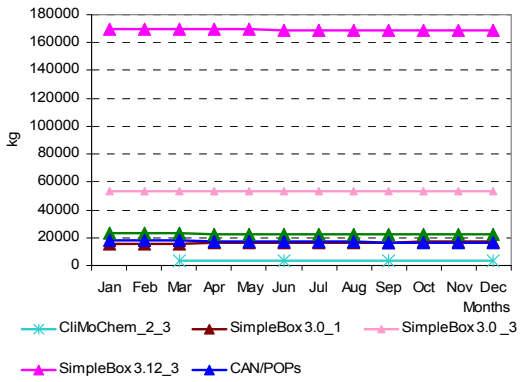


Fig. C.9a. *PCB-180 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

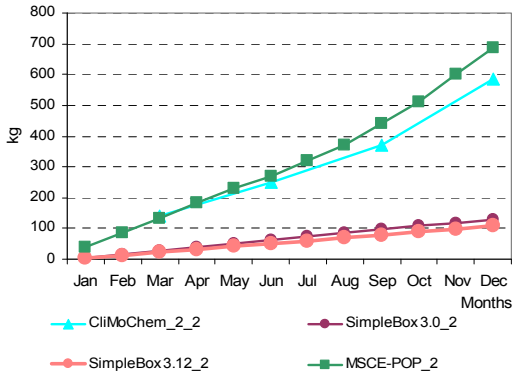


Fig. C.9b. *PCB-180 mass contained in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

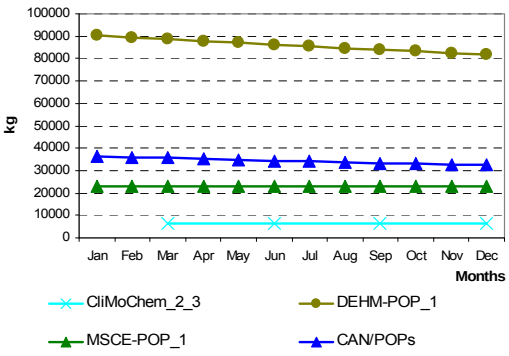


Fig. C.10a. *PCB-180 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

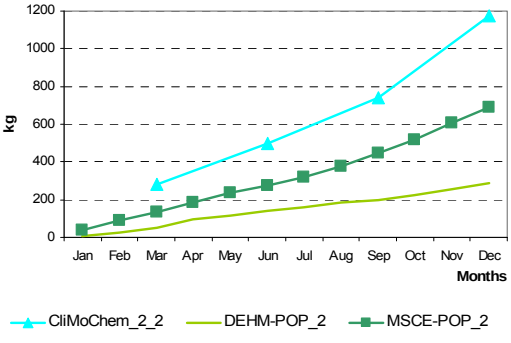


Fig. C.10b. *PCB-180 mass contained in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial condition*

Table C.11. *Calculation results: PCB-180 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	EVN-BETR_1[b]	EVN-BETR_3[b]	CliMoChem_2_3				EVN-BETR_2[a]	CliMo Chem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	90190.0	23078.8	79703.7	18210.8		*52795.8*	*37423.7*	Jan	18.4		8.5	39.3	*22.1*	*15.7*
Feb	89390.0	23012.6	81123.7	18082.0		*52902.1*	*37566.1*	Feb	42.4		29.9	87.3	*53.2*	*30.2*
Mar	88610.0	22940.1	81962.8	17955.7		*52867.1*	*37587.9*	Mar	69.6		56.2	135.2	*87.0*	*42.3*
Seas_1	**89396.7**	**23010.5**	**80930.1**	**18082.8**	**2713.4**	***42826.7***	***39479.9***	**Seas_1**	**43.4**	**354.7**	**31.5**	**87.3**	***129.2***	***152.2***
Apr	87830.0	22874.1	82268.0	17831.6		*52700.9*	*37477.9*	Apr	100.0		96.8	188.0	*128.2*	*51.8*
May	87030.0	22804.7	82195.1	17709.8		*52434.9*	*37266.0*	May	133.6		120.5	240.4	*164.8*	*65.8*
Jun	86240.0	22723.1	81893.1	17590.1		*52111.6*	*37000.5*	Jun	170.2		141.0	286.1	*199.1*	*76.8*
Seas_2	**87033.3**	**22800.6**	**82118.7**	**17710.5**	**2656.9**	***42464.0***	***39188.4***	**Seas_2**	**134.6**	**660.8**	**119.4**	**238.2**	***288.2***	***253.9***
Jul	85470.0	22647.8	81470.8	17475.1		*51766.0*	*36706.4*	Jul	212.0		165.0	341.3	*239.4*	*91.3*
Aug	84700.0	22579.7	80989.4	17369.6		*51409.7*	*36391.9*	Aug	263.4		187.7	397.6	*282.9*	*106.3*
Sep	83930.0	22539.8	80469.3	17271.1		*51052.6*	*36057.5*	Sep	321.4		205.9	465.3	*330.9*	*130.0*
Seas_3	**84700.0**	**22589.1**	**80976.5**	**17371.9**	**2602.6**	***41648.0***	***38331.8***	**Seas_3**	**265.6**	**986.2**	**186.2**	**401.4**	***459.8***	***362.0***
Oct	83190.0	22496.7	79918.1	17172.8		*50694.4*	*35724.9*	Oct	378.7		230.3	531.8	*380.3*	*150.8*
Nov	82440.0	22477.7	79339.4	17069.5		*50331.6*	*35377.0*	Nov	429.8		264.8	610.0	*434.9*	*172.6*
Dec	81710.0	22451.4	78736.5	16959.4		*49964.3*	*35032.9*	Dec	472.6		293.6	682.5	*482.9*	*194.6*
Seas_4	**82446.7**	**22475.3**	**79331.3**	**17067.2**	**2564.3**	***40777.0***	***37350.1***	**Seas_4**	**427.1**	**1550.3**	**262.9**	**608.1**	***712.1***	***576.3***
Annual	**85894.2**	**22718.9**	**80839.2**	**17558.1**	**2634.3**	***41928.9***	***38581.0***	**Annual**	**217.7**	**888.0**	**150.0**	**333.7**	***397.36***	***335.78***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - data of DEHM-POP are given for 15 cm layer of soil;
[b] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.

Table C.12. *Calculation results: PCB-180 mass contained in 5cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	CAN/POPs	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	15442.7	18190.8	22879.2		53549.2	169686.1	*55949.6*	*65387.2*	Jan		5.1	4.2	38.7	*16.0*	*19.7*
Feb	15704.6	18002.5	22858.5		53530.1	169585.5	*55936.3*	*65333.1*	Feb		16.0	13.3	85.8	*38.4*	*41.1*
Mar	15922.3	17800.3	22833.4		53513.9	169487.6	*55911.5*	*65289.8*	Mar		27.0	22.4	132.8	*60.8*	*62.4*
Seas_1	**15689.9**	**17997.9**	**22857.0**	**3334.2**	**53531.1**	**169586.4**	***47166.1***	***62259.1***	**Seas_1**	**139.9**	**16.0**	**13.3**	**85.8**	***63.8***	***60.8***
Apr	16107.8	17599.5	22808.7		53497.3	169418.8	*55886.4*	*65264.2*	Apr		38.3	31.3	183.1	*84.3*	*85.7*
May	16265.9	17387.0	22777.6		53479.6	169288.7	*55839.8*	*65218.9*	May		49.7	41.2	231.4	*107.4*	*107.5*
Jun	16402.4	17183.9	22721.9		53461.1	169188.2	*55791.5*	*65191.8*	Jun		61.1	50.6	270.1	*127.3*	*123.8*
Seas_2	**16258.7**	**17390.1**	**22769.4**	**3331.0**	**53479.3**	**169298.6**	***47087.9***	***62152.6***	**Seas_2**	**247.9**	**49.7**	**41.1**	**228.2**	***141.7***	***111.6***
Jul	16521.2	16991.4	22673.4		53444.2	169088.6	*55743.8*	*65165.4*	Jul		72.6	60.1	318.5	*150.4*	*145.7*
Aug	16626.7	16814.8	22635.9		53427.4	168786.4	*55658.2*	*65049.4*	Aug		84.3	69.8	369.9	*174.6*	*169.2*
Sep	16718.4	16649.8	22642.6		53408.9	168887.4	*55661.4*	*65103.6*	Sep		95.8	79.3	439.1	*204.7*	*203.1*
Seas_3	**16622.1**	**16818.7**	**22650.6**	**3325.9**	**53426.8**	**168920.8**	***46960.8***	***62032.3***	**Seas_3**	**369.1**	**84.2**	**69.7**	**375.8**	***224.7***	***170.7***
Oct	16800.2	16490.0	22654.1		53390.7	168791.1	*55625.2*	*65072.2*	Oct		107.4	88.8	511.0	*235.7*	*238.6*
Nov	16872.9	16339.1	22699.0		53374.4	168690.5	*55595.2*	*65034.8*	Nov		119.0	98.4	599.4	*272.3*	*283.5*
Dec	16936.9	16191.0	22741.3		53357.9	168592.5	*55563.9*	*64999.9*	Dec		130.4	107.9	685.0	*307.8*	*326.9*
Seas_4	**16870.0**	**16340.0**	**22698.1**	**3330.7**	**53374.3**	**168691.3**	***46884.1***	***61959.3***	**Seas_4**	**586.4**	**118.9**	**98.4**	**598.4**	***350.5***	***279.5***
Annual	**16360.2**	**17136.7**	**22743.8**	**3330.4**	**53452.9**	**169124.3**	***47024.7***	***62099.9***	**Annual**	**335.8**	**67.2**	**55.6**	**322.1**	***195.2***	***154.6***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.13. *Calculation results: PCB-180 mass contained in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	DEHM-POP_1[a]	MSCE-POP_1	CAN/POPs[b]	CliMoChem_2_3				CliMoChem_2_2	DEHM-POP_2[a]	MSCE-POP_2		
Jan	90190.0	23129.3	36371.4		*49896.9*	*35517.5*	Jan		7.9	39.1	*23.5*	*22.1*
Feb	89390.0	23108.4	35998.2		*49498.9*	*35142.8*	Feb		28.1	86.8	*57.4*	*41.5*
Mar	88610.0	23083.0	35614.9		*49102.6*	*34783.4*	Mar		53.6	134.3	*94.0*	*57.0*
Seas_1	**89396.7**	**23106.9**	**35994.8**	**6668.3**	***38791.7***	***35807.9***	**Seas_1**	**279.8**	**29.9**	**86.7**	***132.1***	***131.0***
Apr	87830.0	23058.0	35232.7		*48706.9*	*34424.1*	Apr		94.2	185.1	*139.6*	*64.3*
May	87030.0	23026.5	34840.8		*48299.1*	*34058.1*	May		117.5	234.0	*175.7*	*82.3*
Jun	86240.0	22970.2	34459.7		*47890.0*	*33705.3*	Jun		137.5	273.0	*205.3*	*95.8*
Seas_2	**87033.3**	**23018.3**	**34844.4**	**6662.1**	***37889.5***	***34740.4***	**Seas_2**	**495.7**	**116.4**	**230.7**	***280.9***	***194.6***
Jul	85470.0	22921.3	34090.0		*47493.8*	*33359.1*	Jul		160.7	322.0	*241.3*	*114.0*
Aug	84700.0	22883.3	33735.1		*47106.1*	*33006.3*	Aug		182.5	373.9	*278.2*	*135.4*
Sep	83920.0	22890.0	33396.5		*46735.5*	*32628.4*	Sep		200.2	443.9	*322.0*	*172.3*
Seas_3	**84696.7**	**22898.2**	**33740.5**	**6651.8**	***36996.8***	***33692.1***	**Seas_3**	**738.2**	**181.1**	**379.9**	***433.1***	***282.3***
Oct	83180.0	22901.7	33064.9		*46382.2*	*32270.4*	Oct		224.1	516.6	*370.3*	*206.8*
Nov	82440.0	22947.1	32744.1		*46043.7*	*31898.5*	Nov		258.1	605.9	*432.0*	*246.0*
Dec	81700.0	22989.8	32427.5		*45705.8*	*31527.1*	Dec		286.1	692.4	*489.3*	*287.3*
Seas_4	**82440.0**	**22946.2**	**32745.5**	**6661.4**	***36198.3***	***32651.0***	**Seas_4**	**1172.7**	**256.1**	**605.0**	***677.9***	***462.7***
Annual	**85891.7**	**22992.4**	**34331.3**	**6660.9**	***37469.1***	***34221.4***	**Annual**	**671.6**	**145.9**	**325.6**	***381.0***	***267.2***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] – data of DEHM-POP are given for 15 cm layer of soil;
[b] - in CAN/POPs results the second layer of soil is applied as 5cm.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-180 masses contained in soil within 5 and 10 cm layers obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables C.14-C.15.

Table C.14. *The percentage difference between calculation results on PCB-180 masses contained within 5 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			150.7%	-1.6%	-61.7%	224.7%	-37.5%	0.2%	-0.5%
Feb			146.2%	-1.1%	-61.4%	225.7%	-37.2%	0.4%	-0.6%
Mar			143.0%	-0.7%	-61.3%	226.8%	-37.0%	0.6%	-0.7%
Seas_1	**-21.1%**	**145.8%**	**146.5%**	**-0.9%**	**-61.4%**	**225.7%**	**-37.2%**	**0.4%**	**-0.6%**
Apr			140.7%	-0.3%	-61.1%	228.0%	-36.8%	0.8%	-1.5%
May			139.0%	0.0%	-61.0%	229.1%	-36.5%	1.0%	-2.7%
Jun			137.8%	0.3%	-60.9%	230.2%	-36.2%	1.1%	-4.6%
Seas_2	**-25.0%**	**150.8%**	**139.1%**	**0.1%**	**-61.0%**	**229.1%**	**-36.5%**	**1.0%**	**-3.1%**
Jul			137.0%	0.7%	-60.8%	231.3%	-36.0%	1.2%	-5.7%
Aug			136.4%	1.0%	-60.6%	232.5%	-35.2%	1.3%	-6.0%
Sep			136.1%	1.3%	-60.5%	233.6%	-35.4%	1.6%	-4.6%
Seas_3	**-25.1%**	**155.6%**	**136.5%**	**1.0%**	**-60.6%**	**232.5%**	**-35.6%**	**1.4%**	**-5.3%**
Oct			135.9%	1.5%	-60.4%	234.7%	-35.2%	1.8%	-2.9%
Nov			135.9%	1.8%	-60.3%	235.9%	-34.9%	2.1%	-0.7%
Dec			136.0%	2.1%	-60.2%	237.0%	-34.7%	2.4%	1.5%
Seas_4	**-24.4%**	**159.8%**	**135.9%**	**1.9%**	**-60.3%**	**235.9%**	**-34.9%**	**2.1%**	**-0.5%**
Annual	**-24.4%**	**152.9%**	**139.3%**	**1.1%**	**-60.6%**	**230.7%**	**-36.1%**	**1.2%**	**-2.4%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table C.15. *The percentage difference between calculation results on PCB-180 mass contained within 10 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	DEHM-POP_1	DEHM-POP_2	MSCE-POP_1	MSCE-POP_2
Jan			0.00%	-7.91%	0.2%	-0.5%
Feb			0.00%	-6.25%	0.4%	-0.6%
Mar			0.00%	-4.49%	0.6%	-0.7%
Seas_1	**-21.1%**	**145.8%**	**0.00%**	**-5.35%**	**0.4%**	**-0.6%**
Apr			0.00%	-2.70%	0.8%	-1.5%
May			0.00%	-2.49%	1.0%	-2.7%
Jun			0.00%	-2.48%	1.1%	-4.6%
Seas_2	**-25.0%**	**150.8%**	**0.00%**	**-2.54%**	**1.0%**	**-3.1%**
Jul			0.00%	-2.61%	1.2%	-5.7%
Aug			0.00%	-2.77%	1.3%	-6.0%
Sep			-0.01%	-2.77%	1.6%	-4.6%
Seas_3	**-25.1%**	**155.6%**	**0.00%**	**-2.72%**	**1.4%**	**-5.3%**
Oct			-0.01%	-2.69%	1.8%	-2.9%
Nov			0.00%	-2.53%	2.1%	-0.7%
Dec			-0.01%	-2.55%	2.4%	1.5%
Seas_4	**-24.4%**	**159.8%**	**-0.01%**	**-2.59%**	**2.1%**	**-0.5%**
Annual	**-24.4%**	**152.9%**	**0.00%**	**-2.77%**	**1.2%**	**-2.4%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.

C.1.3. Comparison of calculated values of PCB-180 mass in water

According to the programme of Stage II model results of computational experiments on mass balance include masses of PCB-180 contained in sea within a layer of 200 m depth.

Reference data set. Calculation results on PCB-180 mass contained in 200 m layer of seawater (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.16.

Monthly values of PCB-180 mass contained in 200 m layer of seawater calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.11a and b, respectively.

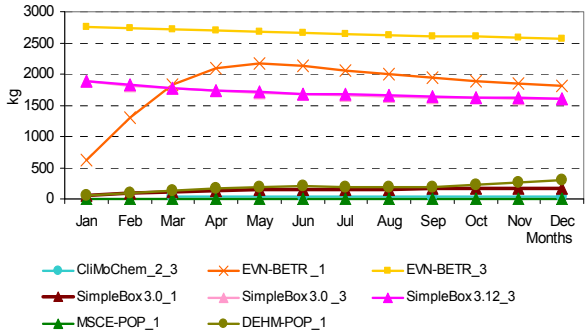


Fig. C.11a. *PCB-180 mass contained in 200 m layer of seawater (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

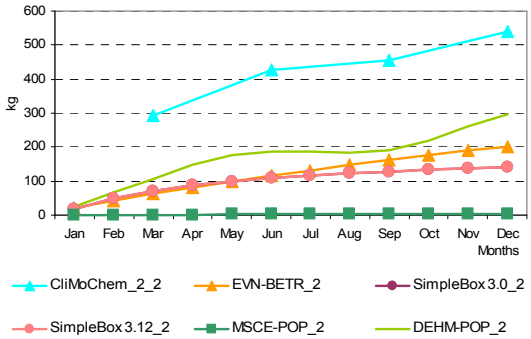


Fig. C.11b. *PCB-180 mass contained in 200 m layer of seawater (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass contained in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.17.

Monthly values of PCB-180 mass contained in 200 m layer of water calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.12a and b, respectively.

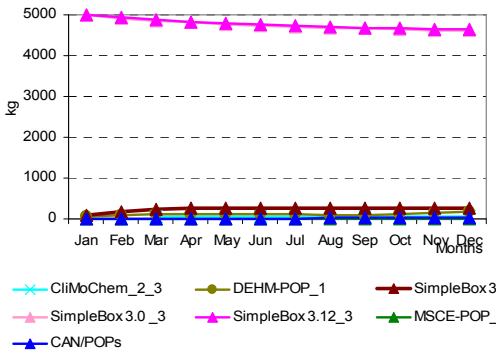


Fig. C.12a. *PCB-180 mass contained in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

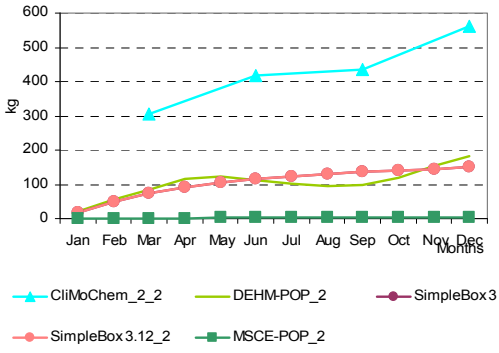


Fig. C.12b. *PCB-180 mass contained in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table C.16. *Calculation results: PCB-180 mass contained in 200 m layer of seawater (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations						*m*	σ
	DEHM-POP_1	MSCE-POP_1	EVN-BETR_1[a]	SimpleBox 3.0_1[b]	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	DEHM-POP_2	MSCE-POP_2		
Jan	51.61	0.46	621.67	52.91	2757.49		1886.26	1888.04	*1036.92*	*1124.87*	Jan	22.70		17.47	17.47	23.19	0.37	16.24	9.29
Feb	92.08	0.67	1302.24	94.37	2738.14		1818.56	1823.46	*1124.22*	*1079.80*	Feb	42.88		48.35	48.34	65.36	0.55	41.09	24.19
Mar	127.70	1.05	1827.46	120.26	2717.57		1768.15	1775.32	*1191.07*	*1088.05*	Mar	62.07		70.92	70.91	104.20	0.88	61.80	37.67
Seas_1	**90.46**	**0.73**	**1250.46**	**89.18**	**2737.74**	**39.02**	**1824.32**	**1828.94**	***982.61***	***1070.75***	**Seas_1**	**42.55**	**292.92**	**45.58**	**45.57**	**64.25**	**0.60**	**81.91**	**105.49**
Apr	168.40	1.85	2097.48	136.70	2697.06		1729.63	1738.48	*1224.23*	*1098.74*	Apr	80.98		87.85	87.85	148.10	1.53	81.26	52.23
May	193.40	2.90	2165.12	146.81	2677.58		1700.27	1710.38	*1228.06*	*1093.58*	May	99.15		100.47	100.47	176.50	2.36	95.79	61.84
Jun	199.70	3.17	2128.66	153.05	2659.35		1677.23	1688.28	*1215.63*	*1079.02*	Jun	115.96		110.09	110.08	186.30	2.54	105.00	65.72
Seas_2	**187.17**	**2.64**	**2130.42**	**145.52**	**2678.00**	**37.73**	**1702.37**	**1712.38**	***1074.53***	***1092.93***	**Seas_2**	**98.69**	**427.21**	**99.47**	**99.47**	**170.30**	**2.15**	**149.55**	**146.19**
Jul	196.40	3.38	2060.32	156.94	2642.34		1658.71	1670.44	*1198.36*	*1062.96*	Jul	131.56		117.58	117.58	186.20	2.71	111.12	66.88
Aug	193.00	3.76	1993.30	159.48	2627.04		1643.08	1655.40	*1182.15*	*1048.41*	Aug	147.04		123.68	123.67	185.20	2.96	116.51	68.28
Sep	197.00	4.97	1934.46	161.23	2611.87		1629.93	1642.72	*1168.88*	*1034.41*	Sep	161.49		128.63	128.62	190.70	3.88	122.66	71.27
Seas_3	**195.47**	**4.04**	**1996.03**	**159.21**	**2627.08**	**34.30**	**1643.90**	**1656.19**	***1039.53***	***1052.27***	**Seas_3**	**146.69**	**455.91**	**123.29**	**123.29**	**187.37**	**3.18**	**173.29**	**151.47**
Oct	225.50	5.54	1885.47	162.57	2596.92		1618.34	1631.53	*1160.84*	*1018.53*	Oct	175.41		132.83	132.83	220.20	4.26	133.11	80.59
Nov	266.00	6.15	1846.40	163.75	2582.40		1607.88	1621.39	*1156.28*	*1002.57*	Nov	189.46		136.53	136.52	261.40	4.72	145.73	94.00
Dec	299.10	6.54	1815.61	164.87	2566.74		1598.34	1612.14	*1151.91*	*988.83*	Dec	202.78		139.79	139.79	295.10	5.10	156.51	105.87
Seas_4	**263.53**	**6.08**	**1849.16**	**163.73**	**2582.02**	**35.13**	**1608.18**	**1621.69**	***1016.19***	***1009.86***	**Seas_4**	**189.22**	**540.14**	**136.38**	**136.38**	**258.90**	**4.69**	**210.95**	**181.55**
Annual	**184.16**	**3.37**	**1806.52**	**139.41**	**2656.21**	**36.55**	**1694.70**	**1704.80**	***1028.21***	***1048.41***	**Annual**	**119.29**	**429.05**	**101.18**	**101.18**	**170.20**	**2.65**	**153.93**	**145.33**

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
[b] - SimpleBox data presented here are masses calculated for continental level.

Table C.17. *Calculation results: PCB-180 mass contained in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data				Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	DEHM-POP_1	SimpleBox 3.0_1[a]	CAN/ POPs	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	DEHM-POP_2	MSCE-POP_2		
Jan	48.88	84.77	9.76	0.49		4996.43	4998.33	*1689.78*	*2562.23*	Jan		17.37	17.37	22.11	0.37	*14.31*	*9.56*
Feb	79.77	175.97	10.17	0.71		4920.35	4927.58	*1685.76*	*2509.09*	Feb		48.76	48.76	57.43	0.55	*38.88*	*25.88*
Mar	103.40	229.26	10.51	1.11		4860.89	4871.73	*1679.48*	*2469.88*	Mar		72.35	72.34	85.84	0.88	*57.85*	*38.51*
Seas_1	**77.35**	**163.33**	**10.14**	**0.77**	**63.47**	**4925.89**	**4932.55**	***1453.36***	***2375.06***	**Seas_1**	**304.02**	**46.16**	**46.16**	**55.13**	**0.60**	***90.41***	***121.30***
Apr	128.40	259.17	10.93	1.93		4812.88	4826.32	*1673.27*	*2438.93*	Apr		90.49	90.48	115.00	1.51	*74.37*	*49.93*
May	132.30	273.68	11.50	2.98		4773.93	4789.37	*1663.96*	*2416.96*	May		104.32	104.31	122.70	2.28	*83.40*	*54.77*
Jun	118.80	279.05	12.48	3.22		4741.78	4758.39	*1652.29*	*2401.61*	Jun		115.06	115.06	112.60	2.42	*86.29*	*55.92*
Seas_2	**126.50**	**270.63**	**11.64**	**2.71**	**60.26**	**4776.20**	**4791.36**	***1434.18***	***2289.98***	**Seas_2**	**416.85**	**103.29**	**103.28**	**116.77**	**2.07**	***148.45***	***156.96***
Jul	104.90	279.09	13.97	3.43		4713.97	4732.12	*1641.25*	*2389.20*	Jul		123.57	123.56	100.80	2.57	*87.62*	*57.71*
Aug	96.90	276.24	15.86	3.82		4689.23	4708.47	*1631.75*	*2377.76*	Aug		130.57	130.56	94.03	2.79	*89.49*	*60.31*
Sep	98.79	272.11	17.58	5.08		4667.50	4687.66	*1624.79*	*2366.61*	Sep		136.28	136.28	96.64	3.66	*93.22*	*62.56*
Seas_3	**100.20**	**275.81**	**15.80**	**4.11**	**54.56**	**4690.24**	**4709.42**	***1407.16***	***2251.13***	**Seas_3**	**436.54**	**130.14**	**130.13**	**97.16**	**3.01**	***159.40***	***163.44***
Oct	122.70	267.55	18.59	5.71		4647.60	4668.46	*1621.77*	*2353.76*	Oct		141.15	141.15	121.00	4.05	*101.84*	*65.88*
Nov	157.60	263.08	19.06	6.40		4628.96	4650.52	*1620.94*	*2340.28*	Nov		145.42	145.41	156.10	4.54	*112.87*	*72.39*
Dec	183.30	259.05	19.39	6.82		4611.61	4633.72	*1618.98*	*2328.64*	Dec		149.18	149.17	182.00	4.93	*121.32*	*79.12*
Seas_4	**154.53**	**263.23**	**19.01**	**6.31**	**55.71**	**4629.39**	**4650.90**	***1397.01***	***2217.26***	**Seas_4**	**563.01**	**145.25**	**145.24**	**153.03**	**4.51**	***202.21***	***211.05***
Annual	**114.65**	**243.25**	**15.48**	**3.47**	**58.50**	**4755.43**	**4771.06**	***1423.12***	***2283.13***	**Annual**	**430.11**	**106.21**	**106.20**	**105.52**	**2.55**	***150.12***	***162.80***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.18.

Table C.18. *The percentage difference between calculation results on PCB-180 mass in water (kg) obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	DEHM-POP_1	DEHM-POP_2	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-5.3%	-4.7%	60.2%	-0.5%	-0.5%	164.9%	164.7%	6.8%	0.6%
Feb			-13.4%	-12.1%	86.5%	0.9%	0.9%	170.6%	170.2%	5.9%	0.2%
Mar			-19.0%	-17.6%	90.6%	2.0%	2.0%	174.9%	174.4%	4.9%	-0.2%
Seas_1	**3.8%**	**62.7%**	**-14.5%**	**-14.2%**	**83.2%**	**1.3%**	**1.3%**	**170.0%**	**169.7%**	**5.6%**	**0.1%**
Apr			-23.8%	-22.3%	89.6%	3.0%	3.0%	178.3%	177.6%	4.2%	-1.3%
May			-31.6%	-30.5%	86.4%	3.8%	3.8%	180.8%	180.0%	2.8%	-3.5%
Jun			-40.5%	-39.6%	82.3%	4.5%	4.5%	182.7%	181.8%	1.8%	-4.8%
Seas_2	**-2.4%**	**59.7%**	**-32.4%**	**-31.4%**	**86.0%**	**3.8%**	**3.8%**	**180.6%**	**179.8%**	**2.7%**	**-3.5%**
Jul			-46.6%	-45.9%	77.8%	5.1%	5.1%	184.2%	183.3%	1.5%	-5.3%
Aug			-49.8%	-49.2%	73.2%	5.6%	5.6%	185.4%	184.4%	1.4%	-5.9%
Sep			-49.9%	-49.3%	68.8%	6.0%	6.0%	186.4%	185.4%	2.1%	-5.6%
Seas_3	**-4.2%**	**59.0%**	**-48.7%**	**-48.1%**	**73.2%**	**5.6%**	**5.5%**	**185.3%**	**184.4%**	**1.7%**	**-5.6%**
Oct			-45.6%	-45.0%	64.6%	6.3%	6.3%	187.2%	186.1%	3.1%	-5.0%
Nov			-40.8%	-40.3%	60.7%	6.5%	6.5%	187.9%	186.8%	4.1%	-3.8%
Dec			-38.7%	-38.3%	57.1%	6.7%	6.7%	188.5%	187.4%	4.2%	-3.2%
Seas_4	**4.2%**	**58.6%**	**-41.4%**	**-40.9%**	**60.8%**	**6.5%**	**6.5%**	**187.9%**	**186.8%**	**3.8%**	**-4.0%**
Annual	**0.2%**	**60.1%**	**-37.7%**	**-38.0%**	**74.5%**	**5.0%**	**5.0%**	**180.6%**	**179.9%**	**3.1%**	**-4.1%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;
DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

C.1.4. Comparison of calculated values of PCB-180 mass in vegetation

Reference data set. Calculation results on PCB-180 mass in vegetation (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.19.

Monthly values of PCB-180 mass in vegetation calculated by all participating models on the basis of "reference" data set are compared in Fig. C.13.

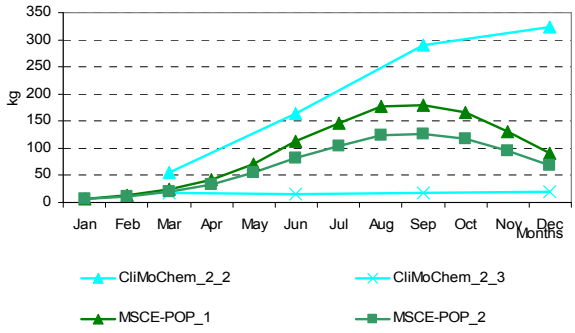


Fig. C.13. *PCB-180 mass in vegetation (kg) calculated by the participating models on the basis of "reference" data set*

Own/alternative data set. Calculation results on PCB-180 mass in vegetation (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.20.

Monthly values of PCB-180 mass in vegetation calculated by all participating models on the basis of "own or alternative" data sets are compared in Fig. C.14.

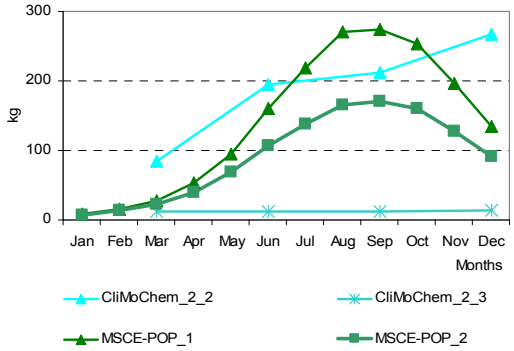


Fig. C.14. *PCB-180 mass in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets*

Table C.19. *Calculation results: PCB-180 mass in vegetation (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	MSCE-POP_2		
Jan	7.74				Jan		6.64		
Feb	13.96				Feb		11.83		
Mar	23.73				Mar		19.72		
Seas_1	**15.14**	**18.20**	***16.67***	***2.16***	**Seas_1**	**54.6**	**12.73**	***33.7***	***29.6***
Apr	42.39				Apr		33.97		
May	70.91				May		55.27		
Jun	112.00				Jun		82.66		
Seas_2	**75.10**	**14.81**	***44.96***	***42.63***	**Seas_2**	**164.7**	**57.30**	***111.0***	***75.9***
Jul	147.19				Jul		103.90		
Aug	178.27				Aug		123.07		
Sep	180.41				Sep		126.24		
Seas_3	**168.62**	**18.29**	***93.45***	***106.30***	**Seas_3**	**291.2**	**117.74**	***204.5***	***122.7***
Oct	167.02				Oct		118.32		
Nov	130.17				Nov		94.45		
Dec	90.57				Dec		67.80		
Seas_4	**129.25**	**19.17**	***74.21***	***77.84***	**Seas_4**	**323.4**	**93.52**	***208.5***	***162.5***
Annual	**97.03**	**17.62**	***57.32***	***56.15***	**Annual**	**208.5**	**70.32**	***139.4***	***97.7***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.20. *Calculation results: PCB-180 mass in vegetation (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	8.68				Jan		7.13		
Feb	16.24				Feb		13.15		
Mar	28.31				Mar		22.34		
Seas_1	**17.74**	**12.70**	***15.22***	***3.57***	**Seas_1**	**84.37**	**14.21**	**49.29**	**49.61**
Apr	54.17				Apr		40.41		
May	95.45				May		68.25		
Jun	160.53				Jun		106.52		
Seas_2	**103.38**	**12.17**	***57.78***	***64.49***	**Seas_2**	**195.02**	**71.73**	**133.37**	**87.18**
Jul	219.37				Jul		137.54		
Aug	270.65				Aug		165.25		
Sep	273.83				Sep		170.39		
Seas_3	**254.61**	**11.73**	***133.17***	***171.74***	**Seas_3**	**211.39**	**157.73**	**184.56**	**37.94**
Oct	252.85				Oct		160.12		
Nov	196.22				Nov		128.27		
Dec	134.26				Dec		91.43		
Seas_4	**194.44**	**14.49**	***104.47***	***127.25***	**Seas_4**	**268.01**	**126.61**	**197.31**	**99.99**
Annual	**142.55**	**12.77**	***77.66***	***91.76***	**Annual**	**189.70**	**92.57**	**141.13**	**68.68**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.21.

Table C.21. *The percentage difference between calculation results on PCB-180 mass in vegetation (kg) obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			12.2%	7.4%
Feb			16.4%	11.1%
Mar			19.3%	13.3%
Seas_1	**54.6%**	**-30.2%**	**17.2%**	**11.6%**
Apr			27.8%	18.9%
May			34.6%	23.5%
Jun			43.3%	28.9%
Seas_2	**18.4%**	**-17.8%**	**37.7%**	**25.2%**
Jul			49.0%	32.4%
Aug			51.8%	34.3%
Sep			51.8%	35.0%
Seas_3	**-27.4%**	**-35.9%**	**51.0%**	**34.0%**
Oct			51.4%	35.3%
Nov			50.7%	35.8%
Dec			48.2%	34.9%
Seas_4	**-17.1%**	**-24.4%**	**50.4%**	**35.4%**
Annual	**-9.0%**	**-27.5%**	**46.9%**	**31.6%**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data.
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

C.1.5. Comparison of distribution of PCB-180 mass between environmental media

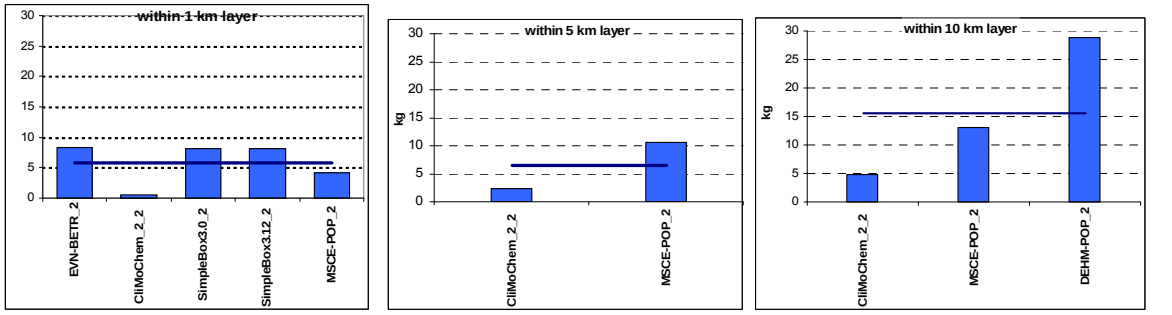
Mass balance estimates presented in Sections 3.1.1-3.1.4 comprise masses of PCB-180 contained in different environmental compartments calculated by the participating models. The considered estimates of mass distribution in 2000 include results of one-year calculation with zero initial concentrations obtained by DEHM-POP, MSCE-POP, SimpleBox 3.0 and 3.12 models and with initial concentrations in media given as input data calculated by CAN/POPs, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP, and SimpleBox 3.0 models; as well as results of long-term calculations for 20-year period with zero initial data with historical emissions carried out by CliMoChem and SimpleBox 3.0 and 3.12 models. Results of CliMoChem, DEHM-POP, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of these models' calculations to the variations in the input data.

A comparison of absolute values and relative fractions of PCB-180 mass contained in the main environmental compartments is presented in this section. The comparison is made separately for results calculated on the basis of initial concentrations or historical emissions (non-zero initial conditions) and for results based on zero initial conditions.

Atmosphere. Comparison of annual values of PCB-180 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "reference" data set is presented in Fig. C.15a. Fig. C.15b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the

basis of initial data; and then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

a



b

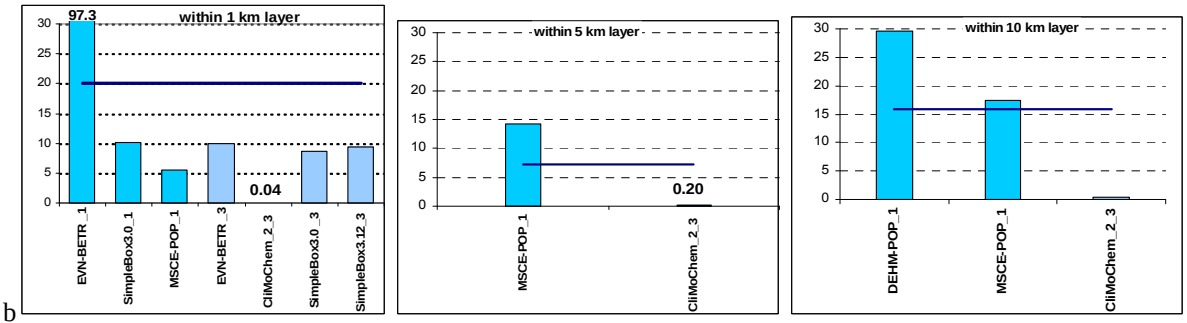


Fig. C.15. *Comparison of annual values of PCB-180 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of air content profiles of annual values of PCB-180 mass calculated by MSCE-POP and CliMoChem models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set is presented in Fig. C.16.

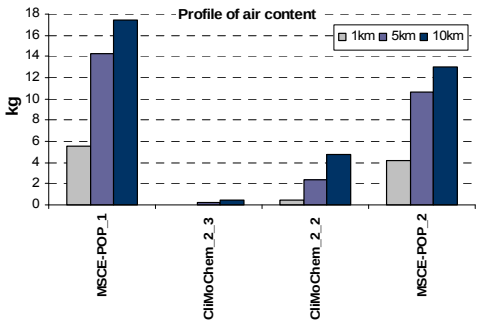


Fig. C.16. *Comparison of air content profiles of annual values of PCB-180 mass calculated by four models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set*

Comparison of annual values of PCB-180 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig. C.17a. Fig. C.17b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

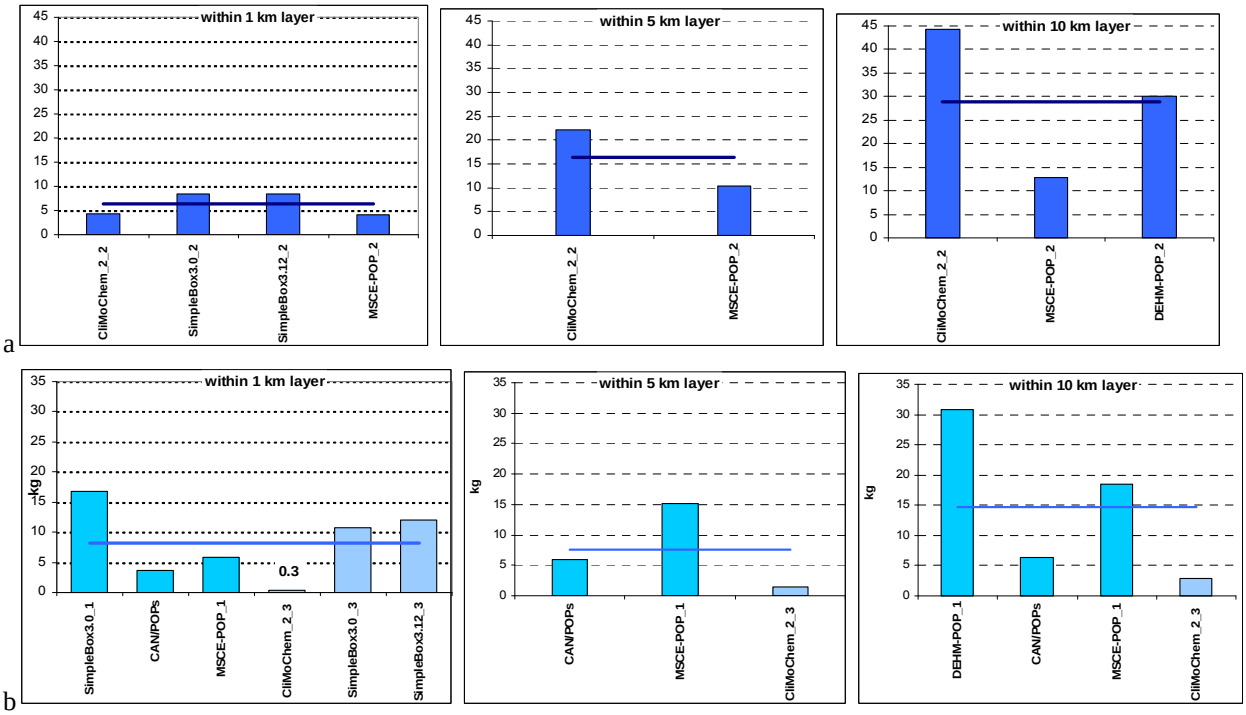


Fig. C.17. *Comparison of annual values of PCB-180 masses contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of air content profiles of annual values of PCB-180 mass calculated by CAN/POPs, MSCE-POP and CliMoChem models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative" data sets is presented in Fig. C.18.

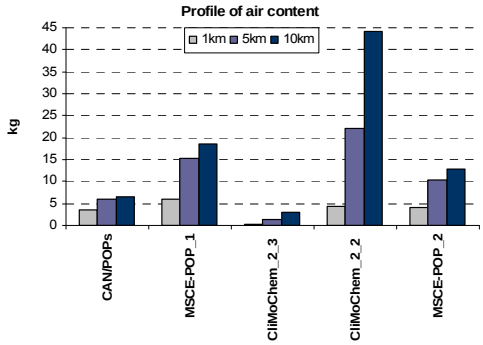


Fig. C.18. *Comparison of air content profiles of annual values of PCB-180 mass calculated by five models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative data sets"*

Comparison of annual values of PCB-180 mass contained in 1, 5 and 10 km layers of the atmosphere obtained by the participating models with the use of "reference" and "own/alternative" data sets is presented in Fig. C.19.

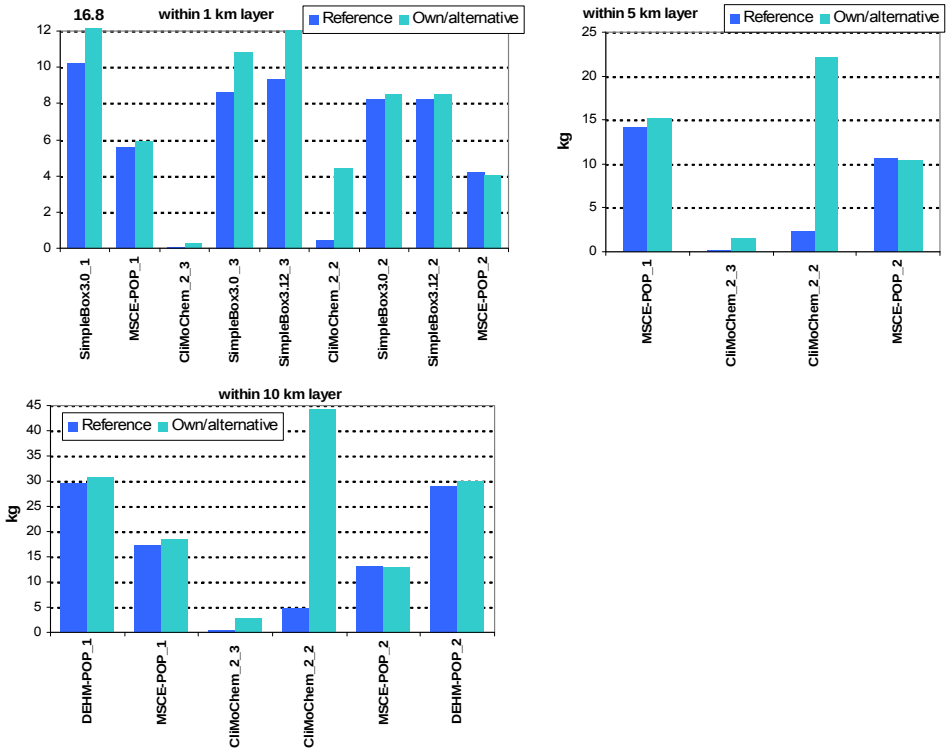


Fig. C.19. *Comparison of PCB-180 mass contained in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of two data set*

Soil. Comparison of annual values of PCB-180 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "reference" data set is presented in Fig. C.20a. Fig. C.20b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

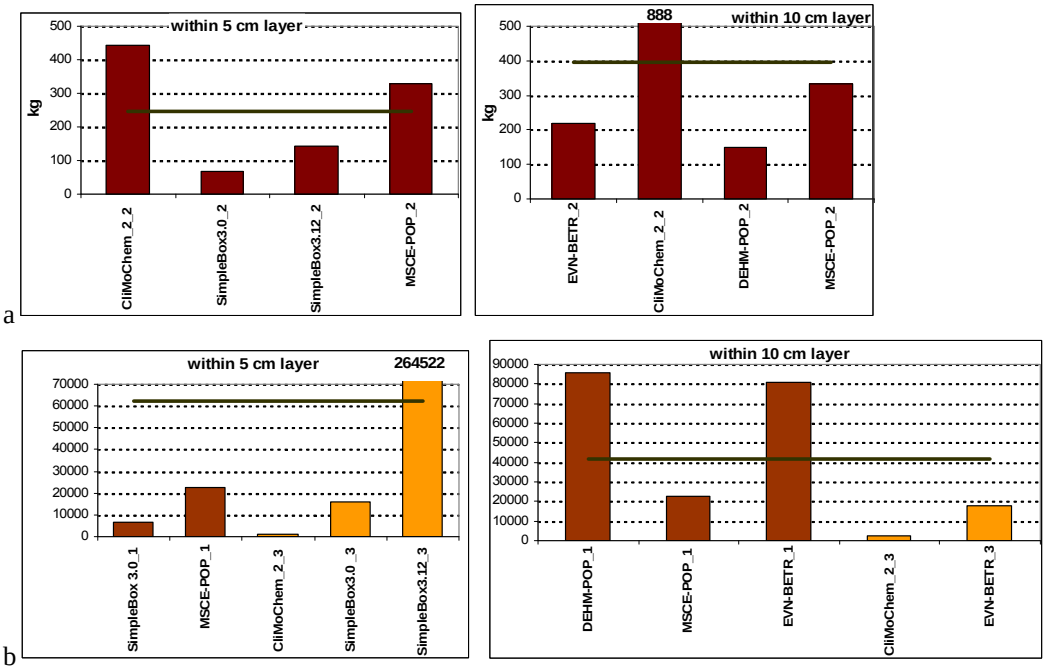


Fig. C.20. *Comparison of annual values of PCB-180 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of soil content profiles of annual values of PCB-180 mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set is presented in Fig. C.21.

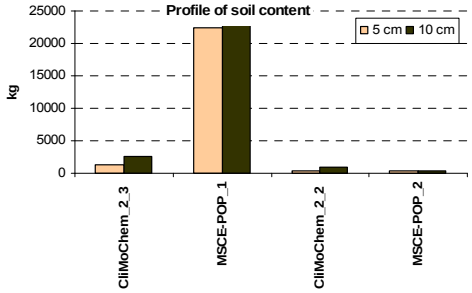
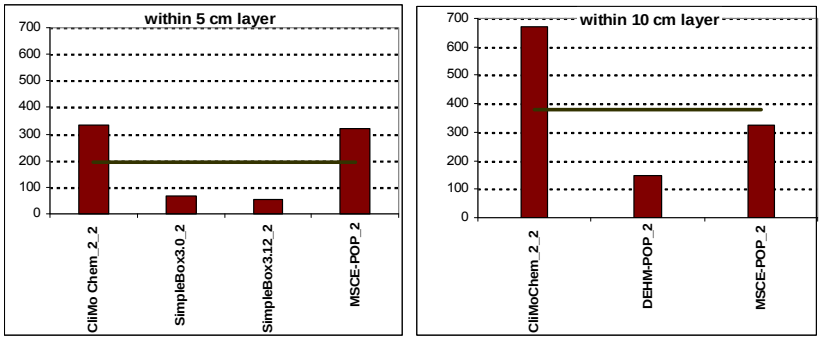


Fig. C.21. *Comparison of soil content profiles of annual values of PCB-180 mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set*

Comparison of annual values of PCB-180 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "own or alternative" data sets is presented in Fig. C.22a. Fig. C.22b shows the same results but obtained on the basis of initial concentrations or historical emissions. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

a



b

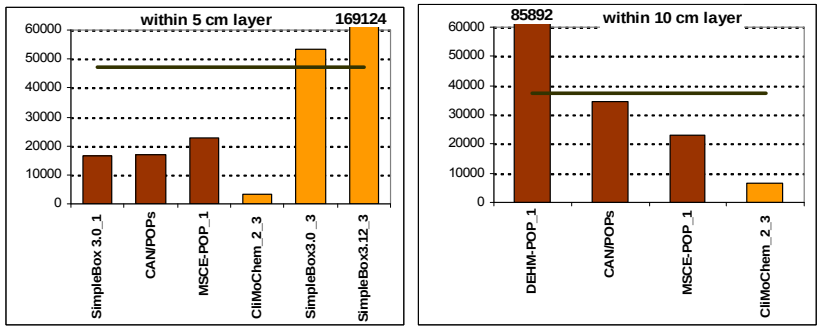


Fig. C.22. *Comparison of annual values of PCB-180 masses contained in soil within 5 and 10 cm layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non- zero initial conditions)*

Comparison of soil content profiles of annual values of PCB-180 mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets is presented in Fig. C.23.

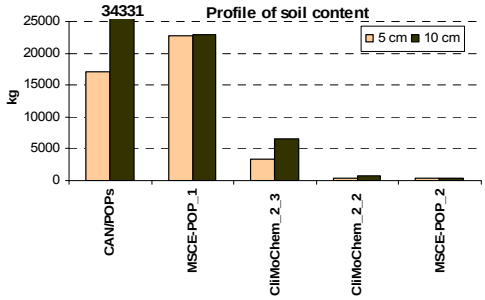


Fig. C.23. *Comparison of soil content profiles of annual values of PCB-180 mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets*

Comparison of annual values of PCB-180 mass contained in the considered different layers of soil obtained with "reference" and "own/alternative" data sets is presented in Fig. C.24.

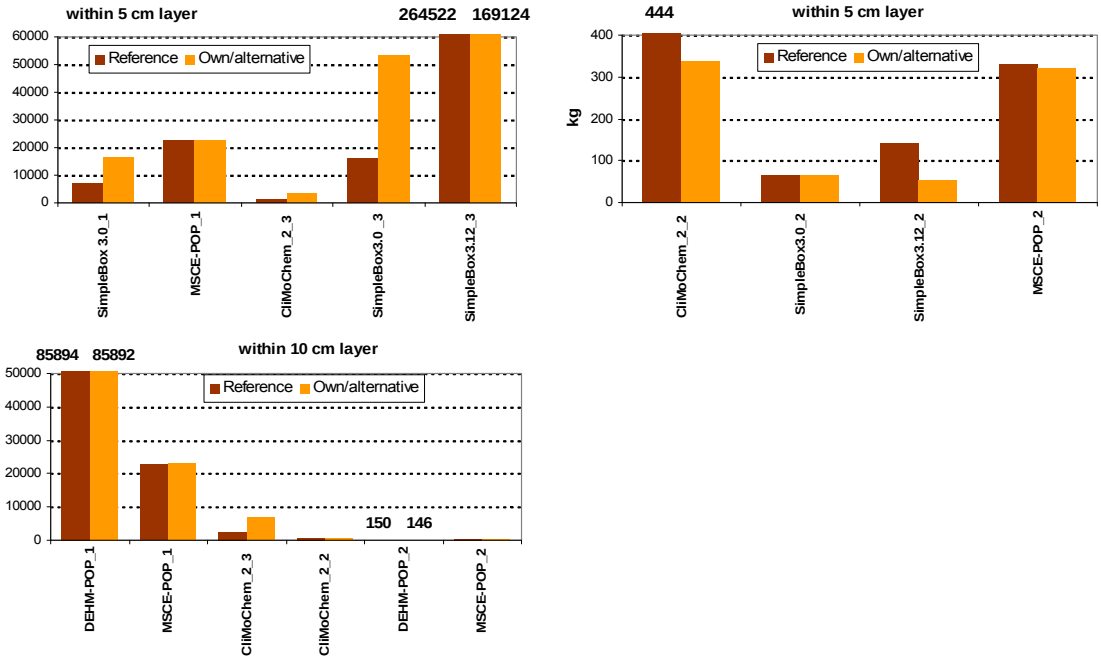


Fig. C.24. *Comparison of PCB-180 mass contained within 5 and 10 cm soil layers calculated by different models on the basis of two data set*

Water. Comparison of annual values of PCB-180 water content calculated by different models on the basis of zero initial concentrations and with the use of "***reference"*** data set is presented in Fig. C.25a. Fig. C.25b shows the same results but obtained on the basis of initial concentrations or historical emissions. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plot shows the value of the corresponding parameter averaged between models.

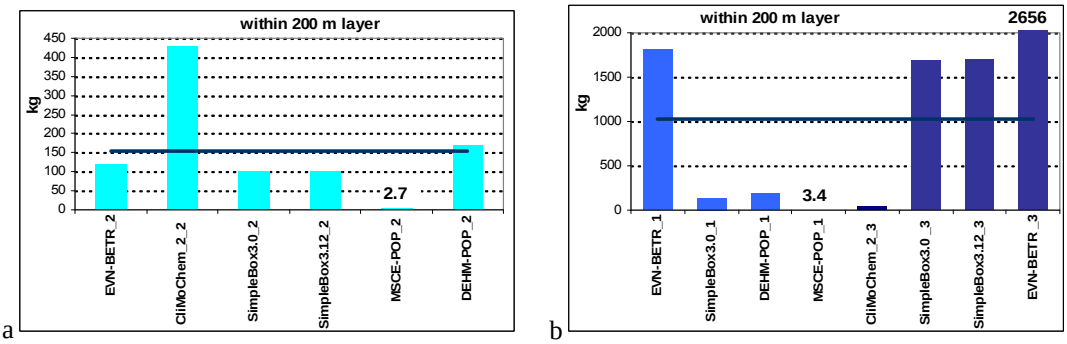


Fig. C.25. *Comparison of annual values of PCB-180 masses contained in water within 200 m layer calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Figs.3.26a and 3.26b show the annual values of PCB-180 masses contained in water layer of 200 m and calculated by different models on the basis of "***own or alternative***" data set and zero and non-zero initial conditions, respectively (blue line corresponds to the averaged value). Different color of columns corresponds to the different types of calculations (a - one-year calculations on the basis of zero initial conditions; b - one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

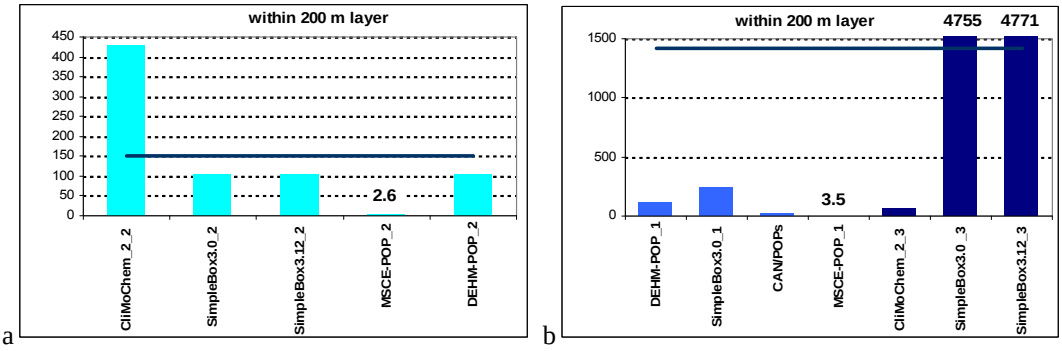


Fig. C.26. *Comparison of annual values of PCB-180 masses contained in water within 200 m layer calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-180 mass contained in the 200m layer of water obtained by the participating models on the basis of "reference" and "own/alternative" data sets is presented in Fig. C.27.

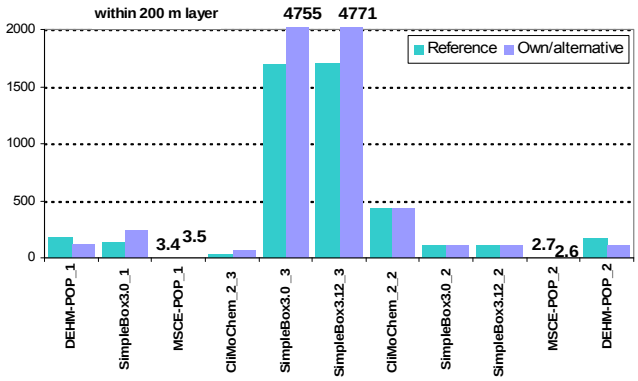


Fig. C.27. *Comparison of PCB-180 mass contained within 200 m water layer calculated by different models on the basis of two data sets*

Vegetation. Annual values of PCB-180 mass contained in vegetation obtained on the basis of zero initial conditions and with the use of "reference" and "own/alternative" data sets are presented in Fig. C.28a.

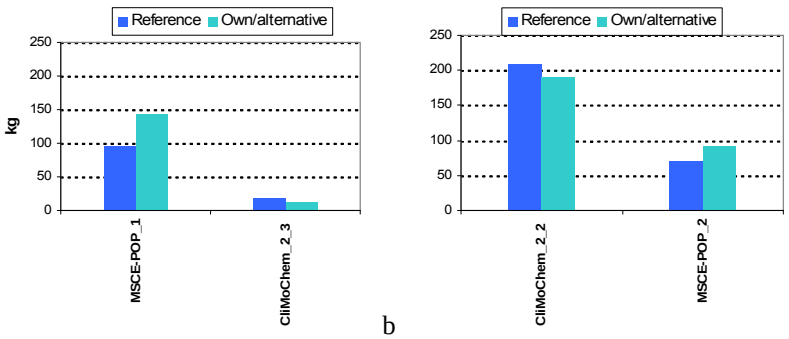
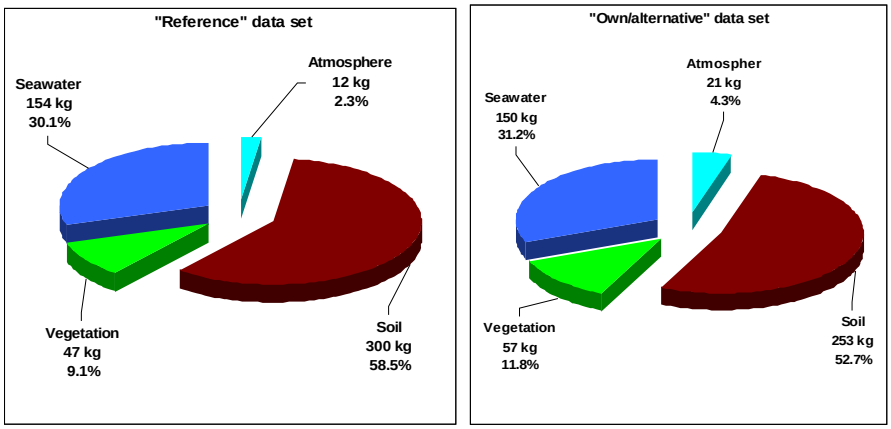


Fig. C.28. *Comparison of PCB-180 mass contained in vegetation calculated by different models on the basis of "reference" and "own/alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Relative distribution of PCB mass. The distribution of PCB-180 mass between main environmental compartments averaged for the results obtained by the participating models on the basis of zero and non-zero initial conditions is presented in Fig. C.29a and b, respectively. In this figure results calculated with the use of “reference” and “own/alternative” data sets are given. Of note, absolute values of averaged mass of PCB-180 in each media calculated with two different data sets of physical-chemical properties could not be directly compared since calculation results of different participating models are enclosed in these averaged figures.

a



b

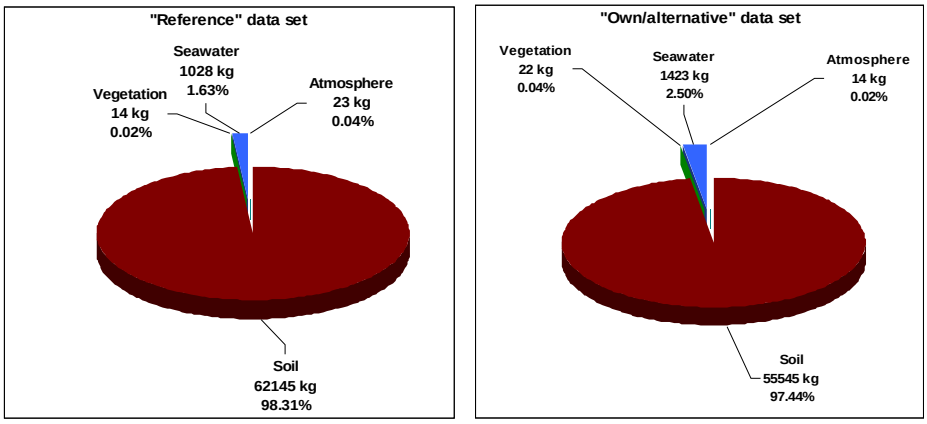
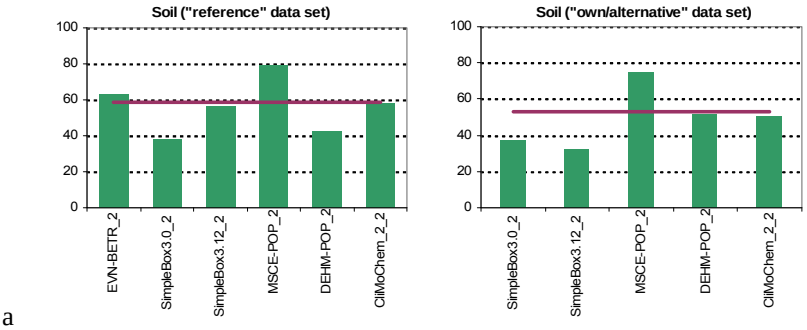
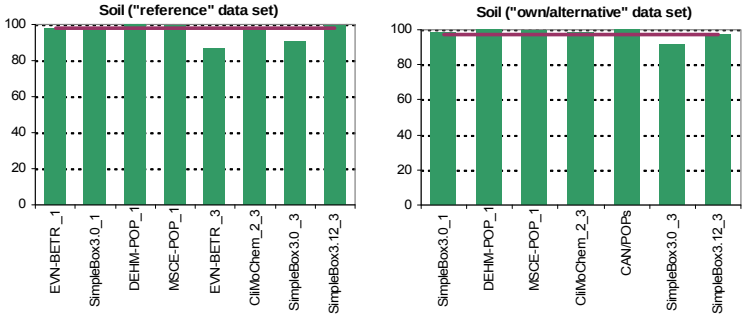


Fig. C.29. *Distribution of PCB-180 mass between environmental compartments (kg) averaged for all participating models and calculated on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

To show redistribution of the pollutant between main environmental compartments for each participating model in more detail, plots of PCB-180 fractions in different environmental compartments calculated by the models on the basis of zero and non-zero initial conditions are presented in Figs. 3.30a and b, respectively. In these figures fractions of PCB-180 mass in soil calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.



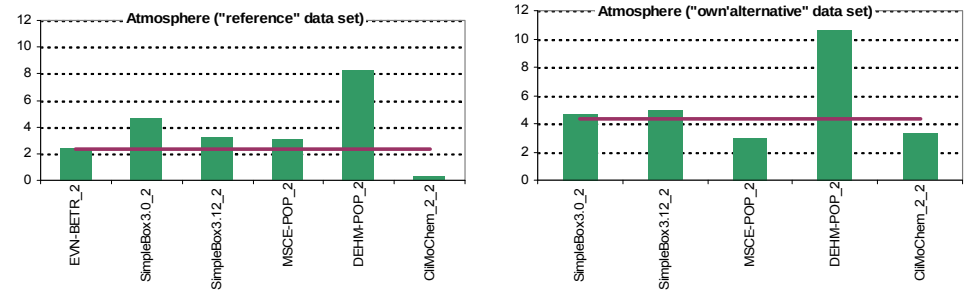
a



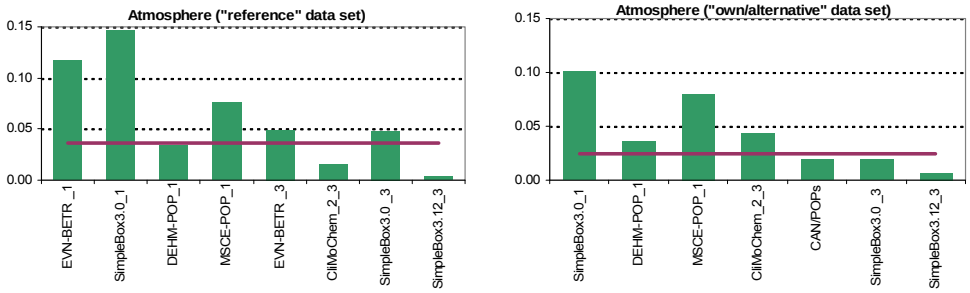
b

Fig. C.30. *Fractions of PCB-180 mass in soil calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of PCB-180 mass in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. C.31a and b, respectively. In these figures fractions of PCB-180 mass in the atmosphere calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.



a



b

Fig. C.31. *Fractions of PCB-180 mass in the atmosphere calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of PCB-180 mass in seawater calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. C.32a and b, respectively. In these figures fractions of PCB-180 mass in seawater calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models.

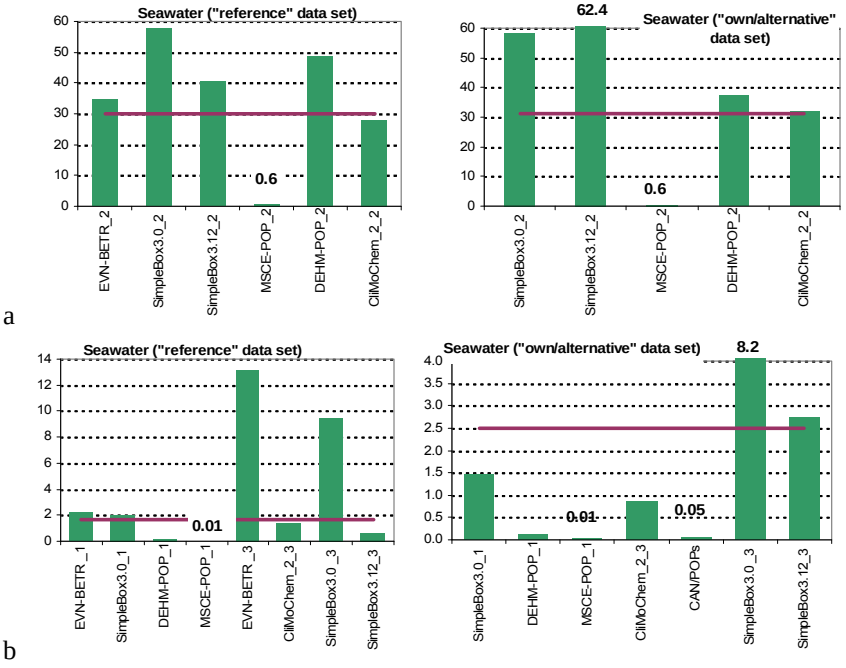


Fig. C.32. *Fractions of PCB-180 mass in seawater calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of total environmental mass of PCB-180 contained in vegetation calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Fig. C.33a and b, respectively. In these figures fractions of PCB-180 mass in vegetation calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared. The red line in the plots shows the value of the corresponding fraction averaged between models. Of note, the models, for which vegetation compartment was not included into calculations of mass balance, are also shown in the plots.

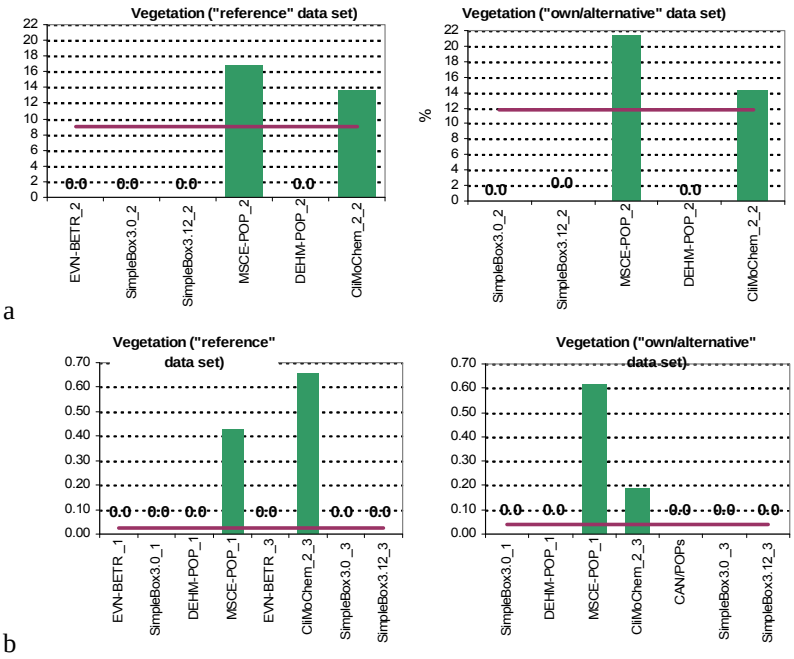


Fig. C.33. *Fractions of PCB-180 mass in vegetation calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

B.2. Masses degraded in the environmental compartments

B.2.1. Comparison of calculated values of PCB-180 mass degraded in the atmosphere

According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-180 degraded in the atmosphere within layers of 1 km, 5 km and 10 km height.

Reference data set. Calculation results on PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.22.

Monthly values of PCB-180 mass degraded in 1 km layer of the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.34 a and b, respectively. Seasonal variations of low values of mass contained in 1 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.34c in more detail.

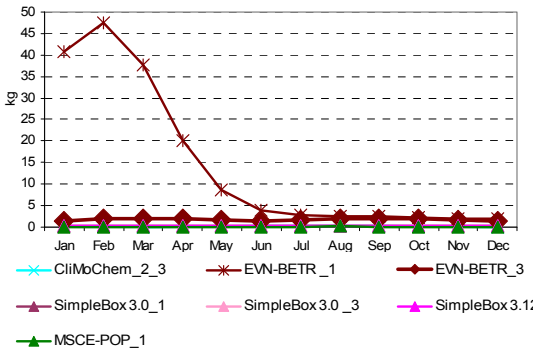


Fig. C.34a. *PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

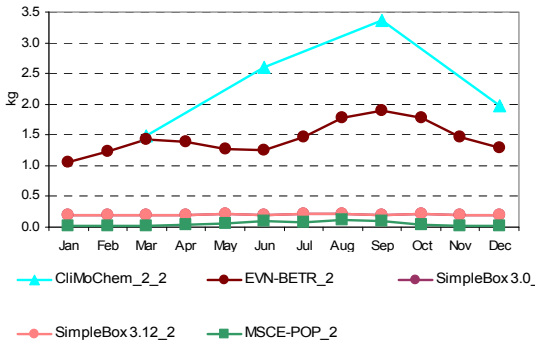


Fig. C.34b. *PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

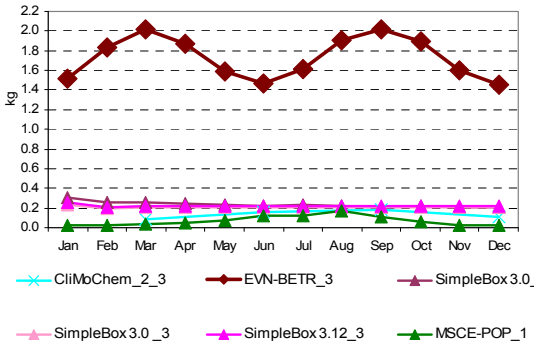


Fig. C.34c. *PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Calculation results on PCB-180 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.23.

Monthly values of PCB-180 mass degraded in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. C.35.

Calculation results on PCB-180 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.24.

Monthly values of PCB-180 mass degraded in 10 km layer of the atmosphere calculated by the participating models on the basis of "reference" data set are compared in Fig. C.36.

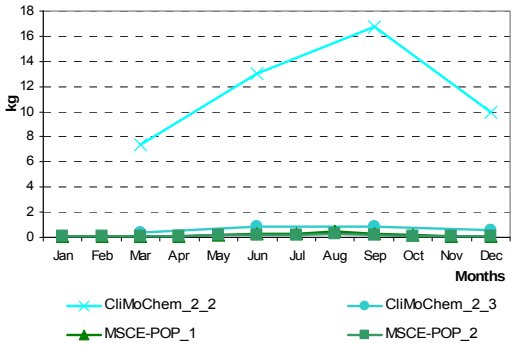


Fig. C.35. *PCB-180 mass degraded in 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

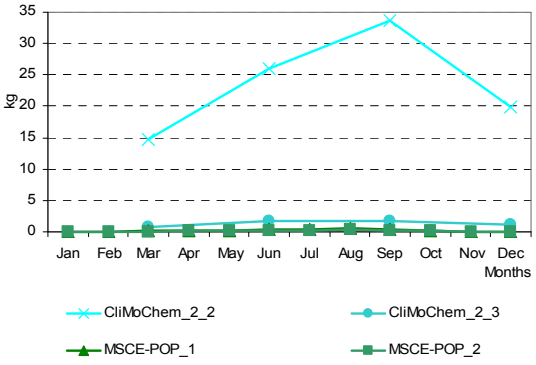


Fig. C.36. *PCB-180 mass degraded in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "reference" data set*

Table C.22. *Calculation results: PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	MSCE-POP_1	EVN-BETR _1[a]	SimpleBox 3.0_1[b]	EVN-BETR _3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	0.03	40.65	0.31	1.51		0.24	0.25	*7.16*	*16.41*	Jan	1.05		0.20	0.20	0.02	*0.37*	*0.46*
Feb	0.03	47.61	0.26	1.83		0.20	0.21	*8.35*	*19.24*	Feb	1.24		0.19	0.19	0.02	*0.41*	*0.56*
Mar	0.03	37.69	0.26	2.02		0.21	0.23	*6.74*	*15.18*	Mar	1.42		0.21	0.21	0.03	*0.46*	*0.64*
Seas_1	**0.08**	**125.94**	**0.83**	**5.36**	**0.08**	**0.65**	**0.69**	***19.09***	***47.15***	**Seas_1**	**3.71**	**1.48**	**0.59**	**0.59**	**0.07**	***1.29***	***1.45***
Apr	0.04	20.16	0.24	1.88		0.20	0.22	*3.79*	*8.05*	Apr	1.40		0.20	0.20	0.03	*0.46*	*0.63*
May	0.08	8.61	0.24	1.58		0.21	0.23	*1.82*	*3.37*	May	1.26		0.21	0.21	0.06	*0.43*	*0.56*
Jun	0.12	3.99	0.22	1.46		0.20	0.22	*1.04*	*1.54*	Jun	1.25		0.20	0.20	0.09	*0.44*	*0.55*
Seas_2	**0.24**	**32.76**	**0.70**	**4.92**	**0.16**	**0.62**	**0.66**	***5.73***	***12.04***	**Seas_2**	**3.91**	**2.61**	**0.60**	**0.60**	**0.19**	***1.58***	***1.61***
Jul	0.12	2.67	0.23	1.62		0.21	0.22	*0.84*	*1.06*	Jul	1.46		0.21	0.21	0.08	*0.49*	*0.65*
Aug	0.17	2.47	0.22	1.91		0.21	0.22	*0.87*	*1.04*	Aug	1.78		0.21	0.21	0.13	*0.58*	*0.80*
Sep	0.11	2.38	0.21	2.02		0.20	0.22	*0.86*	*1.05*	Sep	1.90		0.20	0.20	0.09	*0.60*	*0.87*
Seas_3	**0.40**	**7.52**	**0.66**	**5.54**	**0.18**	**0.63**	**0.67**	***2.23***	***3.00***	**Seas_3**	**5.15**	**3.36**	**0.61**	**0.61**	**0.30**	***2.00***	***2.15***
Oct	0.06	2.20	0.22	1.89		0.21	0.22	*0.80*	*0.97*	Oct	1.78		0.21	0.21	0.04	*0.56*	*0.82*
Nov	0.03	1.93	0.21	1.60		0.20	0.22	*0.70*	*0.84*	Nov	1.47		0.20	0.20	0.02	*0.47*	*0.67*
Dec	0.03	1.92	0.21	1.45		0.20	0.22	*0.67*	*0.80*	Dec	1.30		0.20	0.20	0.02	*0.43*	*0.58*
Seas_4	**0.11**	**6.04**	**0.63**	**4.95**	**0.11**	**0.62**	**0.66**	***1.87***	***2.50***	**Seas_4**	**4.55**	**1.98**	**0.60**	**0.60**	**0.09**	***1.56***	***1.81***
Annual	**0.84**	**172.26**	**2.83**	**20.78**	**0.53**	**2.51**	**2.68**	***28.92***	***63.61***	**Annual**	**17.32**	**9.43**	**2.41**	**2.41**	**0.65**	***6.44***	***6.95***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;

[b] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.23. *Calculation results: PCB-180 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	0.06				Jan		0.06		
Feb	0.07				Feb		0.06		
Mar	0.08				Mar		0.07		
Season_1	**0.21**	**0.41**	***0.31***	***0.14***	**Season_1**	**7.39**	**0.18**	***3.79***	***5.10***
Apr	0.11				Apr		0.09		
May	0.20				May		0.16		
Jun	0.31				Jun		0.23		
Season_2	**0.63**	**0.82**	***0.72***	***0.13***	**Season_2**	**13.03**	**0.48**	***6.76***	***8.88***
Jul	0.30				Jul		0.22		
Aug	0.44				Aug		0.32		
Sep	0.29				Sep		0.23		
Season_3	**1.03**	**0.89**	***0.96***	***0.10***	**Season_3**	**16.79**	**0.77**	***8.78***	***11.33***
Oct	0.14				Oct		0.11		
Nov	0.07				Nov		0.06		
Dec	0.07				Dec		0.06		
Season_4	**0.29**	**0.54**	***0.41***	***0.18***	**Season_4**	**9.91**	**0.23**	***5.07***	***6.85***
Annual	**2.15**	**2.65**	***2.40***	***0.35***	**Annual**	**47.13**	**1.66**	***24.39***	***32.15***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

Table C.24. *Calculation results: PCB-180 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	0.08				Jan		0.07		
Feb	0.08				Feb		0.07		
Mar	0.10				Mar		0.09		
Seas_1	**0.26**	**0.82**	***0.54***	***0.39***	**Seas_1**	**14.79**	**0.23**	***7.51***	***10.30***
Apr	0.13				Apr		0.10		
May	0.25				May		0.20		
Jun	0.38				Jun		0.29		
Seas_2	**0.77**	**1.63**	***1.20***	***0.61***	**Seas_2**	**26.06**	**0.59**	***13.32***	***18.02***
Jul	0.37				Jul		0.27		
Aug	0.53				Aug		0.40		
Sep	0.35				Sep		0.28		
Seas_3	**1.25**	**1.78**	***1.52***	***0.37***	**Seas_3**	**33.58**	**0.94**	***17.26***	***23.08***
Oct	0.18				Oct		0.14		
Nov	0.09				Nov		0.07		
Dec	0.09				Dec		0.07		
Seas_4	**0.35**	**1.07**	***0.71***	***0.51***	**Seas_4**	**19.82**	**0.28**	***10.05***	***13.82***
Annual	**2.63**	**5.30**	***3.97***	***1.89***	**Annual**	**94.25**	**2.03**	***48.14***	***65.21***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Own/alternative data set. Calculation results on PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.25.

Monthly values of PCB-180 mass degraded in 1 km layer of the atmosphere calculated by all participating models on the basis of "own or alternative" and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.37 a and b, respectively.

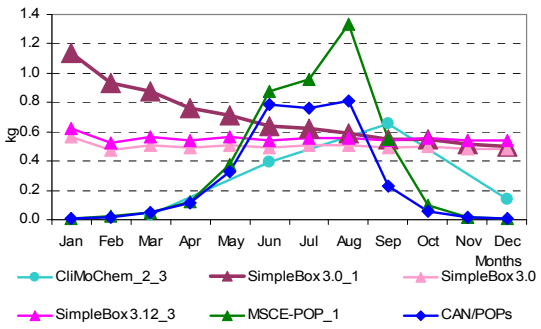


Fig. C.37a. *PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own/alternative" data set and non-zero initial conditions (all models)*

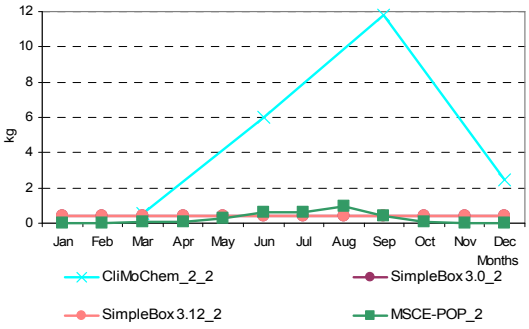


Fig. C.37b. *PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own/alternative" data set and zero-initial conditions*

Calculation results on PCB-180 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data set together with statistical parameters used for evaluation are presented in Table C.26.

Monthly values of PCB-180 mass degraded in 5 km layer of the atmosphere calculated by the models on the basis of "reference" data set are compared in Fig. C.38.

Calculation results on PCB-180 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative data sets" together with statistical parameters used for evaluation are presented in Table C.27.

Monthly values of PCB-180 mass degraded in 10 km layer of the atmosphere calculated by the participating models on the basis of "own or alternative" data sets are compared in Fig. C.39.

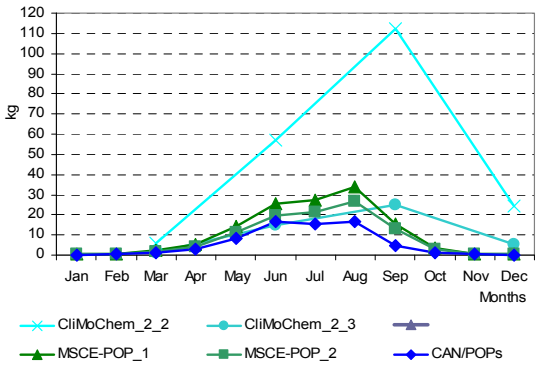


Fig. C.38. *PCB-180 mass degraded in 5 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own/alternative" data set*

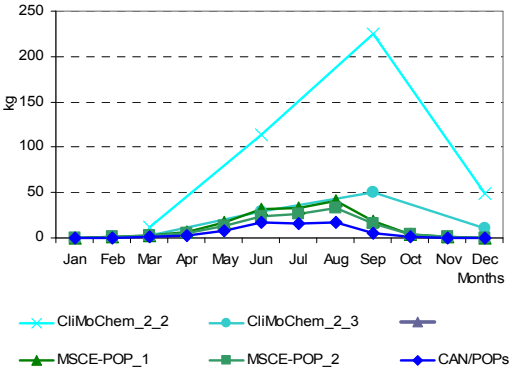


Fig. C.39. *PCB-180 mass degraded in 10 km layer of the atmosphere (kg) calculated by the participating models on the basis of "own/alternative" data set*

Table C.25. *Calculation results: PCB-180 mass degraded in 1 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CAN/ POPs	CliMo Chem_ 2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.01	1.14	0.01		0.56	0.62	*0.47*	*0.47*	Jan		0.39	0.39	0.01	*0.26*	*0.22*
Feb	0.02	0.93	0.02		0.47	0.53	*0.39*	*0.39*	Feb		0.38	0.38	0.02	*0.26*	*0.21*
Mar	0.05	0.87	0.05		0.51	0.56	*0.41*	*0.36*	Mar		0.40	0.40	0.04	*0.28*	*0.21*
Seas_1	**0.08**	**2.95**	**0.08**	**0.03**	**1.55**	**1.71**	***1.07***	***1.20***	**Seas_1**	**0.56**	**1.17**	**1.17**	**0.07**	***0.74***	***0.53***
Apr	0.12	0.76	0.12		0.49	0.54	*0.41*	*0.28*	Apr		0.39	0.39	0.09	*0.29*	*0.18*
May	0.37	0.71	0.33		0.51	0.56	*0.50*	*0.15*	May		0.40	0.40	0.28	*0.36*	*0.07*
Jun	0.88	0.64	0.79		0.49	0.54	*0.67*	*0.16*	Jun		0.39	0.39	0.60	*0.46*	*0.12*
Seas_2	**1.37**	**2.11**	**1.24**	**0.39**	**1.48**	**1.65**	***1.37***	***0.57***	**Seas_2**	**6.02**	**1.19**	**1.19**	**0.96**	***2.34***	***2.45***
Jul	0.96	0.62	0.76		0.50	0.56	*0.68*	*0.18*	Jul		0.41	0.41	0.64	*0.48*	*0.14*
Aug	1.33	0.59	0.81		0.50	0.56	*0.76*	*0.34*	Aug		0.41	0.41	0.93	*0.58*	*0.30*
Sep	0.55	0.55	0.23		0.49	0.54	*0.47*	*0.14*	Sep		0.39	0.39	0.42	*0.40*	*0.02*
Seas_3	**2.84**	**1.76**	**1.80**	**0.65**	**1.50**	**1.66**	***1.70***	***0.70***	**Seas_3**	**11.79**	**1.20**	**1.20**	**1.99**	***4.05***	***5.18***
Oct	0.10	0.55	0.06		0.50	0.56	*0.35*	*0.25*	Oct		0.41	0.41	0.07	*0.29*	*0.19*
Nov	0.02	0.51	0.01		0.49	0.54	*0.31*	*0.27*	Nov		0.39	0.39	0.01	*0.27*	*0.22*
Dec	0.01	0.50	0.01		0.49	0.54	*0.31*	*0.28*	Dec		0.39	0.39	0.01	*0.26*	*0.22*
Seas_4	**0.12**	**1.56**	**0.08**	**0.14**	**1.48**	**1.64**	***0.84***	***0.79***	**Seas_4**	**2.47**	**1.19**	**1.19**	**0.09**	***1.24***	***0.97***
Annual	**4.41**	**8.37**	**3.19**	**1.22**	**6.00**	**6.66**	***4.98***	***2.57***	**Annual**	**20.84**	**4.75**	**4.75**	**3.12**	***8.36***	***8.35***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.26. *Calculation results: PCB-180 mass degraded in 5 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	CAN/POPs	MSCE-POP_1	CliMoChem_2_3				CliMoChem_2_2	MSCE-POP_2		
Jan	0.01	0.03		*0.02*	*0.01*	Jan		0.02		
Feb	0.02	0.06		*0.04*	*0.03*	Feb		0.05		
Mar	0.06	0.13		*0.09*	*0.05*	Mar		0.11		
Seas_1	**0.09**	**0.21**	**0.16**	***0.16***	***0.06***	**Seas_1**	**2.81**	**0.18**	***1.50***	***1.86***
Apr	0.13	0.31		*0.22*	*0.12*	Apr		0.22		
May	0.39	0.96		*0.68*	*0.41*	May		0.72		
Jun	0.96	2.26		*1.61*	*0.92*	Jun		1.54		
Seas_2	**1.48**	**3.53**	**1.97**	***2.33***	***1.07***	**Seas_2**	**30.09**	**2.47**	***16.28***	***19.53***
Jul	0.93	2.46		*1.70*	*1.08*	Jul		1.65		
Aug	1.00	3.42		*2.21*	*1.71*	Aug		2.38		
Sep	0.28	1.41		*0.84*	*0.80*	Sep		1.09		
Seas_3	**2.22**	**7.29**	**3.27**	***4.26***	***2.68***	**Seas_3**	**58.96**	**5.12**	***32.04***	***38.07***
Oct	0.07	0.25		*0.16*	*0.12*	Oct		0.19		
Nov	0.02	0.04		*0.03*	*0.02*	Nov		0.03		
Dec	0.01	0.02		*0.01*	*0.01*	Dec		0.02		
Seas_4	**0.09**	**0.31**	**0.69**	***0.36***	***0.30***	**Seas_4**	**12.33**	**0.24**	***6.28***	***8.55***
Annual	**3.88**	**11.34**	**6.09**	***7.10***	***3.83***	**Annual**	**104.19**	**8.01**	***56.10***	***68.01***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table C.27. *Calculation results: PCB-180 mass degraded in 10 km layer of the atmosphere (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	sults obtained on the basis of itial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	MSCE-POP_1	CAN/POPs	CliMoChem_2_3				CliMo Chem_2_2	MSCE-POP_2		
Jan	0.03	0.01		*0.02*	*0.02*	Jan		0.03		
Feb	0.07	0.02		*0.04*	*0.03*	Feb		0.06		
Mar	0.16	0.06		*0.11*	*0.07*	Mar		0.13		
Seas_1	**0.26**	**0.09**	**0.33**	***0.23***	***0.12***	**Seas_1**	**5.63**	**0.22**	***2.92***	***3.82***
Apr	0.38	0.13		*0.26*	*0.17*	Apr		0.27		
May	1.18	0.39		*0.78*	*0.56*	May		0.88		
Jun	2.76	0.96		*1.86*	*1.27*	Jun		1.88		
Seas_2	**4.31**	**1.48**	**3.94**	***3.25***	***1.54***	**Seas_2**	**60.18**	**3.03**	***31.60***	***40.41***
Jul	3.01	0.93		*1.97*	*1.47*	Jul		2.02		
Aug	4.18	1.00		*2.59*	*2.25*	Aug		2.91		
Sep	1.72	0.28		*1.00*	*1.02*	Sep		1.33		
Seas_3	**8.91**	**2.22**	**6.54**	***5.89***	***3.39***	**Seas_3**	**117.91**	**6.26**	***62.08***	***78.95***
Oct	0.30	0.07		*0.19*	*0.16*	Oct		0.23		
Nov	0.05	0.02		*0.03*	*0.03*	Nov		0.04		
Dec	0.02	0.01		*0.02*	*0.01*	Dec		0.02		
Seas_4	**0.38**	**0.09**	**1.38**	***0.62***	***0.68***	**Seas_4**	**24.66**	**0.29**	***12.47***	***17.23***
Annual	**13.87**	**3.88**	**12.19**	***9.98***	***5.35***	**Annual**	**208.38**	**9.79**	***109.09***	***140.42***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-180 mass degraded in 1, 5 and 10 km layers of obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables 3.28 – 3.30.

Table C.28. *The percentage difference between calculation results on PCB-180 mass degraded in 1 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			272%	96%	96%	138%	146%	-56%	-57%
Feb			259%	97%	97%	140%	150%	-15%	-18%
Mar			236%	97%	97%	140%	149%	59%	54%
Season_1	-62%	-60%	257%	97%	97%	139%	148%	1%	-3%
Apr			217%	97%	97%	140%	149%	180%	161%
May			200%	97%	97%	140%	149%	379%	348%
Jun			186%	97%	97%	140%	149%	617%	556%
Season_2	131%	142%	201%	97%	97%	140%	149%	464%	417%
Jul			174%	97%	97%	139%	149%	713%	660%
Aug			165%	97%	97%	139%	149%	685%	634%
Sep			157%	97%	97%	139%	149%	390%	374%
Season_3	251%	267%	165%	97%	97%	139%	149%	611%	564%
Oct			150%	98%	97%	139%	149%	70%	67%
Nov			145%	98%	98%	139%	149%	-41%	-41%
Dec			140%	98%	98%	139%	149%	-71%	-72%
Season_4	24%	29%	145%	98%	98%	139%	149%	7%	4%
Annual	121%	130%	196%	97%	97%	139%	149%	427%	381%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Table C.29. *The percentage difference between calculation results on PCB-180 mass degraded in 5 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			-56%	-57%
Feb			-15%	-18%
Mar			59%	54%
Season_1	-62%	-60%	1%	-3%
Apr			180%	161%
May			379%	348%
Jun			617%	556%
Season_2	131%	142%	464%	417%
Jul			713%	660%
Aug			685%	634%
Sep			390%	374%
Season_3	251%	267%	611%	564%
Oct			70%	67%
Nov			-41%	-41%
Dec			-71%	-72%
Season_4	24%	29%	7%	4%
Annual	121%	130%	427%	381%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

Table C.30. *The percentage difference between calculation results on PCB-180 mass degraded in 10 km layer of the atmosphere obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			-56%	-57%
Feb			-15%	-18%
Mar			59%	54%
Season_1	-62%	-60%	1%	-3%
Apr			180%	161%
May			379%	348%
Jun			617%	556%
Season_2	131%	142%	464%	417%
Jul			713%	660%
Aug			685%	634%
Sep			390%	374%
Season_3	251%	267%	611%	564%
Oct			70%	67%
Nov			-41%	-41%
Dec			-71%	-72%
Season_4	24%	29%	7%	4%
Annual	121%	130%	427%	381%

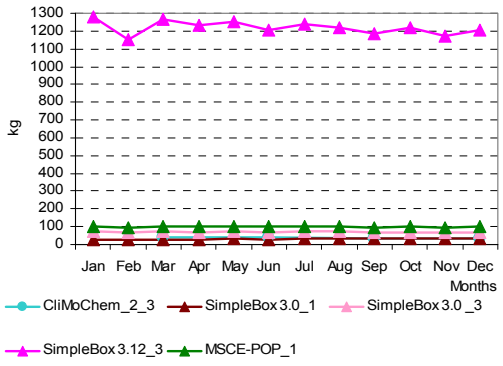
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

C.2.2. Comparison of calculated values of PCB-180 mass degraded in soil

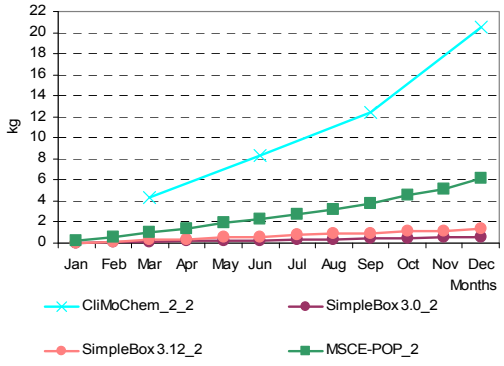
According to the programme of Stage II results of computational experiments on mass balance include masses of PCB-180 degraded in soil within 5 cm and 10 cm depth.

Reference data set. Calculation results on PCB-180 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.31.

Monthly values of PCB-180 mass degraded in 5cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.40a and b, respectively. Seasonal variations of low values of mass in 5cm layer of soil calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.40c in more detail.



a



b

Fig. C.40a. *PCB-180 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. C.40b. *PCB-180 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

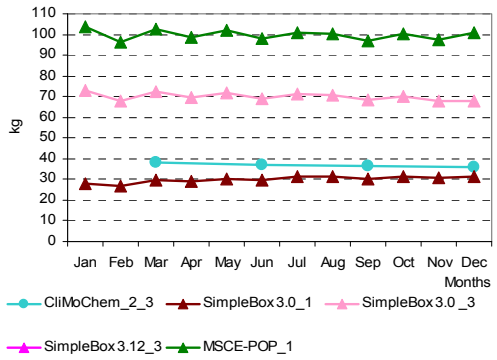


Fig. C.40c. *PCB-180 mass degraded in 5 cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Calculation results on PCB-180 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.32.

Monthly values of PCB-180 mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.41a and b, respectively. Seasonal variations of low values of mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.41c in more detail.

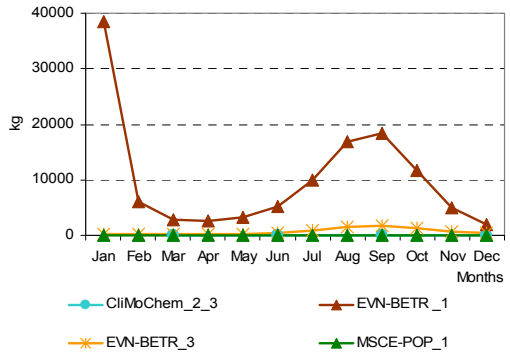


Fig. C.41a. *PCB-180 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

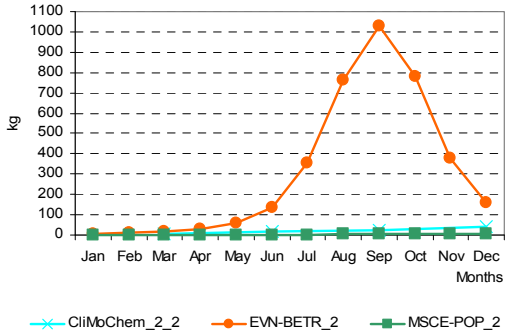


Fig. C.41b. *PCB-180 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

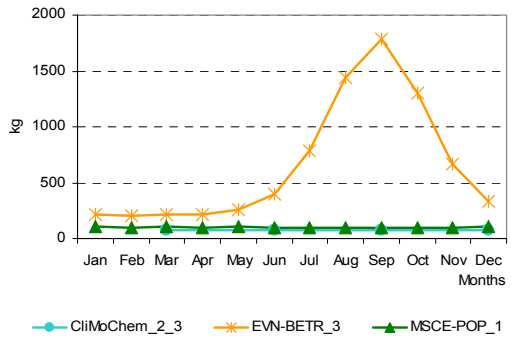


Fig. C.41c. *PCB-153 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Table C.31. *Calculation results: PCB-180 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	103.54	27.68		73.04	1278.43	*370.7*	*606.0*	Jan		0.02	0.1	0.2	*0.1*	*0.1*
Feb	96.39	26.79		68.04	1148.52	*334.9*	*543.1*	Feb		0.1	0.2	0.5	*0.3*	*0.3*
Mar	102.59	29.38		72.42	1264.76	*367.3*	*599.1*	Mar		0.1	0.3	1.0	*0.5*	*0.5*
Seas_1	**302.52**	**83.8**	**37.91**	**213.5**	**3691.7**	***865.9***	***1583.1***	**Seas_1**	**4.3**	**0.2**	**0.5**	**1.7**	***1.7***	***1.9***
Apr	98.88	29.00		69.77	1232.42	*357.5*	*584.0*	Apr		0.2	0.4	1.4	*0.7*	*0.7*
May	101.75	30.43		71.78	1251.02	*363.7*	*592.2*	May		0.2	0.5	1.9	*0.9*	*0.9*
Jun	97.99	29.80		69.16	1204.08	*350.3*	*569.9*	Jun		0.3	0.6	2.2	*1.0*	*1.0*
Seas_2	**298.62**	**89.2**	**37.11**	**210.7**	**3687.5**	***864.6***	***1581.4***	**Seas_2**	**8.4**	**0.7**	**1.5**	**5.5**	***4.0***	***3.6***
Jul	100.78	31.08		71.16	1237.47	*360.1*	*585.6*	Jul		0.3	0.8	2.7	*1.3*	*1.3*
Aug	100.40	31.31		70.84	1222.31	*356.2*	*578.1*	Aug		0.4	0.9	3.2	*1.5*	*1.5*
Sep	97.09	30.47		68.26	1184.53	*345.1*	*560.3*	Sep		0.4	1.0	3.7	*1.7*	*1.8*
Seas_3	**298.27**	**92.9**	**36.33**	**210.3**	**3644.3**	***856.4***	***1561.8***	**Seas_3**	**12.4**	**1.2**	**2.6**	**9.7**	***6.4***	***5.4***
Oct	100.44	31.62		70.22	1217.40	*354.9*	*575.7*	Oct		0.5	1.1	4.5	*2.0*	*2.2*
Nov	97.47	30.70		67.66	1171.75	*341.9*	*553.9*	Nov		0.5	1.2	5.2	*2.3*	*2.5*
Dec	101.12	31.18		67.76	1204.36	*351.1*	*569.6*	Dec		0.6	1.3	6.2	*2.7*	*3.0*
Seas_4	**299.03**	**93.5**	**35.80**	**205.6**	**3593.5**	***845.5***	***1539.5***	**Seas_4**	**20.5**	**1.6**	**3.6**	**15.9**	***10.4***	***9.2***
Annual	**1198.43**	**359.44**	**147.16**	**840.11**	**14617.05**	***3432.4***	***6265.8***	**Annual**	**45.5**	**3.7**	**8.2**	**32.8**	***22.6***	***20.0***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Table C.32. *Calculation results: PCB-180 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	EVN- BETR_1[a]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_ 2_3				EVN-BETR_2[a]	CliMo Chem_2_2	MSCE-POP_2		
Jan	38411.4	104.7	214.3		*12910.1*	*22084.8*	Jan	7.3		0.2	*3.7*	*5.0*
Feb	6077.2	97.4	204.3		*2126.3*	*3422.0*	Feb	13.2		0.5	*6.9*	*9.0*
Mar	2776.1	103.7	212.5		*1030.7*	*1512.5*	Mar	19.5		1.0	*10.3*	*13.1*
Seas_1	**47264.6**	**305.8**	**631.1**	**75.8**	***12069.3***	***23464.6***	**Seas_1**	**40.1**	**8.6**	**1.7**	***16.8***	***20.4***
Apr	2531.3	100.0	220.1		*950.5*	*1370.4*	Apr	31.2		1.4	*16.3*	*21.1*
May	3139.3	102.9	256.0		*1166.0*	*1710.6*	May	59.0		1.9	*30.4*	*40.4*
Jun	5175.2	99.1	398.6		*1891.0*	*2848.2*	Jun	138.0		2.3	*70.1*	*96.0*
Seas_2	**10845.8**	**301.9**	**874.8**	**74.2**	***3024.2***	***5225.3***	**Seas_2**	**228.2**	**16.7**	**5.6**	***83.5***	***125.5***
Jul	10011.3	101.9	788.3		*3633.8*	*5533.7*	Jul	356.6		2.8	*179.7*	*250.2*
Aug	16873.2	101.5	1445.1		*6140.0*	*9319.5*	Aug	763.6		3.2	*383.4*	*537.7*
Sep	18483.8	98.2	1780.9		*6787.6*	*10164.1*	Sep	1026.8		3.8	*515.3*	*723.4*
Seas_3	**45368.3**	**301.5**	**4014.4**	**72.7**	*12439.2*	*22027.0*	**Seas_3**	**2147.0**	**24.8**	**9.8**	*727.2*	*1229.6*
Oct	11735.9	101.5	1305.9		*4381.1*	*6397.9*	Oct	777.9		4.6	*391.2*	*546.8*
Nov	4998.2	98.5	665.3		*1920.7*	*2680.2*	Nov	380.3		5.2	*192.8*	*265.2*
Dec	2045.9	102.2	333.9		*827.3*	*1061.7*	Dec	162.5		6.2	*84.4*	*110.5*
Seas_4	**18780.1**	**302.3**	**2305.1**	**71.6**	***5364.8***	***8999.6***	**Seas_4**	**1320.7**	**41.0**	**16.0**	***459.2***	***746.1***
Annual	**122258.8**	**1211.5**	**7825.3**	**294.3**	***32897.5***	***59668.6***	**Annual**	**3736.0**	**91.1**	**33.1**	***1286.7***	***2121.3***

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
a - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model.

Own/alternative data set. Calculation results on PCB-180 mass degraded in 5cm layer of soil (kg) calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.33.

Monthly values of PCB-180 mass degraded in 5cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.42a and b, respectively.

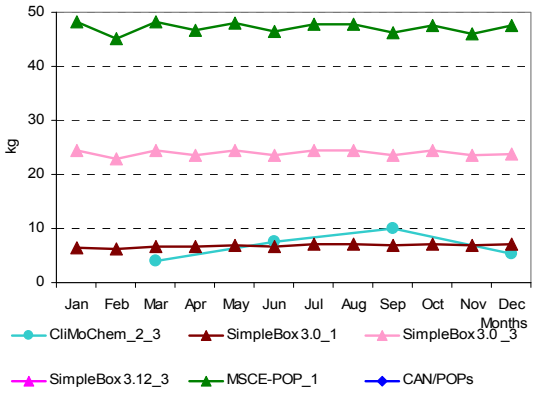


Fig. C.42a. *PCB-180 mass degraded in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

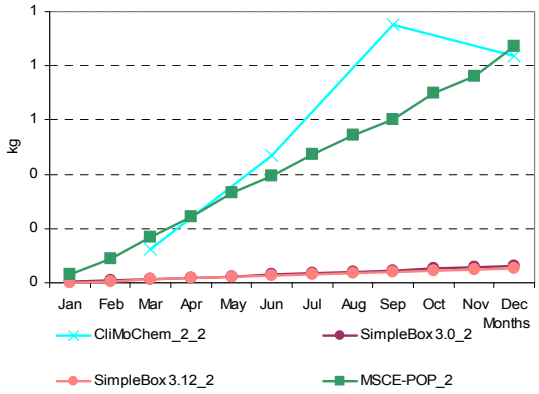


Fig. C.42b. *PCB-180 mass degraded in 5cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Table C.33. *Calculation results: PCB-180 mass degraded in 5cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	166.4	48.3	6.6		24.5	98.1	*68.8*	*64.5*	Jan		0.003	0.002	0.03	*0.01*	*0.02*
Feb	154.0	45.1	6.2		22.9	88.5	*63.4*	*59.3*	Feb		0.01	0.01	0.1	*0.03*	*0.05*
Mar	162.7	48.2	6.8		24.4	98.0	*68.0*	*63.1*	Mar		0.01	0.01	0.2	*0.1*	*0.1*
Seas_ 1	**483.1**	**141.6**	**19.6**	4.1	**71.8**	**284.6**	***167.5***	***185.3***	**Seas_1**	**0.1**	**0.02**	**0.02**	**0.3**	***0.1***	***0.1***
Apr	155.6	46.6	6.6		23.7	96.4	*65.8*	*60.5*	Apr		0.02	0.02	0.2	*0.1*	*0.1*
May	158.8	48.1	6.9		24.4	97.8	*67.2*	*61.6*	May		0.02	0.02	0.3	*0.1*	*0.2*
Jun	151.9	46.4	6.8		23.6	94.6	*64.7*	*58.9*	Jun		0.03	0.03	0.4	*0.1*	*0.2*
Seas_ 2	**466.3**	**141.1**	**20.3**	7.6	**71.7**	**288.9**	***166.0***	***179.5***	**Seas_2**	**0.5**	**0.07**	**0.06**	**1.0**	***0.4***	***0.4***
Jul	155.1	47.9	7.1		24.4	97.7	*66.4*	*60.2*	Jul		0.04	0.03	0.5	*0.2*	*0.3*
Aug	153.5	47.8	7.1		24.4	97.5	*66.1*	*59.5*	Aug		0.04	0.04	0.5	*0.2*	*0.3*
Sep	147.0	46.2	6.9		23.6	94.4	*63.6*	*57.1*	Sep		0.05	0.04	0.6	*0.2*	*0.3*
Seas_ 3	**455.6**	**141.8**	**21.1**	9.9	**72.4**	**289.6**	***165.1***	***175.4***	**Seas_3**	**1.0**	**0.12**	**0.11**	**1.6**	***0.7***	***0.7***
Oct	150.4	47.6	7.2		24.4	97.5	*65.4*	*58.4*	Oct		0.05	0.05	0.7	*0.3*	*0.4*
Nov	144.2	46.0	7.0		23.6	94.3	*63.0*	*56.0*	Nov		0.06	0.05	0.8	*0.3*	*0.4*
Dec	147.6	47.5	7.1		23.7	97.3	*64.6*	*57.5*	Dec		0.06	0.06	0.9	*0.3*	*0.5*
Seas_ 4	**442.2**	**141.2**	**21.2**	5.3	**71.7**	**289.1**	***161.8***	***171.8***	**Seas_4**	**0.8**	**0.17**	**0.15**	**2.3**	***0.9***	***1.0***
Annual	**1847.1**	**519.1**	**82.2**	**26.9**	**287.6**	**1152.2**	***652.5***	***713.4***	**Annual**	**2.4**	**0.39**	**0.34**	**5.0**	***2.0***	***2.2***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Calculation results on PCB-180 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.34.

Table C.34. *Calculation results: PCB-180 mass degraded in 10 cm layer of soil (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions	*m*	σ	Month	Results obtained on the basis of zero initial concentrations		*m*	σ
	CAN/POPs	MSCE-POP_1	CliMoChem_2_3				CliMo Chem_2_2	MSCE- POP_2		
Jan	332.7	48.8		*190.8*	*200.7*	Jan		0.03		
Feb	307.9	45.6		*176.8*	*185.5*	Feb		0.1		
Mar	325.6	48.7		*187.1*	*195.8*	Mar		0.2		
Seas_1	**966.2**	**143.2**	**8.1**	***372.5***	***518.5***	**Seas_1**	**0.2**	**0.3**	***0.3***	***0.0***
Apr	311.6	47.1		*179.3*	*187.0*	Apr		0.2		
May	318.3	48.6		*183.4*	*190.7*	May		0.3		
Jun	304.6	47.0		*175.8*	*182.2*	Jun		0.4		
Seas_2	**934.4**	**142.7**	**15.2**	***364.1***	***498.0***	**Seas_2**	**0.9**	**1.0**	***1.0***	***0.0***
Jul	311.2	48.4		*179.8*	*185.8*	Jul		0.5		
Aug	307.9	48.3		*178.1*	*183.6*	Aug		0.6		
Sep	294.9	46.7		*170.8*	*175.5*	Sep		0.6		
Seas_3	**914.0**	**143.4**	**19.9**	***359.1***	***484.5***	**Seas_3**	**1.9**	**1.6**	***1.8***	***0.2***
Oct	301.6	48.1		*174.9*	*179.2*	Oct		0.7		
Nov	288.9	46.5		*167.7*	*171.4*	Nov		0.8		
Dec	295.6	48.0		*171.8*	*175.1*	Dec		0.9		
Seas_4	**886.1**	**142.7**	**10.6**	***346.5***	***472.0***	**Seas_4**	**1.7**	**2.4**	***2.0***	***0.5***
Annual	**3700.7**	**571.9**	**53.8**	***1442.1***	***1973.1***	**Annual**	**4.8**	**5.3**	***5.0***	***0.4***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
a - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model on the basis of initial concentrations given as input data;
[b]– in CAN/POPs results the second layer of soil is applied as 5cm;

Monthly values of PCB-180 mass degraded in 10 cm layer of soil calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.43a and b, respectively.

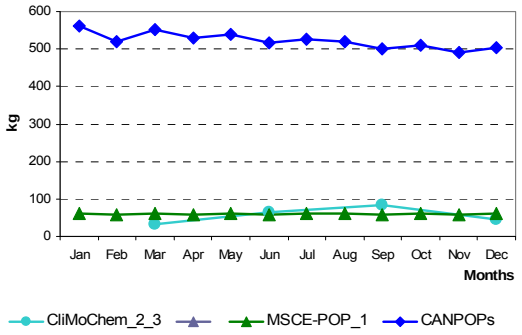


Fig. C.43a. *PCB-180 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

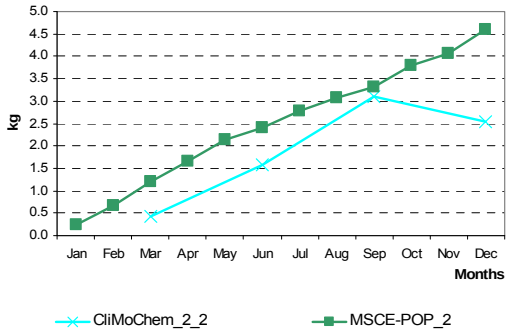


Fig. C.43b. *PCB-180 mass degraded in 10cm layer of soil (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results on PCB-180 mass degraded in soil within 5 and 10 cm layers obtained with two different data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Tables 3.35-3.36.

Table C.35. *The percentage difference between calculation results on PCB-180 mass degraded within 5 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-76%	-90%	-96%	-66%	-92%	-53%	-83%
Feb			-77%	-90%	-96%	-66%	-92%	-53%	-83%
Mar			-77%	-90%	-96%	-66%	-92%	-53%	-83%
Season_1	-97%	-89%	-77%	-90%	-96%	-66%	-92%	-53%	-83%
Apr			-77%	-90%	-96%	-66%	-92%	-53%	-83%
May			-77%	-90%	-96%	-66%	-92%	-53%	-82%
Jun			-77%	-90%	-96%	-66%	-92%	-53%	-82%
Season_2	-94%	-80%	-77%	-90%	-96%	-66%	-92%	-53%	-83%
Jul			-77%	-90%	-96%	-66%	-92%	-52%	-83%
Aug			-77%	-89%	-96%	-66%	-92%	-52%	-83%
Sep			-77%	-89%	-96%	-65%	-92%	-52%	-84%
Season_3	-92%	-73%	-77%	-89%	-96%	-66%	-92%	-52%	-83%
Oct			-77%	-89%	-96%	-65%	-92%	-53%	-85%
Nov			-77%	-89%	-96%	-65%	-92%	-53%	-85%
Dec			-77%	-89%	-96%	-65%	-92%	-53%	-86%
Season_4	-96%	-85%	-77%	-89%	-96%	-65%	-92%	-53%	-85%
Annual	-95%	-82%	-77%	-89%	-96%	-66%	-92%	-57%	-85%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations; SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data; SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations; SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Table C.36. *The percentage difference between calculation results on PCB-180 mass degraded within 10 cm soil layer obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMoChem_2_2	CliMoChem_2_3	MSCE-POP_1	MSCE-POP_2
Jan			-53%	-83%
Feb			-53%	-83%
Mar			-53%	-83%
Season_1	-97%	-89%	-53%	-83%
Apr			-53%	-83%
May			-53%	-82%
Jun			-53%	-82%
Season_2	-94%	-80%	-53%	-83%
Jul			-52%	-83%
Aug			-52%	-83%
Sep			-52%	-84%
Season_3	-92%	-73%	-52%	-83%
Oct			-53%	-85%
Nov			-53%	-85%
Dec			-53%	-86%
Season_4	-96%	-85%	-53%	-85%
Annual	-95%	-82%	-53%	-84%

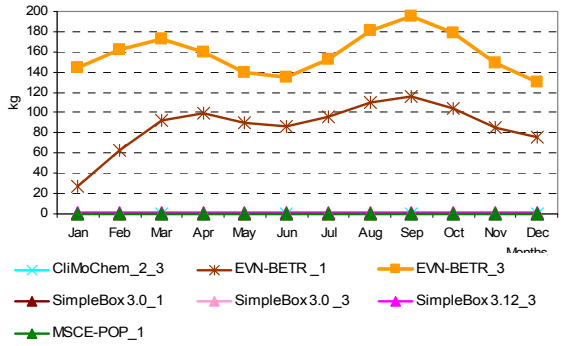
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations; CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period; MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data; MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations.

C.2.3. Comparison of calculated values of PCB-180 mass degraded in water

According to the programme of Stage II model results of computational experiments on mass balance include masses of PCB-180 degraded in sea within a layer of 200 m depth.

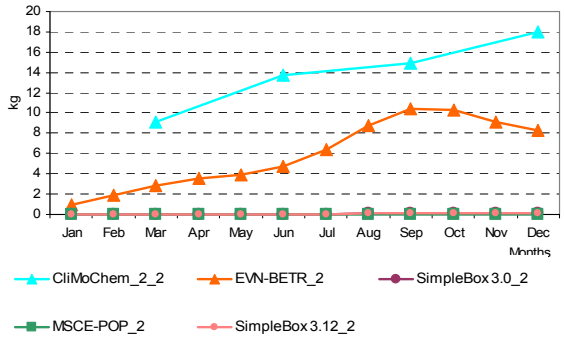
Reference data set. Calculation results on PCB-180 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.37.

Monthly values of PCB-180 mass degraded in 200 m layer of water calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.44a and b, respectively. Seasonal variations of low values of mass degraded in 200 m layer of water calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.44c in more detail.



a

Fig. C.44a. *PCB-180 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*



b

Fig. C.44b. *PCB-180 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

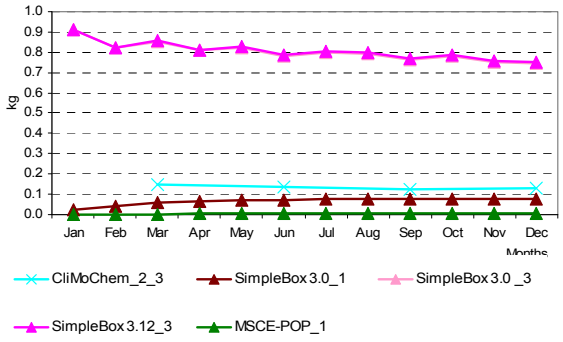


Fig. C.44c. *PCB-180 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

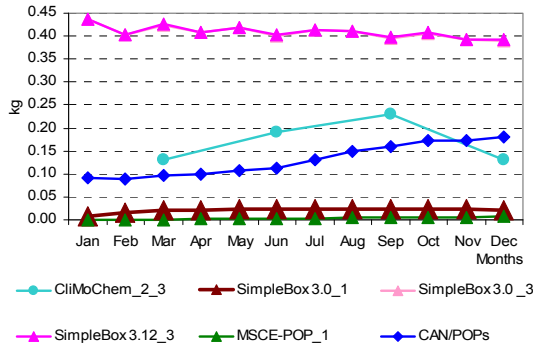
Table C.37. *Calculation results: PCB-180 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions				*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	EVN-BETR_1[a]	SimpleBox 3.0_1[b]	MSCE-POP_1	EVN-BETR_3[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[b]	SimpleBox 3.12_3[b]				EVN-BETR_2[a]	CliMo Chem_2_2	SimpleBox 3.0_2[b]	SimpleBox 3.12_2[b]	MSCE-POP_2		
Jan	27.08	0.03	0.002	144.08		0.91	0.91	*28.83*	*57.45*	Jan	0.90		0.01	0.01	0.001	0.23	0.45
Feb	62.32	0.04	0.002	162.60		0.82	0.82	*37.77*	*65.98*	Feb	1.86		0.02	0.02	0.002	0.48	0.92
Mar	92.70	0.06	0.003	173.03		0.85	0.86	*44.58*	*72.95*	Mar	2.87		0.03	0.03	0.002	0.74	1.43
Seas_1	**182.10**	**0.13**	**0.006**	**479.71**	**0.15**	**2.59**	**2.59**	***95.32***	***182.43***	**Seas_1**	**5.64**	**9.09**	**0.06**	**0.06**	**0.005**	**2.97**	**4.19**
Apr	99.23	0.06	0.004	160.06		0.81	0.81	*43.50*	*69.45*	Apr	3.55		0.04	0.04	0.003	0.91	1.76
May	90.44	0.07	0.004	139.70		0.82	0.83	*38.64*	*61.22*	May	3.96		0.05	0.05	0.004	1.02	1.96
Jun	86.88	0.07	0.005	135.02		0.78	0.79	*37.26*	*59.08*	Jun	4.72		0.05	0.05	0.004	1.21	2.34
Seas_2	**276.55**	**0.21**	**0.01**	**434.79**	**0.14**	**2.41**	**2.43**	***102.36***	***178.97***	**Seas_2**	**12.24**	**13.70**	**0.14**	**0.14**	**0.011**	**5.25**	**7.07**
Jul	95.81	0.08	0.01	152.37		0.80	0.81	*41.64*	*66.32*	Jul	6.37		0.06	0.06	0.004	1.62	3.17
Aug	110.63	0.08	0.01	180.75		0.79	0.80	*48.84*	*78.23*	Aug	8.74		0.06	0.06	0.004	2.22	4.35
Sep	115.94	0.08	0.01	194.95		0.76	0.77	*52.08*	*83.87*	Sep	10.47		0.06	0.06	0.01	2.65	5.21
Seas_3	**322.37**	**0.23**	**0.02**	**528.07**	**0.12**	**2.36**	**2.37**	***122.22***	***215.34***	**Seas_3**	**25.58**	**14.91**	**0.18**	**0.18**	**0.01**	**8.17**	**11.65**
Oct	103.84	0.08	0.01	179.05		0.78	0.79	*47.43*	*76.62*	Oct	10.32		0.06	0.06	0.01	2.61	5.14
Nov	85.65	0.08	0.01	149.21		0.75	0.76	*39.41*	*63.69*	Nov	9.08		0.06	0.06	0.01	2.30	4.52
Dec	75.56	0.08	0.01	130.30		0.75	0.75	*34.57*	*55.71*	Dec	8.34		0.07	0.07	0.01	2.12	4.15
Seas_4	**265.05**	**0.23**	**0.03**	**458.56**	**0.13**	**2.28**	**2.30**	***104.08***	***184.71***	**Seas_4**	**27.75**	**18.00**	**0.19**	**0.19**	**0.02**	**9.23**	**12.92**
Annual	**1046.07**	**0.79**	**0.06**	**1901.13**	**0.54**	**9.63**	**9.69**	***423.99***	***758.33***	**Annual**	**71.20**	**55.70**	**0.58**	**0.58**	**0.05**	**25.62**	**34.96**

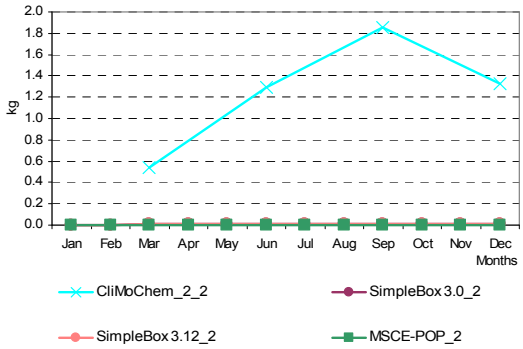
EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data;
EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;
EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - EVN-BETR and UK-MODEL results were calculated with the help of a single box version of European model;
b - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-180 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.38.

Monthly values of PCB-180 mass degraded in 200 m layer of water calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.45a and b, respectively. Seasonal variations of low values of mass degraded in 200 m layer of water calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions are also shown in Fig. C.45c in more detail.



a



b

Fig. C.45a. *PCB-180 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

Fig. C.45b. *PCB-180 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "own or alternative" data sets and zero initial conditions*

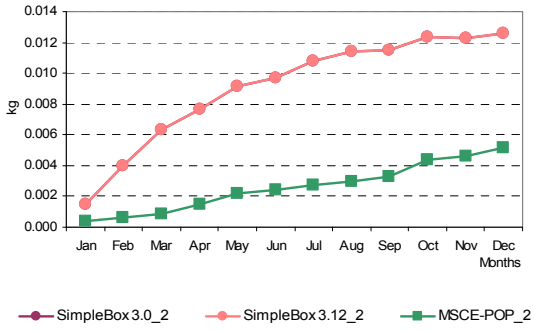


Fig. C.45c. *PCB-180 mass degraded in 200 m layer of water (kg) calculated by the participating models on the basis of "reference" data set and zero initial conditions (models with low values)*

Table C.38. *Calculation results: PCB-180 mass degraded in 200 m layer of water (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	0.09	0.01	0.0005		0.44	0.44	*0.19*	*0.22*	Jan		0.002	0.002	0.0004	*0.001*	*0.001*
Feb	0.09	0.01	0.001		0.40	0.40	*0.18*	*0.20*	Feb		0.004	0.004	0.001	*0.003*	*0.002*
Mar	0.10	0.02	0.001		0.42	0.43	*0.19*	*0.21*	Mar		0.006	0.006	0.001	*0.005*	*0.003*
Seas_1	**0.28**	**0.04**	**0.002**	**0.13**	**1.26**	**1.27**	***0.50***	***0.60***	**Seas_1**	**0.54**	**0.012**	**0.012**	**0.002**	***0.14***	***0.27***
Apr	0.10	0.02	0.002		0.41	0.41	*0.19*	*0.20*	Apr		0.008	0.008	0.001	*0.01*	*0.00*
May	0.11	0.02	0.003		0.42	0.42	*0.19*	*0.21*	May		0.009	0.009	0.002	*0.01*	*0.00*
Jun	0.11	0.02	0.003		0.40	0.40	*0.19*	*0.20*	Jun		0.010	0.010	0.002	*0.01*	*0.00*
Seas_2	**0.32**	**0.07**	**0.008**	**0.19**	**1.23**	**1.23**	***0.51***	***0.57***	**Seas_2**	**1.29**	**0.027**	**0.027**	**0.006**	***0.34***	***0.63***
Jul	0.13	0.02	0.004		0.41	0.41	*0.20*	*0.20*	Jul		0.011	0.011	0.003	*0.01*	*0.00*
Aug	0.15	0.02	0.004		0.41	0.41	*0.20*	*0.20*	Aug		0.011	0.011	0.003	*0.01*	*0.00*
Sep	0.16	0.02	0.005		0.39	0.40	*0.20*	*0.19*	Sep		0.012	0.012	0.003	*0.01*	*0.00*
Seas_3	**0.44**	**0.07**	**0.012**	**0.23**	**1.22**	**1.22**	***0.53***	***0.55***	**Seas_3**	**1.85**	**0.034**	**0.034**	**0.009**	***0.48***	***0.91***
Oct	0.17	0.02	0.006		0.41	0.41	*0.20*	*0.20*	Oct		0.012	0.012	0.004	*0.01*	*0.00*
Nov	0.17	0.02	0.007		0.39	0.39	*0.20*	*0.19*	Nov		0.012	0.012	0.005	*0.01*	*0.00*
Dec	0.18	0.02	0.007		0.39	0.39	*0.20*	*0.19*	Dec		0.013	0.013	0.005	*0.01*	*0.00*
Seas_4	**0.53**	**0.07**	**0.020**	**0.13**	**1.19**	**1.19**	***0.52***	***0.55***	**Seas_4**	**1.32**	**0.037**	**0.037**	**0.014**	***0.35***	***0.65***
Annual	**1.56**	**0.25**	**0.043**	**0.68**	**4.89**	**4.91**	***2.06***	***2.27***	**Annual**	**5.01**	**0.109**	**0.109**	**0.031**	***1.31***	***2.46***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data presented here are overall masses calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.39.

Table C.39. *The percentage difference between calculation results on PCB-180 mass degraded in 200 m layer of water obtained by models on the basis of two data sets: "own or alternative" and "reference"*

Month	CliMo Chem_2_2	CliMo Chem_2_3	Simple Box 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			-71%	-82%	-82%	-52%	-52%	-69%	-71%
Feb			-66%	-82%	-82%	-51%	-51%	-63%	-65%
Mar			-65%	-82%	-82%	-50%	-50%	-57%	-59%
Seas_1	-94%	-9%	-67%	-82%	-82%	-51%	-51%	-62%	-64%
Apr			-66%	-81%	-81%	-50%	-50%	-51%	-54%
May			-66%	-81%	-81%	-49%	-49%	-37%	-41%
Jun			-67%	-81%	-81%	-49%	-49%	-33%	-37%
Seas_2	-91%	38%	-66%	-81%	-81%	-49%	-49%	-40%	-43%
Jul			-68%	-81%	-81%	-49%	-49%	-32%	-36%
Aug			-69%	-81%	-81%	-48%	-48%	-29%	-34%
Sep			-69%	-81%	-81%	-48%	-48%	-28%	-34%
Seas_3	-88%	84%	-69%	-81%	-81%	-48%	-49%	-30%	-35%
Oct			-70%	-81%	-81%	-48%	-48%	-25%	-32%
Nov			-71%	-81%	-81%	-48%	-48%	-25%	-32%
Dec			-72%	-81%	-81%	-48%	-48%	-17%	-25%
Seas_4	-93%	1%	-71%	-81%	-81%	-48%	-48%	-22%	-29%
Annual	-91%	27%	-68%	-81%	-81%	-49%	-49%	-32%	-38%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

B.2.4. Comparison of calculated values of PCB-180 mass degraded in vegetation

Reference data set. Values of PCB-180 mass degraded in vegetation (kg) obtained by CliMoChem_2_2 and CliMoChem_2_3 models on the basis of "reference" data set are equal to zero.

Own/alternative data set. Calculation results on PCB-180 mass degraded in vegetation (kg) calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.40.

Table C.40. *Calculation results: PCB-180 mass degraded in vegetation (kg) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of historical emissions	Results obtained on the basis of zero initial concentrations	*m*	σ
	CliMoChem_2_3	CliMoChem_2_2		
Jan				
Feb				
Mar				
Seas_1	**3.35**	**18.38**	***10.86***	***7.52***
Apr				
May				
Jun				
Seas_2	**8.05**	**123.10**	***65.57***	***57.53***
Jul				
Aug				
Sep				
Seas_3	**15.18**	**274.91**	***145.04***	***129.87***
Oct				
Nov				
Dec				
Seas_4	**7.77**	**142.38**	***75.08***	***67.31***
Annual	**34.34**	**558.78**	***296.56***	***262.22***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
* - In MSCE-POP model degradation in vegetation is not taken into account.

Monthly values of PCB-180 mass degraded in vegetation calculated by the participating models on the basis of "own or alternative" data sets are compared in Fig. C.46.

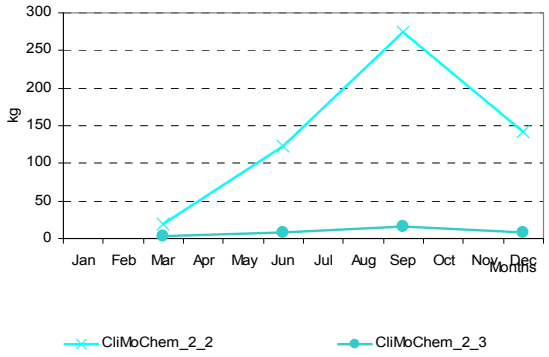


Fig. C.46. *PCB-180 mass degraded in vegetation (kg) calculated by the participating models on the basis of "own or alternative" data sets*

C.2.5. Comparison of distribution of PCB-180 mass degraded in the environment

Sections from 3.2.1 to 3.2.4 above are devoted to the comparison between the results of participating models on PCB-180 mass degraded in the main environmental compartments (atmosphere, soil, water and vegetation). The comparison includes results of one-year calculations made on the basis of initial conditions (CAN/POPs, EVN-BETR and UK-MODEL, MSCE-POP, SimpleBox) and zero initial concentrations (CliMoChem, MSCE-POP and SimpleBox) along with results of long-term calculations performed with historical emissions (CliMoChem, EVN-BETR and UK-MODEL, and SimpleBox).

Calculation results obtained with the use of two different physical-chemical data sets are submitted by CliMoChem, MSCE-POP and SimpleBox models.

A preliminary analysis of the main results on comparison of absolute and relative values of PCB-180 mass degraded in the main environmental compartments is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions and for results based on zero-initial conditions.

Atmosphere. Comparison of annual values of PCB-180 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. C.47a. Fig. C.47b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

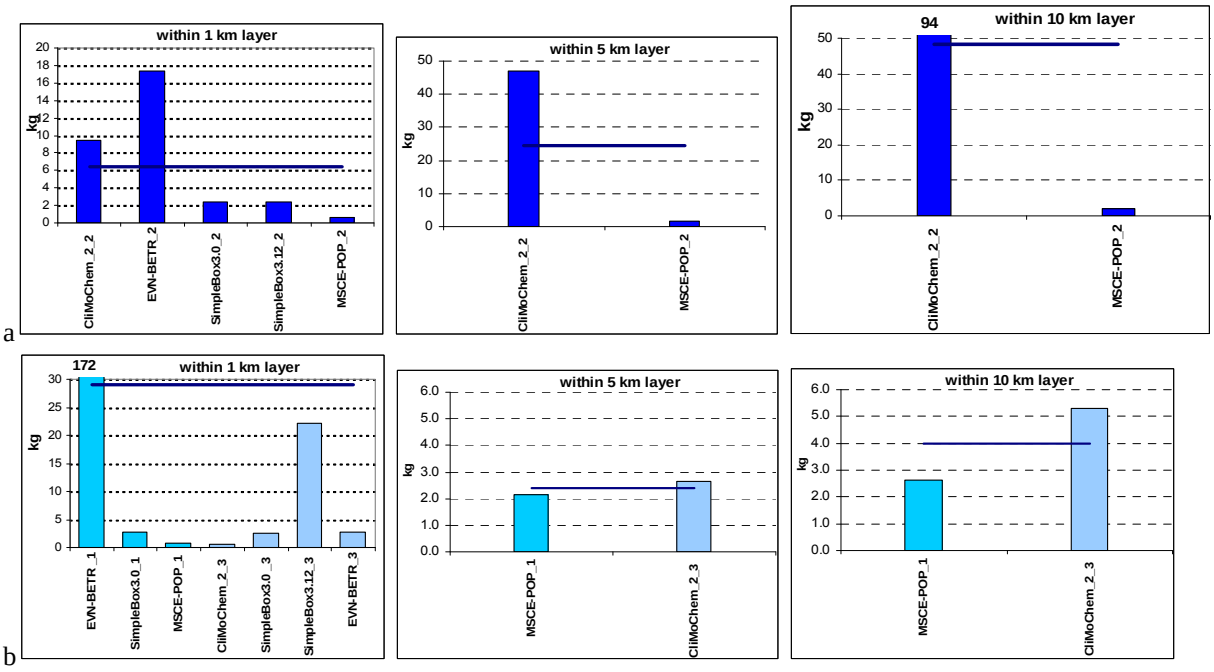


Fig. C.47. *Comparison of annual values of PCB-180 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-180 degraded mass calculated by CliMoChem and MSCE-POP models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference" data set is presented in Fig. C.48.

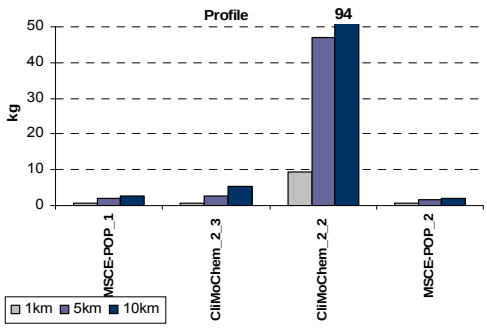


Fig. C.48. *Comparison of profiles of annual values of PCB-180 degraded mass calculated by four models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "reference data set»*

Comparison of annual values of PCB-180 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of zero initial concentrations and with the use of "***own***

or alternative" data sets is presented in Fig. C.49a. Fig. C.49b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

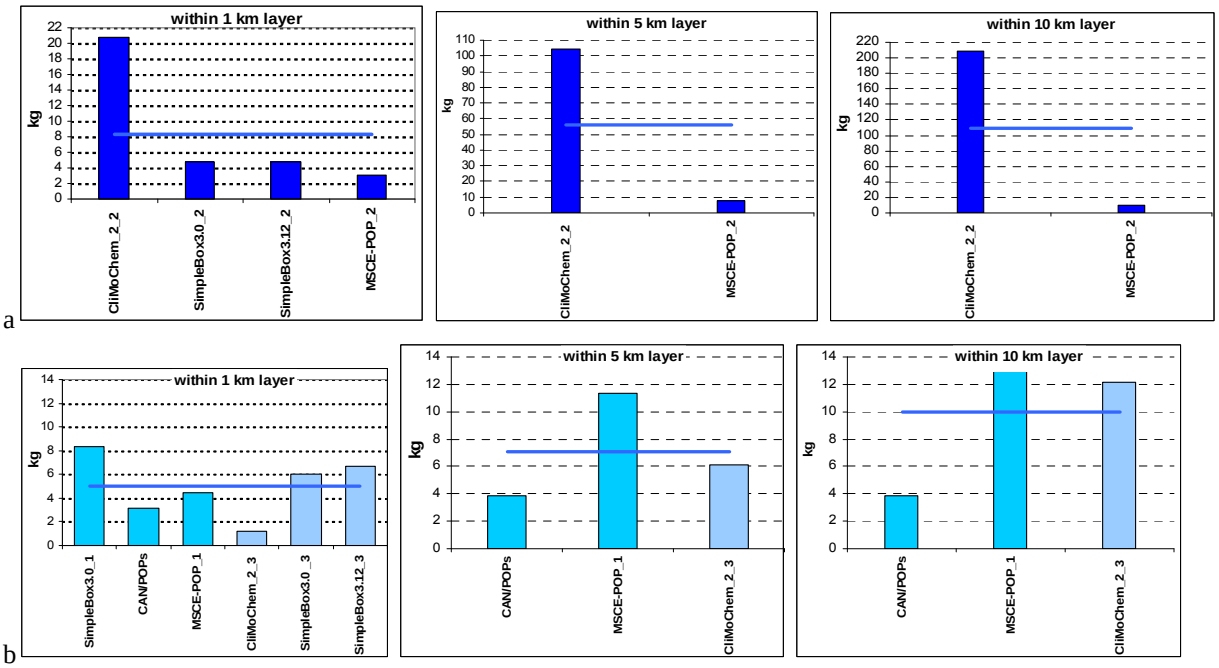


Fig. C.49. *Comparison of annual values of PCB-180 masses degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-180 degraded mass calculated by three models (CAN/POPs, CliMoChem and MSCE-POP) for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative" data sets is presented in Fig. C.50.

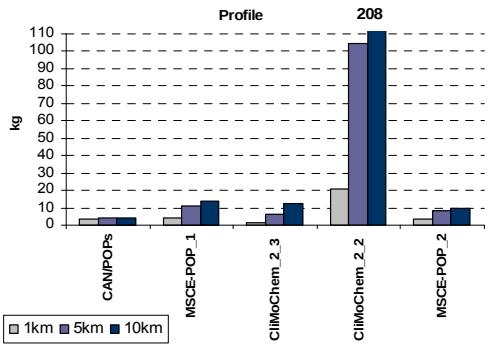


Fig. C.50. *Comparison of profiles of annual values of PCB-180 degraded mass calculated by the models for the considered atmospheric layers (1, 5 and 10 km) on the basis of "own or alternative data sets"*

Comparison of annual values of PCB-180 mass degraded in the considered different layers of the atmosphere obtained with "reference" and "own/alternative" data sets is presented in Fig. C.51.

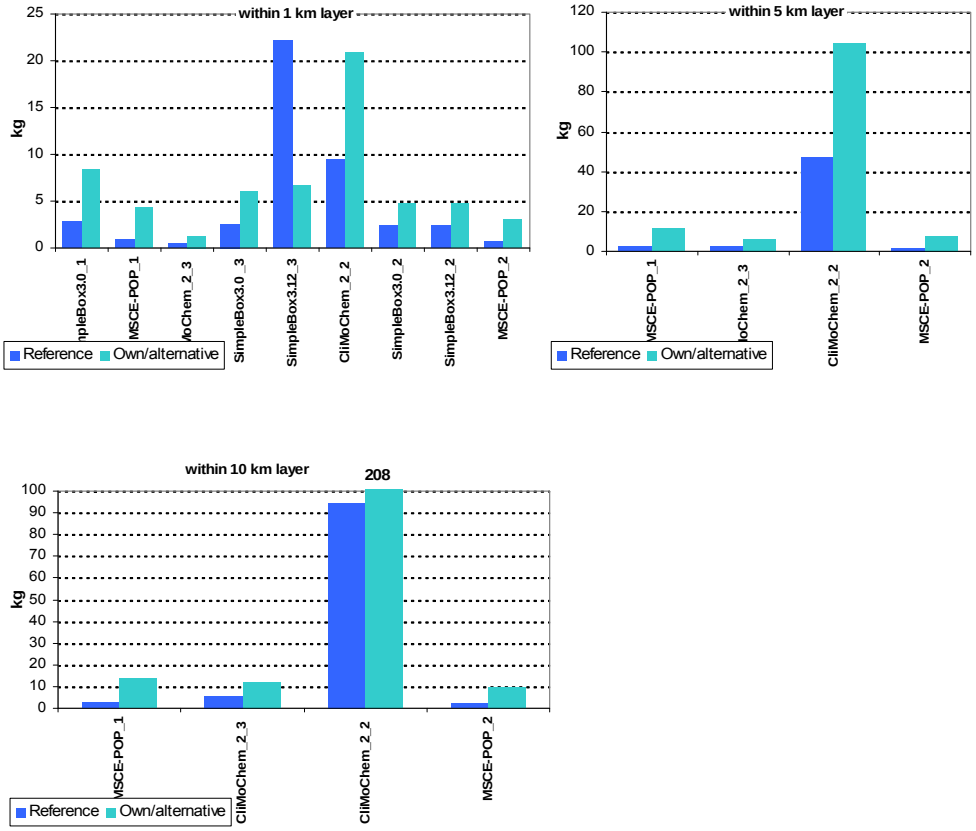


Fig. C.51. *Comparison of PCB-180 mass degraded in the atmosphere within 1, 5 and 10 km layers calculated by different models on the basis of two data set*

Soil. Comparison of annual values of PCB-180 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. C.52a. Fig. C.52b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

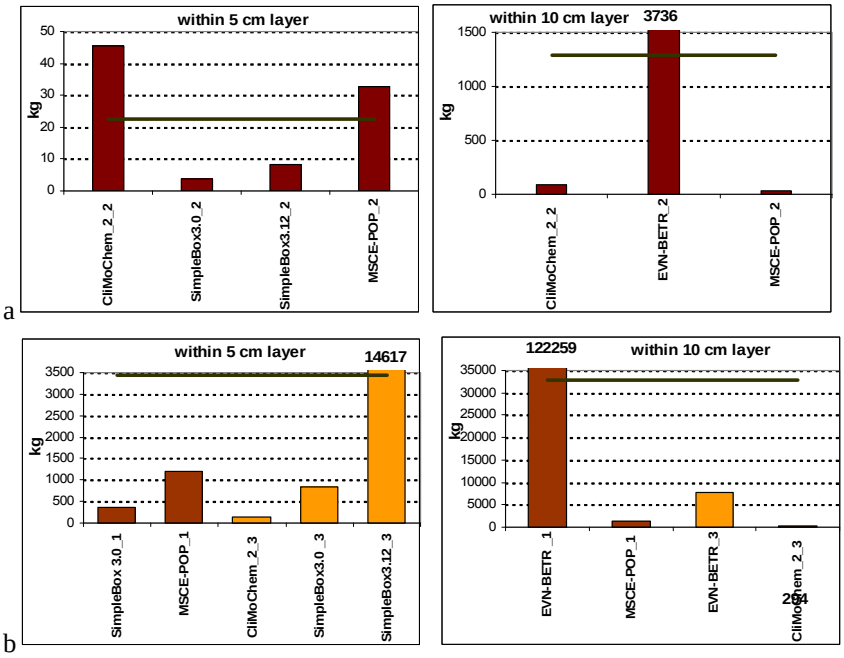


Fig. C.52. *Comparison of annual values of PCB-180 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-180 degraded mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "reference" data set is presented in Fig. C.53.

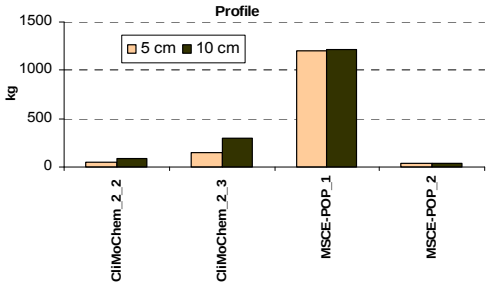


Fig. C.53. *Comparison of profiles of annual values of PCB-180 degraded mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "reference data set"*

Comparison of annual values of PCB-180 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative***" data sets is presented in Fig. C.54a. Fig. C.54b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The black line in the plots shows the value of the corresponding parameter averaged between models.

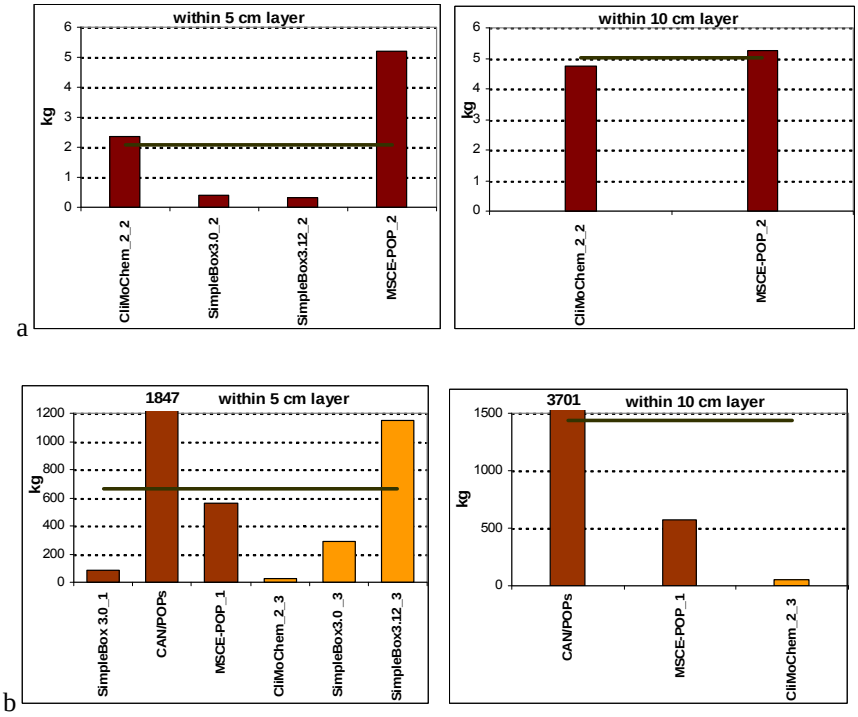


Fig. C.54. *Comparison of annual values of PCB-180 masses degraded in soil within 5 and 10 cm layers calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of profiles of annual values of PCB-180 degraded mass calculated by the participating models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative" data sets is presented in Fig. C.55.

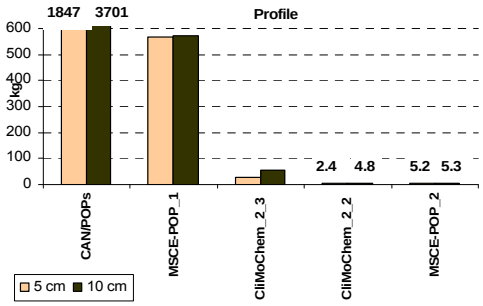


Fig. C.55. *Comparison of profiles of annual values of PCB-180 degraded mass calculated by the models for the considered soil layers (5 and 10 cm) on the basis of "own or alternative data sets"*

Comparison of annual values of PCB-180 mass degraded in the considered different layers of soil obtained with "reference" and "own/alternative" data sets is presented in Fig. C.56.

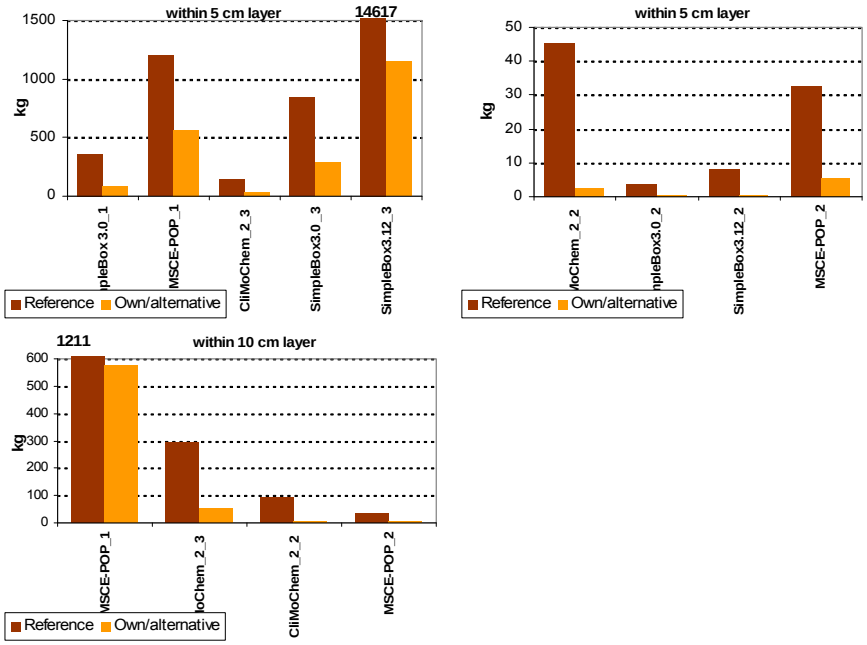
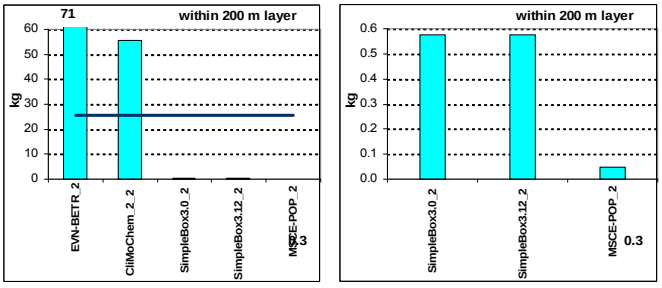


Fig. C.56. *Comparison of PCB-180 mass degraded within 5 and 10 cm soil layers calculated by different models on the basis of two data set*

Water. Comparison of annual values of PCB-180 masses degraded in water layer of 200 m calculated by different models on the basis of zero initial concentrations and with the use of "***reference"*** data set is presented in Fig. C.57a. Fig. C.57b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plot shows the value of the corresponding parameter averaged between models.

a



b

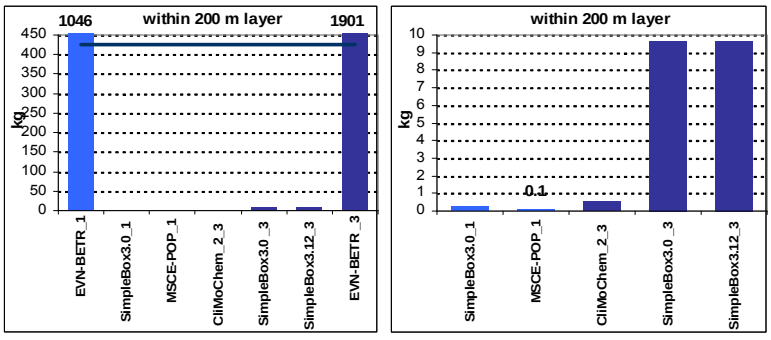


Fig. C.57. *Comparison of annual values of PCB-180 masses degraded in water within 200 m layer calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-180 masses degraded in water layer of 200 m calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative"*** data sets is presented in Fig. C.58a (blue line corresponds to the averaged value). Fig. C.58b shows the same results but obtained on the basis of initial concentrations or historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

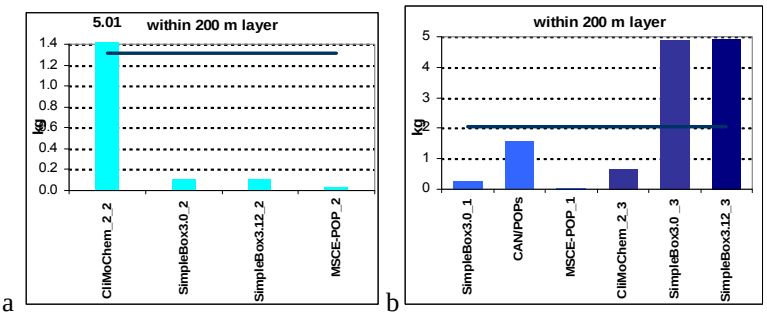


Fig. C.58. *Comparison of annual values of PCB-180 masses degraded in water within 200 m layer calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Annual values of PCB-180 mass degraded in the 200m layer of water obtained by the participating models on the basis of "reference" and "own/alternative" data sets are compared in Fig. C.59.

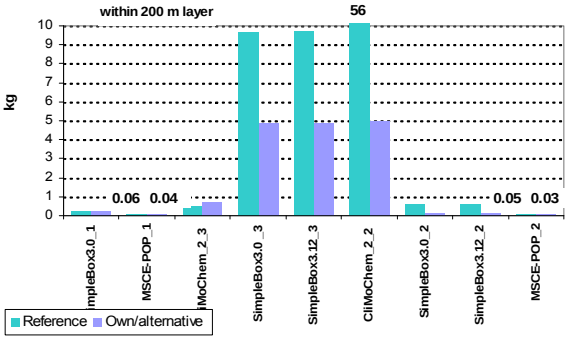


Fig. C.59. *Comparison of PCB-180 mass degraded within 200 m water layer calculated by different models on the basis of two data sets*

Vegetation. Annual values of PCB-180 mass degraded in vegetation obtained by the participating models on the basis of "reference" and "own/alternative" data sets are shown in Fig. C.60.

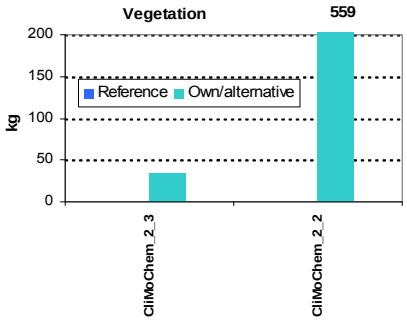


Fig. C.60. *Comparison of PCB-180 mass degraded in vegetation calculated by different models on the basis of two data sets*

Relative distribution of PCB mass degraded in the environmental compartments

The presented estimates of PCB-180 masses degraded in the main environmental compartments allow one to reveal the relative contributions of degradation process occurs in this or that media to the overall mass of PCB-180 in the whole environment. Below, the comparison of relative fractions of PCB-180 mass degraded in the main environmental media in relation to the mass balance estimates is presented. Of note, here and hereinafter fractions of mass degraded in different media are the ratios of the degraded mass and the mass contained in the considered compartment (taking into account also degraded mass).

Fractions of PCB-180 mass degraded in the atmosphere calculated by the participating models on the basis of zero and non-zero initial conditions are presented in Figs. 3.61a and b, respectively. In these figures fractions of PCB-180 mass degraded in the atmosphere calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared.

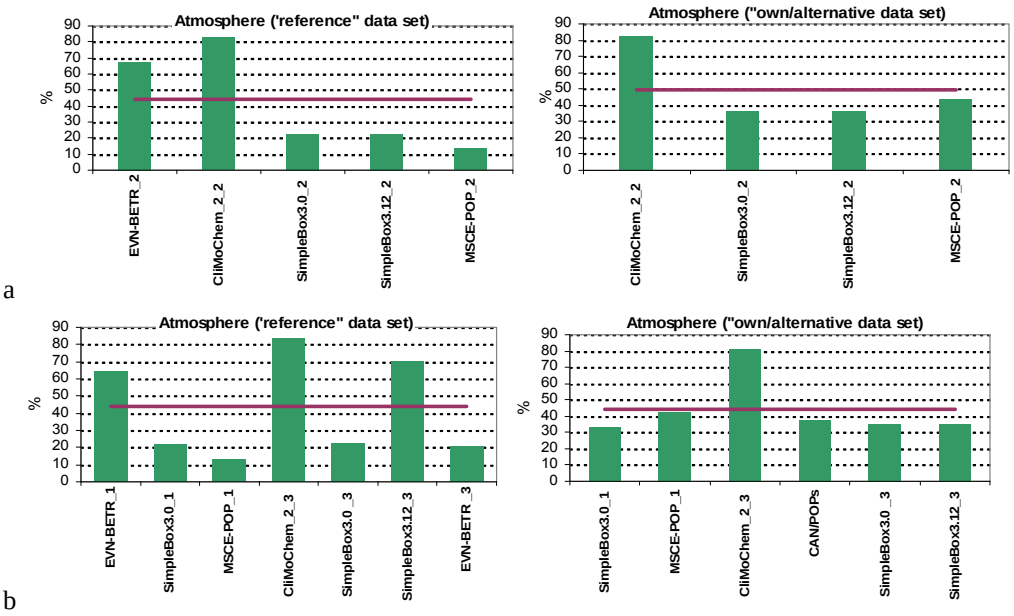


Fig. C.61. *Fractions of PCB-180 mass degraded in the atmosphere calculated by the participating models on the basis of “reference” and “own or alternative” data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

In Fig. C.62 a and b fractions of PCB-180 mass degraded in soil calculated by the different models on the basis of zero and non-zero initial conditions are presented, respectively. In these figures fractions of PCB-180 mass degraded in soil calculated by the different models with the use of “reference” and “own/alternative” data sets are also compared.

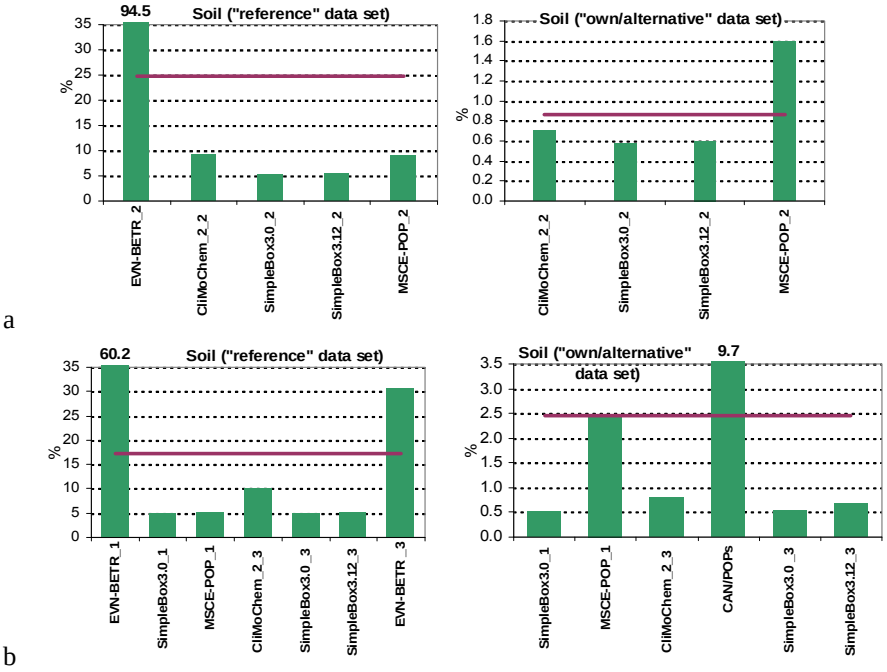


Fig. C.62. *Fractions of PCB-180 mass degraded in soil calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fractions of PCB-180 mass degraded in seawater calculated by the participating on the basis of zero and non-zero initial conditions are presented in Figs. 3.63a and b, respectively. In these figures fractions of PCB-180 mass degraded in the atmosphere calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.

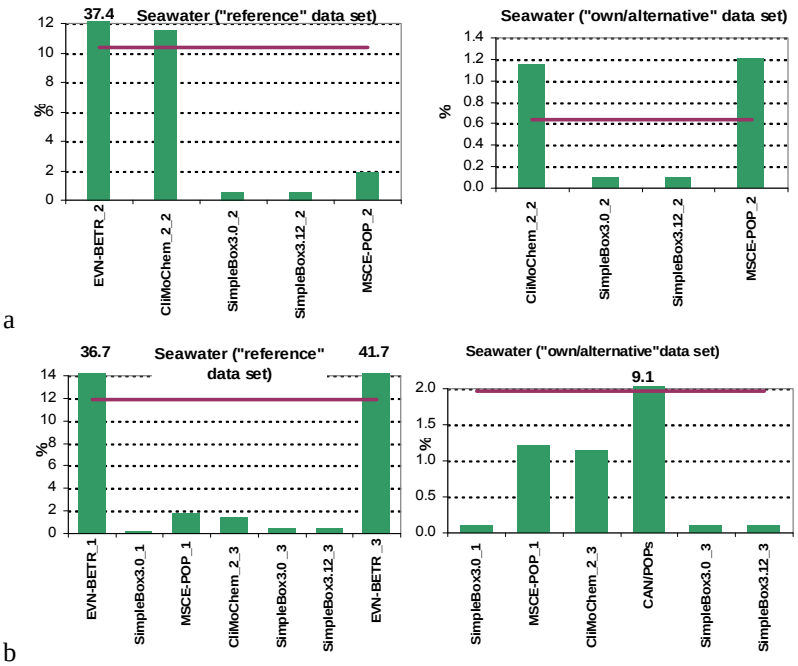


Fig. C.63. *Fractions of PCB-180 mass degraded in seawater calculated by the participating models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

For the participating models, which consider process of degradation in vegetation, fractions of PCB-180 mass degraded in vegetation calculated on the basis of zero and non-zero initial conditions are presented in Figs. 3.64.

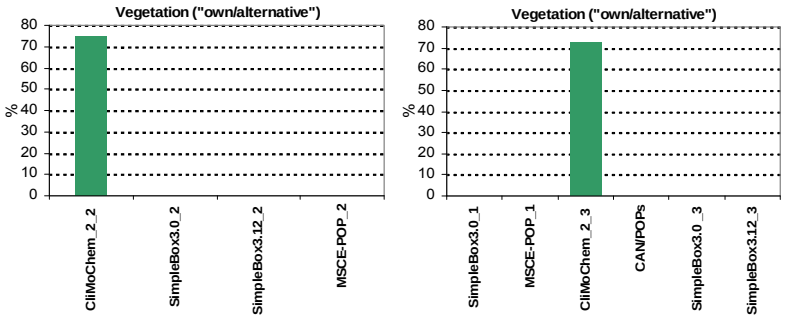


Fig. C.64. *Fractions of PCB-180 mass degraded in vegetation calculated by the participating models on the basis of "own or alternative" data sets*

3.2.6. Comparison of calculated values of PCB-180 mass deposited into deep sea

In this section a comparison of results calculated by CliMoChem model with historical emission scenario on the basis of their own Land Cover Data [*DeFries and Townshend*, 1994] and Land Cover Data given as input data for this intercomparison study [*Guo and Chen*, 1994] is presented. Of note, contrary to the calculations discussed in the previous and subsequent sections in this simulation, PCB-180 is emitted as pulse emission into air each year at the beginning of season one.

Reference data set. Two sets of calculated values of PCB-180 mass deposited into deep sea (kg) obtained by CliMoChem model on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.41.

Table C.41. *Calculation results: PCB-180 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "reference" data set and statistical parameters used for evaluation*

Month	CliMoChem_1_3	CliMoChem_2_3	*m*	σ
Season_1	37.38	41.72	*39.55*	*3.07*
Season_2	23.75	26.39	*25.07*	*1.87*
Season_3	14.31	15.85	*15.08*	*1.09*
Season_4	10.31	11.48	*10.90*	*0.83*
Annual	**85.75**	**95.45**	***90.60***	***6.86***

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

Seasonal values of PCB-180 mass deposited into deep sea calculated by CliMoChem model on the basis of "reference" data set are compared in Fig. C.65.

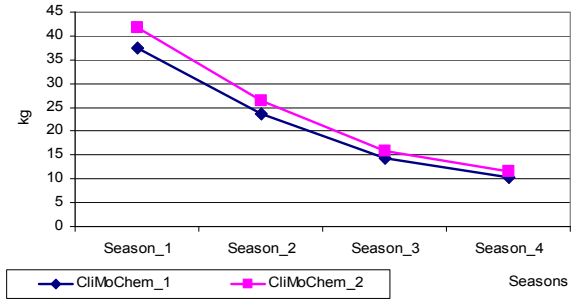


Fig. C.65. *PCB-180 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "reference" data set*

Own/alternative data set. Two versions of calculation results on PCB-180 mass deposited into deep sea (kg) obtained by CliMoChem model on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.42.

Table C.42. *Calculation results: PCB-180 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	CliMoChem_1_3	CliMoChem_2_3	*m*	σ
Season_1	27.70	32.71	*30.20*	*3.54*
Season_2	22.39	26.62	*24.51*	*2.99*
Season_3	16.39	19.57	*17.98*	*2.25*
Season_4	13.67	16.48	*15.08*	*1.98*
Annual	**80.16**	**95.37**	***87.77***	***10.76***

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

Seasonal values of PCB-180 mass deposited into deep sea calculated by CliMoChem model on the basis of "own or alternative" data sets are compared in Fig. C.66.

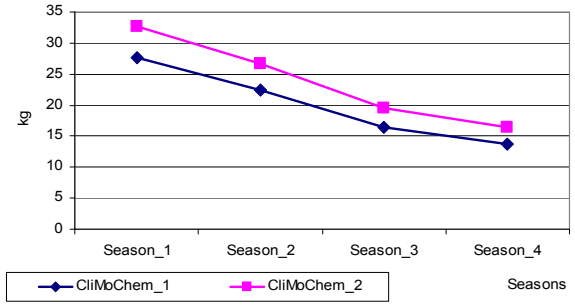


Fig. C.66. *PCB-180 mass deposited into deep sea (kg) calculated by CliMoChem model on the basis of "own or alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.45.

Table C.45. *The percentage difference between calculation results on PCB-180 mass deposited into deep sea obtained by CliMoChem model on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_1_3	CliMoChem_2_3
Season_1	-26%	-22%
Season_2	-6%	1%
Season_3	15%	23%
Season_4	33%	43%
Annual	**-7%**	**-0.1%**

CliMoChem_1_3 – CliMoChem results calculated on the basis of their own Land Cover Data;
CliMoChem_2_3 – CliMoChem results calculated on the basis of Land Cover Data given as input data for this intercomparison study

C.3. Mass flows transported in/out the specified domain: inflow and outflow

Mass flows of PCB-180 transported in/out the specified domain (inflow and outflow) are calculated by the participating models on the basis of atmospheric emission estimates presented by [*Breivik et al*. 2002a] (see also www.nilu.no/projects/globalpcb/). The higher (or worst-case) emission estimates for 1981-2000 are applied.

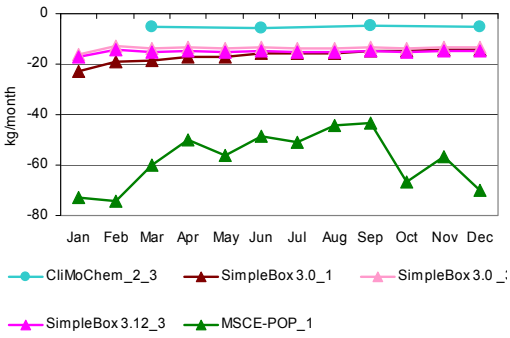
All amount of emissions is released into the atmosphere and is uniformly distributed throughout a year. In calculations of CAN/POPs, SimpleBox and MSCE-POP models, a value of PCB-180 total annual emissions in 2000 equals on average 1511 kg. In CliMoChem model the global emission data were summarized to zone-specific emissions (10 zones) and for the specified domain emission data for the model zones 2 and 3 (of 10) are used. At that emission value in 2000 used by CliMoChem for PCB-180 totals to 2216 kg.

It should be noted that transport into the calculation domain is supposed to be positive.

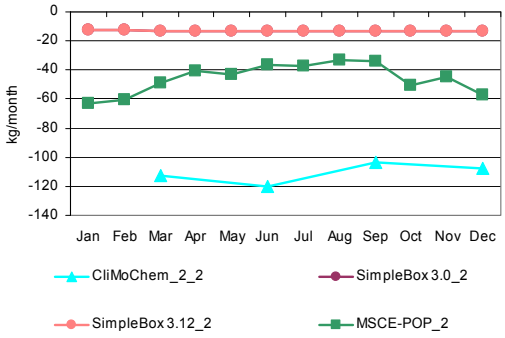
C.3.1. Comparison of calculated values of PCB-180 mass flows transported in/out the calculation domain through the atmosphere.

Reference data set. Calculation results on PCB-180 mass flows transported in/out the calculation domain through the atmosphere calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.44.

Monthly values of PCB-180 mass flows transported in/out the calculation domain through the atmosphere calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.67 a and b, respectively.



a



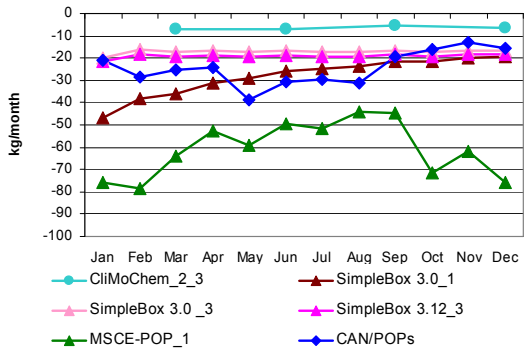
b

Fig. C.67a. *PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

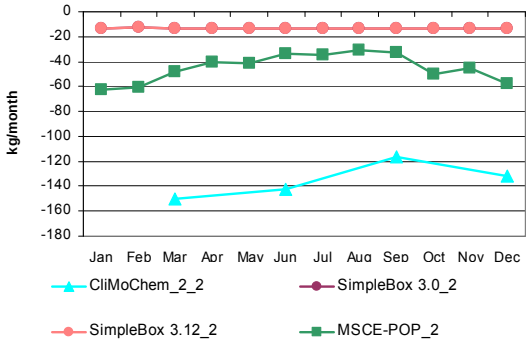
Fig. C.67b. *PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported in/out the calculation domain through the atmosphere calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.45.

Monthly values of PCB-180 mass flows transported in/out of the calculation domain through atmosphere calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.68 a and b, respectively.



a



b

Fig. C.68a. *PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

Fig. C.68b. *PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.46.

Table C.44. *Calculation results: PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-22.7	-72.7		-16.1	-17.4	*-32.2*	*27.1*	Jan		-12.7	-12.7	-62.7	*-29.3*	*28.9*
Feb	-18.9	-74.1		-12.9	-14.2	*-30.0*	*29.5*	Feb		-12.5	-12.5	-60.3	*-28.4*	*27.6*
Mar	-18.8	-60.0		-13.8	-15.1	*-26.9*	*22.1*	Mar		-13.4	-13.4	-48.5	*-25.1*	*20.3*
Seas_1	**-60.4**	**-206.7**	**-16.1**	**-42.9**	**-46.7**	***-74.5***	***75.6***	**Seas_1**	**-339.2**	**-38.5**	**-38.5**	**-171.4**	***-146.9***	***142.7***
Apr	-17.2	-49.9		-13.4	-14.6	*-23.8*	*17.5*	Apr		-12.9	-12.9	-40.8	*-22.2*	*16.1*
May	-16.9	-56.2		-13.8	-15.1	*-25.5*	*20.5*	May		-13.4	-13.4	-43.4	*-23.4*	*17.3*
Jun	-15.8	-48.6		-13.4	-14.6	*-23.1*	*17.0*	Jun		-12.9	-12.9	-36.3	*-20.7*	*13.5*
Seas_2	**-49.9**	**-154.7**	**-17.3**	**-40.5**	**-44.3**	***-61.4***	***53.6***	**Seas_2**	**-360.0**	**-39.3**	**-39.3**	**-120.5**	***-139.7***	***151.7***
Jul	-15.9	-50.7		-13.8	-15.1	*-23.9*	*17.9*	Jul		-13.4	-13.4	-37.3	*-21.4*	*13.8*
Aug	-15.5	-44.2		-13.8	-15.1	*-22.1*	*14.7*	Aug		-13.4	-13.4	-33.1	*-20.0*	*11.4*
Sep	-14.7	-43.4		-13.3	-14.6	*-21.5*	*14.6*	Sep		-13.0	-13.0	-33.9	*-20.0*	*12.1*
Seas_3	**-46.1**	**-138.4**	**-14.9**	**-40.9**	**-44.7**	***-57.0***	***47.2***	**Seas_3**	**-310.3**	**-39.7**	**-39.7**	**-104.4**	***-123.5***	***128.2***
Oct	-15.0	-66.5		-13.8	-15.0	*-27.6*	*25.9*	Oct		-13.4	-13.4	-50.5	*-25.7*	*21.4*
Nov	-14.3	-56.9		-13.3	-14.6	*-24.8*	*21.4*	Nov		-13.0	-13.0	-44.5	*-23.5*	*18.2*
Dec	-14.1	-70.2		-13.3	-14.5	*-28.1*	*28.1*	Dec		-13.0	-13.0	-56.8	*-27.6*	*25.3*
Seas_4	**-43.4**	**-193.5**	**-15.7**	**-40.4**	**-44.2**	***-67.4***	***71.4***	**Seas_4**	**-322.3**	**-39.3**	**-39.3**	**-151.8**	***-138.2***	***133.7***
Annual	**-199.8**	**-693.3**	**-64.1**	**-164.8**	**-179.9**	***-260.4***	***247.6***	**Annual**	**-1331.7**	**-156.9**	**-156.9**	**-548.0**	***-548.4***	***553.8***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data are presented for moderate scale.

Table C.45. *Calculation results: PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-21.00	-46.81	-75.86		-19.81	-21.68	*-37.0*	*24.5*	Jan		-13.05	-13.05	-62.57	*-29.6*	*28.6*
Feb	-28.42	-38.23	-78.56		-16.24	-18.08	*-35.9*	*25.4*	Feb		-12.93	-12.93	-60.19	*-28.7*	*27.3*
Mar	-25.49	-35.87	-63.74		-17.32	-19.29	*-32.3*	*19.0*	Mar		-13.84	-13.84	-48.35	*-25.3*	*19.9*
Seas_1	**-74.91**	**-120.91**	**-218.15**	**-21.33**	**-53.37**	**-59.05**	***-91.3***	***70.2***	**Seas_1**	**-450.21**	**-39.82**	**-39.82**	**-171.11**	***-175.2***	***193.5***
Apr	-24.05	-30.99	-52.85		-16.73	-18.64	*-28.7*	*14.6*	Apr		-13.41	-13.41	-40.54	*-22.5*	*15.7*
May	-38.70	-29.08	-58.89		-17.26	-19.23	*-32.6*	*17.0*	May		-13.87	-13.87	-41.66	*-23.1*	*16.0*
Jun	-30.43	-25.92	-49.34		-16.68	-18.59	*-28.2*	*13.1*	Jun		-13.43	-13.43	-33.75	*-20.2*	*11.7*
Seas_2	**-93.17**	**-86.00**	**-161.08**	**-20.74**	**-50.66**	**-56.46**	***-78.0***	***48.3***	**Seasl_2**	**-427.65**	**-40.71**	**-40.71**	**-115.94**	***-156.3***	***184.4***
Jul	-29.54	-24.98	-51.52		-17.21	-19.19	*-28.5*	*13.8*	Jul		-13.89	-13.89	-34.89	*-20.9*	*12.1*
Aug	-31.18	-23.51	-43.91		-17.20	-19.17	*-27.0*	*10.9*	Aug		-13.90	-13.90	-30.33	*-19.4*	*9.5*
Sep	-19.10	-21.60	-44.45		-16.63	-18.54	*-24.1*	*11.5*	Sep		-13.46	-13.46	-32.26	*-19.7*	*10.9*
Seas_3	**-79.82**	**-70.09**	**-139.87**	**-16.75**	**-51.04**	**-56.90**	***-69.1***	***40.8***	**Seas_3**	**-349.14**	**-41.24**	**-41.24**	**-97.49**	***-132.3***	***147.0***
Oct	-16.18	-21.35	-71.46		-17.17	-19.14	*-29.1*	*23.8*	Oct		-13.91	-13.91	-50.02	*-25.9*	*20.9*
Nov	-12.66	-19.86	-61.86		-16.60	-18.51	*-25.9*	*20.3*	Nov		-13.47	-13.47	-45.06	*-24.0*	*18.2*
Dec	-15.81	-19.20	-75.95		-16.59	-18.50	*-29.2*	*26.2*	Dec		-13.47	-13.47	-57.69	*-28.2*	*25.5*
Seas_4	**-44.65**	**-60.40**	**-209.27**	**-19.08**	**-50.35**	**-56.15**	***-73.3***	***68.2***	**Seas_4**	**-395.73**	**-40.85**	**-40.85**	**-152.78**	***-157.6***	***167.3***
Annual	**-292.55**	**-337.40**	**-728.38**	**-77.89**	**-205.42**	**-228.57**	***-311.7***	***222.5***	**Annual**	**-1622.73**	**-162.61**	**-162.61**	**-537.32**	***-621.3***	***690.6***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table C.46. *Comparison of the calculation results on PCB-180 mass flows transported in/out the calculation domain through the atmosphere (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative"*

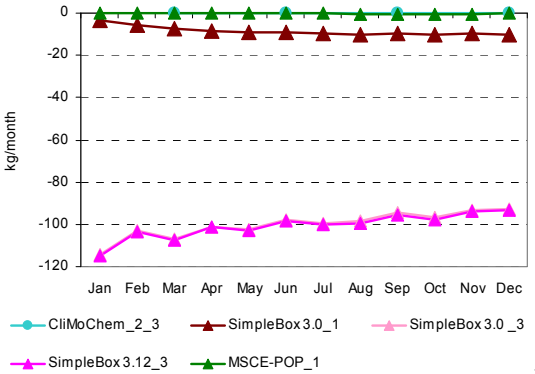
Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	own	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-22.74	-46.81	-12.7	-13.05	-12.7	-13.05	-16.10	-19.81	-17.35	-21.68	-72.68	-75.86	-62.7	-62.57		
Feb			-18.85	-38.23	-12.5	-12.93	-12.5	-12.93	-12.94	-16.24	-14.17	-18.08	-74.06	-78.56	-60.3	-60.19		
Mar			-18.77	-35.87	-13.4	-13.84	-13.4	-13.84	-13.82	-17.32	-15.13	-19.29	-59.97	-63.74	-48.5	-48.35		
Seas_1	**-16.12**	**-21.33**	**-60.37**	**-120.91**	**-38.5**	**-39.82**	**-38.5**	**-39.82**	**-42.87**	**-53.37**	**-46.66**	**-59.05**	**-206.71**	**-218.15**	**-171.4**	**-171.11**	**-339.21**	**-450.21**
Apr			-17.16	-30.99	-12.9	-13.41	-12.9	-13.41	-13.37	-16.73	-14.63	-18.64	-49.90	-52.85	-40.8	-40.54		
May			-16.94	-29.08	-13.4	-13.87	-13.4	-13.87	-13.81	-17.26	-15.10	-19.23	-56.19	-58.89	-43.4	-41.66		
Jun			-15.82	-25.92	-12.9	-13.43	-12.9	-13.43	-13.35	-16.68	-14.60	-18.59	-48.58	-49.34	-36.3	-33.75		
Seas_2	**-17.35**	**-20.74**	**-49.92**	**-86.00**	**-39.3**	**-40.71**	**-39.3**	**-40.71**	**-40.53**	**-50.66**	**-44.34**	**-56.46**	**-154.68**	**-161.08**	**-120.5**	**-115.94**	**-359.97**	**-427.65**
Jul			-15.88	-24.98	-13.4	-13.89	-13.4	-13.89	-13.79	-17.21	-15.08	-19.19	-50.74	-51.52	-37.3	-34.89		
Aug			-15.50	-23.51	-13.4	-13.90	-13.4	-13.90	-13.79	-17.20	-15.07	-19.17	-44.21	-43.91	-33.1	-30.33		
Sep			-14.72	-21.60	-13.0	-13.46	-13.0	-13.46	-13.34	-16.63	-14.57	-18.54	-43.40	-44.45	-33.9	-32.26		
Seas_3	**-14.92**	**-16.75**	**-46.10**	**-70.09**	**-39.7**	**-41.24**	**-39.7**	**-41.24**	**-40.92**	**-51.04**	**-44.72**	**-56.90**	**-138.36**	**-139.87**	**-104.4**	**-97.49**	**-310.28**	**-349.14**
Oct			-14.96	-21.35	-13.4	-13.91	-13.4	-13.91	-13.78	-17.17	-15.05	-19.14	-66.46	-71.46	-50.5	-50.02		
Nov			-14.29	-19.86	-13.0	-13.47	-13.0	-13.47	-13.33	-16.60	-14.56	-18.51	-56.86	-61.86	-44.5	-45.06		
Dec			-14.13	-19.20	-13.0	-13.47	-13.0	-13.47	-13.33	-16.59	-14.55	-18.50	-70.20	-75.95	-56.8	-57.69		
Seas_4	**-15.74**	**-19.08**	**-43.38**	**-60.40**	**-39.3**	**-40.85**	**-39.3**	**-40.85**	**-40.44**	**-50.35**	**-44.15**	**-56.15**	**-193.52**	**-209.27**	**-151.8**	**-152.78**	**-322.25**	**-395.73**
Annual	**-64.13**	**-77.89**	**-199.76**	**-337.40**	**-156.9**	**-162.61**	**-156.9**	**-162.61**	**-164.76**	**-205.42**	**-179.87**	**-228.57**	**-693.27**	**-728.38**	**-548.0**	**-537.32**	**-1331.71**	**-1622.73**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

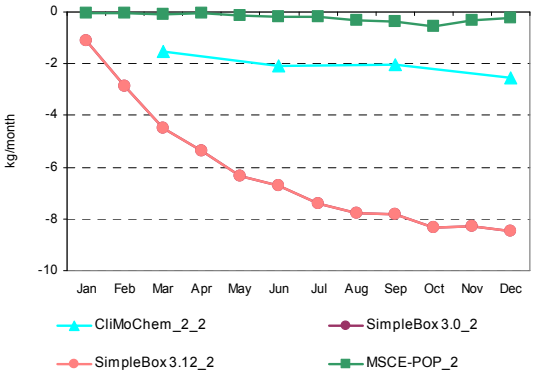
C.3.2. Comparison of calculated values of PCB-180 mass flows transported in/out the calculation domain through ocean

Reference data set. Calculation results on PCB-180 mass flows transported in/out the calculation domain through ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.47.

Monthly values of PCB-180 mass flows transported in/out the calculation domain through ocean calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.69 a and b, respectively.



a



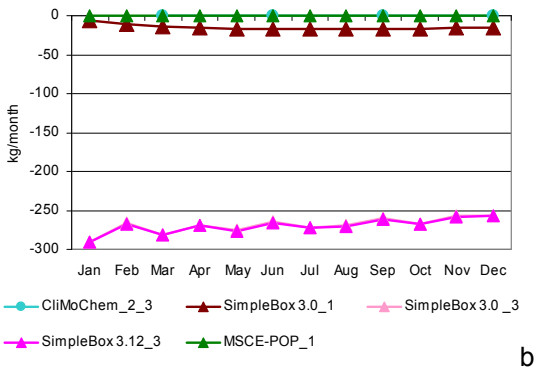
b

Fig. C.69a. *PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

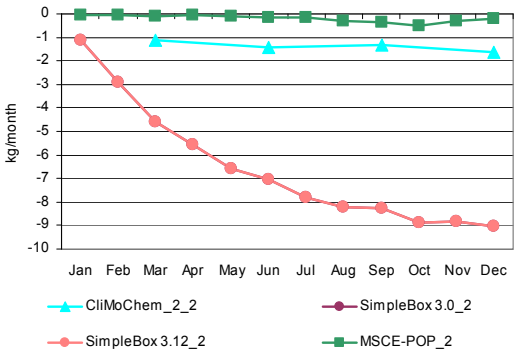
Fig. C.69b. *PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported in/out the calculation domain through ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.48.

Monthly values of PCB-180 mass flows transported in/out the calculation domain through ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.70 a and b, respectively.



a



b

Fig. C.70a. *PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

Fig. C.70b. *PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.49.

Table C.47. *Calculation results: PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	MSCE-POP_1	SimpleBox 3.0_1[a]	CliMoChem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-0.03	-3.37		-114.59	-114.64	*-58.16*	*65.21*	Jan		-1.11	-1.11	-0.03	*-0.75*	*0.63*
Feb	-0.06	-5.60		-103.08	-103.30	*-53.01*	*57.98*	Feb		-2.87	-2.87	-0.06	*-1.93*	*1.62*
Mar	-0.09	-7.62		-106.89	-107.27	*-55.47*	*59.68*	Mar		-4.49	-4.49	-0.08	*-3.02*	*2.55*
Seas_1	**-0.18**	**-16.59**	**-0.58**	**-324.56**	**-325.20**	***-133.42***	***174.90***	**Seas_1**	**-4.61**	**-8.48**	**-8.47**	**-0.16**	***-5.43***	***3.96***
Apr	-0.08	-8.37		-100.99	-101.46	*-52.72*	*56.11*	Apr		-5.38	-5.38	-0.07	*-3.61*	*3.07*
May	-0.14	-9.27		-102.42	-102.98	*-53.70*	*56.70*	May		-6.35	-6.35	-0.12	*-4.27*	*3.60*
Jun	-0.21	-9.34		-97.64	-98.23	*-51.36*	*53.92*	Jun		-6.72	-6.72	-0.17	*-4.54*	*3.78*
Seas_2	**-0.42**	**-26.98**	**-0.66**	**-301.06**	**-302.67**	***-126.36***	***160.58***	**Seas_2**	**-6.26**	**-18.46**	**-18.44**	**-0.36**	***-10.88***	***9.07***
Jul	-0.21	-9.88		-99.66	-100.31	*-52.51*	*54.96*	Jul		-7.41	-7.41	-0.17	*-4.99*	*4.18*
Aug	-0.41	-10.02		-98.62	-99.30	*-52.09*	*54.26*	Aug		-7.78	-7.78	-0.33	*-5.30*	*4.30*
Sep	-0.49	-9.79		-94.58	-95.27	*-50.03*	*51.98*	Sep		-7.82	-7.82	-0.37	*-5.34*	*4.30*
Seas_3	**-1.11**	**-29.69**	**-0.63**	**-292.86**	**-294.88**	***-123.83***	***155.67***	**Seas_3**	**-6.17**	**-23.02**	**-23.00**	**-0.86**	***-13.26***	***11.46***
Oct	-0.73	-10.19		-96.95	-97.68	*-51.39*	*53.18*	Oct		-8.34	-8.33	-0.56	*-5.74*	*4.49*
Nov	-0.42	-9.92		-93.14	-93.87	*-49.34*	*51.15*	Nov		-8.28	-8.28	-0.32	*-5.63*	*4.59*
Dec	-0.27	-9.97		-92.52	-93.26	*-49.00*	*50.83*	Dec		-8.47	-8.47	-0.21	*-5.72*	*4.77*
Seas_4	**-1.42**	**-30.07**	**-0.54**	**-282.61**	**-284.80**	***-119.89***	***150.02***	**Seas_4**	**-7.68**	**-25.09**	**-25.08**	**-1.10**	***-14.74***	***12.25***
Annual	**-3.13**	**-103.33**	**-2.42**	**-1201.09**	**-1207.55**	***-503.51***	***641.07***	**Annual**	**-24.72**	**-75.04**	**-75.00**	**-2.48**	***-44.31***	***36.61***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
[a] - SimpleBox data are presented for moderate scale.

Table C.48. *Calculation results: PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-5.39	-0.03		-290.09	-290.03	*-146.39*	*165.92*	Jan		-1.10	-1.10	-0.03	*-0.74*	*0.62*
Feb	-10.45	-0.07		-266.74	-267.00	*-136.06*	*151.10*	Feb		-2.90	-2.89	-0.06	*-1.95*	*1.64*
Mar	-14.53	-0.09		-281.26	-281.76	*-144.41*	*158.42*	Mar		-4.59	-4.58	-0.08	*-3.08*	*2.60*
Seas_1	**-30.36**	**-0.19**	**-0.61**	**-838.09**	**-838.79**	***-341.61***	***453.71***	**Seas_1**	**-3.37**	**-8.58**	**-8.58**	**-0.16**	***-5.17***	***4.15***
Apr	-15.86	-0.08		-269.14	-269.79	*-138.72*	*151.11*	Apr		-5.54	-5.54	-0.07	*-3.72*	*3.16*
May	-17.28	-0.13		-275.55	-276.34	*-142.33*	*154.45*	May		-6.59	-6.59	-0.11	*-4.43*	*3.74*
Jun	-17.02	-0.21		-264.61	-265.44	*-136.82*	*148.20*	Jun		-7.03	-7.02	-0.16	*-4.74*	*3.96*
Seas_2	**-50.16**	**-0.42**	**-0.68**	**-809.30**	**-811.58**	***-334.43***	***435.01***	**Seas_2**	**-4.32**	**-19.16**	**-19.15**	**-0.34**	***-10.74***	***9.85***
Jul	-17.56	-0.21		-271.59	-272.55	*-140.48*	*152.12*	Jul		-7.79	-7.78	-0.16	*-5.24*	*4.41*
Aug	-17.34	-0.41		-269.95	-270.97	*-139.67*	*151.18*	Aug		-8.22	-8.21	-0.30	*-5.58*	*4.57*
Sep	-16.50	-0.49		-259.84	-260.88	*-134.43*	*145.56*	Sep		-8.29	-8.28	-0.34	*-5.64*	*4.59*
Seas_3	**-51.40**	**-1.12**	**-0.60**	**-801.38**	**-804.40**	***-331.78***	***430.56***	**Seas_3**	**-3.91**	**-24.30**	**-24.28**	**-0.80**	***-13.32***	***12.73***
Oct	-16.74	-0.74		-267.18	-268.30	*-138.24*	*149.68*	Oct		-8.86	-8.86	-0.51	*-6.08*	*4.82*
Nov	-15.90	-0.42		-257.35	-258.48	*-133.04*	*144.33*	Nov		-8.82	-8.82	-0.30	*-5.98*	*4.92*
Dec	-15.63	-0.26		-256.23	-257.39	*-132.38*	*143.82*	Dec		-9.04	-9.03	-0.19	*-6.09*	*5.11*
Seas_4	**-48.27**	**-1.42**	**-0.55**	**-780.76**	**-784.16**	***-323.03***	***419.85***	**Seas_4**	**-4.91**	**-26.72**	**-26.71**	**-1.00**	***-14.84***	***13.81***
Annual	**-180.20**	**-3.15**	**-2.44**	**-3229.53**	**-3238.93**	***-1330.85***	***1739.06***	**Annual**	**-16.51**	**-78.77**	**-78.72**	**-2.30**	***-44.08***	***40.45***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

a - SimpleBox data are presented for moderate scale.

Table C.49. *Comparison of the calculation results on PCB-180 mass flows transported in/out the calculation domain through ocean (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-3.37	-5.39	-1.11	-1.10	-1.11	-1.10	-114.59	-290.09	-114.64	-290.03	-0.03	-0.03	-0.03	-0.03		
Feb			-5.60	-10.45	-2.87	-2.90	-2.87	-2.89	-103.08	-266.74	-103.30	-267.00	-0.06	-0.07	-0.06	-0.06		
Mar			-7.62	-14.53	-4.49	-4.59	-4.49	-4.58	-106.89	-281.26	-107.27	-281.76	-0.09	-0.09	-0.08	-0.08		
Seas_1	**-0.58**	**-0.61**	**-16.59**	**-30.36**	**-8.48**	**-8.58**	**-8.47**	**-8.58**	**-324.56**	**-838.09**	**-325.20**	**-838.79**	**-0.18**	**-0.19**	**-0.16**	**-0.16**	**-4.61**	**-3.37**
Apr			-8.37	-15.86	-5.38	-5.54	-5.38	-5.54	-100.99	-269.14	-101.46	-269.79	-0.08	-0.08	-0.07	-0.07		
May			-9.27	-17.28	-6.35	-6.59	-6.35	-6.59	-102.42	-275.55	-102.98	-276.34	-0.14	-0.13	-0.12	-0.11		
Jun			-9.34	-17.02	-6.72	-7.03	-6.72	-7.02	-97.64	-264.61	-98.23	-265.44	-0.21	-0.21	-0.17	-0.16		
Seas_2	**-0.66**	**-0.68**	**-26.98**	**-50.16**	**-18.46**	**-19.16**	**-18.44**	**-19.15**	**-301.06**	**-809.30**	**-302.67**	**-811.58**	**-0.42**	**-0.42**	**-0.36**	**-0.34**	**-6.26**	**-4.32**
Jul			-9.88	-17.56	-7.41	-7.79	-7.41	-7.78	-99.66	-271.59	-100.31	-272.55	-0.21	-0.21	-0.17	-0.16		
Aug			-10.02	-17.34	-7.78	-8.22	-7.78	-8.21	-98.62	-269.95	-99.30	-270.97	-0.41	-0.41	-0.33	-0.30		
Sep			-9.79	-16.50	-7.82	-8.29	-7.82	-8.28	-94.58	-259.84	-95.27	-260.88	-0.49	-0.49	-0.37	-0.34		
Seas_3	**-0.63**	**-0.60**	**-29.69**	**-51.40**	**-23.02**	**-24.30**	**-23.00**	**-24.28**	**-292.86**	**-801.38**	**-294.88**	**-804.40**	**-1.11**	**-1.12**	**-0.86**	**-0.80**	**-6.17**	**-3.91**
Oct			-10.19	-16.74	-8.34	-8.86	-8.33	-8.86	-96.95	-267.18	-97.68	-268.30	-0.73	-0.74	-0.56	-0.51		
Nov			-9.92	-15.90	-8.28	-8.82	-8.28	-8.82	-93.14	-257.35	-93.87	-258.48	-0.42	-0.42	-0.32	-0.30		
Dec			-9.97	-15.63	-8.47	-9.04	-8.47	-9.03	-92.52	-256.23	-93.26	-257.39	-0.27	-0.26	-0.21	-0.19		
Seas_4	**-0.54**	**-0.55**	**-30.07**	**-48.27**	**-25.09**	**-26.72**	**-25.08**	**-26.71**	**-282.61**	**-780.76**	**-284.80**	**-784.16**	**-1.42**	**-1.42**	**-1.10**	**-1.00**	**-7.68**	**-4.91**
Annual	**-2.42**	**-2.44**	**-103.33**	**-180.20**	**-75.04**	**-78.77**	**-75.00**	**-78.72**	**-1201.09**	**-3229.53**	**-1207.55**	**-3238.93**	**-3.13**	**-3.15**	**-2.48**	**-2.30**	**-24.72**	**-16.51**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.3.3. Calculated values of PCB-180 mass flows transported in/out the calculation domain through other compartments

Reference data set. Calculation results on PCB-180 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.50.

Monthly values of PCB-180 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "reference" data set are presented in Fig. C.71.

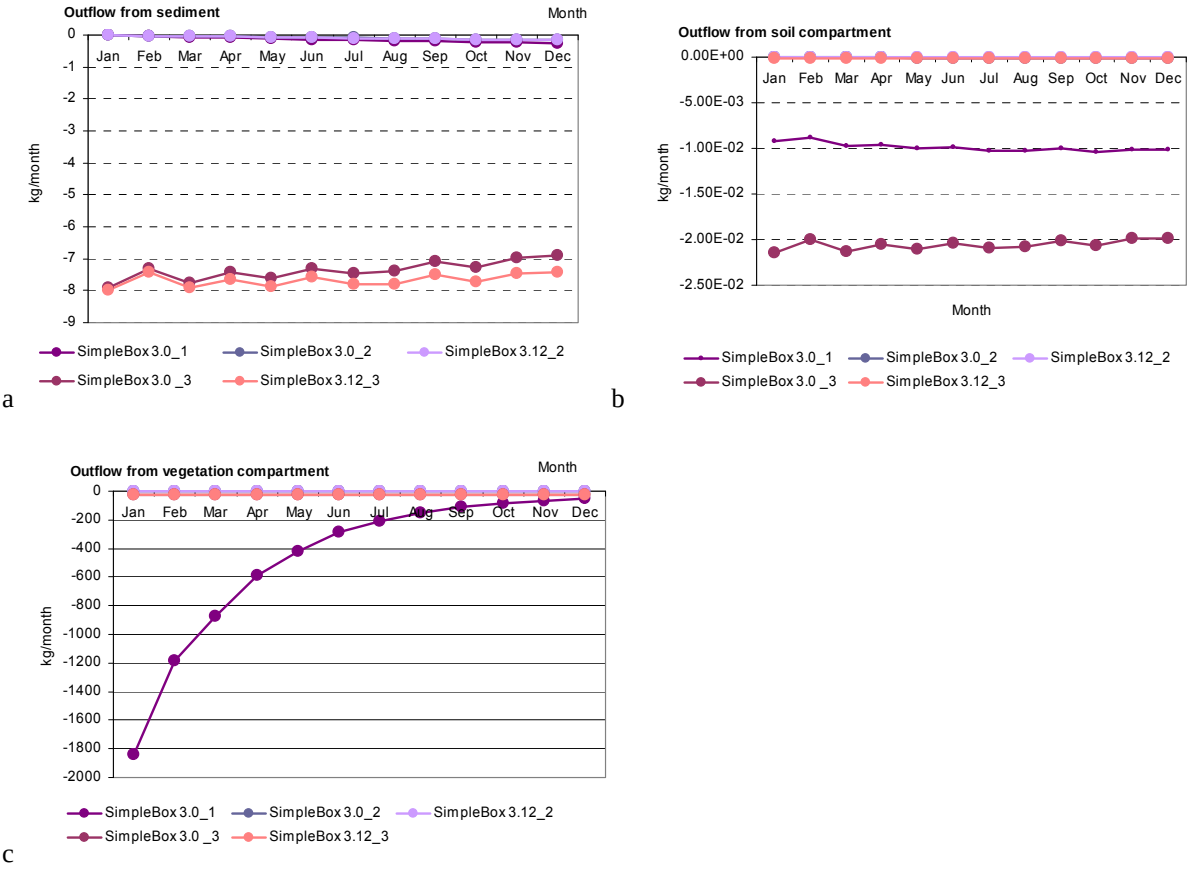


Fig. C.71. *PCB-180 mass flows transported in/out the calculation domain through sediment (a), soil (b) and vegetation(c) calculated by SimpleBox on the basis of "reference" data set*

Own/alternative data set. Calculation results on PCB-180 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "alternative" data sets together with statistical parameters used for evaluation are presented in Table C.51.

Monthly values of PCB-180 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of "alternative" data set are compared in Fig. C.72.

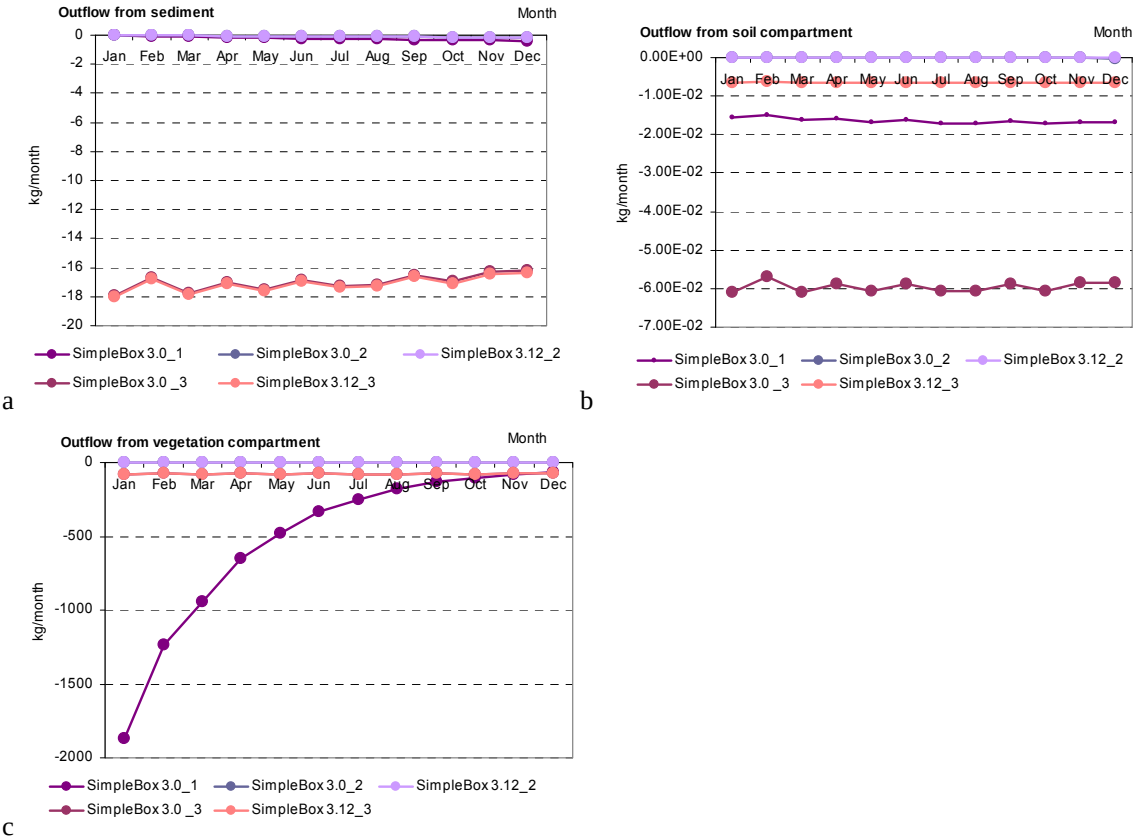


Fig. C.72. *PCB-180 mass flows transported in/out the calculation domain through sediment (a), soil (b) and vegetation(c) calculated by SimpleBox on the basis of "alternative" data sets*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two different data sets of physical-chemical properties (for SimpleBox model) is shown in Table C.52.

Table C.50. *Calculation results: PCB-180 mass flows transported in/out the calculation domain through sediments, soil and vegetation (kg/month) calculated by SimpleBox on the basis of "reference" data set*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	-0.02	-0.01	-0.01	-7.89	-7.98	-9.15E-03	-7.32E-06	-2.09E-09	-2.15E-02	-8.69E-05	-1842.5	-0.2	-0.2	-29.0	-29.1
Feb	-0.04	-0.02	-0.02	-7.32	-7.44	-8.85E-03	-2.13E-05	-5.98E-09	-2.00E-02	-8.06E-05	-1185.1	-0.4	-0.4	-26.4	-26.4
Mar	-0.07	-0.04	-0.04	-7.75	-7.92	-9.70E-03	-3.84E-05	-1.07E-08	-2.13E-02	-8.54E-05	-875.6	-0.7	-0.6	-27.5	-27.6
Apr	-0.09	-0.05	-0.05	-7.44	-7.64	-9.57E-03	-5.24E-05	-1.45E-08	-2.05E-02	-8.19E-05	-584.4	-0.8	-0.7	-26.2	-26.2
May	-0.12	-0.06	-0.07	-7.61	-7.87	-1.00E-02	-7.00E-05	-1.92E-08	-2.11E-02	-8.39E-05	-419.8	-1.0	-0.9	-26.7	-26.7
Jun	-0.14	-0.08	-0.08	-7.30	-7.59	-9.82E-03	-8.30E-05	-2.27E-08	-2.03E-02	-8.05E-05	-285.0	-1.0	-0.9	-25.6	-25.6
Jul	-0.16	-0.09	-0.09	-7.48	-7.81	-1.02E-02	-1.01E-04	-2.77E-08	-2.09E-02	-8.24E-05	-209.6	-1.1	-1.0	-26.2	-26.2
Aug	-0.19	-0.11	-0.11	-7.41	-7.78	-1.03E-02	-1.17E-04	-3.19E-08	-2.09E-02	-8.16E-05	-150.9	-1.2	-1.0	-26.0	-26.0
Sep	-0.20	-0.12	-0.12	-7.10	-7.51	-1.00E-02	-1.29E-04	-3.49E-08	-2.01E-02	-7.83E-05	-108.1	-1.2	-1.0	-25.0	-25.0
Oct	-0.23	-0.14	-0.14	-7.27	-7.73	-1.04E-02	-1.49E-04	-4.01E-08	-2.07E-02	-8.02E-05	-85.1	-1.3	-1.1	-25.6	-25.7
Nov	-0.24	-0.14	-0.15	-6.98	-7.45	-1.01E-02	-1.59E-04	-4.27E-08	-1.99E-02	-7.69E-05	-64.7	-1.2	-1.0	-24.7	-24.7
Dec	-0.26	-0.16	-0.16	-6.91	-7.43	-1.01E-02	-1.73E-04	-4.66E-08	-1.98E-02	-7.62E-05	-52.9	-1.3	-1.0	-24.5	-24.6
Annual	**-1.75**	**-1.01**	**-1.02**	**-88.46**	**-92.14**	**-1.18E-01**	**-1.10E-03**	**-2.99E-07**	**-2.47E-01**	**-9.75E-04**	**-5863.8**	**-11.4**	**-9.9**	**-313.3**	**-313.8**

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

* - SimpleBox data are presented for moderate scale

Table C.51. *Calculation results: PCB-180 mass flows transported in/out the calculation domain through sediment, soil and vegetation (kg/month) calculated by SimpleBox on the basis of "alternative" data set*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	-0.03	-0.01	-0.01	-17.96	-18.05	-1.56E-02	-6.93E-06	-1.51E-07	-6.09E-02	-6.68E-03	-1870.7	-0.2	-0.2	-80.2	-80.3
Feb	-0.07	-0.02	-0.02	-16.70	-16.78	-1.50E-02	-2.02E-05	-4.42E-07	-5.70E-02	-6.25E-03	-1239.8	-0.6	-0.5	-74.4	-74.5
Mar	-0.12	-0.03	-0.04	-17.73	-17.83	-1.63E-02	-3.65E-05	-7.99E-07	-6.08E-02	-6.68E-03	-942.8	-0.9	-0.8	-79.1	-79.2
Apr	-0.15	-0.05	-0.05	-17.05	-17.15	-1.60E-02	-5.00E-05	-1.10E-06	-5.88E-02	-6.46E-03	-647.2	-1.0	-1.0	-76.2	-76.4
May	-0.19	-0.06	-0.06	-17.50	-17.61	-1.67E-02	-6.69E-05	-1.47E-06	-6.08E-02	-6.67E-03	-477.4	-1.2	-1.2	-78.4	-78.7
Jun	-0.22	-0.08	-0.08	-16.83	-16.94	-1.63E-02	-7.96E-05	-1.75E-06	-5.88E-02	-6.45E-03	-332.1	-1.3	-1.2	-75.7	-75.9
Jul	-0.26	-0.09	-0.09	-17.28	-17.40	-1.70E-02	-9.76E-05	-2.14E-06	-6.07E-02	-6.66E-03	-249.3	-1.4	-1.3	-78.0	-78.3
Aug	-0.29	-0.11	-0.11	-17.16	-17.29	-1.71E-02	-1.13E-04	-2.49E-06	-6.07E-02	-6.65E-03	-182.6	-1.5	-1.4	-77.9	-78.2
Sep	-0.30	-0.12	-0.12	-16.50	-16.63	-1.66E-02	-1.25E-04	-2.73E-06	-5.87E-02	-6.44E-03	-132.4	-1.5	-1.4	-75.3	-75.6
Oct	-0.34	-0.14	-0.14	-16.94	-17.08	-1.72E-02	-1.44E-04	-3.16E-06	-6.06E-02	-6.65E-03	-104.7	-1.6	-1.4	-77.7	-78.0
Nov	-0.35	-0.14	-0.15	-16.29	-16.43	-1.67E-02	-1.54E-04	-3.39E-06	-5.86E-02	-6.43E-03	-79.6	-1.6	-1.4	-75.1	-75.4
Dec	-0.38	-0.16	-0.16	-16.18	-16.33	-1.68E-02	-1.69E-04	-3.72E-06	-5.86E-02	-6.42E-03	-64.6	-1.6	-1.4	-75.0	-75.4
Annual	**-2.69**	**-1.00**	**-1.02**	**-204.13**	**-205.50**	**-1.97E-01**	**-1.06E-03**	**-2.33E-05**	**-7.15E-01**	**-7.84E-02**	**-6323.2**	**-14.4**	**-13.3**	**-922.9**	**-926.0**

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

* - SimpleBox data are presented for moderate scale.

Table C.52. *The percentage difference between calculation results on PCB-180 mass flows transported in/out the calculation domain through sediments, soil and vegetation calculated by SimpleBox model on the basis of two data sets: "reference" and "alternative"*

Month	Sediment					Soil					Vegetation				
	Outflow from sediment compartment = burial					Outflow from soil compartment = leaching					Outflow from vegetation compartment = harvest of agricultural vegetation				
	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan	66.8%	-2.6%	-2.6%	127.6%	126.3%	71%	-5%	7109%	184%	7588%	2%	24%	28%	176%	176%
Feb	72.3%	-1.9%	-1.9%	128.1%	125.7%	69%	-5%	7304%	185%	7651%	5%	26%	30%	182%	183%
Mar	69.8%	-1.6%	-1.5%	128.7%	125.1%	68%	-5%	7395%	186%	7715%	8%	27%	31%	187%	187%
Apr	66.4%	-1.3%	-1.2%	129.3%	124.5%	67%	-5%	7466%	187%	7781%	11%	27%	33%	191%	191%
May	62.9%	-1.1%	-1.0%	129.9%	123.9%	66%	-4%	7528%	188%	7847%	14%	27%	34%	194%	194%
Jun	59.7%	-0.8%	-0.8%	130.5%	123.3%	66%	-4%	7585%	189%	7914%	16%	28%	35%	196%	197%
Jul	56.7%	-0.6%	-0.5%	131.1%	122.7%	66%	-4%	7639%	190%	7982%	19%	27%	36%	198%	199%
Aug	54.0%	-0.4%	-0.3%	131.7%	122.1%	66%	-3%	7691%	191%	8051%	21%	27%	36%	200%	201%
Sep	51.6%	-0.2%	-0.1%	132.3%	121.5%	66%	-3%	7740%	192%	8119%	22%	27%	37%	201%	202%
Oct	49.3%	0.0%	0.2%	132.9%	120.9%	66%	-3%	7787%	193%	8189%	23%	26%	37%	203%	204%
Nov	47.3%	0.3%	0.4%	133.5%	120.4%	66%	-3%	7833%	194%	8259%	23%	25%	37%	204%	205%
Dec	45.5%	0.5%	0.6%	134.1%	119.8%	67%	-2%	7877%	195%	8328%	22%	25%	37%	205%	207%
Annual	**54.0%**	**-0.3%**	**-0.2%**	**130.8%**	**123.0%**	**67%**	**-3%**	**7702%**	**189%**	**7945%**	**8%**	**26%**	**35%**	**195%**	**195%**

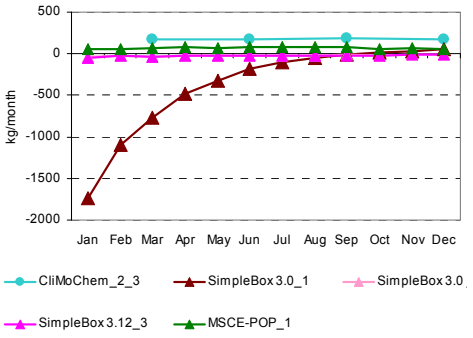
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

C.3.4. Comparison of calculated values of PCB-180 total mass flows transported in/out the specified domain

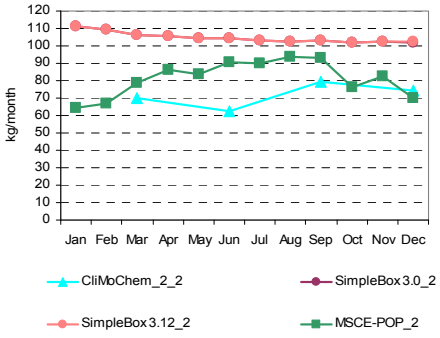
Values of total mass flow transported in/out the calculation domain are calculated as sum of inflow (emissions) and all outflows through the main transport media.

Reference data set. Calculation results on PCB-180 total mass flows transported in/out the specified domain calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.53.

Monthly values of PCB-180 total mass flows transported in/out the specified domain calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.73 a and b, respectively.



a



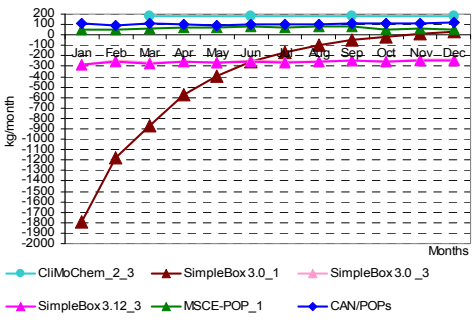
b

Fig. C.73a. *PCB-180 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

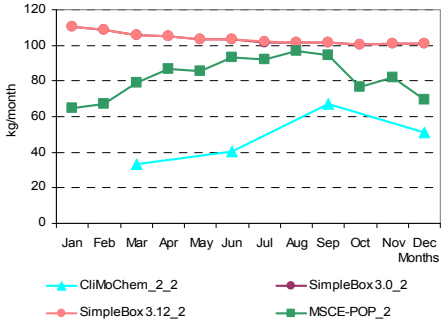
Fig. C.73b. *PCB-180 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "reference" data set and zero initial conditions*

Own/alternative data set. Calculation results on PCB-180 total mass flows transported in/out the specified domain calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.54.

Monthly values of PCB-180 mass flows transported in/out the specified domain calculated by the participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.74 a and b, respectively.



a



b

Fig. C.74a. *PCB-180 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions*

Fig. C.74b. *PCB-180 mass flows transported in/out the specified domain (kg/month) calculated by the participating models on the basis of "own or alternative" data set and zero initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.55.

Table C.53. *Calculation results: PCB-180 total mass flows transported in/out the specified domain (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-1741.2	54.5		-42.6	-44.0	*-443.3*	*866.5*	Jan		111.0	111.1	64.6	*95.6*	*26.8*
Feb	-1094.5	53.1		-24.7	-26.3	*-273.1*	*548.9*	Feb		109.2	109.2	66.9	*95.1*	*24.4*
Mar	-774.7	67.2		-31.0	-32.9	*-192.8*	*390.7*	Mar		106.4	106.5	78.7	*97.2*	*16.0*
Seas_1	**-3610.4**	**174.9**	**537.3**	**-98.3**	**-103.2**	***-620.0***	***1692.1***	**Seas_1**	**210.1**	**326.6**	**326.7**	**210.2**	***268.4***	***67.3***
Apr	-486.7	77.3		-23.0	-24.9	*-114.3*	*252.8*	Apr		105.8	105.9	86.4	*99.4*	*11.2*
May	-318.7	70.9		-25.5	-27.7	*-75.3*	*168.7*	May		104.3	104.4	83.7	*97.5*	*11.9*
Jun	-187.0	78.5		-18.9	-21.0	*-37.1*	*110.2*	Jun		104.2	104.4	90.8	*99.8*	*7.8*
Seas_2	**-992.5**	**226.7**	**536.0**	**-67.4**	**-73.6**	***-74.2***	***571.4***	**Seas_2**	**187.7**	**314.3**	**314.6**	**260.9**	***269.4***	***60.0***
Jul	-108.1	76.3		-22.1	-24.4	*-19.6*	*75.4*	Jul		103.0	103.1	89.8	*98.6*	*7.7*
Aug	-49.2	82.6		-20.8	-23.2	*-2.6*	*58.3*	Aug		102.6	102.7	93.8	*99.7*	*5.1*
Sep	-9.5	83.4		-15.0	-17.3	*10.4*	*48.8*	Sep		102.9	103.1	92.9	*99.7*	*5.8*
Seas_3	**-166.9**	**242.3**	**538.4**	**-57.9**	**-64.9**	***98.2***	***289.7***	**Seas_3**	**237.5**	**308.5**	**309.0**	**276.5**	***282.9***	***33.9***
Oct	16.9	60.1		-18.7	-21.1	*9.3*	*38.0*	Oct		101.9	102.1	76.2	*93.4*	*14.9*
Nov	34.1	70.0		-13.1	-15.6	*18.8*	*41.0*	Nov		102.4	102.6	82.4	*95.8*	*11.6*
Dec	50.2	56.8		-12.3	-14.8	*20.0*	*38.8*	Dec		102.1	102.4	70.3	*91.6*	*18.5*
Seas_4	**101.2**	**186.8**	**537.7**	**-44.1**	**-51.5**	***146.0***	***241.0***	**Seas_4**	**224.0**	**306.4**	**307.1**	**228.9**	***266.6***	***46.4***
Annual	**-4668.6**	**830.7**	**2149.3**	**-267.7**	**-293.2**	***-449.9***	***2561.8***	**Annual**	**859.4**	**1255.9**	**1257.4**	**976.6**	***1087.3***	***201.3***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table C.54. *Calculation results: PCB-180 total mass flows transported in/out the specified domain (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	110.9	-1795.6	51.4		-283.1	-285.0	*-440.3*	*779.6*	Jan		110.6	110.6	64.7	*95.3*	*26.5*
Feb	95.0	-1173.5	48.6		-249.1	-251.4	*-306.1*	*511.2*	Feb		108.6	108.6	67.0	*94.8*	*24.0*
Mar	106.4	-865.9	63.4		-270.4	-273.1	*-247.9*	*389.1*	Mar		105.7	105.7	78.8	*96.7*	*15.5*
Seas_1	**312.2**	**-3835.0**	**163.4**	**532.0**	**-802.7**	**-809.5**	***-739.9***	***1620.4***	**Seas_1**	**100.4**	**324.9**	**325.0**	**210.5**	***240.2***	***107.7***
Apr	103.6	-571.0	74.3		-254.1	-256.9	*-180.8*	*278.1*	Apr		105.0	105.0	86.7	*98.9*	*10.6*
May	93.2	-396.6	68.2		-263.8	-266.8	*-153.2*	*220.3*	May		103.3	103.3	85.5	*97.4*	*10.3*
Jun	97.2	-251.9	77.7		-248.8	-251.9	*-115.6*	*185.5*	Jun		103.2	103.3	93.3	*99.9*	*5.7*
Seas_2	**294.0**	**-1219.5**	**220.3**	**532.5**	**-766.7**	**-775.7**	***-285.9***	***721.8***	**Seas_2**	**122.0**	**311.4**	**311.6**	**265.5**	***252.6***	***89.8***
Jul	102.3	-164.7	75.5		-259.2	-262.5	*-101.7*	*178.6*	Jul		101.8	101.9	92.2	*98.7*	*5.6*
Aug	100.7	-96.4	82.9		-257.2	-260.6	*-86.1*	*175.6*	Aug		101.3	101.4	96.6	*99.8*	*2.7*
Sep	108.5	-47.5	82.3		-243.3	-246.6	*-69.3*	*170.9*	Sep		101.7	101.8	94.6	*99.4*	*4.1*
Seas_3	**311.6**	**-308.5**	**240.8**	**536.6**	**-759.7**	**-769.7**	***-124.8***	***568.2***	**Seas_3**	**200.9**	**304.8**	**305.1**	**283.5**	***273.6***	***49.5***
Oct	115.7	-15.8	55.1		-254.0	-257.5	*-71.3*	*174.7*	Oct		100.5	100.7	76.7	*92.6*	*13.8*
Nov	115.0	7.6	65.0		-240.4	-243.9	*-59.3*	*171.1*	Nov		101.0	101.2	81.9	*94.7*	*11.1*
Dec	116.1	27.6	51.1		-239.0	-242.6	*-57.4*	*170.6*	Dec		100.8	100.9	69.4	*90.3*	*18.2*
Seas_4	**346.7**	**19.5**	**171.1**	**534.3**	**-733.4**	**-744.0**	***-67.6***	***547.6***	**Seas_4**	**153.3**	**302.3**	**302.8**	**228.0**	***246.6***	***71.4***
Annual	**1264.5**	**-5343.5**	**795.6**	**2135.5**	**-3062.5**	**-3098.9**	***-1218.2***	***3014.1***	**Annual**	**576.6**	**1243.4**	**1244.5**	**987.5**	***1013.0***	***315.1***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data are presented for moderate scale.

Table C.55. *Comparison of the calculation results on PCB-180 mass flows transported in/out the specified domain (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative"*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0_3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-1741.2	-1795.6	111.0	110.6	111.1	110.6	-42.6	-283.1	-44.0	-285.0	54.5	51.4	64.6	64.7		
Feb			-1094.5	-1173.5	109.2	108.6	109.2	108.6	-24.7	-249.1	-26.3	-251.4	53.1	48.6	66.9	67.0		
Mar			-774.7	-865.9	106.4	105.7	106.5	105.7	-31.0	-270.4	-32.9	-273.1	67.2	63.4	78.7	78.8		
Seas_1	**537.3**	**532.0**	**-3610.4**	**-3835.0**	**326.6**	**324.9**	**326.7**	**325.0**	**-98.3**	**-802.7**	**-103.2**	**-809.5**	**174.9**	**163.4**	**210.2**	**210.5**	**210.1**	**100.4**
Apr			-486.7	-571.0	105.8	105.0	105.9	105.0	-23.0	-254.1	-24.9	-256.9	77.3	74.3	86.4	86.7		
May			-318.7	-396.6	104.3	103.3	104.4	103.3	-25.5	-263.8	-27.7	-266.8	70.9	68.2	83.7	85.5		
Jun			-187.0	-251.9	104.2	103.2	104.4	103.3	-18.9	-248.8	-21.0	-251.9	78.5	77.7	90.8	93.3		
Seas_2	**536.0**	**532.5**	**-992.5**	**-1219.5**	**314.3**	**311.4**	**314.6**	**311.6**	**-67.4**	**-766.7**	**-73.6**	**-775.7**	**226.7**	**220.3**	**260.9**	**265.5**	**187.7**	**122.0**
Jul			-108.1	-164.7	103.0	101.8	103.1	101.9	-22.1	-259.2	-24.4	-262.5	76.3	75.5	89.8	92.2		
Aug			-49.2	-96.4	102.6	101.3	102.7	101.4	-20.8	-257.2	-23.2	-260.6	82.6	82.9	93.8	96.6		
Sep			-9.5	-47.5	102.9	101.7	103.1	101.8	-15.0	-243.3	-17.3	-246.6	83.4	82.3	92.9	94.6		
Seas_3	**538.4**	**536.6**	**-166.9**	**-308.5**	**308.5**	**304.8**	**309.0**	**305.1**	**-57.9**	**-759.7**	**-64.9**	**-769.7**	**242.3**	**240.8**	**276.5**	**283.5**	**237.5**	**200.9**
Oct			16.9	-15.8	101.9	100.5	102.1	100.7	-18.7	-254.0	-21.1	-257.5	60.1	55.1	76.2	76.7		
Nov			34.1	7.6	102.4	101.0	102.6	101.2	-13.1	-240.4	-15.6	-243.9	70.0	65.0	82.4	81.9		
Dec			50.2	27.6	102.1	100.8	102.4	100.9	-12.3	-239.0	-14.8	-242.6	56.8	51.1	70.3	69.4		
Seas_4	**537.7**	**534.3**	**101.2**	**19.5**	**306.4**	**302.3**	**307.1**	**302.8**	**-44.1**	**-733.4**	**-51.5**	**-744.0**	**186.8**	**171.1**	**228.9**	**228.0**	**224.0**	**153.3**
Annual	**2149.3**	**2135.5**	**-4668.6**	**-5343.5**	**1255.9**	**1243.4**	**1257.4**	**1244.5**	**-267.7**	**-3062.5**	**-293.2**	**-3098.9**	**830.7**	**795.6**	**976.6**	**987.5**	**859.4**	**576.6**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

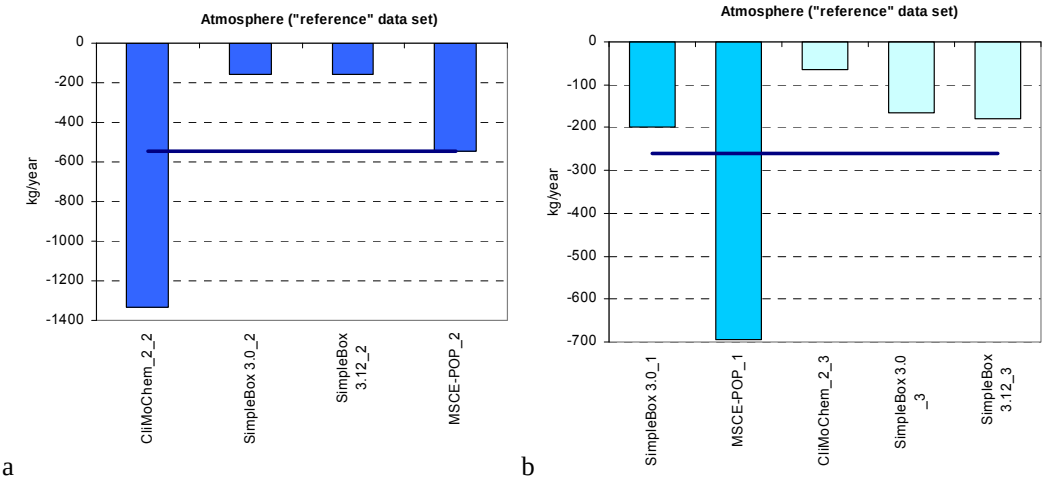
C.3.5. Comparison of PCB-180 mass flows transported in/out the specified domain

The calculation results on PCB-180 transport inside and outside the calculation domain through main transport media such as atmosphere and seawater are discussed in this subsection. Transport of this pollutant from sediment, soil and vegetation compartments due to such processes as burial, leaching and harvest of agricultural vegetation, respectively, is considered in SimpleBox model.

The results considered in Sections 3.3.1-3.3.4 above are obtained with one-year calculations with zero initial concentrations (CliMoChem, MSCE-POP, SimpleBox) and with initial concentrations in media (CAN/POPs, MSCE-POP, SimpleBox); and with long-term calculations with historical emissions (CliMoChem, SimpleBox). CliMoChem, MSCE-POP, and SimpleBox models presented results obtained on the basis of two different physical-chemical data sets. Of note, the calculated values compared below are negative in the case if a model predicted PCB-180 transport out the calculation domain through the considered media.

A preliminary analysis of the comparison of absolute values PCB-180 transport mass flows inside and outside the calculation domain through main transport media is presented in this section. The analysis is made separately for results calculated on the basis of initial concentrations or historical emissions and for results based on zero initial conditions.

Transport through the atmosphere. Comparison of annual values of PCB-180 mass flows transported out the calculation domain through the atmosphere calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. C.75a together with the averaged value given as the blue line. Fig. C.75b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).

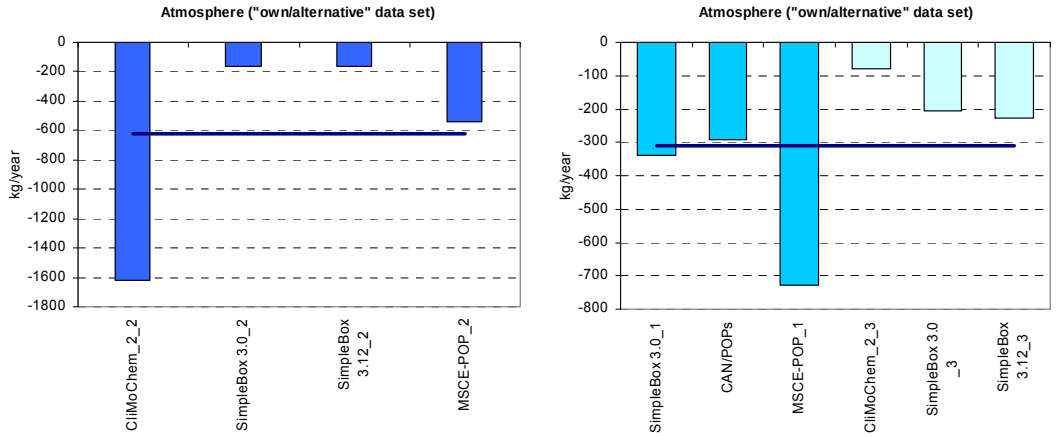


a b

Fig. C.75. *Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Fig. C.76a demonstrates the comparison of the annual values of PCB-180 mass flows transported out the calculation domain through the atmosphere calculated on the basis of zero initial concentrations and with the use of "***own or alternative*****"** data sets. Fig. C.76b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial

data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig. C.76. *Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-180 mass flows transported out the calculation domain through the atmosphere obtained with "reference" and "own/alternative" data sets is presented in and in Fig. C.77 (see also Table C.46 given in Section 3.3.1).

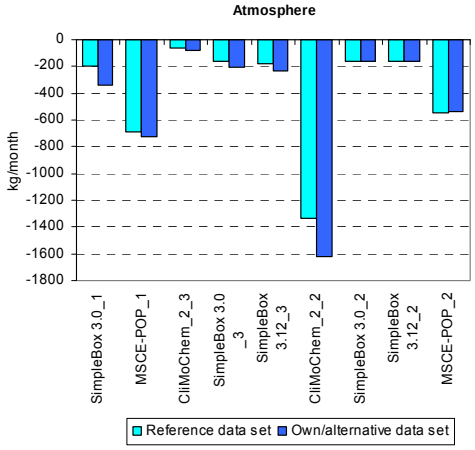
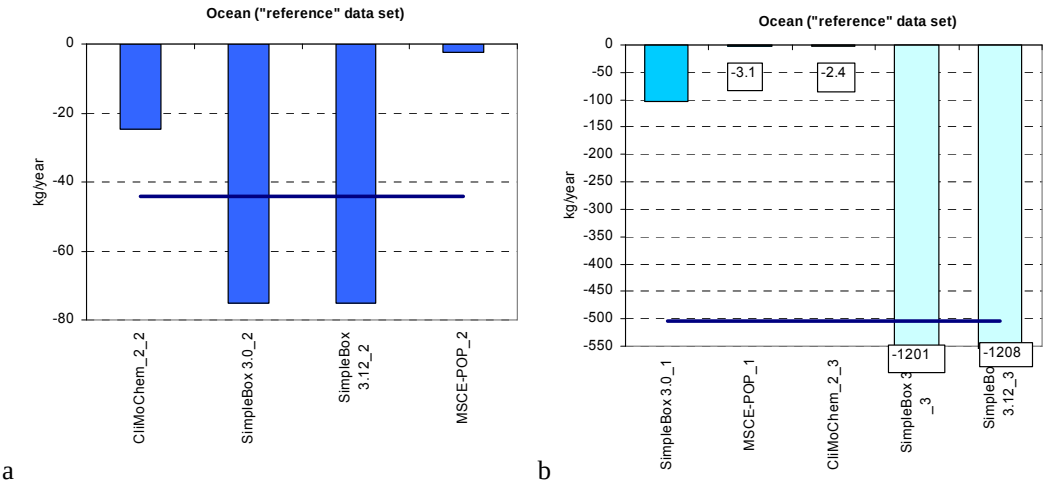


Fig. C.77. *Comparison of PCB-180 mass flows transported in/out the calculation domain through the atmosphere calculated by different models on the basis of two physical-chemical data sets*

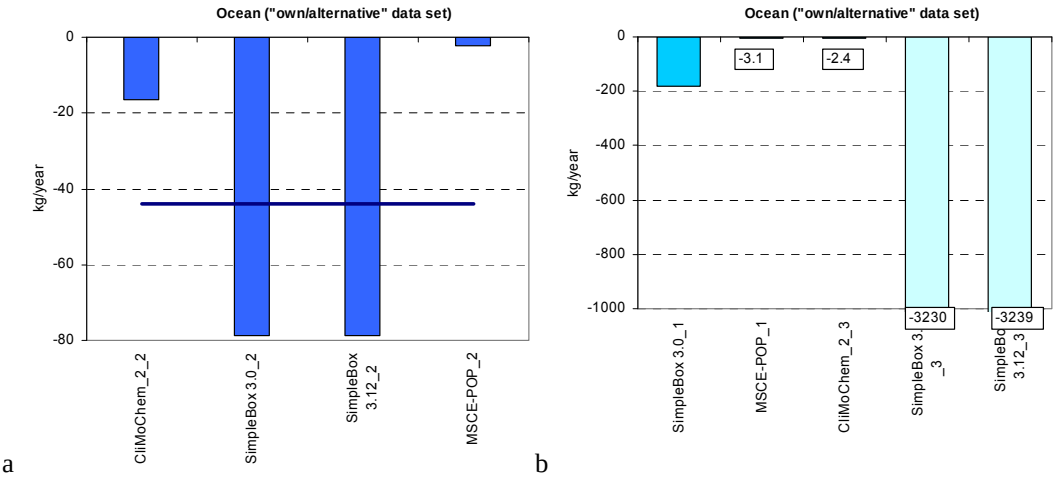
Transport through ocean. Comparison of annual values of PCB-180 mass flows transported out the calculation domain through ocean calculated by different models on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. C.78a. Fig. C.78b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig. C.78. *Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-180 mass flows transported out the calculation domain through ocean calculated by different models on the basis of zero initial concentrations and with the use of "***own or alternative***" data sets is presented in Fig. C.79a. Fig. C.79b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig. C.79. *Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-180 mass flows transported out the calculation domain through ocean obtained with "reference" and "own/alternative" data sets is presented in Table C.49 given in Section 3.3.2 and in Fig. C.80a below. The same data for models with low values of mass flows transported out the calculation domain through ocean are also shown in Fig. C.80b in more detail.

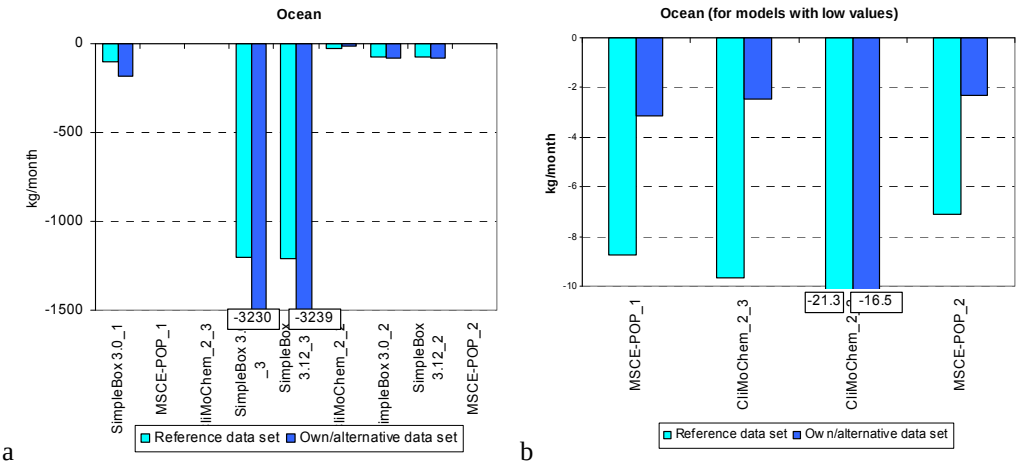


Fig. C.80. *Comparison of PCB-180 mass flows transported in/out the calculation domain through ocean calculated by different models on the basis of two data sets (a - all models; b – models with low values of PCB-180 mass flows transported in/out of ocean).*

Transport through other media. In addition to the results on mass flows of PCB-180 transported out the calculation domain via the atmosphere and ocean, Simple Box model presented calculated values of outflows from sediments, soil and vegetation. Transport of this pollutant from these compartments is considered to be due to such processes as burial, leaching and harvest of agricultural vegetation, respectively.

Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of zero initial concentrations and with the use of "***reference***" data set is presented in Fig. C.81a. Fig. C.81b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between calculations of different types.

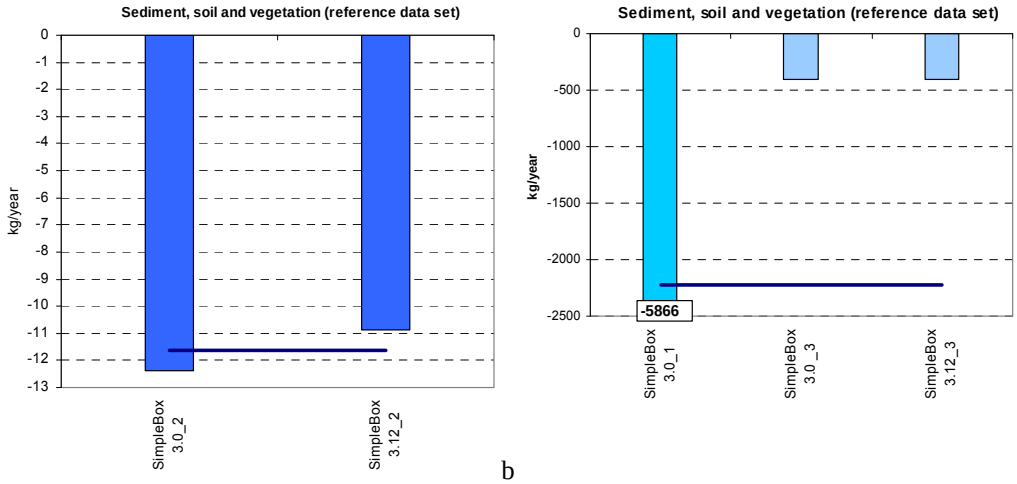
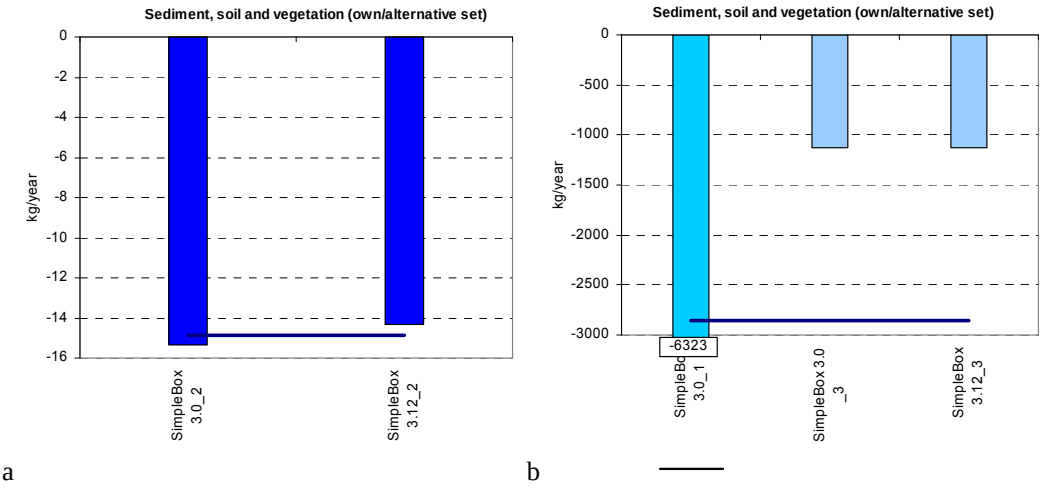


Fig. C.81. *Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions).*

The annual values of PCB-180 mass flows transported out the calculation domain through three considered media calculated by SimpleBox model on the basis of zero initial concentrations and "***alternative***" data set are compared in Fig. C.82a. Fig. C.82b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between different versions of this model.



a b

Fig. C.82. *Comparison of annual values of PCB-180 mass flows transported in/out the calculation domain through three media as a whole (sediment, soil and vegetation) calculated by SimpleBox model on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Annual values of PCB-180 mass flows transported out the calculation domain through such media as sediment, soil and vegetation obtained with "reference" and "own/alternative" data sets are compared in Fig. C.83.

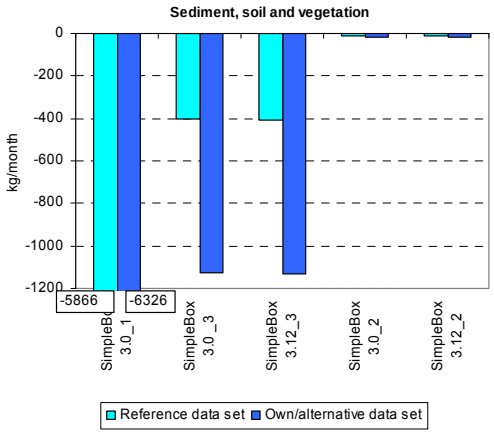
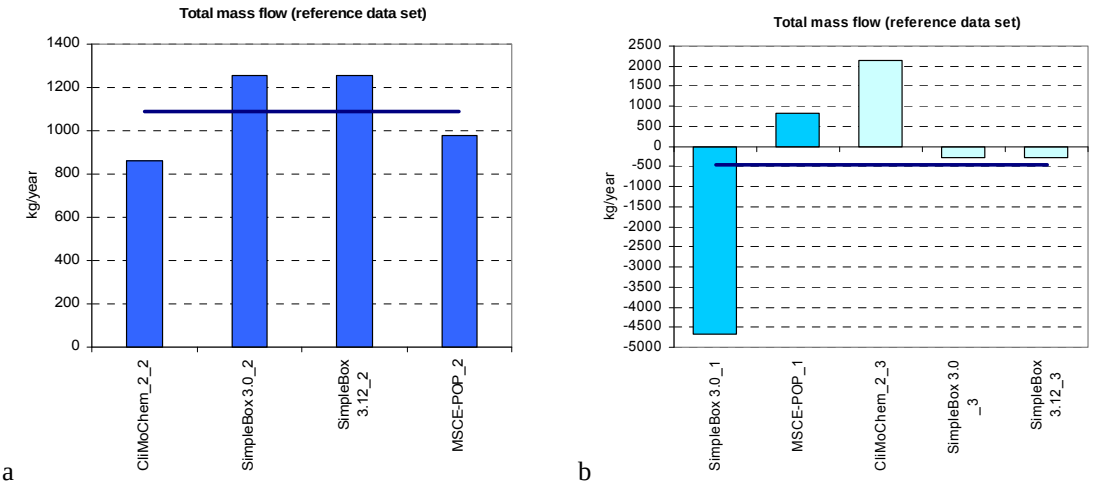


Fig. C.83. *Comparison of PCB-180 mass flows transported in/out the calculation domain through the atmosphere (a), other media (sediment, soil and vegetation)(b) and seawater(c, d) calculated by different models on the basis of two data sets*

Total mass flow. Comparison of annual values of PCB-180 total mass flows transported in/out the calculation domain calculated by different models on the basis of zero initial concentrations and with the use of "***reference*****"** data set is presented in Fig. C.84a. Fig. C.84b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different

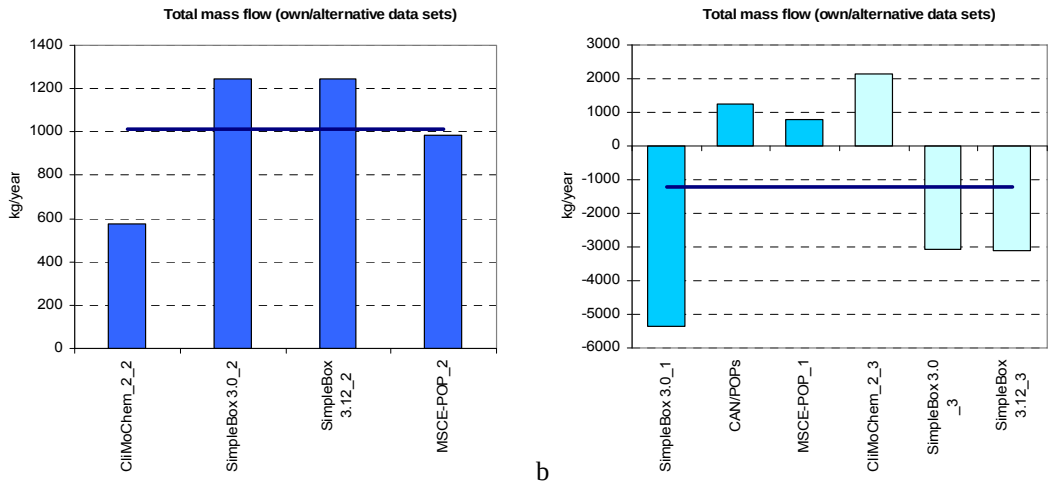
color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig. C.84. *Comparison of annual values of PCB-180 total mass flows transported in/out the calculation domain calculated by different models on the basis of "reference" data set (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

Comparison of annual values of PCB-180 total mass flows transported in/out the calculation domain calculated by different models on the basis of zero initial concentrations and "***own or alternative***" data sets is presented in Fig. C.85a. Fig. C.85b shows the same results but obtained on the basis of initial concentrations and historical emissions. In the latter figure different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.



a b

Fig. C.85. *Comparison of annual values of PCB-180 total mass flows transported in/out the calculation domain calculated by different models on the basis of "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

For models performed calculations on two data sets, the annual values of PCB-180 mass flow transported inside and outside the calculation domain (taking into account emissions) obtained with

"reference" and "own/alternative" data sets are compared in Fig. C.86a. Fig. C.86b presents also the comparison of absolute values of overall mass flow transported outside the calculation domain (not taking into account emission value).

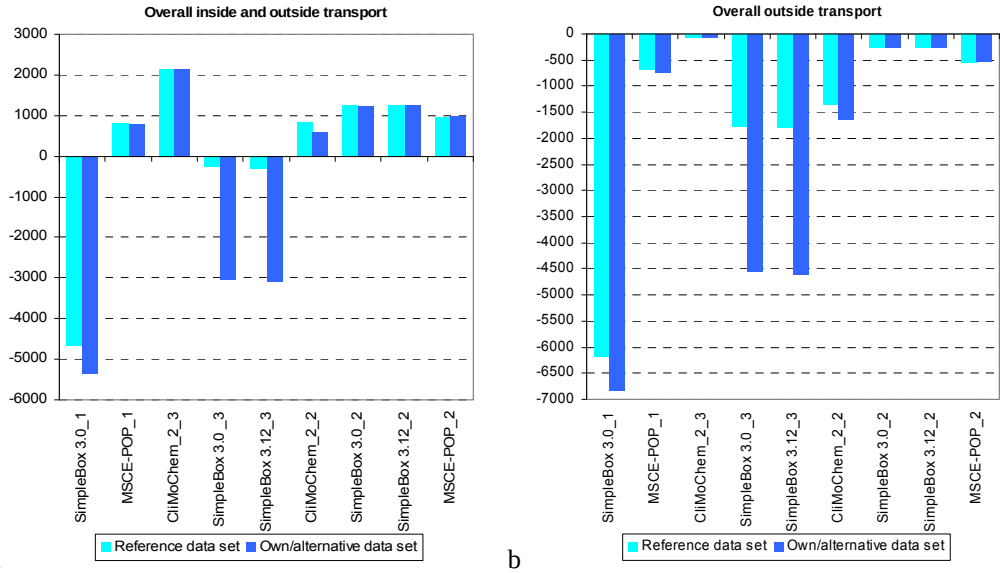
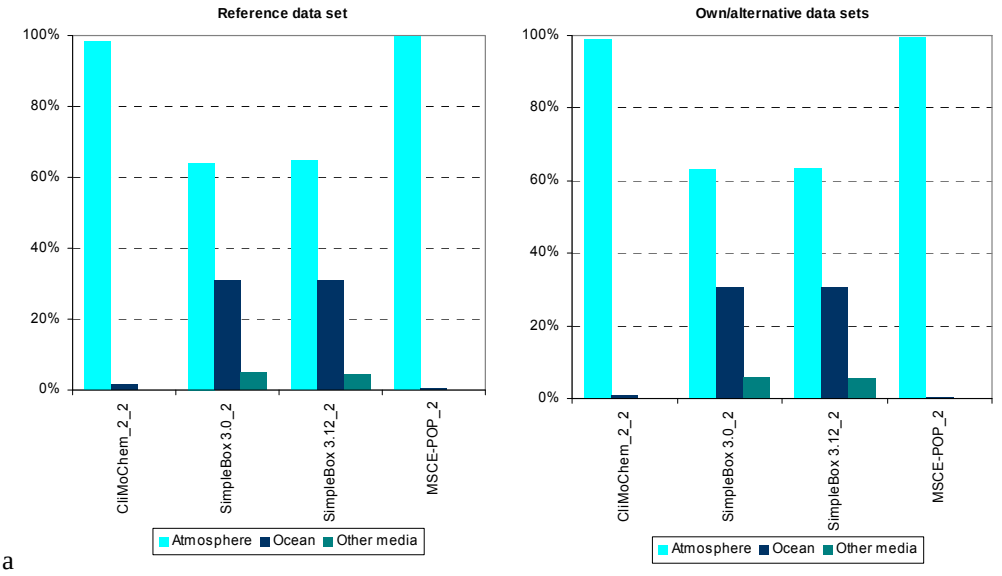
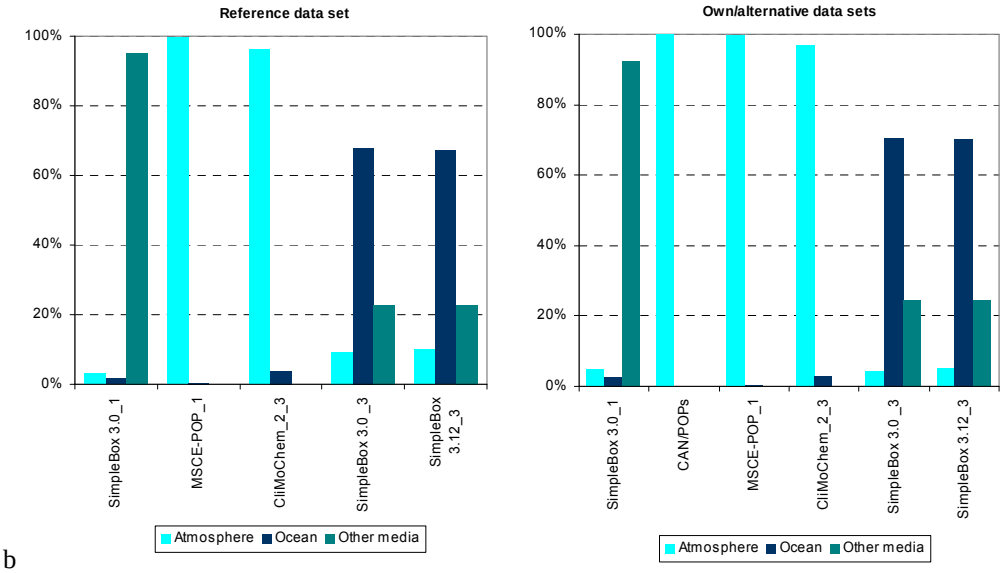


Fig. C.86. *Comparison of PCB-180 overall transport inside and outside the calculation domain (taking into account emissions) (a) and overall transport outside the calculation domain (b) calculated by different models on the basis of two data sets*

Fractions of overall outside transport through atmosphere, ocean and other media (sediment, soil and vegetation) calculated on the basis of zero and non-zero initial conditions are presented in Figs. 3.87a and b, respectively. In these figures fractions of PCB-180 mass in soil calculated by the different models with the use of "reference" and "own/alternative" data sets are also compared.



a



b

Fig. C.87. *Comparison of PCB-180 fractions of overall outside transport through atmosphere, ocean and other media (sediment, soil and vegetation) calculated by different models on the basis of "reference" and "own or alternative" data sets (a – results obtained on the basis of zero initial conditions; b – results based on non-zero initial conditions)*

C.4. Mass flows transported from one compartment to another in both directions

C.4.1. Comparison of calculated values of PCB-180 mass flows transported from the atmosphere to soil

Dry deposition

Reference data set. Calculation results on PCB-180 mass flows transported from the atmosphere to soil: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.56.

Monthly values of PCB-180 mass flows transported from the atmosphere to soil: dry deposition calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.88 a and b, respectively.

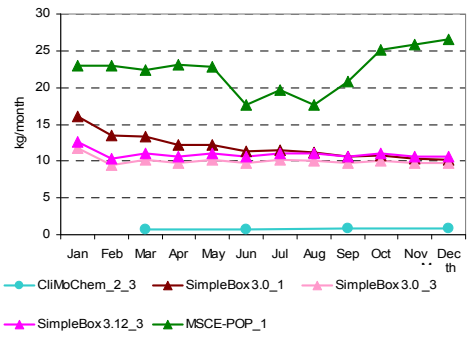


Fig. C.88a. *PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

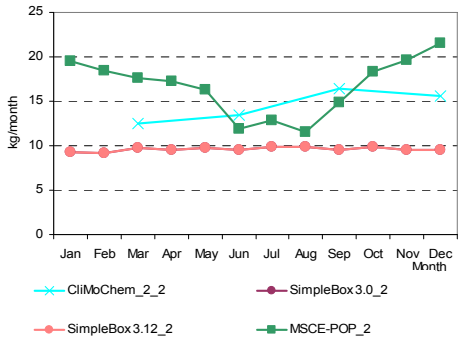


Fig. C.88b. *PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from the atmosphere to soil: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.57.

Monthly values of PCB-180 mass flows transported from the atmosphere to soil: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.89 a and b, respectively.

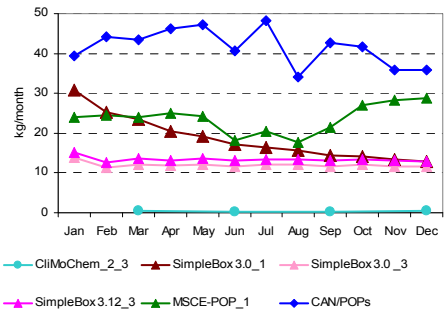


Fig. C.89a. *PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

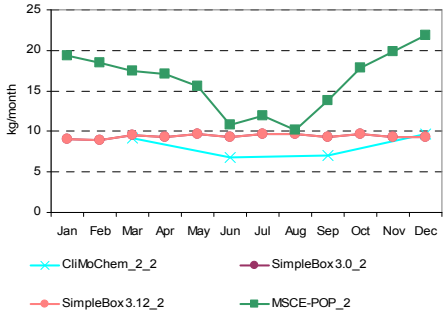


Fig. C.89b. *PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.56. *Calculation results: PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	16.10	23.00		11.72	12.60	*15.85*	*5.13*	Jan		9.32	9.32	19.50	*12.72*	*5.88*
Feb	13.44	23.00		9.50	10.36	*14.07*	*6.19*	Feb		9.18	9.18	18.50	*12.29*	*5.38*
Mar	13.40	22.40		10.14	11.06	*14.25*	*5.60*	Mar		9.81	9.81	17.60	*12.41*	*4.49*
Seas_1	**42.94**	**68.40**	**1.94**	**31.36**	**34.01**	***35.73***	***23.89***	**Seas_1**	**37.42**	**28.32**	**28.32**	**55.60**	***37.41***	***12.86***
Apr	12.27	23.10		9.81	10.69	*13.97*	*6.17*	Apr		9.50	9.50	17.30	*12.10*	*4.50*
May	12.15	22.80		10.13	11.04	*14.03*	*5.91*	May		9.82	9.82	16.30	*11.98*	*3.74*
Jun	11.36	17.70		9.80	10.67	*12.38*	*3.60*	Jun		9.50	9.50	11.90	*10.30*	*1.38*
Seas_2	**35.78**	**63.60**	**2.08**	**29.74**	**32.40**	***32.72***	***21.86***	**Seas_2**	**40.45**	**28.82**	**28.82**	**45.50**	***35.90***	***8.43***
Jul	11.43	19.60		10.12	11.02	*13.04*	*4.41*	Jul		9.82	9.82	12.80	*10.82*	*1.72*
Aug	11.18	17.60		10.12	11.01	*12.48*	*3.45*	Aug		9.82	9.82	11.60	*10.42*	*1.02*
Sep	10.63	20.80		9.79	10.65	*12.97*	*5.24*	Sep		9.51	9.51	14.90	*11.31*	*3.11*
Seas_3	**33.24**	**58.00**	**2.51**	**30.03**	**32.68**	***31.29***	***19.68***	**Seas_3**	**49.17**	**29.16**	**29.16**	**39.30**	***36.70***	***9.59***
Oct	10.83	25.10		10.11	11.00	*14.26*	*7.24*	Oct		9.83	9.83	18.30	*12.65*	*4.89*
Nov	10.35	25.80		9.78	10.64	*14.14*	*7.78*	Nov		9.51	9.51	19.60	*12.87*	*5.82*
Dec	10.25	26.60		9.78	10.63	*14.32*	*8.20*	Dec		9.51	9.51	21.50	*13.51*	*6.92*
Seas_4	**31.43**	**77.50**	**2.39**	**29.68**	**32.27**	***34.65***	***27.01***	**Seas_4**	**46.88**	**28.85**	**28.85**	**59.40**	***41.00***	***14.93***
Annual	**143.38**	**267.50**	**8.93**	**120.80**	**131.36**	***134.40***	***91.83***	**Annual**	**173.93**	**115.14**	**115.15**	**199.80**	***151.01***	***42.73***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.57. *Calculation results: PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			***m***	**σ**	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	39.36	30.75	24.10		13.80	15.11	*24.62*	*10.75*	Jan		9.08	9.08	19.40	*12.52*	*5.96*
Feb	44.28	25.14	24.50		11.40	12.70	*23.61*	*13.22*	Feb		8.97	8.97	18.50	*12.15*	*5.50*
Mar	43.51	23.59	24.00		12.17	13.55	*23.36*	*12.53*	Mar		9.60	9.60	17.50	*12.23*	*4.56*
Seas_1	**127.15**	**79.48**	**72.60**	**1.49**	**37.37**	**41.36**	***59.9***	***43.2***	**Seas_1**	**27.39**	**27.66**	**27.66**	**55.40**	***34.5***	***13.9***
Apr	46.21	20.40	24.90		11.75	13.09	*23.27*	*13.90*	Apr		9.30	9.30	17.10	*11.90*	*4.50*
May	47.17	19.17	24.30		12.13	13.51	*23.26*	*14.21*	May		9.62	9.62	15.60	*11.61*	*3.45*
Jun	40.69	17.12	18.10		11.72	13.06	*20.14*	*11.80*	Jun		9.32	9.32	10.80	*9.81*	*0.86*
Seas_2	**134.07**	**56.68**	**67.30**	**1.06**	**35.61**	**39.67**	***55.7***	***44.5***	**Seas_2**	**20.22**	**28.24**	**28.24**	**43.50**	***30.1***	***9.7***
Jul	48.29	16.53	20.50		12.10	13.49	*22.18*	*14.95*	Jul		9.63	9.63	11.90	*10.39*	*1.31*
Aug	34.11	15.59	17.70		12.09	13.48	*18.59*	*8.93*	Aug		9.64	9.64	10.20	*9.83*	*0.32*
Sep	42.75	14.36	21.50		11.69	13.03	*20.67*	*12.91*	Sep		9.33	9.33	13.80	*10.82*	*2.58*
Seas_3	**125.15**	**46.49**	**59.70**	**1.11**	**35.88**	**39.99**	***51.4***	***41.1***	**Seas_3**	**21.07**	**28.61**	**28.61**	**35.90**	***28.5***	***6.1***
Oct	41.76	14.23	26.90		12.07	13.46	*21.68*	*12.71*	Oct		9.65	9.65	17.90	*12.40*	*4.76*
Nov	35.76	13.27	28.20		11.67	13.01	*20.38*	*10.94*	Nov		9.34	9.34	19.80	*12.83*	*6.04*
Dec	35.97	12.86	28.70		11.66	13.00	*20.44*	*11.17*	Dec		9.34	9.34	21.80	*13.50*	*7.19*
Seas_4	**113.49**	**40.36**	**83.80**	**1.49**	**35.41**	**39.47**	***52.3***	***39.8***	**Seas_4**	**29.01**	**28.33**	**28.33**	**59.50**	***36.3***	***15.5***
Annual	**499.86**	**223.01**	**283.40**	**5.15**	**144.27**	**160.50**	***219.37***	***166.00***	**Annual**	**97.69**	**112.84**	**112.83**	**194.30**	***129.41***	***43.84***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.58.

Table C.58. *The percentage difference between calculation results on PCB-180 mass flows transported from the atmosphere to soil: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			90.9%	-2.6%	-2.6%	17.8%	20.0%	4.8%	-0.5%
Feb			87.1%	-2.3%	-2.3%	20.1%	22.6%	6.5%	0.0%
Mar			76.1%	-2.2%	-2.2%	19.9%	22.5%	7.1%	-0.6%
Seas_1	-26.8%	-23.5%	85.1%	-2.3%	-2.3%	19.2%	21.6%	6.1%	-0.4%
Apr			66.2%	-2.1%	-2.1%	19.8%	22.5%	7.8%	-1.2%
May			57.8%	-2.0%	-2.0%	19.7%	22.4%	6.6%	-4.3%
Jun			50.7%	-2.0%	-2.0%	19.6%	22.4%	2.3%	-9.2%
Seas_2	-50.0%	-49.0%	58.4%	-2.0%	-2.0%	19.7%	22.4%	5.8%	-4.4%
Jul			44.7%	-1.9%	-1.9%	19.6%	22.4%	4.6%	-7.0%
Aug			39.5%	-1.9%	-1.9%	19.5%	22.4%	0.6%	-12.1%
Sep			35.1%	-1.8%	-1.8%	19.4%	22.3%	3.4%	-7.4%
Seas_3	-57.2%	-55.8%	39.9%	-1.9%	-1.9%	19.5%	22.4%	2.9%	-8.7%
Oct			31.4%	-1.8%	-1.8%	19.4%	22.3%	7.2%	-2.2%
Nov			28.2%	-1.8%	-1.8%	19.3%	22.3%	9.3%	1.0%
Dec			25.4%	-1.8%	-1.8%	19.2%	22.3%	7.9%	1.4%
Seas_4	-38.1%	-37.6%	28.4%	-1.8%	-1.8%	19.3%	22.3%	8.1%	0.2%
Annual	-43.8%	-42.3%	55.5%	-2.0%	-2.0%	19.4%	22.2%	5.9%	-2.8%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Wet deposition

Reference data set. Calculation results on PCB-180 mass flows transported from the atmosphere to soil: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.59.

Monthly values of PCB-180 mass flows transported from the atmosphere to soil: wet deposition calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.90 a and b, respectively.

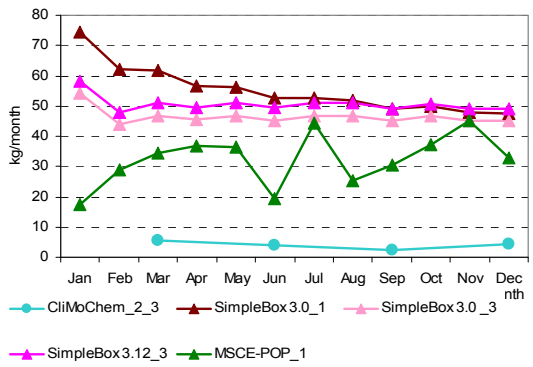


Fig. C.90a. *PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

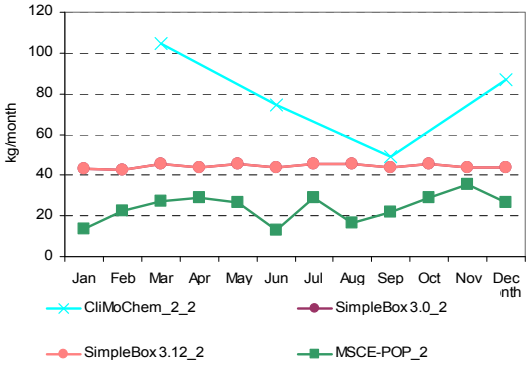


Fig. C.90b. *PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from the atmosphere to soil: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.60.

Monthly values of PCB-180 mass flows transported from the atmosphere to soil: wet deposition calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.91 a and b, respectively.

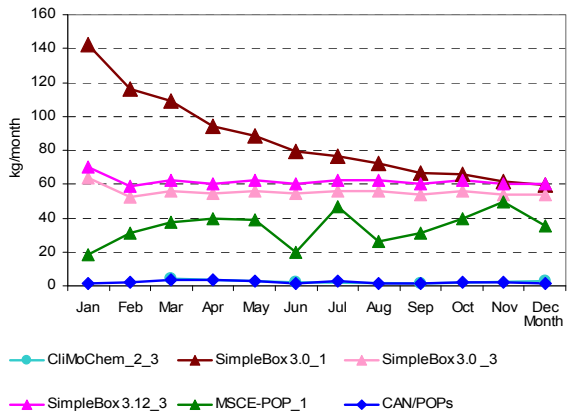


Fig. C.91a. *PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

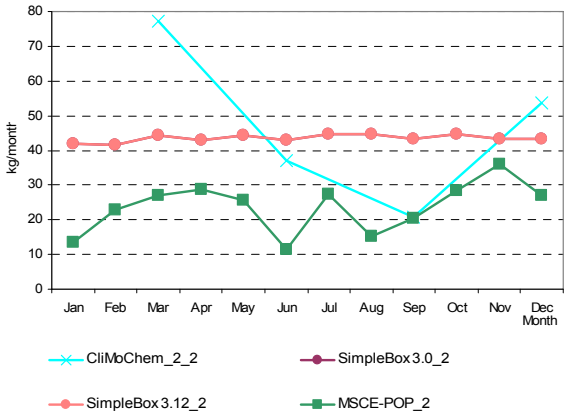


Fig. C.91b. *PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.59. *Calculation results: PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by models on the basis of "reference" data set" and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	MSCE-POP_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	74.49	17.30		54.20	58.25	*51.06*	*24.15*	Jan		13.50	43.11	43.11	*33.24*	*17.10*
Feb	62.14	29.10		43.92	47.89	*45.76*	*13.59*	Feb		22.60	42.44	42.44	*35.83*	*11.46*
Mar	61.98	34.60		46.91	51.14	*48.66*	*11.32*	Mar		26.90	45.39	45.39	*39.22*	*10.67*
Seas_1	**198.60**	**81.00**	**16.34**	**145.02**	**157.28**	***119.65***	***71.52***	**Seas_1**	**314.64**	**63.00**	**130.94**	**130.94**	***159.88***	***108.03***
Apr	56.75	37.00		45.36	49.44	*47.14*	*8.24*	Apr		29.10	43.93	43.93	*38.99*	*8.56*
May	56.17	36.40		46.85	51.04	*47.62*	*8.39*	May		26.50	45.41	45.41	*39.11*	*10.92*
Jun	52.54	19.40		45.31	49.36	*41.65*	*15.13*	Jun		12.80	43.95	43.95	*33.57*	*17.98*
Seas_2	**165.47**	**92.80**	**11.49**	**137.53**	**149.84**	***111.42***	***62.07***	**Seas_2**	**223.52**	**68.40**	**133.30**	**133.30**	***139.63***	***63.75***
Jul	52.85	44.30		46.81	50.96	*48.73*	*3.89*	Jul		29.10	45.43	45.43	*39.99*	*9.43*
Aug	51.70	25.50		46.79	50.93	*43.73*	*12.34*	Aug		16.70	45.43	45.43	*35.86*	*16.59*
Sep	49.16	30.30		45.27	49.26	*43.50*	*8.99*	Sep		22.00	43.97	43.97	*36.65*	*12.68*
Seas_3	**153.71**	**100.10**	**7.50**	**138.86**	**151.15**	***110.27***	***61.32***	**Seas_3**	**146.76**	**67.80**	**134.83**	**134.83**	***121.05***	***35.95***
Oct	50.07	37.20		46.76	50.86	*46.22*	*6.27*	Oct		28.80	45.43	45.44	*39.89*	*9.60*
Nov	47.88	45.30		45.24	49.19	*46.90*	*1.96*	Nov		35.50	43.98	43.98	*41.16*	*4.90*
Dec	47.40	32.90		45.23	49.17	*43.67*	*7.36*	Dec		26.50	43.99	43.99	*38.16*	*10.10*
Seas_4	**145.35**	**115.40**	**13.28**	**137.24**	**149.22**	***112.10***	***56.77***	**Seas_4**	**260.26**	**90.80**	**133.40**	**133.41**	***154.47***	***73.33***
Annual	**663.13**	**389.30**	**48.61**	**558.65**	**607.49**	***453.44***	***248.38***	**Annual**	**945.18**	**290.00**	**532.47**	**532.48**	***575.03***	***271.95***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.60. *Calculation results: PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.72	142.12	18.60		63.78	69.84	*59.21*	*54.69*	Jan		41.96	41.96	13.50	*32.48*	*16.43*
Feb	2.15	116.19	31.30		52.70	58.68	*52.20*	*42.07*	Feb		41.45	41.45	22.70	*35.20*	*10.82*
Mar	3.67	109.05	37.20		56.22	62.61	*53.75*	*38.48*	Mar		44.37	44.37	26.90	*38.54*	*10.08*
Seas_1	**7.54**	**367.36**	**87.10**	**12.55**	**172.69**	**191.13**	***139.7***	***135.6***	**Seas_1**	**231.36**	**127.78**	**127.78**	**63.10**	***137.5***	***69.6***
Apr	3.53	94.28	39.50		54.31	60.51	*50.43*	*33.01*	Apr		42.98	42.98	28.80	*38.26*	*8.19*
May	2.83	88.59	38.80		56.04	62.45	*49.74*	*31.74*	May		44.46	44.45	25.50	*38.14*	*10.94*
Jun	1.63	79.11	19.90		54.17	60.37	*43.03*	*31.53*	Jun		43.05	43.05	11.60	*32.57*	*18.16*
Seas_2	**7.99**	**261.98**	**98.20**	**5.82**	**164.52**	**183.32**	***120.3***	***102.2***	**Seas_2**	**110.96**	**130.49**	**130.49**	**65.90**	***109.5***	***30.5***
Jul	3.07	76.40	47.00		55.91	62.32	*48.94*	*27.79*	Jul		44.51	44.51	27.30	*38.78*	*9.94*
Aug	1.32	72.06	26.20		55.86	62.27	*43.54*	*29.15*	Aug		44.54	44.54	15.10	*34.72*	*17.00*
Sep	1.76	66.39	31.50		54.01	60.21	*42.77*	*26.45*	Sep		43.12	43.12	20.60	*35.61*	*13.00*
Seas_3	**6.14**	**214.84**	**104.70**	**3.28**	**165.79**	**184.80**	***113.3***	***91.5***	**Seas_3**	**62.32**	**132.17**	**132.17**	**63.00**	***97.4***	***40.1***
Oct	2.19	65.76	39.80		55.77	62.17	*45.14*	*25.99*	Oct		44.58	44.58	28.40	*39.18*	*9.34*
Nov	2.24	61.33	49.30		53.93	60.13	*45.39*	*24.61*	Nov		43.16	43.15	35.90	*40.74*	*4.19*
Dec	1.60	59.42	35.60		53.89	60.09	*42.12*	*24.72*	Dec		43.17	43.17	27.00	*37.78*	*9.33*
Seas_4	**6.02**	**186.51**	**124.70**	**8.27**	**163.59**	**182.38**	***111.9***	***84.0***	**Seas_4**	**160.83**	**130.90**	**130.90**	**91.30**	***128.5***	***28.5***
Annual	**27.69**	**1030.69**	**414.70**	**29.93**	**666.59**	**741.63**	***485.2***	***404.4***	**Annual**	**565.48**	**521.35**	**521.34**	**283.30**	***472.87***	***128.08***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.61.

Table C.61. *The percentage difference between calculation results on PCB-180 mass flows transported from the atmosphere to soil: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			90.8%	-2.7%	-2.7%	17.7%	19.9%	7.5%	0.0%
Feb			87.0%	-2.3%	-2.3%	20.0%	22.5%	7.6%	0.4%
Mar			75.9%	-2.2%	-2.2%	19.8%	22.4%	7.5%	0.0%
Seas_1	-26.5%	-23.2%	85.0%	-2.4%	-2.4%	19.1%	21.5%	7.5%	0.2%
Apr			66.1%	-2.2%	-2.2%	19.7%	22.4%	6.8%	-1.0%
May			57.7%	-2.1%	-2.1%	19.6%	22.3%	6.6%	-3.8%
Jun			50.6%	-2.0%	-2.0%	19.5%	22.3%	2.6%	-9.4%
Seas_2	-50.4%	-49.4%	58.3%	-2.1%	-2.1%	19.6%	22.3%	5.8%	-3.7%
Jul			44.6%	-2.0%	-2.0%	19.5%	22.3%	6.1%	-6.2%
Aug			39.4%	-2.0%	-2.0%	19.4%	22.3%	2.7%	-9.6%
Sep			35.0%	-1.9%	-1.9%	19.3%	22.2%	4.0%	-6.4%
Seas_3	-57.5%	-56.2%	39.8%	-2.0%	-2.0%	19.4%	22.3%	4.6%	-7.1%
Oct			31.3%	-1.9%	-1.9%	19.3%	22.2%	7.0%	-1.4%
Nov			28.1%	-1.9%	-1.9%	19.2%	22.2%	8.8%	1.1%
Dec			25.4%	-1.9%	-1.9%	19.1%	22.2%	8.2%	1.9%
Seas_4	-38.2%	-37.7%	28.3%	-1.9%	-1.9%	19.2%	22.2%	8.1%	0.6%
Annual	-40.2%	-38.4%	55.4%	-2.1%	-2.1%	19.3%	22.1%	6.5%	-2.3%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Gaseous exchange

Reference data set. Calculation results on PCB-180 mass flows between the atmosphere and soil: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.62.

Monthly values of PCB-180 mass flows between the atmosphere and soil: gaseous exchange calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.92 a and b, respectively.

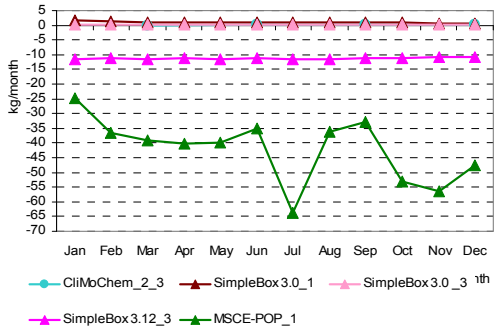


Fig. C.92a. *PCB-180 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

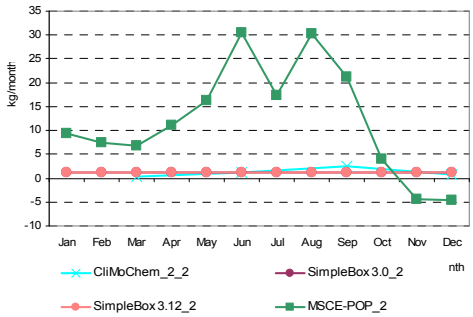


Fig. C.92b. *PCB-180 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows between the atmosphere and soil: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.63.

Monthly values of PCB-180 mass flows between the atmosphere and soil: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.93 a and b, respectively.

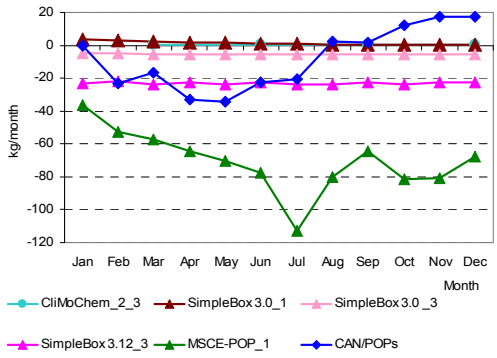


Fig. C.93a. *PCB-180 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

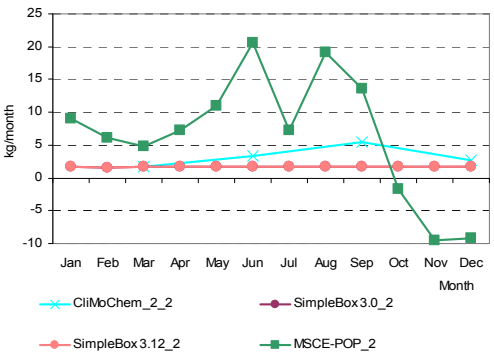


Fig. C.93b. *PCB-180 mass between the atmosphere and soil: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.64.

Table C.62. *Calculation results: PCB-180 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMoChem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE- POP_2		
Jan	1.53	-24.60		0.35	-11.61	*-8.58*	*12.22*	Jan		1.15	1.15	9.45	*3.92*	*4.79*
Feb	1.18	-36.50		0.12	-11.01	*-11.55*	*17.52*	Feb		1.11	1.11	7.48	*3.23*	*3.68*
Mar	1.14	-39.30		0.14	-11.72	*-12.44*	*18.84*	Mar		1.19	1.19	6.69	*3.02*	*3.18*
Seas_1	**3.85**	**-100.40**	**0.07**	**0.61**	**-34.35**	***-26.0***	***44.4***	**Seas_1**	**1.29**	**3.45**	**3.45**	**23.62**	***8.0***	***10.5***
Apr	1.00	-40.10		0.14	-11.28	*-12.56*	*19.19*	Apr		1.15	1.15	11.00	*4.43*	*5.69*
May	0.96	-39.70		0.14	-11.60	*-12.55*	*18.99*	May		1.19	1.18	16.20	*6.19*	*8.67*
Jun	0.88	-34.90		0.14	-11.17	*-11.26*	*16.70*	Jun		1.15	1.14	30.50	*10.93*	*16.95*
Seas_2	**2.85**	**-114.70**	**0.20**	**0.42**	**-34.05**	***-29.1***	***50.3***	**Seas_2**	**3.78**	**3.48**	**3.48**	**57.70**	***17.1***	***27.1***
Jul	0.87	-63.70		0.15	-11.48	*-18.54*	*30.63*	Jul		1.19	1.18	17.30	*6.56*	*9.30*
Aug	0.83	-36.00		0.16	-11.42	*-11.61*	*17.21*	Aug		1.18	1.18	30.30	*10.89*	*16.81*
Sep	0.78	-32.80		0.16	-11.00	*-10.72*	*15.69*	Sep		1.15	1.14	21.20	*7.83*	*11.58*
Seas_3	**2.48**	**-132.50**	**0.38**	**0.46**	**-33.91**	***-32.6***	***57.9***	**Seas_3**	**7.24**	**3.52**	**3.50**	**68.80**	***20.8***	***32.1***
Oct	0.78	-53.00		0.16	-11.31	*-15.84*	*25.39*	Oct		1.18	1.18	4.06	*2.14*	*1.66*
Nov	0.74	-56.30		0.16	-10.89	*-16.57*	*27.02*	Nov		1.14	1.14	-4.37	*-0.70*	*3.18*
Dec	0.73	-47.60		0.17	-10.83	*-14.39*	*22.77*	Dec		1.14	1.14	-4.64	*-0.79*	*3.34*
Seas_4	**2.25**	**-156.90**	**0.13**	**0.49**	**-33.03**	***-37.4***	***68.4***	**Seas_4**	**2.47**	**3.47**	**3.46**	**-4.95**	***1.1***	***4.1***
Annual	**11.43**	**-504.50**	**0.78**	**2.00**	**-135.33**	***-125.13***	***220.62***	**Annual**	**14.78**	**13.92**	**13.88**	**145.17**	*46.94*	*65.49*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.63. *Calculation results: PCB-180 mass flows between the atmosphere and soil: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-0.44	3.69	-36.30		-5.16	-23.31	*-12.30*	*16.91*	Jan		1.65	1.66	9.05	*4.12*	*4.27*
Feb	-23.34	2.66	-52.80		-5.15	-22.10	*-20.15*	*21.36*	Feb		1.60	1.60	6.09	*3.10*	*2.59*
Mar	-16.92	2.22	-57.50		-5.50	-23.62	*-20.26*	*23.09*	Mar		1.71	1.71	4.81	*2.75*	*1.79*
Seas_1	**-40.70**	**8.57**	**-146.60**	**0.29**	**-15.82**	**-69.03**	***-43.9***	***57.8***	**Seas_1**	**5.28**	**4.97**	**4.97**	**19.95**	***8.79***	***7.44***
Apr	-32.67	1.68	-64.50		-5.33	-22.84	*-24.73*	*26.09*	Apr		1.66	1.66	7.33	*3.55*	*3.27*
May	-34.61	1.36	-70.20		-5.50	-23.59	*-26.51*	*28.29*	May		1.71	1.72	11.00	*4.81*	*5.36*
Jun	-22.49	1.04	-77.70		-5.32	-22.82	*-25.46*	*31.03*	Jun		1.66	1.66	20.60	*7.97*	*10.94*
Seas_2	**-89.77**	**4.08**	**-212.40**	**0.46**	**-16.15**	**-69.25**	***-63.8***	***82.2***	**Seas_2**	**10.20**	**5.03**	**5.03**	**38.93**	***14.80***	***16.27***
Jul	-20.35	0.85	-113.00		-5.50	-23.56	*-32.31*	*46.23*	Jul		1.71	1.71	7.22	*3.55*	*3.18*
Aug	2.61	0.66	-80.40		-5.49	-23.55	*-21.23*	*34.65*	Aug		1.71	1.71	19.20	*7.54*	*10.10*
Sep	1.97	0.50	-64.20		-5.31	-22.78	*-17.96*	*27.65*	Sep		1.65	1.66	13.60	*5.64*	*6.90*
Seas_3	**-15.77**	**2.01**	**-257.60**	**0.59**	**-16.31**	**-69.89**	***-59.5***	***100.5***	**Seas_3**	**16.29**	**5.08**	**5.09**	**40.02**	***16.62***	***16.47***
Oct	12.40	0.40	-81.70		-5.49	-23.52	*-19.58*	*37.06*	Oct		1.71	1.71	-1.63	*0.60*	*1.93*
Nov	17.22	0.28	-80.80		-5.31	-22.75	*-18.27*	*37.76*	Nov		1.65	1.66	-9.57	*-2.09*	*6.48*
Dec	17.64	0.20	-67.90		-5.31	-22.74	*-15.62*	*32.58*	Dec		1.65	1.66	-9.26	*-1.98*	*6.30*
Seas_4	**47.26**	**0.88**	**-230.40**	**0.41**	**-16.10**	**-69.01**	***-44.5***	***98.4***	**Seas_4**	**8.29**	**5.01**	**5.02**	**-20.46**	***-0.53***	***13.37***
Annual	**-98.97**	**15.54**	**-847.00**	**1.75**	**-64.37**	**-277.17**	***-211.71***	***328.48***	**Annual**	**40.06**	**20.09**	**20.12**	**78.44**	***39.68***	***27.50***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.64. *Comparison of the calculation results on PCB-180 mass flows between the atmosphere and soil: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets.*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			1.53	3.69	1.15	**1.65**	1.15	1.66	0.35	-5.16	-11.61	-23.31	-24.60	-36.30	9.45	9.05		
Feb			1.18	2.66	1.11	**1.60**	1.11	1.60	0.12	-5.15	-11.01	-22.10	-36.50	-52.80	7.48	6.09		
Mar			1.14	2.22	1.19	**1.71**	1.19	1.71	0.14	-5.50	-11.72	-23.62	-39.30	-57.50	6.69	4.81		
Seas_1	**0.07**	**0.29**	**3.85**	**8.57**	**3.45**	**4.97**	**3.45**	**4.97**	**0.61**	**-15.82**	**-34.35**	**-69.03**	**-100.40**	**-146.60**	**23.62**	**19.95**	**1.29**	**5.28**
Apr			1.00	1.68	1.15	**1.66**	1.15	1.66	0.14	-5.33	-11.28	-22.84	-40.10	-64.50	11.00	7.33		
May			0.96	1.36	1.19	**1.71**	1.18	1.72	0.14	-5.50	-11.60	-23.59	-39.70	-70.20	16.20	11.00		
Jun			0.88	1.04	1.15	**1.66**	1.14	1.66	0.14	-5.32	-11.17	-22.82	-34.90	-77.70	30.50	20.60		
Seas_2	**0.20**	**0.46**	**2.85**	**4.08**	**3.48**	**5.03**	**3.48**	**5.03**	**0.42**	**-16.15**	**-34.05**	**-69.25**	**-114.70**	**-212.40**	**57.70**	**38.93**	**3.78**	**10.20**
Jul			0.87	0.85	1.19	**1.71**	1.18	1.71	0.15	-5.50	-11.48	-23.56	-63.70	-113.00	17.30	7.22		
Aug			0.83	0.66	1.18	**1.71**	1.18	1.71	0.16	-5.49	-11.42	-23.55	-36.00	-80.40	30.30	19.20		
Sep			0.78	0.50	1.15	**1.65**	1.14	1.66	0.16	-5.31	-11.00	-22.78	-32.80	-64.20	21.20	13.60		
Seas_3	**0.38**	**0.59**	**2.48**	**2.01**	**3.52**	**5.08**	**3.50**	**5.09**	**0.46**	**-16.31**	**-33.91**	**-69.89**	**-132.50**	**-257.60**	**68.80**	**40.02**	**7.24**	**16.29**
Oct			0.78	0.40	1.18	**1.71**	1.18	1.71	0.16	-5.49	-11.31	-23.52	-53.00	-81.70	4.06	-1.63		
Nov			0.74	0.28	1.14	**1.65**	1.14	1.66	0.16	-5.31	-10.89	-22.75	-56.30	-80.80	-4.37	-9.57		
Dec			0.73	0.20	1.14	**1.65**	1.14	1.66	0.17	-5.31	-10.83	-22.74	-47.60	-67.90	-4.64	-9.26		
Seas_4	**0.13**	**0.41**	**2.25**	**0.88**	**3.47**	**5.01**	**3.46**	**5.02**	**0.49**	**-16.10**	**-33.03**	**-69.01**	**-156.90**	**-230.40**	**-4.95**	**-20.46**	**2.47**	**8.29**
Annual	**0.78**	**1.75**	**11.43**	**15.54**	**13.92**	**20.09**	**13.88**	**20.12**	**2.00**	**-64.37**	**-135.33**	**-277.17**	**-504.50**	**-847.00**	**145.17**	**78.44**	**14.78**	**40.06**

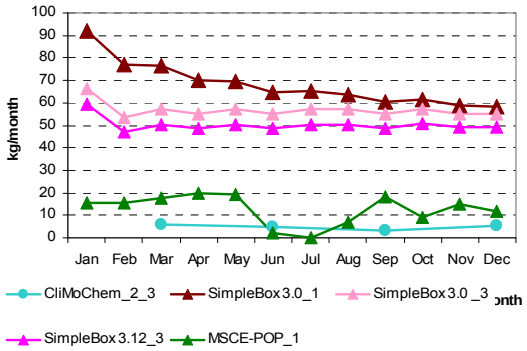
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Net mass flows between the atmosphere and soil

Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

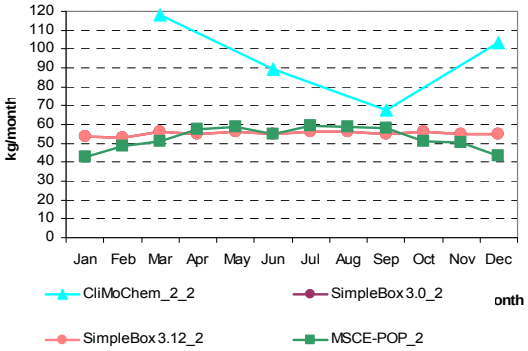
Reference data set. Calculation results on PCB-180 net mass flows between the atmosphere and soil calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.65.

Monthly values of PCB-180 net mass flows between the atmosphere and soil calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.94 a and b, respectively.



a

Fig. C.94a. *PCB-180 net mass flows between the atmosphere and soil (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*



b

Fig. C.94b. *PCB-180 net mass flows between the atmosphere and soil (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table C.65. *Calculation results: PCB-180 net mass flows between the atmosphere and soil (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	92.12	15.70		66.27	59.23	*58.33*	*31.74*	Jan		53.59	53.59	42.45	*49.88*	*6.43*
Feb	76.76	15.60		53.54	47.24	*48.28*	*25.22*	Feb		52.73	52.73	48.58	*51.35*	*2.40*
Mar	76.51	17.70		57.19	50.48	*50.47*	*24.48*	Mar		56.39	56.39	51.19	*54.66*	*3.00*
Seas_1	**245.40**	**49.00**	**18.35**	**176.99**	**156.95**	***129.34***	***93.91***	**Seas_1**	**353.36**	**162.71**	**162.71**	**142.22**	***205.25***	***99.21***
Apr	70.03	20.00		55.31	48.85	*48.55*	*20.99*	Apr		54.58	54.58	57.40	*55.52*	*1.63*
May	69.28	19.50		57.12	50.48	*49.10*	*21.21*	May		56.42	56.42	59.00	*57.28*	*1.49*
Jun	64.78	2.20		55.26	48.86	*42.78*	*27.83*	Jun		54.60	54.60	55.20	*54.80*	*0.35*
Seas_2	**204.09**	**41.70**	**13.78**	**167.69**	**148.19**	***115.09***	***82.82***	**Seas_2**	**267.76**	**165.60**	**165.60**	**171.60**	***192.64***	***50.16***
Jul	65.14	0.20		57.08	50.50	*43.23*	*29.31*	Jul		56.44	56.44	59.20	*57.36*	*1.60*
Aug	63.71	7.10		57.06	50.52	*44.60*	*25.57*	Aug		56.44	56.44	58.60	*57.16*	*1.25*
Sep	60.57	18.30		55.21	48.91	*45.75*	*18.91*	Sep		54.62	54.62	58.10	*55.78*	*2.01*
Seas_3	**189.43**	**25.60**	**10.39**	**169.36**	**149.93**	***108.94***	***84.36***	**Seas_3**	**203.17**	**167.50**	**167.49**	**175.90**	***178.51***	***16.90***
Oct	61.68	9.30		57.04	50.55	*44.64*	*24.00*	Oct		56.44	56.44	51.16	*54.68*	*3.05*
Nov	58.97	14.80		55.19	48.94	*44.48*	*20.21*	Nov		54.64	54.64	50.73	*53.33*	*2.26*
Dec	58.37	11.90		55.18	48.96	*43.60*	*21.49*	Dec		54.64	54.64	43.36	*50.88*	*6.51*
Seas_4	**179.03**	**36.00**	**15.81**	**167.41**	**148.46**	***109.34***	***77.28***	**Seas_4**	**309.61**	**165.72**	**165.71**	**145.25**	***196.57***	***75.97***
Annual	**817.94**	**152.30**	**58.33**	**681.45**	**603.52**	*462.71*	*336.80*	**Annual**	**1133.90**	**661.53**	**661.51**	**634.97**	***772.98***	***240.94***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates;

C.4.2. Comparison of calculated values of PCB-180 mass flows transported from vegetation to soil: Litterfall

Reference data set. Calculation results on PCB-180 mass flows transported from the vegetation to soil: litterfall calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.66.

Monthly values of PCB-180 mass flows transported from vegetation to soil: litterfall calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.95 a and b, respectively. Seasonal variations of low values of mass flows transported from vegetation to soil calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.95c in more detail.

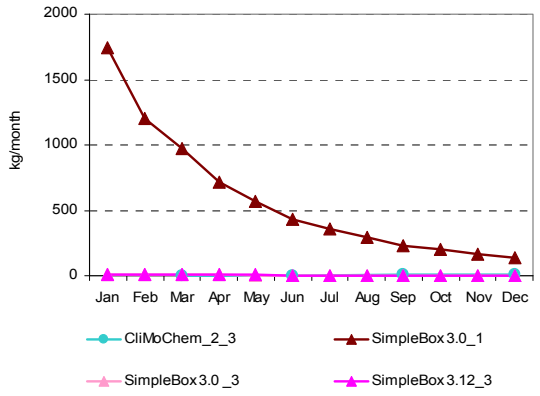


Fig. C.95a. *PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

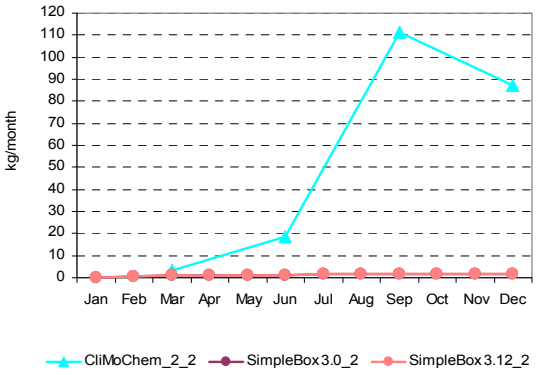


Fig. C.95b. *PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

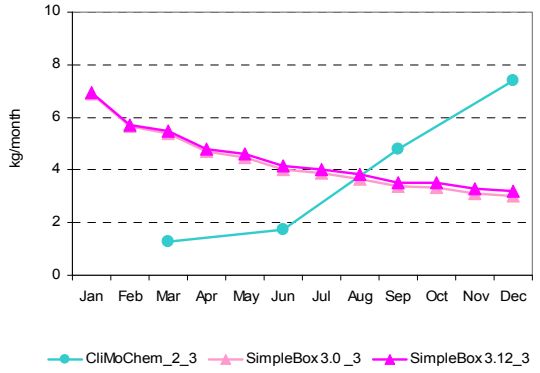
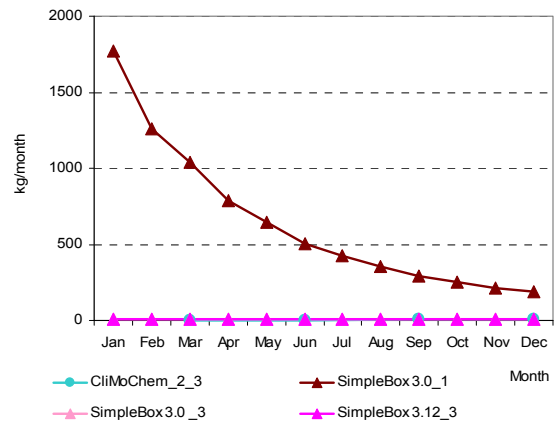


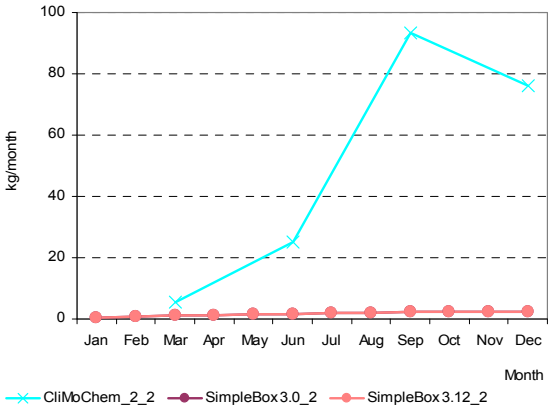
Fig. C.95c. *PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from vegetation to soil: litterfall calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.67.

Monthly values of PCB-180 mass flows transported from vegetation to soil: litterfall calculated by all participating models on the basis of “own or alternative” data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.96 a and b, respectively. Seasonal variations of low values of mass flows transported from vegetation to soil calculated by the participating models on the basis of “reference” data set and non-zero initial conditions are also shown in Fig. C.96c in more detail.



a



b

Fig. C.96a. *PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (all models)*

Fig. C.96b. *PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and zero-initial conditions*

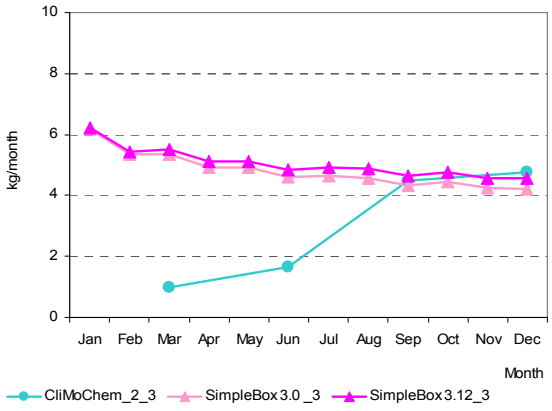


Fig. C.96c. *PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by the participating models on the basis of “own or alternative” data sets and non-zero initial conditions (models with low values)*

Table C.66. *Calculation results: PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	CliMoChem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	1744.67		6.91	6.93	*586.17*	*1003.29*	Jan		0.20	0.20	*581.69*	*1007.17*
Feb	1206.19		5.66	5.71	*405.85*	*693.11*	Feb		0.52	0.52	*0.52*	*0.00*
Mar	968.83		5.39	5.47	*326.56*	*556.22*	Mar		0.83	0.83	*0.83*	*0.00*
Seas_1	**3919.68**	**3.82**	**17.97**	**18.11**	***989.90***	***1953.20***	**Seas_1**	**10.15**	**1.55**	**1.55**	***4.42***	***4.96***
Apr	712.54		4.72	4.82	*240.69*	*408.63*	Apr		1.02	1.02	*1.02*	*0.00*
May	569.84		4.47	4.59	*192.97*	*326.38*	May		1.24	1.24	*1.24*	*0.00*
Jun	434.30		4.02	4.14	*147.49*	*248.39*	Jun		1.34	1.34	*1.34*	*0.00*
Seas_2	**1716.68**	**5.27**	**13.21**	**13.55**	***437.18***	***853.01***	**Seas_2**	**55.36**	**3.59**	**3.59**	***20.85***	***29.89***
Jul	359.70		3.89	4.03	*122.54*	*205.39*	Jul		1.50	1.50	*1.50*	*0.00*
Aug	292.04		3.67	3.82	*99.84*	*166.44*	Aug		1.60	1.60	*1.60*	*0.00*
Sep	233.63		3.38	3.53	*80.18*	*132.89*	Sep		1.63	1.63	*1.63*	*0.00*
Seas_3	**885.37**	**14.41**	**10.95**	**11.39**	***230.53***	***436.56***	**Seas_3**	**333.12**	**4.73**	**4.73**	***114.19***	***189.59***
Oct	202.27		3.35	3.51	*69.71*	*114.80*	Oct		1.76	1.76	*1.76*	*0.00*
Nov	165.82		3.11	3.28	*57.40*	*93.89*	Nov		1.76	1.76	*1.76*	*0.00*
Dec	142.20		3.01	3.18	*49.46*	*80.31*	Dec		1.81	1.81	*1.81*	*0.00*
Seas_4	**510.29**	**22.18**	**9.47**	**9.96**	***137.98***	***248.28***	**Seas_4**	**261.83**	**5.33**	**5.33**	***90.83***	***148.09***
Annual	**7032.02**	**45.68**	**51.59**	**53.01**	*1795.58*	*3490.96*	**Annual**	**660.46**	**15.21**	**15.21**	*230.29*	*372.53*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.67. *Calculation results: PCB-180 mass flows transported from vegetation to soil: litterfall (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1a	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a		
Jan	1770.31		6.18	6.22	*594.24*	*1018.51*	Jan		0.25	0.25	*0.25*	*0.00*
Feb	1258.80		5.34	5.44	*423.19*	*723.66*	Feb		0.65	0.65	*0.65*	*0.00*
Mar	1038.49		5.36	5.52	*349.79*	*596.43*	Mar		1.06	1.06	*1.06*	*0.00*
Seas_1	**4067.60**	**2.98**	**16.89**	**17.17**	***1026.16***	***2027.64***	**Seas_1**	**16.11**	**1.96**	**1.96**	***6.68***	***8.17***
Apr	783.91		4.94	5.13	*264.66*	*449.69*	Apr		1.31	1.31	*1.31*	*0.00*
May	642.62		4.91	5.14	*217.56*	*368.12*	May		1.60	1.60	*1.60*	*0.00*
Jun	501.44		4.61	4.86	*170.30*	*286.78*	Jun		1.74	1.74	*1.74*	*0.00*
Seas_2	**1927.98**	**4.92**	**14.45**	**15.12**	***490.62***	***958.25***	**Seas_2**	**75.74**	**4.65**	**4.65**	***28.35***	***41.05***
Jul	424.79		4.65	4.93	*144.79*	*242.49*	Jul		1.97	1.97	*1.97*	*0.00*
Aug	352.56		4.56	4.86	*120.66*	*200.83*	Aug		2.12	2.12	*2.12*	*0.00*
Sep	288.07		4.34	4.66	*99.02*	*163.72*	Sep		2.17	2.17	*2.17*	*0.00*
Seas_3	**1065.42**	**13.48**	**13.55**	**14.45**	***276.73***	***525.80***	**Seas_3**	**279.85**	**6.25**	**6.25**	***97.45***	***157.96***
Oct	254.57		4.43	4.77	*87.92*	*144.32*	Oct		2.35	2.35	*2.35*	*0.00*
Nov	212.98		4.25	4.59	*73.94*	*120.41*	Nov		2.36	2.36	*2.36*	*0.00*
Dec	186.27		4.21	4.56	*65.02*	*105.01*	Dec		2.44	2.44	*2.44*	*0.00*
Seas_4	**653.82**	**14.25**	**12.89**	**13.92**	***173.72***	***320.07***	**Seas_4**	**228.28**	**7.16**	**7.15**	***80.86***	***127.66***
Annual	**7714.83**	**35.63**	**57.77**	**60.66**	***1967.22***	***3831.75***	**Annual**	**599.98**	**20.02**	**20.02**	*213.34*	*334.84*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.68.

Table C.68. *The percentage difference between calculation results on PCB-180 mass flows transported from vegetation to soil: litterfall obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_2	CliMoChem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan			1.5%	24.1%	24.1%	-10.6%	-10.3%
Feb			4.4%	25.7%	25.7%	-5.6%	-4.8%
Mar			7.2%	27.0%	27.0%	-0.6%	0.8%
Seas_1	58.6%	-22.1%	3.8%	26.2%	26.2%	-6.0%	-5.2%
Apr			10.0%	28.3%	28.3%	4.6%	6.4%
May			12.8%	29.3%	29.3%	9.7%	11.9%
Jun			15.5%	30.3%	30.3%	14.6%	17.2%
Seas_2	36.8%	-6.5%	12.3%	29.4%	29.4%	9.4%	11.6%
Jul			18.1%	31.2%	31.2%	19.4%	22.3%
Aug			20.7%	32.1%	32.1%	24.1%	27.2%
Sep			23.3%	32.8%	32.8%	28.4%	31.7%
Seas_3	-16.0%	-6.4%	20.3%	32.1%	32.1%	23.8%	26.9%
Oct			25.9%	33.6%	33.6%	32.5%	36.0%
Nov			28.4%	34.2%	34.2%	36.4%	39.9%
Dec			31.0%	34.9%	34.8%	39.9%	43.6%
Seas_4	-12.8%	-35.8%	28.1%	34.2%	34.2%	36.1%	39.7%
Annual	-9.2%	-22.0%	9.7%	31.6%	31.6%	12.0%	14.4%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.4.3. Comparison of calculated values of PCB-180 mass flows transported from the atmosphere to water

Dry deposition

Reference data set. Calculation results on PCB-180 mass flows transported from the atmosphere to water: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.69.

Monthly values of PCB-180 mass flows transported from the atmosphere to water: dry deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.97 a and b, respectively.

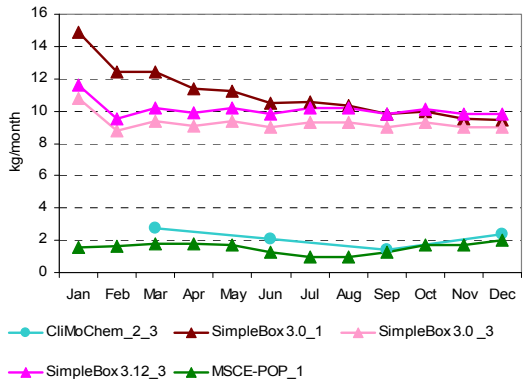


Fig. C.97a. *PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

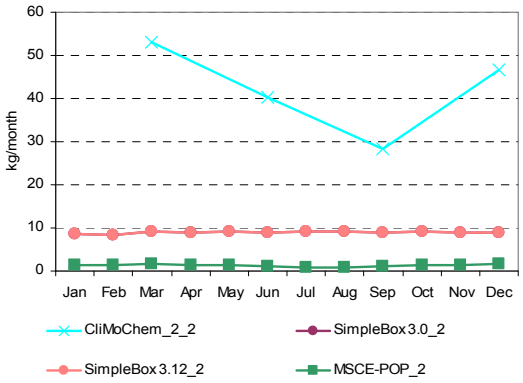


Fig. C.97b. *PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from the atmosphere to water: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.70.

Monthly values of PCB-180 mass flows transported from the atmosphere to water: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.98 a and b, respectively.

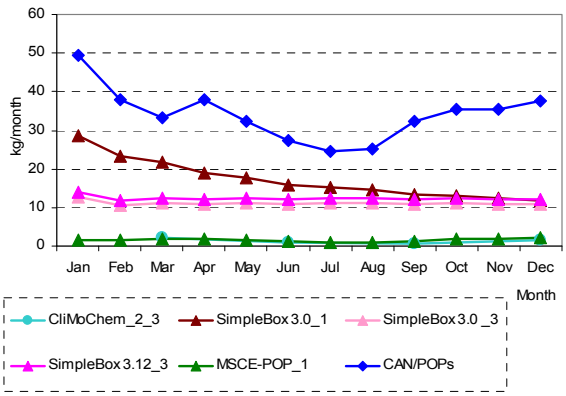


Fig. C.98a. *PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

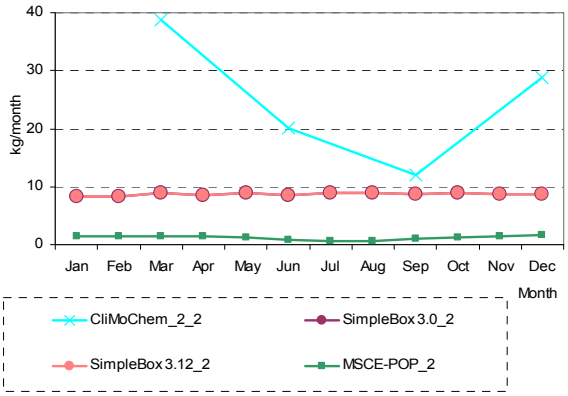


Fig. C.98b. *PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.69. *Calculation results: PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	14.91	1.60		10.82	11.64	*9.74*	*5.71*	Jan		8.59	8.59	1.39	*6.19*	*4.16*
Feb	12.43	1.63		8.76	9.56	*8.09*	*4.59*	Feb		8.46	8.46	1.40	*6.11*	*4.08*
Mar	12.40	1.82		9.35	10.21	*8.44*	*4.60*	Mar		9.05	9.05	1.57	*6.56*	*4.32*
Seas_1	**39.74**	**5.05**	**8.27**	**28.93**	**31.40**	***22.68***	***15.21***	**Seas_1**	**159.08**	**26.10**	**26.10**	**4.36**	***53.91***	***70.86***
Apr	11.35	1.80		9.05	9.87	*8.02*	*4.25*	Apr		8.76	8.76	1.51	*6.34*	*4.18*
May	11.23	1.68		9.34	10.19	*8.11*	*4.36*	May		9.05	9.05	1.40	*6.50*	*4.42*
Jun	10.50	1.23		9.04	9.85	*7.65*	*4.32*	Jun		8.76	8.76	0.98	*6.17*	*4.49*
Seas_2	**33.08**	**4.71**	**6.22**	**27.42**	**29.90**	***20.27***	***13.67***	**Seas_2**	**120.94**	**26.57**	**26.57**	**3.89**	***44.49***	***52.07***
Jul	10.56	0.96		9.33	10.17	*7.76*	*4.56*	Jul		9.06	9.06	0.77	*6.30*	*4.78*
Aug	10.33	0.95		9.33	10.16	*7.69*	*4.51*	Aug		9.06	9.06	0.76	*6.29*	*4.79*
Sep	9.82	1.29		9.03	9.83	*7.49*	*4.15*	Sep		8.77	8.77	1.02	*6.18*	*4.47*
Seas_3	**30.71**	**3.21**	**4.34**	**27.69**	**30.17**	***19.22***	***14.16***	**Seas_3**	**84.83**	**26.88**	**26.88**	**2.55**	***35.28***	***34.96***
Oct	10.00	1.68		9.32	10.15	*7.79*	*4.09*	Oct		9.06	9.06	1.31	*6.48*	*4.47*
Nov	9.56	1.74		9.02	9.82	*7.53*	*3.88*	Nov		8.77	8.77	1.41	*6.32*	*4.25*
Dec	9.46	1.99		9.02	9.81	*7.57*	*3.73*	Dec		8.77	8.77	1.71	*6.42*	*4.08*
Seas_4	**29.02**	**5.41**	**7.16**	**27.37**	**29.78**	***19.75***	***12.34***	**Seas_4**	**140.16**	**26.60**	**26.60**	**4.43**	***49.45***	***61.37***
Annual	**132.55**	**18.38**	**25.98**	**111.41**	**121.25**	*81.91*	*55.11*	**Annual**	**505.00**	**106.15**	**106.15**	**15.23**	*183.13*	*218.82*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.70. *Calculation results: PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	49.46	28.55	1.65		12.75	13.96	*21.27*	*18.43*	Jan		8.37	8.37	1.38	*6.04*	*4.04*
Feb	37.90	23.34	1.69		10.52	11.72	*17.03*	*13.97*	Feb		8.27	8.27	1.38	*5.97*	*3.98*
Mar	33.14	21.91	1.88		11.23	12.51	*16.13*	*11.86*	Mar		8.85	8.85	1.55	*6.42*	*4.22*
Seas_1	**120.50**	**73.80**	**5.22**	**6.32**	**34.50**	**38.18**	***46.42***	***44.16***	**Seas_1**	**116.43**	**25.50**	**25.50**	**4.31**	***42.93***	***50.01***
Apr	37.94	18.94	1.87		10.85	12.08	*16.34*	*13.52*	Apr		8.58	8.58	1.48	*6.21*	*4.10*
May	32.28	17.79	1.70		11.19	12.47	*15.09*	*11.23*	May		8.87	8.87	1.33	*6.36*	*4.35*
Jun	27.35	15.88	1.22		10.82	12.06	*13.46*	*9.45*	Jun		8.59	8.59	0.91	*6.03*	*4.44*
Seas_2	**97.57**	**52.61**	**4.79**	**3.17**	**32.85**	**36.61**	***37.93***	***34.95***	**Seas_2**	**60.45**	**26.04**	**26.04**	**3.72**	***29.06***	***23.42***
Jul	24.42	15.33	0.94		11.17	12.45	*12.86*	*8.44*	Jul		8.88	8.88	0.71	*6.16*	*4.72*
Aug	25.10	14.46	0.91		11.15	12.44	*12.81*	*8.64*	Aug		8.89	8.89	0.67	*6.15*	*4.75*
Sep	32.42	13.32	1.29		10.79	12.03	*13.97*	*11.35*	Sep		8.61	8.61	0.95	*6.05*	*4.42*
Seas_3	**81.94**	**43.11**	**3.14**	**1.92**	**33.11**	**36.91**	***33.35***	***29.56***	**Seas_3**	**36.34**	**26.38**	**26.38**	**2.32**	***22.86***	***14.47***
Oct	35.38	13.19	1.75		11.14	12.42	*14.78*	*12.41*	Oct		8.90	8.90	1.27	*6.35*	*4.40*
Nov	35.36	12.30	1.86		10.77	12.01	*14.46*	*12.45*	Nov		8.61	8.61	1.41	*6.21*	*4.16*
Dec	37.68	11.91	2.10		10.76	12.00	*14.89*	*13.39*	Dec		8.62	8.62	1.72	*6.32*	*3.98*
Seas_4	**108.42**	**37.39**	**5.71**	**4.47**	**32.67**	**36.42**	***37.51***	***37.83***	**Seas_4**	**86.73**	**26.13**	**26.13**	**4.40**	***35.85***	***35.44***
Annual	**408.43**	**206.92**	**18.86**	**15.88**	**133.13**	**148.13**	***155.22***	***145.14***	**Annual**	**299.96**	**104.05**	**104.05**	**14.75**	***130.70***	***120.43***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.71.

Table C.71. *The percentage difference between calculation results on PCB-180 mass flows transported from the atmosphere to water: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			91.4%	-2.6%	-2.6%	17.8%	20.0%	3.1%	-0.7%
Feb			87.8%	-2.2%	-2.2%	20.2%	22.6%	3.7%	-1.4%
Mar			76.7%	-2.1%	-2.1%	20.0%	22.5%	3.3%	-1.3%
Seas_1	-26.8%	-23.5%	85.7%	-2.3%	-2.3%	19.2%	21.6%	3.4%	-1.1%
Apr			66.9%	-2.0%	-2.1%	19.9%	22.5%	3.9%	-2.0%
May			58.4%	-2.0%	-2.0%	19.8%	22.4%	1.2%	-5.0%
Jun			51.3%	-1.9%	-1.9%	19.7%	22.4%	-0.8%	-7.8%
Seas_2	-50.0%	-49.0%	59.0%	-2.0%	-2.0%	19.8%	22.4%	1.7%	-4.5%
Jul			45.2%	-1.9%	-1.9%	19.6%	22.4%	-2.2%	-8.7%
Aug			40.0%	-1.9%	-1.9%	19.6%	22.3%	-4.5%	-11.4%
Sep			35.6%	-1.8%	-1.8%	19.5%	22.3%	0.0%	-7.0%
Seas_3	-57.2%	-55.8%	40.4%	-1.9%	-1.9%	19.6%	22.3%	-2.0%	-8.8%
Oct			31.9%	-1.8%	-1.8%	19.4%	22.3%	4.2%	-3.1%
Nov			28.6%	-1.8%	-1.8%	19.4%	22.3%	6.9%	0.0%
Dec			25.9%	-1.7%	-1.7%	19.3%	22.3%	5.5%	0.6%
Seas_4	-38.1%	-37.6%	28.9%	-1.8%	-1.8%	19.4%	22.3%	5.5%	-0.7%
Annual	-40.6%	-38.9%	56.1%	-2.0%	-2.0%	19.5%	22.2%	2.6%	-3.2%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Wet deposition

Reference data set. Calculation results on PCB-180 mass flows transported from the atmosphere to water: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.72.

Monthly values of PCB-180 mass flows transported from the atmosphere to water: wet deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.99 a and b, respectively.

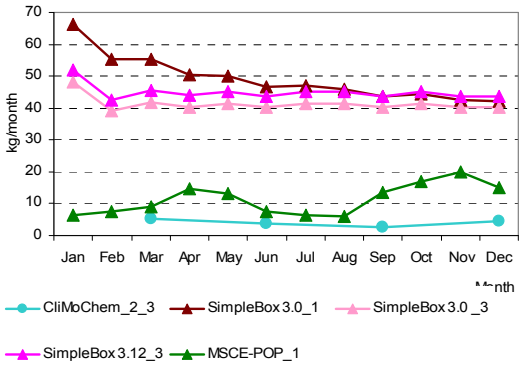


Fig. C.99a. *PCB-180 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "reference data set" and non-zero initial conditions*

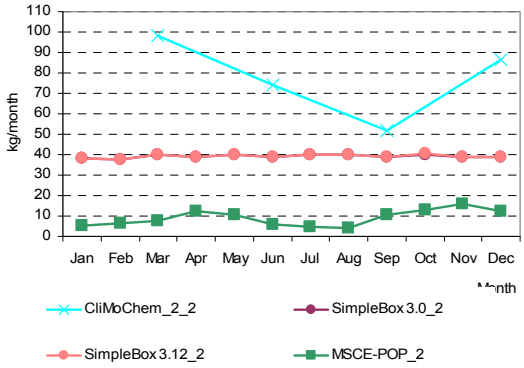


Fig. C.99b. *PCB-180 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "reference data set" and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from the atmosphere to water: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.73.

Monthly values of PCB-180 mass flows transported from the atmosphere to water: wet deposition calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.100 a and b, respectively.

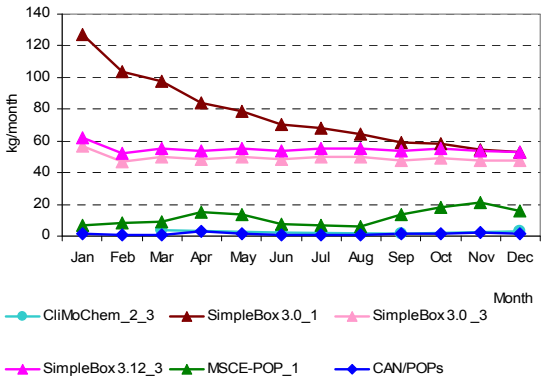


Fig. C.100a. *PCB-180 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

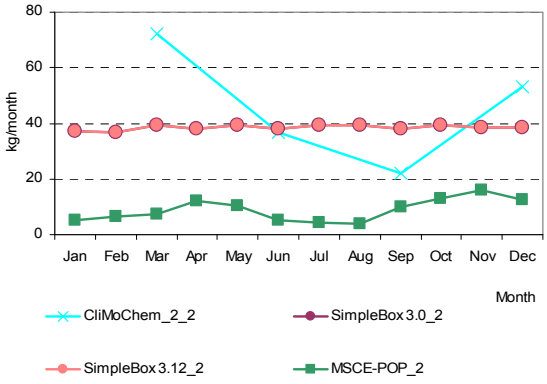


Fig. C.100b. *PCB-180 mass flows transported from the atmosphere to water: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.74.

Gaseous exchange

Reference data set. Calculation results on PCB-180 mass flows between the atmosphere and water: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.75.

Monthly values of PCB-180 mass flows between the atmosphere and water: gaseous exchange calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.101 a and b, respectively.

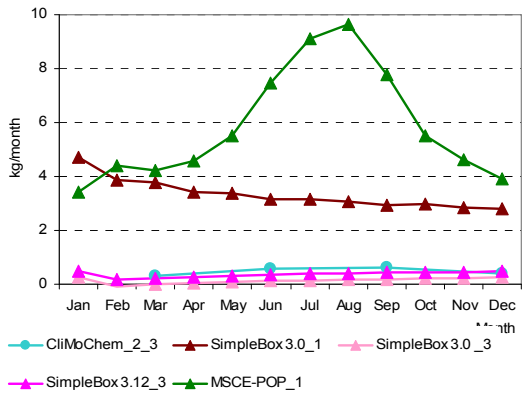


Fig. C.101a. *PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

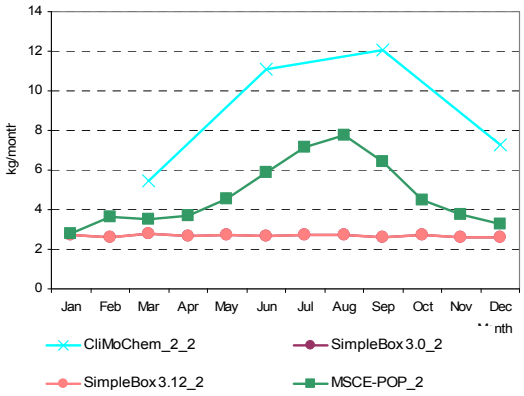


Fig. C.101b. *PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table C.72. *Calculation results: PCB-180 mass flows between the atmosphere and water: wet deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	66.34	6.38		48.13	51.77	*43.15*	*25.75*	Jan		38.22	38.22	5.44	*27.29*	*18.93*
Feb	55.30	7.71		38.96	42.52	*36.12*	*20.20*	Feb		37.64	37.64	6.36	*27.21*	*18.06*
Mar	55.15	8.88		41.61	45.40	*37.76*	*20.08*	Mar		40.25	40.25	7.61	*29.37*	*18.85*
Seas_1	**176.79**	**22.97**	**15.33**	**128.70**	**139.69**	***96.69***	***73.05***	**Seas_1**	**295.19**	**116.11**	**116.11**	**19.41**	***136.71***	***115.07***
Apr	50.49	14.70		40.24	43.89	*37.33*	*15.67*	Apr		38.96	38.96	12.40	*30.11*	*15.34*
May	49.96	13.20		41.56	45.32	*37.51*	*16.56*	May		40.28	40.28	10.80	*30.45*	*17.02*
Jun	46.72	7.41		40.20	43.82	*34.54*	*18.28*	Jun		38.98	38.98	5.74	*27.90*	*19.19*
Seas_2	**147.16**	**35.31**	**11.44**	**121.99**	**133.03**	***89.79***	***61.86***	**Seas_2**	**222.54**	**118.21**	**118.21**	**28.94**	***121.98***	***79.16***
Jul	46.98	6.31		41.52	45.25	*35.01*	*19.27*	Jul		40.29	40.29	4.83	*28.47*	*20.47*
Aug	45.95	5.96		41.50	45.22	*34.66*	*19.23*	Aug		40.29	40.29	4.34	*28.31*	*20.76*
Sep	43.68	13.40		40.15	43.73	*35.24*	*14.66*	Sep		38.99	38.99	10.50	*29.50*	*16.45*
Seas_3	**136.61**	**25.67**	**7.96**	**123.18**	**134.19**	***85.52***	***63.24***	**Seas_3**	**155.64**	**119.57**	**119.58**	**19.67**	***103.61***	***58.49***
Oct	44.48	16.90		41.48	45.16	*37.00*	*13.50*	Oct		40.29	40.30	13.20	*31.26*	*15.64*
Nov	42.53	19.80		40.13	43.68	*36.53*	*11.25*	Nov		39.01	39.01	15.90	*31.30*	*13.34*
Dec	42.09	15.00		40.12	43.65	*35.22*	*13.55*	Dec		39.01	39.01	12.60	*30.21*	*15.25*
Seas_4	**129.10**	**51.70**	**13.22**	**121.74**	**132.48**	***89.65***	***54.09***	**Seas_4**	**259.11**	**118.31**	**118.32**	**41.70**	***134.36***	***90.67***
Annual	**589.66**	**135.65**	**47.95**	**495.60**	**539.40**	***361.65***	***250.50***	**Annual**	**932.48**	**472.21**	**472.22**	**109.72**	*496.66*	*337.07*

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.73. *Calculation results: PCB-180 mass flows between the atmosphere and water: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3a	SimpleBox 3.12_3a				CliMo Chem_2_2	SimpleBox 3.0_2a	SimpleBox 3.12_2a	MSCE-POP_2		
Jan	1.29	126.90	6.63		56.66	62.05	*50.71*	*50.88*	Jan		*37.21*	*37.21*	5.39	*26.60*	*18.37*
Feb	1.07	103.75	8.12		46.78	52.09	*42.36*	*41.11*	Feb		*36.77*	*36.77*	6.33	*26.62*	*17.57*
Mar	0.97	97.37	9.22		49.90	55.59	*42.61*	*38.95*	Mar		*39.36*	*39.36*	7.54	*28.75*	*18.37*
Seas_1	**3.32**	**328.01**	**23.97**	**11.78**	**153.34**	**169.73**	***115.02***	***127.48***	**Seas_1**	***217.05***	***113.34***	***113.34***	**19.26**	***115.75***	***80.80***
Apr	3.37	84.17	15.20		48.21	53.71	*40.93*	*32.24*	Apr		*38.13*	*38.13*	12.30	*29.52*	*14.91*
May	1.42	79.08	13.50		49.74	55.43	*39.83*	*31.82*	May		*39.44*	*39.44*	10.30	*29.73*	*16.82*
Jun	0.74	70.60	7.53		48.08	53.59	*36.11*	*30.44*	Jun		*38.19*	*38.19*	5.38	*27.26*	*18.95*
Seas_2	**5.54**	**233.85**	**36.23**	**5.79**	**146.03**	**162.74**	***98.36***	***95.73***	**Seas_2**	***110.47***	***115.76***	***115.76***	**27.98**	***92.49***	***43.08***
Jul	0.54	68.16	6.47		49.63	55.32	*36.02*	*30.51*	Jul		*39.49*	*39.49*	4.54	*27.84*	*20.18*
Aug	0.71	64.27	6.04		49.58	55.28	*35.18*	*29.56*	Aug		*39.51*	*39.51*	3.97	*27.66*	*20.52*
Sep	1.31	59.20	13.70		47.94	53.45	*35.12*	*25.89*	Sep		*38.26*	*38.25*	9.93	*28.81*	*16.35*
Seas_3	**2.56**	**191.63**	**26.21**	**3.48**	**147.15**	**164.05**	***89.18***	***87.49***	**Seas_3**	***66.09***	***117.26***	***117.26***	**18.44**	***79.76***	***47.47***
Oct	1.70	58.62	17.80		49.50	55.19	*36.56*	*25.34*	Oct		*39.55*	*39.55*	12.90	*30.66*	*15.38*
Nov	1.89	54.66	21.20		47.87	53.37	*35.80*	*23.31*	Nov		*38.29*	*38.29*	16.00	*30.86*	*12.87*
Dec	1.30	52.93	16.00		47.83	53.34	*34.28*	*24.07*	Dec		*38.30*	*38.30*	12.70	*29.77*	*14.78*
Seas_4	**4.90**	**166.21**	**55.00**	**8.24**	**145.20**	**161.90**	***90.24***	***76.39***	**Seas_4**	***160.13***	***116.13***	***116.13***	**41.60**	***108.50***	***49.18***
Annual	**16.31**	**919.71**	**141.41**	**29.29**	**591.72**	**658.41**	***392.81***	***380.75***	**Annual**	***553.75***	***462.49***	***462.48***	**107.28**	***396.50***	***197.55***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.74. *The percentage difference between calculation results on PCB-180 mass flows between the atmosphere and water: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			91.3%	-2.6%	-2.6%	17.7%	19.9%	3.9%	-0.9%
Feb			87.6%	-2.3%	-2.3%	20.1%	22.5%	5.3%	-0.5%
Mar			76.6%	-2.2%	-2.2%	19.9%	22.4%	3.8%	-0.9%
Seas_1	-26.5%	-23.2%	85.5%	-2.4%	-2.4%	19.1%	21.5%	4.4%	-0.8%
Apr			66.7%	-2.1%	-2.1%	19.8%	22.4%	3.4%	-0.8%
May			58.3%	-2.1%	-2.1%	19.7%	22.3%	2.3%	-4.6%
Jun			51.1%	-2.0%	-2.0%	19.6%	22.3%	1.6%	-6.3%
Seas_2	-50.4%	-49.4%	58.9%	-2.1%	-2.1%	19.7%	22.3%	2.6%	-3.3%
Jul			45.1%	-2.0%	-2.0%	19.5%	22.3%	2.5%	-6.0%
Aug			39.9%	-1.9%	-1.9%	19.5%	22.2%	1.3%	-8.5%
Sep			35.5%	-1.9%	-1.9%	19.4%	22.2%	2.2%	-5.4%
Seas_3	-57.5%	-56.2%	40.3%	-1.9%	-1.9%	19.5%	22.2%	2.1%	-6.3%
Oct			31.8%	-1.9%	-1.9%	19.3%	22.2%	5.3%	-2.3%
Nov			28.5%	-1.8%	-1.9%	19.3%	22.2%	7.1%	0.6%
Dec			25.8%	-1.8%	-1.8%	19.2%	22.2%	6.7%	0.8%
Seas_4	-38.2%	-37.7%	28.7%	-1.8%	-1.8%	19.3%	22.2%	6.4%	-0.2%
Annual	-40.6%	-38.9%	56.0%	-2.1%	-2.1%	19.4%	22.1%	4.2%	-2.2%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Own/alternative data set. Calculation results on PCB-180 mass flows between the atmosphere and water: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.76.

Monthly values of PCB-180 mass flows between the atmosphere and water: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.102 a and b, respectively.

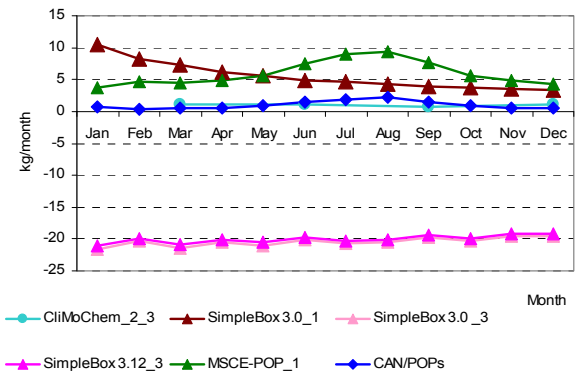


Fig. C.102a. *PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

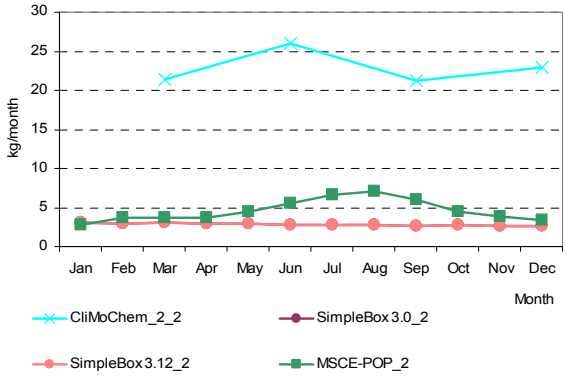


Fig. C.102b. *PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.77.

Table C.75. *Calculation results: PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	4.70	3.41		0.26	0.51	*2.22*	*2.19*	Jan		2.72	2.72	2.77	*2.74*	*0.03*
Feb	3.85	4.39		-0.09	0.16	*2.08*	*2.37*	Feb		2.64	2.64	3.62	*2.96*	*0.57*
Mar	3.79	4.23		-0.02	0.23	*2.06*	*2.26*	Mar		2.79	2.79	3.52	*3.03*	*0.42*
Seas_1	**12.33**	**12.03**	**0.89**	**0.15**	**0.90**	***5.26***	***6.33***	**Seas_1**	**16.38**	**8.14**	**8.14**	**9.91**	***10.64***	***3.91***
Apr	3.44	4.56		0.04	0.28	*2.08*	*2.27*	Apr		2.68	2.68	3.67	*3.01*	*0.57*
May	3.38	5.49		0.08	0.33	*2.32*	*2.59*	May		2.75	2.75	4.57	*3.36*	*1.05*
Jun	3.14	7.47		0.12	0.35	*2.77*	*3.42*	Jun		2.65	2.65	5.89	*3.73*	*1.87*
Seas_2	**9.96**	**17.52**	**1.76**	**0.24**	**0.96**	***6.09***	***7.50***	**Seas_2**	**33.19**	**8.07**	**8.07**	**14.13**	***15.86***	***11.90***
Jul	3.15	9.09		0.15	0.39	*3.20*	*4.16*	Jul		2.72	2.72	7.18	*4.21*	*2.57*
Aug	3.07	9.64		0.18	0.42	*3.33*	*4.41*	Aug		2.71	2.71	7.78	*4.40*	*2.92*
Sep	2.91	7.77		0.20	0.42	*2.83*	*3.52*	Sep		2.62	2.62	6.43	*3.89*	*2.20*
Seas_3	**9.13**	**26.50**	**1.87**	**0.53**	**1.23**	***7.85***	***10.99***	**Seas_3**	**36.11**	**8.06**	**8.06**	**21.39**	***18.41***	***13.37***
Oct	2.96	5.49		0.22	0.46	*2.28*	*2.47*	Oct		2.70	2.70	4.51	*3.30*	*1.04*
Nov	2.82	4.61		0.24	0.46	*2.03*	*2.08*	Nov		2.61	2.61	3.77	*3.00*	*0.67*
Dec	2.79	3.91		0.25	0.47	*1.86*	*1.79*	Dec		2.60	2.60	3.26	*2.82*	*0.38*
Seas_4	**8.57**	**14.01**	**1.17**	**0.71**	**1.39**	***5.17***	***5.91***	**Seas_4**	**21.85**	**7.91**	**7.91**	**11.54**	***12.31***	***6.59***
Annual	**40.01**	**70.06**	**5.69**	**1.63**	**4.47**	***24.37***	***29.97***	**Annual**	**107.54**	**32.18**	**32.19**	**56.97**	***57.22***	***35.52***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.76. *Calculation results: PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	CAN/POPs	SimpleBox 3.0_1[a]	MSCE- POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.67	10.52	3.69		-21.54	-21.10	*-5.55*	*14.83*	Jan		3.10	3.10	2.84	*3.01*	*0.15*
Feb	0.39	8.16	4.73		-20.27	-19.85	*-5.37*	*13.69*	Feb		2.92	2.92	3.71	*3.19*	*0.45*
Mar	0.57	7.33	4.57		-21.39	-20.96	*-5.98*	*14.08*	Mar		3.03	3.03	3.62	*3.23*	*0.34*
Seas_1	**1.63**	**26.01**	**12.99**	**3.22**	**-63.20**	**-61.91**	***-13.54***	***38.95***	**Seas_1**	**64.29**	**9.05**	**9.05**	**10.17**	***23.14***	***27.44***
Apr	0.53	6.11	4.86		-20.49	-20.08	*-5.81*	*13.37*	Apr		2.86	2.86	3.69	*3.14*	*0.48*
May	0.87	5.57	5.67		-20.98	-20.57	*-5.89*	*13.73*	May		2.90	2.90	4.46	*3.42*	*0.90*
Jun	1.45	4.86	7.45		-20.15	-19.76	*-5.23*	*13.61*	Jun		2.76	2.76	5.48	*3.67*	*1.57*
Seas_2	**2.85**	**16.55**	**17.98**	**3.53**	**-61.62**	**-60.41**	***-13.52***	***37.33***	**Seas_2**	**77.78**	**8.51**	**8.51**	**13.63**	***27.11***	***33.87***
Jul	1.80	4.61	8.97		-20.68	-20.28	*-5.12*	*14.26*	Jul		2.81	2.81	6.65	*4.09*	*2.21*
Aug	2.22	4.28	9.34		-20.55	-20.16	*-4.97*	*14.28*	Aug		2.78	2.78	7.11	*4.23*	*2.50*
Sep	1.50	3.90	7.73		-19.78	-19.40	*-5.21*	*13.31*	Sep		2.67	2.67	6.07	*3.80*	*1.96*
Seas_3	**5.53**	**12.79**	**26.04**	**2.27**	**-61.02**	**-59.85**	***-12.37***	***38.11***	**Seas_3**	**63.50**	**8.27**	**8.27**	**19.83**	***24.97***	***26.26***
Oct	0.96	3.82	5.68		-20.33	-19.94	*-5.96*	*13.05*	Oct		2.74	2.74	4.44	*3.30*	*0.98*
Nov	0.54	3.54	4.88		-19.57	-19.20	*-5.96*	*12.36*	Nov		2.63	2.63	3.81	*3.02*	*0.68*
Dec	0.49	3.40	4.21		-19.48	-19.11	*-6.10*	*12.13*	Dec		2.61	2.61	3.38	*2.87*	*0.44*
Seas_4	**1.99**	**10.76**	**14.77**	**3.32**	**-59.38**	**-58.26**	***-14.47***	***34.68***	**Seas_4**	**68.61**	**7.98**	**7.98**	**11.63**	***24.05***	***29.76***
Annual	**11.99**	**66.11**	**71.78**	**12.35**	**-245.23**	**-240.42**	***-53.90***	***148.54***	**Annual**	**274.18**	**33.81**	**33.81**	**55.26**	***99.27***	***117.05***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.77. *Comparison of the calculation results on PCB-180 mass flows between the atmosphere and water: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0 _3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			4.70	10.52	2.72	3.10	2.72	3.10	0.26	-21.54	0.51	-21.10	3.41	3.69	2.77	2.84		
Feb			3.85	8.16	2.64	2.92	2.64	2.92	-0.09	-20.27	0.16	-19.85	4.39	4.73	3.62	3.71		
Mar			3.79	7.33	2.79	3.03	2.79	3.03	-0.02	-21.39	0.23	-20.96	4.23	4.57	3.52	3.62		
Seas_1	**0.89**	**3.22**	**12.33**	**26.01**	**8.14**	**9.05**	**8.14**	**9.05**	**0.15**	**-63.20**	**0.90**	**-61.91**	**12.03**	**12.99**	**9.91**	**10.17**	**16.38**	**64.29**
Apr			3.44	6.11	2.68	2.86	2.68	2.86	0.04	-20.49	0.28	-20.08	4.56	4.86	3.67	3.69		
May			3.38	5.57	2.75	2.90	2.75	2.90	0.08	-20.98	0.33	-20.57	5.49	5.67	4.57	4.46		
Jun			3.14	4.86	2.65	2.76	2.65	2.76	0.12	-20.15	0.35	-19.76	7.47	7.45	5.89	5.48		
Seas_2	**1.76**	**3.53**	**9.96**	**16.55**	**8.07**	**8.51**	**8.07**	**8.51**	**0.24**	**-61.62**	**0.96**	**-60.41**	**17.52**	**17.98**	**14.13**	**13.63**	**33.19**	**77.78**
Jul			3.15	4.61	2.72	2.81	2.72	2.81	0.15	-20.68	0.39	-20.28	9.09	8.97	7.18	6.65		
Aug			3.07	4.28	2.71	2.78	2.71	2.78	0.18	-20.55	0.42	-20.16	9.64	9.34	7.78	7.11		
Sep			2.91	3.90	2.62	2.67	2.62	2.67	0.20	-19.78	0.42	-19.40	7.77	7.73	6.43	6.07		
Seas_3	**1.87**	**2.27**	**9.13**	**12.79**	**8.06**	**8.27**	**8.06**	**8.27**	**0.53**	**-61.02**	**1.23**	**-59.85**	**26.50**	**26.04**	**21.39**	**19.83**	**36.11**	**63.50**
Oct			2.96	3.82	2.70	2.74	2.70	2.74	0.22	-20.33	0.46	-19.94	5.49	5.68	4.51	4.44		
Nov			2.82	3.54	2.61	2.63	2.61	2.63	0.24	-19.57	0.46	-19.20	4.61	4.88	3.77	3.81		
Dec			2.79	3.40	2.60	2.61	2.60	2.61	0.25	-19.48	0.47	-19.11	3.91	4.21	3.26	3.38		
Seas_4	**1.17**	**3.32**	**8.57**	**10.76**	**7.91**	**7.98**	**7.91**	**7.98**	**0.71**	**-59.38**	**1.39**	**-58.26**	**14.01**	**14.77**	**11.54**	**11.63**	**21.85**	**68.61**
Annual	**5.69**	**12.35**	**40.01**	**66.11**	**32.18**	**33.81**	**32.19**	**33.81**	**1.63**	**-245.23**	**4.47**	**-240.42**	**70.06**	**71.78**	**56.97**	**55.26**	**107.54**	**274.18**

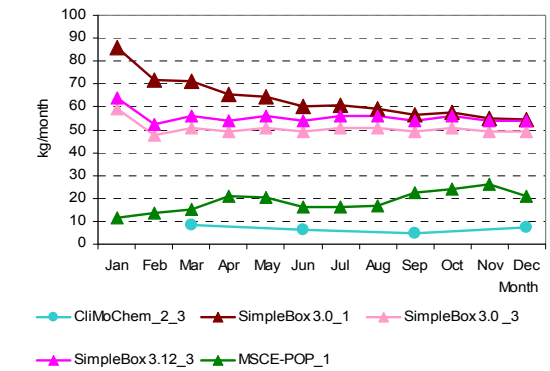
CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Net mass flows between the atmosphere and water

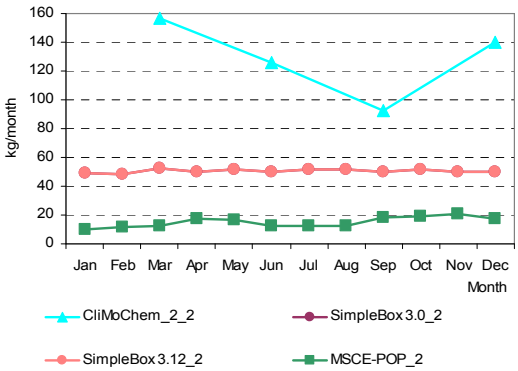
Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-180 net mass flows PCB-180 between the atmosphere and water calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.78.

Monthly values of PCB-180 net mass flows PCB-180 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.103 a and b, respectively.



a



b

Fig. C.103a. *PCB-180 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

Fig. C.103b. *PCB-180 net mass flows between the atmosphere and water (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Table C.78. *Calculation results: PCB-180 net mass flows between the atmosphere and water (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	85.94	11.39		59.21	63.91	*55.11*	*31.39*	Jan		49.53	49.53	9.60	*36.22*	*23.05*
Feb	71.58	13.73		47.63	52.24	*46.29*	*24.06*	Feb		48.74	48.74	11.38	*36.28*	*21.57*
Mar	71.34	14.93		50.94	55.84	*48.26*	*23.86*	Mar		52.09	52.09	12.70	*38.96*	*22.74*
Seas_1	**228.86**	**40.05**	**24.48**	**157.78**	**171.99**	***124.63***	***88.59***	**Seas_1**	**470.65**	**150.35**	**150.36**	**33.68**	***201.26***	***187.83***
Apr	65.28	21.06		49.32	54.04	*47.42*	*18.81*	Apr		50.39	50.40	17.58	*39.46*	*18.95*
May	64.56	20.37		50.98	55.83	*47.94*	*19.22*	May		52.08	52.08	16.77	*40.31*	*20.38*
Jun	60.36	16.11		49.35	54.02	*44.96*	*19.76*	Jun		50.38	50.38	12.61	*37.79*	*21.81*
Seas_2	**190.20**	**57.54**	**19.42**	**149.65**	**163.89**	***116.14***	***73.62***	**Seas_2**	**376.67**	**152.86**	**152.86**	**46.96**	***182.34***	***138.84***
Jul	60.69	16.36		51.00	55.81	*45.97*	*20.13*	Jul		52.07	52.07	12.78	*38.97*	*22.68*
Aug	59.35	16.55		51.01	55.79	*45.68*	*19.71*	Aug		52.07	52.07	12.88	*39.00*	*22.63*
Sep	56.41	22.46		49.38	53.98	*45.56*	*15.67*	Sep		50.38	50.38	17.95	*39.57*	*18.72*
Seas_3	**176.45**	**55.38**	**14.17**	**151.39**	**165.59**	***112.59***	***73.06***	**Seas_3**	**276.58**	**154.51**	**154.52**	**43.61**	***157.30***	***95.16***
Oct	57.44	24.07		51.03	55.76	*47.08*	*15.58*	Oct		52.05	52.06	19.02	*41.04*	*19.07*
Nov	54.91	26.15		49.39	53.95	*46.10*	*13.52*	Nov		50.38	50.39	21.08	*40.62*	*16.92*
Dec	54.34	20.90		49.40	53.94	*44.64*	*15.99*	Dec		50.38	50.38	17.57	*39.45*	*18.94*
Seas_4	**166.70**	**71.12**	**21.55**	**149.81**	**163.65**	***114.57***	***65.02***	**Seas_4**	**421.12**	**152.82**	**152.83**	**57.67**	***196.11***	***156.57***
Annual	**762.22**	**224.09**	**79.62**	**608.64**	**665.12**	***467.94***	***298.13***	**Annual**	**1545.02**	**610.54**	**610.56**	**181.92**	***737.01***	***575.32***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates;

C.4.4. Comparison of calculated values of PCB-180 mass flows transported from the atmosphere to vegetation

Dry deposition

Reference data set. Calculation results on PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.79.

Monthly values of PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.104 a and b, respectively.

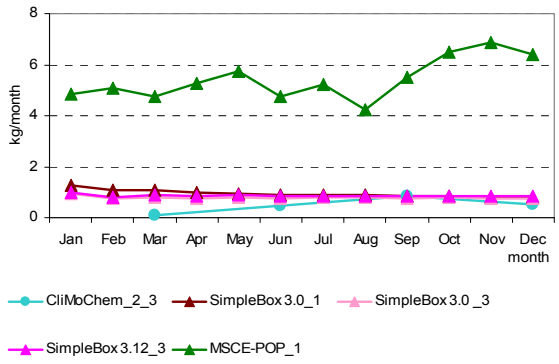


Fig. C.104a. *PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

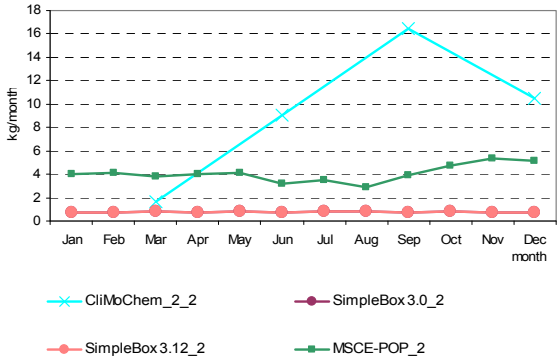


Fig. C.104b. *PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.80.

Monthly values of PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.105 a and b, respectively.

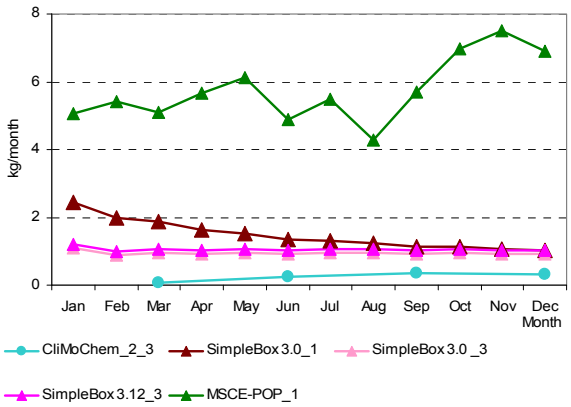


Fig. C.105a. *PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

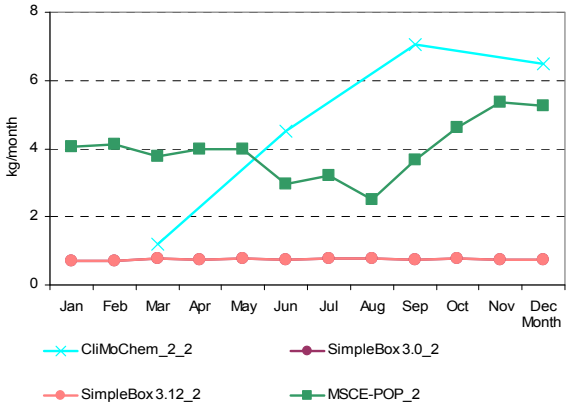


Fig. C.105b. *PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.79 *Calculation results: PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.28	4.84		0.93	1.00	*2.01*	*1.89*	Jan		0.74	0.74	4.06	*1.84*	*1.92*
Feb	1.06	5.10		0.75	0.82	*1.93*	*2.12*	Feb		0.72	0.72	4.12	*1.86*	*1.96*
Mar	1.06	4.77		0.80	0.87	*1.88*	*1.93*	Mar		0.77	0.77	3.77	*1.77*	*1.73*
Seas_1	**3.40**	**14.71**	**0.26**	**2.48**	**2.69**	***4.71***	***5.71***	**Seas_1**	**4.91**	**2.23**	**2.23**	**11.95**	***5.33***	***4.59***
Apr	0.97	5.29		0.77	0.84	*1.97*	*2.21*	Apr		0.75	0.75	4.05	*1.85*	*1.91*
May	0.96	5.73		0.80	0.87	*2.09*	*2.43*	May		0.77	0.77	4.16	*1.90*	*1.95*
Jun	0.90	4.75		0.77	0.84	*1.82*	*1.96*	Jun		0.75	0.75	3.24	*1.58*	*1.44*
Seas_2	**2.83**	**15.77**	**1.40**	**2.35**	**2.56**	***4.98***	***6.06***	**Seas_2**	**27.14**	**2.27**	**2.27**	**11.45**	***10.78***	***11.73***
Jul	0.90	5.24		0.80	0.87	*1.95*	*2.19*	Jul		0.77	0.78	3.45	*1.67*	*1.54*
Aug	0.88	4.25		0.80	0.87	*1.70*	*1.70*	Aug		0.78	0.78	2.83	*1.46*	*1.19*
Sep	0.84	5.49		0.77	0.84	*1.99*	*2.34*	Sep		0.75	0.75	3.94	*1.81*	*1.84*
Seas_3	**2.63**	**14.98**	**2.52**	**2.37**	**2.58**	***5.02***	***5.57***	**Seas_3**	**49.24**	**2.30**	**2.30**	**10.22**	***16.01***	***22.46***
Oct	0.86	6.48		0.80	0.87	*2.25*	*2.82*	Oct		0.78	0.78	4.73	*2.09*	*2.28*
Nov	0.82	6.88		0.77	0.84	*2.33*	*3.04*	Nov		0.75	0.75	5.30	*2.27*	*2.63*
Dec	0.81	6.39		0.77	0.84	*2.20*	*2.79*	Dec		0.75	0.75	5.18	*2.23*	*2.56*
Seas_4	**2.48**	**19.75**	**1.61**	**2.34**	**2.55**	***5.75***	***7.84***	**Seas_4**	**31.45**	**2.28**	**2.28**	**15.21**	***12.80***	***13.85***
Annual	**11.35**	**65.21**	**5.77**	**9.53**	**10.38**	***20.45***	***25.11***	**Annual**	**112.74**	**9.08**	**9.08**	**48.83**	***44.93***	***48.93***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.80. *Calculation results: PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.45	5.07		1.09	1.19	*2.45*	*1.85*	Jan		0.72	0.72	4.05	*1.83*	*1.92*
Feb	2.00	5.41		0.90	1.00	*2.33*	*2.11*	Feb		0.71	0.71	4.12	*1.85*	*1.97*
Mar	1.88	5.11		0.96	1.07	*2.25*	*1.95*	Mar		0.76	0.76	3.77	*1.76*	*1.74*
Seas_1	**6.32**	**15.59**	**0.20**	**2.95**	**3.27**	***5.67***	***5.96***	**Seas_1**	**3.60**	**2.18**	**2.18**	**11.94**	***4.97***	***4.69***
Apr	1.62	5.67		0.93	1.03	*2.31*	*2.26*	Apr		0.73	0.73	4.00	*1.82*	*1.89*
May	1.52	6.13		0.96	1.07	*2.42*	*2.49*	May		0.76	0.76	4.00	*1.84*	*1.87*
Jun	1.36	4.88		0.93	1.03	*2.05*	*1.90*	Jun		0.74	0.74	2.95	*1.47*	*1.28*
Seas_2	**4.51**	**16.68**	**0.71**	**2.81**	**3.13**	***5.57***	***6.36***	**Seas_2**	**13.56**	**2.23**	**2.23**	**10.95**	***7.24***	***5.89***
Jul	1.31	5.50		0.96	1.07	*2.21*	*2.20*	Jul		0.76	0.76	3.22	*1.58*	*1.42*
Aug	1.24	4.29		0.95	1.06	*1.89*	*1.61*	Aug		0.76	0.76	2.51	*1.34*	*1.01*
Sep	1.14	5.69		0.92	1.03	*2.20*	*2.33*	Sep		0.74	0.74	3.68	*1.72*	*1.70*
Seas_3	**3.69**	**15.48**	**1.11**	**2.83**	**3.16**	***5.26***	***5.80***	**Seas_3**	**21.10**	**2.26**	**2.26**	**9.41**	***8.76***	***8.89***
Oct	1.13	6.96		0.95	1.06	*2.53*	*2.96*	Oct		0.76	0.76	4.63	*2.05*	*2.23*
Nov	1.05	7.50		0.92	1.03	*2.63*	*3.25*	Nov		0.74	0.74	5.36	*2.28*	*2.67*
Dec	1.02	6.90		0.92	1.03	*2.47*	*2.96*	Dec		0.74	0.74	5.26	*2.24*	*2.61*
Seas_4	**3.20**	**21.36**	**1.00**	**2.80**	**3.12**	***6.30***	***8.47***	**Seas_4**	**19.46**	**2.24**	**2.24**	**15.25**	***9.80***	***8.90***
Annual	**17.72**	**69.11**	**3.02**	**11.39**	**12.68**	***22.78***	***26.43***	**Annual**	**57.72**	**8.90**	**8.90**	**47.55**	***30.77***	***25.59***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.81.

Table C.81. *The percentage difference between calculation results on PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMo Chem_2_2	CliMo Chem_2_3	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan			91.5%	-2.6%	-2.6%	17.8%	20.0%	4.8%	-0.2%
Feb			87.8%	-2.2%	-2.2%	20.2%	22.6%	6.1%	0.0%
Mar			76.8%	-2.1%	-2.1%	20.0%	22.5%	7.1%	0.0%
Seas_1	-26.8%	-23.5%	85.8%	-2.3%	-2.3%	19.3%	21.6%	6.0%	-0.1%
Apr			66.9%	-2.0%	-2.0%	19.9%	22.5%	7.2%	-1.2%
May			58.5%	-2.0%	-2.0%	19.8%	22.4%	7.0%	-3.8%
Jun			51.3%	-1.9%	-1.9%	19.7%	22.4%	2.7%	-9.0%
Seas_2	-50.0%	-49.0%	59.1%	-2.0%	-2.0%	19.8%	22.4%	5.8%	-4.4%
Jul			45.3%	-1.9%	-1.9%	19.6%	22.4%	5.0%	-6.7%
Aug			40.1%	-1.9%	-1.9%	19.6%	22.3%	0.9%	-11.3%
Sep			35.7%	-1.8%	-1.8%	19.5%	22.3%	3.6%	-6.6%
Seas_3	-57.2%	-55.8%	40.5%	-1.9%	-1.9%	19.6%	22.3%	3.3%	-7.9%
Oct			31.9%	-1.8%	-1.8%	19.4%	22.3%	7.4%	-2.1%
Nov			28.7%	-1.8%	-1.8%	19.4%	22.3%	9.0%	1.1%
Dec			25.9%	-1.7%	-1.7%	19.3%	22.3%	8.0%	1.5%
Seas_4	-38.1%	-37.6%	28.9%	-1.8%	-1.8%	19.4%	22.3%	8.2%	0.3%
Annual	-48.8%	-47.7%	56.2%	-2.0%	-2.0%	19.5%	22.2%	6.0%	-2.6%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Wet deposition

Reference data set. Calculation results on PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.82.

Monthly values of PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.106 a and b, respectively.

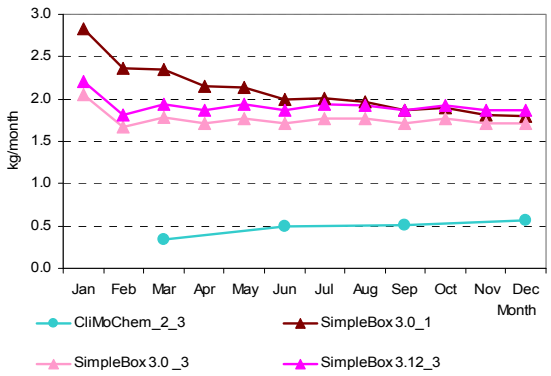


Fig. C.106a. *PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

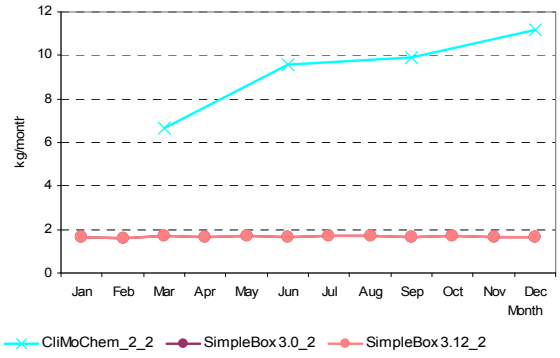


Fig. C.106b. *PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.83.

Monthly values of PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.107 a and b, respectively.

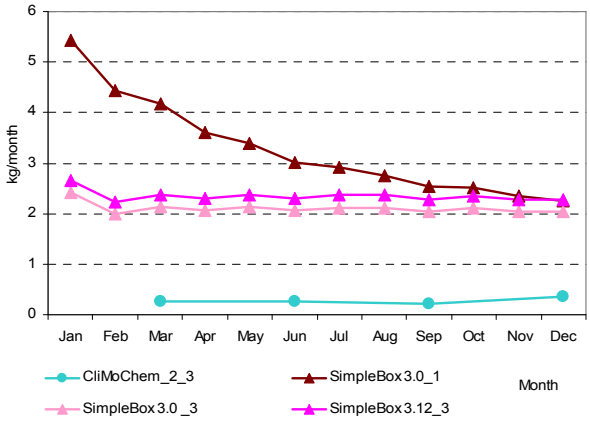


Fig. C.107a. *PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

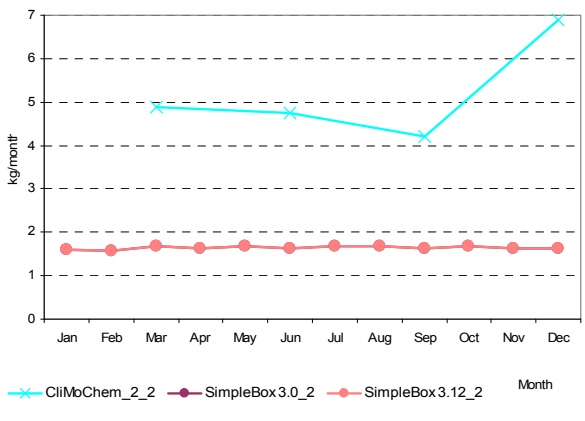


Fig. C.107b. *PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.82. *Calculation results: PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	2.83		2.06	2.21	*2.37*	*0.41*	Jan		1.63	1.63	*1.63*	*0.00*
Feb	2.36		1.66	1.82	*1.95*	*0.37*	Feb		1.61	1.61	*1.61*	*0.00*
Mar	2.36		1.78	1.94	*2.02*	*0.30*	Mar		1.72	1.72	*1.72*	*0.00*
Seas_1	**7.55**	**1.04**	**5.50**	**5.97**	***5.01***	***2.79***	**Seas_1**	**19.97**	**4.96**	**4.96**	***9.96***	***8.67***
Apr	2.16		1.72	1.87	*1.92*	*0.22*	Apr		1.66	1.66	*1.66*	*0.00*
May	2.13		1.77	1.94	*1.95*	*0.18*	May		1.72	1.72	*1.72*	*0.00*
Jun	2.00		1.72	1.87	*1.86*	*0.14*	Jun		1.66	1.66	*1.66*	*0.00*
Seas_2	**6.29**	**1.48**	**5.21**	**5.68**	***4.66***	***2.17***	**Seas_2**	**28.74**	**5.05**	**5.05**	***12.94***	***13.68***
Jul	2.01		1.77	1.93	*1.90*	*0.12*	Jul		1.72	1.72	*1.72*	*0.00*
Aug	1.96		1.77	1.93	*1.89*	*0.10*	Aug		1.72	1.72	*1.72*	*0.00*
Sep	1.87		1.71	1.87	*1.82*	*0.09*	Sep		1.66	1.66	*1.66*	*0.00*
Seas_3	**5.83**	**1.52**	**5.26**	**5.73**	***4.59***	***2.06***	**Seas_3**	**29.67**	**5.11**	**5.11**	***13.29***	***14.18***
Oct	1.90		1.77	1.93	*1.87*	*0.08*	Oct		1.72	1.72	*1.72*	*0.00*
Nov	1.82		1.71	1.87	*1.80*	*0.08*	Nov		1.67	1.67	*1.67*	*0.00*
Dec	1.80		1.71	1.86	*1.79*	*0.08*	Dec		1.67	1.67	*1.67*	*0.00*
Seas_4	**5.51**	**1.71**	**5.20**	**5.66**	***4.52***	***1.88***	**Seas_4**	**33.46**	**5.05**	**5.05**	***14.52***	***16.40***
Annual	**25.19**	**5.74**	**21.16**	**23.03**	***18.78***	***8.85***	**Annual**	**111.84**	**20.16**	**20.16**	***50.72***	***52.93***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.
* - In MSCE-POP model wet deposition on vegetation is not taken into account since it is considered as a part of deposition directly to soil.

Table C.83. *Calculation results: PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis o initial concentrations given as input data	Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]		
Jan	5.43		2.42	2.65	*3.50*	*1.67*	Jan		1.59	1.59	*1.59*	*0.00*
Feb	4.44		2.00	2.23	*2.89*	*1.35*	Feb		1.57	1.57	*1.57*	*0.00*
Mar	4.16		2.13	2.38	*2.89*	*1.11*	Mar		1.68	1.68	*1.68*	*0.00*
Seas_1	**14.03**	**0.80**	**6.55**	**7.25**	***7.16***	***5.42***	**Seas_1**	**14.69**	**4.84**	**4.84**	***8.12***	***5.68***
Apr	3.60		2.06	2.30	*2.65*	*0.83*	Apr		1.63	1.63	*1.63*	*0.00*
May	3.38		2.13	2.37	*2.63*	*0.67*	May		1.69	1.69	*1.69*	*0.00*
Jun	3.02		2.05	2.29	*2.45*	*0.50*	Jun		1.63	1.63	*1.63*	*0.00*
Seas_2	**10.00**	**0.75**	**6.24**	**6.95**	***5.99***	***3.85***	**Seas_2**	**14.27**	**4.95**	**4.95**	***8.05***	***5.38***
Jul	2.91		2.12	2.36	*2.47*	*0.41*	Jul		1.69	1.69	*1.69*	*0.00*
Aug	2.75		2.12	2.36	*2.41*	*0.32*	Aug		1.69	1.69	*1.69*	*0.00*
Sep	2.53		2.05	2.28	*2.29*	*0.24*	Sep		1.63	1.63	*1.63*	*0.00*
Seas_3	**8.19**	**0.66**	**6.29**	**7.01**	***5.54***	***3.34***	**Seas_3**	**12.60**	**5.01**	**5.01**	***7.54***	***4.38***
Oct	2.51		2.12	2.36	*2.33*	*0.20*	Oct		1.69	1.69	*1.69*	*0.00*
Nov	2.34		2.05	2.28	*2.22*	*0.15*	Nov		1.64	1.64	*1.64*	*0.00*
Dec	2.26		2.04	2.28	*2.20*	*0.13*	Dec		1.64	1.64	*1.64*	*0.00*
Seas_4	**7.11**	**1.06**	**6.21**	**6.92**	***5.32***	***2.87***	**Seas_4**	**20.68**	**4.96**	**4.96**	***10.20***	***9.07***
Annual	**39.33**	**3.27**	**25.29**	**28.14**	***24.01***	***15.09***	**Annual**	**62.23**	**19.76**	**19.76**	***33.92***	***24.52***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.
* - In MSCE-POP model wet deposition on vegetation is not taken into account since it is considered as a part of deposition directly to soil.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.84.

Table C.84. *The percentage difference between calculation results on PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_ 2_2	CliMoChem_ 2_3	Simple Box 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3
Jan			91.5%	-2.6%	-2.6%	17.8%	20.0%
Feb			87.8%	-2.2%	-2.2%	20.2%	22.6%
Mar			76.8%	-2.1%	-2.1%	20.0%	22.5%
Seas_1	-26.5%	-23.2%	85.8%	-2.3%	-2.3%	19.3%	21.6%
Apr			66.9%	-2.0%	-2.0%	19.9%	22.5%
May			58.5%	-2.0%	-2.0%	19.8%	22.4%
Jun			51.3%	-1.9%	-1.9%	19.7%	22.4%
Seas_2	-50.4%	-49.4%	59.1%	-2.0%	-2.0%	19.8%	22.4%
Jul			45.3%	-1.9%	-1.9%	19.6%	22.4%
Aug			40.1%	-1.9%	-1.9%	19.6%	22.3%
Sep			35.7%	-1.8%	-1.8%	19.5%	22.3%
Seas_3	-57.5%	-56.2%	40.5%	-1.9%	-1.9%	19.6%	22.3%
Oct			31.9%	-1.8%	-1.8%	19.4%	22.3%
Nov			28.7%	-1.8%	-1.8%	19.4%	22.3%
Dec			25.9%	-1.7%	-1.7%	19.3%	22.3%
Seas_4	-38.2%	-37.7%	28.9%	-1.8%	-1.8%	19.4%	22.3%
Annual	-44.4%	-43.0%	56.2%	-2.0%	-2.0%	19.5%	22.2%

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

Gaseous exchange

Reference data set. Calculation results on PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.85.

Monthly values of PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.108a and b, respectively. Seasonal variations for models with positive values of gaseous exchange flows between the atmosphere and vegetation calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.108c in more detail.

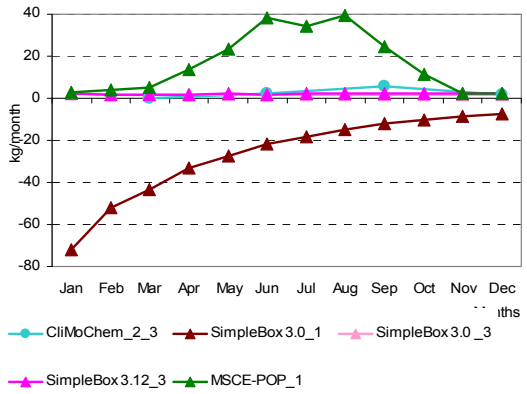


Fig. C.108a. *PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

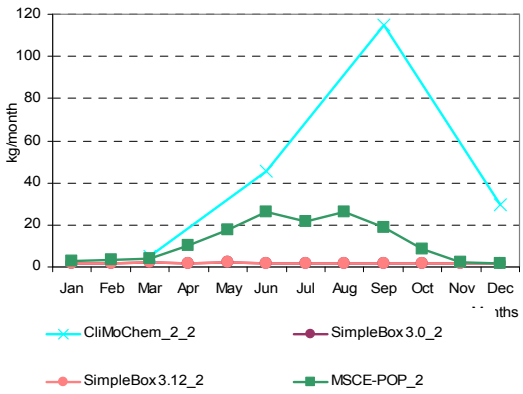


Fig. C.108b. *PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

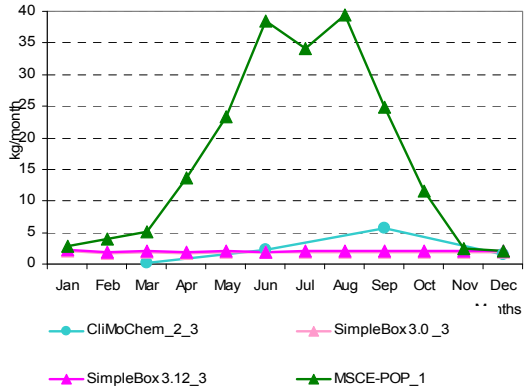


Fig. C.108c. *PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with positive values)*

Own/alternative data set. Calculation results on PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.86.

Monthly values of PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.109a and b, respectively. Seasonal variations for models with positive values of gaseous exchange flows between the atmosphere and vegetation calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions are also shown in Fig. C.109c in more detail.

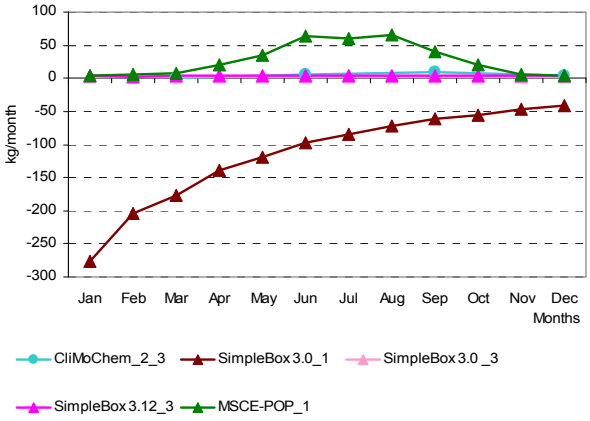


Fig. C.109a. *PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

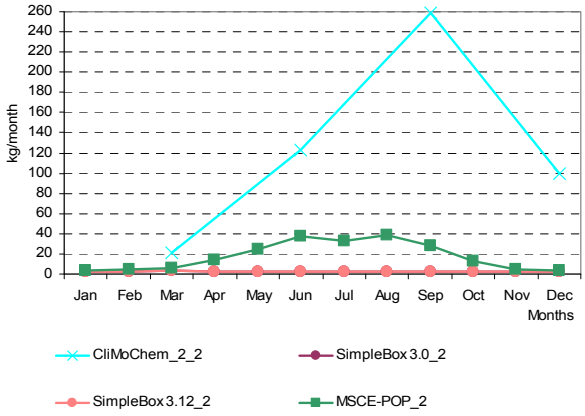


Fig. C.109b. *PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

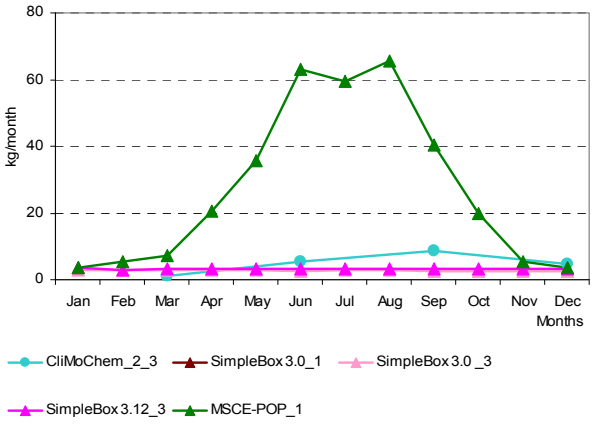


Fig. C.109c. *PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by the participating models on the basis of "own or alternative" data set and non-zero initial conditions (models with positive values)*

Comparison between results obtained on the basis of two data sets. A comparison of the calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.87.

Table C.85. *Calculation results: PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMoChem_2_3	SimpleBox 3.0 _3	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-72.18	2.89		2.06	2.24	*-16.25*	*37.29*	Jan		1.95	1.95	2.58	*2.16*	*0.36*
Feb	-51.88	3.98		1.66	1.83	*-11.10*	*27.21*	Feb		1.90	1.90	3.38	*2.39*	*0.85*
Mar	-43.28	5.12		1.80	1.99	*-8.59*	*23.18*	Mar		2.02	2.02	4.22	*2.75*	*1.27*
Seas_1	**-167.34**	**11.99**	**0.85**	**5.52**	**6.07**	***-28.58***	***77.67***	**Seas_1**	**15.78**	**5.87**	**5.87**	**10.18**	***9.42***	***4.70***
Apr	-33.03	13.60		1.77	1.95	*-3.93*	*20.18*	Apr		1.94	1.94	10.40	*4.76*	*4.88*
May	-27.32	23.30		1.85	2.03	*-0.03*	*20.79*	May		2.00	2.00	17.60	*7.20*	*9.01*
Jun	-21.43	38.40		1.81	1.98	*5.19*	*24.72*	Jun		1.92	1.92	26.00	*9.95*	*13.90*
Seas_2	**-81.79**	**75.30**	**7.05**	**5.43**	**5.97**	***2.39***	***55.78***	**Seas_2**	**136.41**	**5.86**	**5.86**	**54.00**	***50.53***	***61.58***
Jul	-18.16	34.20		1.88	2.06	*5.00*	*21.66*	Jul		1.98	1.98	21.40	*8.45*	*11.21*
Aug	-14.97	39.50		1.90	2.07	*7.12*	*23.02*	Aug		1.97	1.97	26.40	*10.12*	*14.10*
Sep	-12.07	24.80		1.85	2.02	*4.15*	*15.27*	Sep		1.91	1.91	18.90	*7.57*	*9.81*
Seas_3	**-45.19**	**98.50**	**16.91**	**5.63**	**6.15**	***16.40***	***51.85***	**Seas_3**	**344.44**	**5.86**	**5.86**	**66.70**	***105.72***	***161.71***
Oct	-10.44	11.50		1.92	2.09	*1.27*	*9.00*	Oct		1.96	1.96	8.43	*4.12*	*3.73*
Nov	-8.48	2.52		1.86	2.03	*-0.52*	*5.32*	Nov		1.90	1.90	2.22	*2.01*	*0.19*
Dec	-7.14	2.03		1.87	2.04	*-0.30*	*4.56*	Dec		1.89	1.89	1.87	*1.89*	*0.01*
Seas_4	**-26.06**	**16.05**	**4.64**	**5.65**	**6.16**	***1.29***	***15.97***	**Seas_4**	**88.91**	**5.76**	**5.76**	**12.52**	***28.24***	***40.57***
Annual	**-320.38**	**201.84**	**29.45**	**22.22**	**24.34**	***-8.51***	***190.38***	**Annual**	**585.53**	**23.35**	**23.35**	**143.40**	***193.91***	***267.15***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.86. *Calculation results: PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1a	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				CliMo Chem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-275.75	3.60		3.24	3.66	*-66.31*	*139.63*	Jan		2.92	2.92	3.08	*2.98*	*0.09*
Feb	-204.43	5.31		2.61	3.01	*-48.38*	*104.05*	Feb		2.81	2.81	4.30	*3.31*	*0.86*
Mar	-176.15	7.10		2.83	3.25	*-40.74*	*90.29*	Mar		2.94	2.94	5.53	*3.80*	*1.50*
Seas_1	**-656.33**	**16.01**	**3.46**	**8.68**	**9.93**	***-123.65***	***297.81***	**Seas_1**	**64.42**	**8.67**	**8.67**	**12.91**	***23.67***	***27.24***
Apr	-138.99	20.40		2.77	3.17	*-28.16*	*74.34*	Apr		2.79	2.79	14.20	*6.59*	*6.59*
May	-118.89	35.70		2.89	3.30	*-19.25*	*68.18*	May		2.83	2.83	24.30	*9.99*	*12.40*
Jun	-96.52	63.10		2.81	3.20	*-6.85*	*66.15*	Jun		2.70	2.70	37.70	*14.37*	*20.21*
Seas_2	**-354.40**	**119.20**	**16.60**	**8.47**	**9.67**	***-40.09***	***181.80***	**Seas_2**	**367.72**	**8.32**	**8.32**	**76.20**	***115.14***	***171.40***
Jul	-84.72	59.30		2.92	3.32	*-4.79*	*59.50*	Jul		2.75	2.75	32.70	*12.73*	*17.29*
Aug	-72.53	65.50		2.94	3.33	*-0.19*	*56.48*	Aug		2.72	2.72	38.80	*14.75*	*20.83*
Sep	-60.78	40.30		2.85	3.22	*-3.60*	*41.97*	Sep		2.60	2.60	28.00	*11.07*	*14.66*
Seas_3	**-218.03**	**165.10**	**26.08**	**8.71**	**9.87**	***-1.65***	***137.51***	**Seas_3**	**776.06**	**8.08**	**8.08**	**99.50**	***222.93***	***371.26***
Oct	-54.80	20.00		2.95	3.34	*-7.13*	*32.76*	Oct		2.67	2.67	13.40	*6.24*	*6.20*
Nov	-46.54	5.32		2.86	3.23	*-8.78*	*25.20*	Nov		2.56	2.56	4.24	*3.12*	*0.97*
Dec	-41.12	3.64		2.87	3.23	*-7.84*	*22.18*	Dec		2.54	2.54	3.12	*2.73*	*0.34*
Seas_4	**-142.45**	**28.96**	**14.37**	**8.69**	**9.80**	***-16.13***	***71.08***	**Seas_4**	**298.99**	**7.76**	**7.76**	**20.76**	***83.82***	***143.58***
Annual	**-1371.21**	**329.27**	**60.52**	**34.55**	**39.27**	***-181.52***	***676.44***	**Annual**	**1507.19**	**32.83**	**32.83**	**209.37**	***445.55***	***712.63***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

Table C.87. *Comparison of the calculation results on PCB-180 mass flows between the atmosphere and vegetation: gaseous exchange (kg/month) obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	CliMoChem_2_3		SimpleBox 3.0_1		SimpleBox 3.0_2		SimpleBox 3.12_2		SimpleBox 3.0_3		SimpleBox 3.12_3		MSCE-POP_1		MSCE-POP_2		CliMoChem_2_2	
	ref	own	ref	alt	ref	alt	ref	alt	ref	alt	ref	alt	ref	own	ref	own	ref	own
Jan			-72.18	-275.75	1.95	2.92	1.95	2.92	2.06	3.24	2.24	3.66	2.89	3.60	2.58	3.08		
Feb			-51.88	-204.43	1.90	2.81	1.90	2.81	1.66	2.61	1.83	3.01	3.98	5.31	3.38	4.30		
Mar			-43.28	-176.15	2.02	2.94	2.02	2.94	1.80	2.83	1.99	3.25	5.12	7.10	4.22	5.53		
Seas_1	**0.85**	**3.46**	**-167.34**	**-656.33**	**5.87**	**8.67**	**5.87**	**8.67**	**5.52**	**8.68**	**6.07**	**9.93**	**11.99**	**16.01**	**10.18**	**12.91**	**15.78**	**64.42**
Apr			-33.03	-138.99	1.94	2.79	1.94	2.79	1.77	2.77	1.95	3.17	13.60	20.40	10.40	14.20		
May			-27.32	-118.89	2.00	2.83	2.00	2.83	1.85	2.89	2.03	3.30	23.30	35.70	17.60	24.30		
Jun			-21.43	-96.52	1.92	2.70	1.92	2.70	1.81	2.81	1.98	3.20	38.40	63.10	26.00	37.70		
Seas_2	**7.05**	**16.60**	**-81.79**	**-354.40**	**5.86**	**8.32**	**5.86**	**8.32**	**5.43**	**8.47**	**5.97**	**9.67**	**75.30**	**119.20**	**54.00**	**76.20**	**136.41**	**367.72**
Jul			-18.16	-84.72	1.98	2.75	1.98	2.75	1.88	2.92	2.06	3.32	34.20	59.30	21.40	32.70		
Aug			-14.97	-72.53	1.97	2.72	1.97	2.72	1.90	2.94	2.07	3.33	39.50	65.50	26.40	38.80		
Sep			-12.07	-60.78	1.91	2.60	1.91	2.60	1.85	2.85	2.02	3.22	24.80	40.30	18.90	28.00		
Seas_3	**16.91**	**26.08**	**-45.19**	**-218.03**	**5.86**	**8.08**	**5.86**	**8.08**	**5.63**	**8.71**	**6.15**	**9.87**	**98.50**	**165.10**	**66.70**	**99.50**	**344.44**	**776.06**
Oct			-10.44	-54.80	1.96	2.67	1.96	2.67	1.92	2.95	2.09	3.34	11.50	20.00	8.43	13.40		
Nov			-8.48	-46.54	1.90	2.56	1.90	2.56	1.86	2.86	2.03	3.23	2.52	5.32	2.22	4.24		
Dec			-7.14	-41.12	1.89	2.54	1.89	2.54	1.87	2.87	2.04	3.23	2.03	3.64	1.87	3.12		
Seas_4	**4.64**	**14.37**	**-26.06**	**-142.45**	**5.76**	**7.76**	**5.76**	**7.76**	**5.65**	**8.69**	**6.16**	**9.80**	**16.05**	**28.96**	**12.52**	**20.76**	**88.91**	**298.99**
Annual	**29.45**	**60.52**	**-320.38**	**-1371.21**	**23.35**	**32.83**	**23.35**	**32.83**	**22.22**	**34.55**	**24.34**	**39.27**	**201.84**	**329.27**	**143.40**	**209.37**	**585.53**	**1507.19**

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;

Net mass flows between the atmosphere and vegetation

Net mass flows are equal to the total mass flows resulted from summing up of dry and wet depositions and gaseous exchange.

Reference data set. Calculation results on PCB-180 net mass flows between the atmosphere and vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.89.

Monthly values of PCB-180 net mass flows between the atmosphere and vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.110a and b, respectively. Seasonal variations for models with low positive values of net mass flows between the atmosphere and vegetation calculated by the participating models on the basis of "reference" data set and non-zero initial conditions are also shown in Fig. C.110c in more detail.

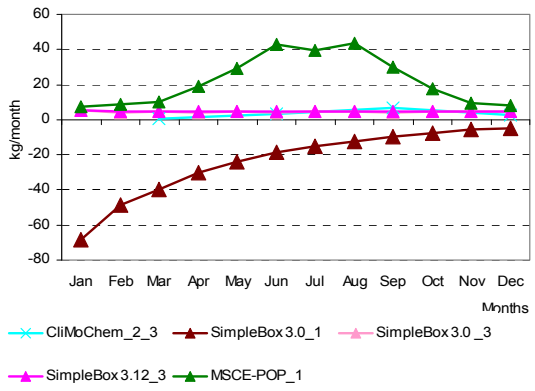


Fig. C.110a. *PCB-180 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

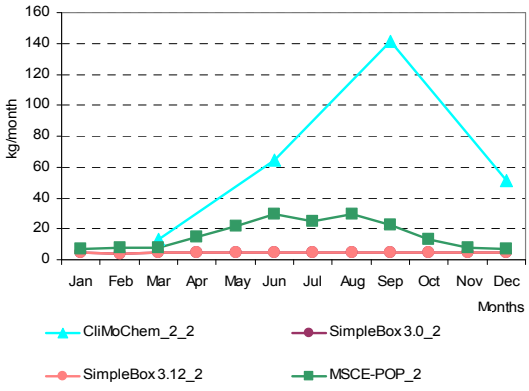


Fig. C.110b. *PCB-180 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

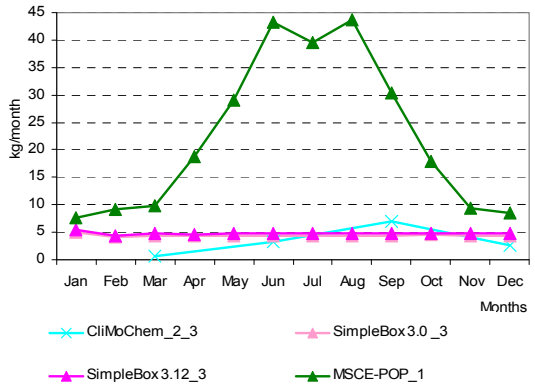


Fig. C.110c. *PCB-180 net mass flows between the atmosphere and vegetation (kg/month) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (models with low values)*

Table C.89. *Calculation results: PCB-180 net mass flows between the atmosphere and vegetation (kg/month) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions			*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	CliMo Chem_2_3	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				CliMoChem_2_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	-68.07	7.73		5.04	5.45	*-12.46*	*37.09*	Jan		4.32	4.32	6.64	*5.09*	*1.34*
Feb	-48.46	9.08		4.07	4.47	*-7.71*	*27.26*	Feb		4.23	4.23	7.50	*5.32*	*1.89*
Mar	-39.86	9.89		4.38	4.80	*-5.20*	*23.25*	Mar		4.51	4.51	7.99	*5.67*	*2.01*
Seas_1	**-156.39**	**26.70**	**2.14**	**13.49**	**14.72**	***-19.87***	***76.81***	**Seas_1**	**40.66**	**13.06**	**13.06**	**22.13**	***22.23***	***13.01***
Apr	-29.90	18.89		4.26	4.67	*-0.52*	*20.74*	Apr		4.35	4.35	14.45	*7.72*	*5.83*
May	-24.23	29.03		4.42	4.84	*3.52*	*21.78*	May		4.49	4.49	21.76	*10.25*	*9.97*
Jun	-18.54	43.15		4.30	4.70	*8.40*	*25.59*	Jun		4.34	4.34	29.24	*12.64*	*14.38*
Seas_2	**-72.67**	**91.07**	**9.93**	**12.99**	**14.21**	***11.10***	***57.94***	**Seas_2**	**192.28**	**13.18**	**13.18**	**65.45**	***71.02***	***84.51***
Jul	-15.25	39.44		4.45	4.87	*8.38*	*22.73*	Jul		4.48	4.48	24.85	*11.27*	*11.76*
Aug	-12.12	43.75		4.47	4.87	*10.24*	*23.70*	Aug		4.47	4.47	29.23	*12.72*	*14.30*
Sep	-9.36	30.29		4.33	4.73	*7.50*	*16.55*	Sep		4.32	4.32	22.84	*10.49*	*10.69*
Seas_3	**-36.73**	**113.48**	**20.95**	**13.25**	**14.47**	***25.08***	***54.55***	**Seas_3**	**423.34**	**13.27**	**13.27**	**76.92**	***131.70***	***196.73***
Oct	-7.68	17.98		4.49	4.89	*4.92*	*10.48*	Oct		4.46	4.46	13.16	*7.36*	*5.02*
Nov	-5.84	9.40		4.35	4.74	*3.16*	*6.43*	Nov		4.31	4.31	7.52	*5.38*	*1.85*
Dec	-4.54	8.42		4.35	4.74	*3.24*	*5.50*	Dec		4.31	4.31	7.05	*5.22*	*1.58*
Seas_4	**-18.06**	**35.80**	**7.95**	**13.19**	**14.36**	***10.65***	***19.26***	**Seas_4**	**153.82**	**13.08**	**13.08**	**27.73**	***51.93***	***68.28***
Annual	**-283.85**	**267.05**	**40.96**	**52.92**	**57.76**	***26.97***	***197.52***	**Annual**	**810.11**	**52.59**	**52.59**	**192.23**	***276.88***	***361.53***

CliMoChem_2_2 – CliMoChem results calculated on the basis of Land Cover Data given as input data and with zero initial concentrations;
CliMoChem_2_3 - CliMoChem results calculated on the basis of Land Cover Data given as input data and with historical emissions for 20-year period;
MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
a - SimpleBox data presented here are overall mass flows (to regional and continental cells) calculated as sum of regional and continental level estimates.

C.5. Concentrations at each interface

C.5.1. Comparison of calculated values of PCB-180 concentration in the atmosphere at its interface with soil

Reference data set. Calculation results on PCB-180 concentration in the atmosphere at its interface with soil calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.90.

Monthly values of PCB-180 concentration in the atmosphere at its interface with soil calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.111 a and b, respectively.

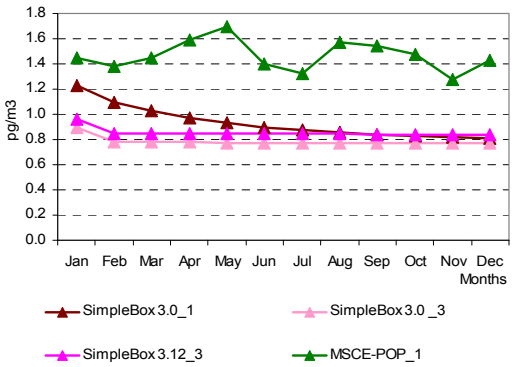


Fig. C.111a. *PCB-180 concentration in the atmosphere at its interface with soil (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

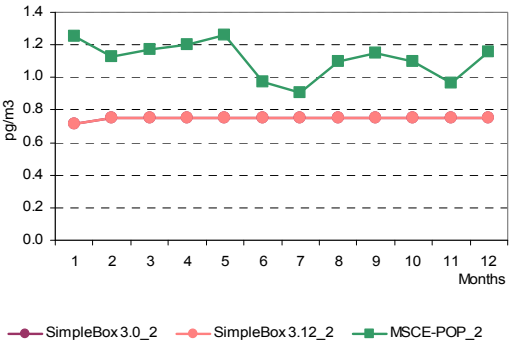


Fig. C.111b. *PCB-180 concentration in the atmosphere at its interface with soil (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 concentration in the atmosphere at its interface with soil calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.91.

Monthly values of PCB-180 concentration in the atmosphere at its interface with soil calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.112 a and b, respectively.

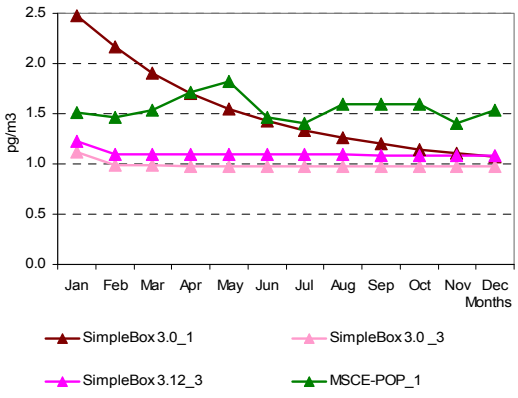


Fig. C.112a. *PCB-180 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

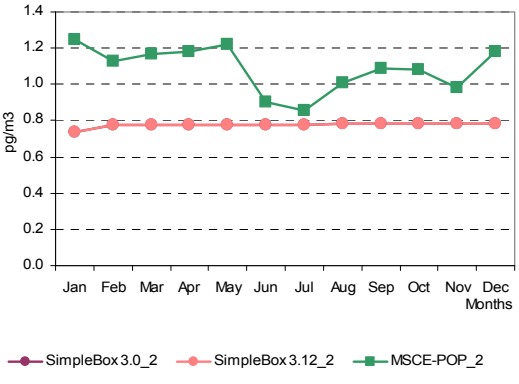


Fig. C.112b. *PCB-180 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.90. *Calculation results: PCB-180 concentration in the atmosphere at interface with soil (pg/m3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1	MSCE-POP_1	SimpleBox 3.0_3	SimpleBox 3.12_3				SimpleBox 3.0_2	SimpleBox 3.12_2	MSCE-POP_2		
Jan	1.23	1.45	0.90	0.96	*1.14*	*0.25*	Jan	0.71	0.71	1.25	*0.89*	*0.31*
Feb	1.10	1.38	0.78	0.85	*1.03*	*0.27*	Feb	0.75	0.75	1.13	*0.88*	*0.22*
Mar	1.02	1.45	0.78	0.85	*1.02*	*0.30*	Mar	0.75	0.75	1.17	*0.89*	*0.24*
Apr	0.97	1.59	0.78	0.85	*1.05*	*0.37*	Apr	0.75	0.75	1.20	*0.90*	*0.26*
May	0.93	1.70	0.78	0.84	*1.06*	*0.43*	May	0.75	0.75	1.26	*0.92*	*0.29*
Jun	0.90	1.40	0.78	0.84	*0.98*	*0.28*	Jun	0.75	0.75	0.97	*0.82*	*0.13*
Jul	0.87	1.32	0.78	0.84	*0.95*	*0.25*	Jul	0.75	0.75	0.91	*0.80*	*0.09*
Aug	0.86	1.57	0.77	0.84	*1.01*	*0.37*	Aug	0.75	0.75	1.10	*0.87*	*0.20*
Sep	0.84	1.54	0.77	0.84	*1.00*	*0.36*	Sep	0.75	0.75	1.15	*0.89*	*0.23*
Oct	0.83	1.48	0.77	0.84	*0.98*	*0.33*	Oct	0.75	0.75	1.10	*0.87*	*0.20*
Nov	0.82	1.28	0.77	0.84	*0.93*	*0.24*	Nov	0.75	0.75	0.97	*0.82*	*0.12*
Dec	0.81	1.43	0.77	0.84	*0.96*	*0.31*	Dec	0.75	0.75	1.16	*0.89*	*0.24*
Annual	**0.93**	**1.49**	**0.79**	**0.85**	***1.01***	***0.32***	**Annual**	**0.75**	**0.75**	**1.12**	***0.87***	***0.22***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table C.91. *Calculation results: PCB-180 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.48	1.51	1.12	1.22	*1.58*	*0.62*	Jan	0.73	0.73	1.25	*0.91*	*0.30*
Feb	2.16	1.47	0.99	1.10	*1.43*	*0.53*	Feb	0.78	0.78	1.13	*0.89*	*0.20*
Mar	1.90	1.54	0.98	1.10	*1.38*	*0.42*	Mar	0.78	0.78	1.17	*0.91*	*0.23*
Apr	1.70	1.72	0.98	1.09	*1.37*	*0.39*	Apr	0.78	0.78	1.18	*0.91*	*0.23*
May	1.54	1.82	0.98	1.09	*1.36*	*0.39*	May	0.78	0.78	1.22	*0.93*	*0.26*
Jun	1.43	1.47	0.98	1.09	*1.24*	*0.24*	Jun	0.78	0.78	0.90	*0.82*	*0.07*
Jul	1.33	1.40	0.98	1.09	*1.20*	*0.20*	Jul	0.78	0.78	0.86	*0.81*	*0.05*
Aug	1.26	1.60	0.98	1.09	*1.23*	*0.27*	Aug	0.78	0.78	1.01	*0.86*	*0.13*
Sep	1.20	1.60	0.98	1.09	*1.22*	*0.27*	Sep	0.78	0.78	1.09	*0.88*	*0.18*
Oct	1.15	1.59	0.98	1.09	*1.20*	*0.27*	Oct	0.78	0.78	1.08	*0.88*	*0.17*
Nov	1.11	1.40	0.98	1.09	*1.14*	*0.18*	Nov	0.78	0.78	0.98	*0.85*	*0.11*
Dec	1.07	1.54	0.97	1.09	*1.17*	*0.25*	Dec	0.78	0.78	1.18	*0.91*	*0.23*
Annual	**1.53**	**1.56**	**0.99**	**1.10**	***1.29***	***0.29***	**Annual**	**0.78**	**0.78**	**1.09**	***0.88***	***0.18***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.92.

Table C.92. *The percentage difference between calculation results on PCB-180 concentration in the atmosphere at its interface with soil obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	101.3%	2.9%	2.9%	24.4%	26.8%	4.1%	0.0%
Feb	97.2%	3.2%	3.2%	26.8%	29.5%	6.5%	0.0%
Mar	85.6%	3.3%	3.3%	26.6%	29.4%	6.2%	0.0%
Apr	75.2%	3.4%	3.4%	26.5%	29.4%	8.2%	-1.7%
May	66.3%	3.5%	3.5%	26.4%	29.3%	7.1%	-3.2%
Jun	58.8%	3.5%	3.5%	26.3%	29.3%	5.0%	-6.8%
Jul	52.4%	3.6%	3.6%	26.2%	29.3%	6.1%	-5.1%
Aug	47.0%	3.6%	3.6%	26.2%	29.3%	1.9%	-8.2%
Sep	42.4%	3.7%	3.6%	26.1%	29.2%	3.9%	-5.2%
Oct	38.5%	3.7%	3.7%	26.0%	29.2%	7.4%	-1.8%
Nov	35.1%	3.7%	3.7%	26.0%	29.2%	9.4%	1.3%
Dec	32.2%	3.7%	3.7%	25.9%	29.2%	7.7%	1.7%
Annual	64.0%	3.5%	3.5%	26.1%	29.1%	4.5%	-3.2%

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.5.2. Comparison of calculated values of PCB-180 concentration in the atmosphere at its interface with ocean

Reference data set. Calculation results on PCB-180 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.93.

Monthly values of PCB-180 concentration in the atmosphere at its interface with ocean calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.113 a and b, respectively.

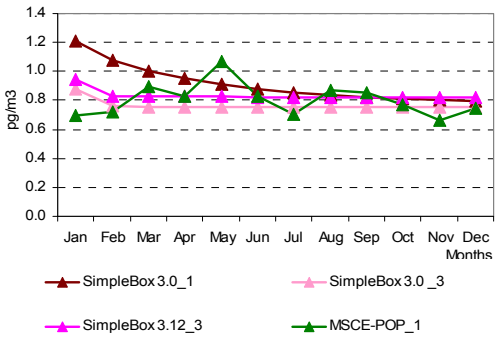


Fig. C.113a. *PCB-180 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

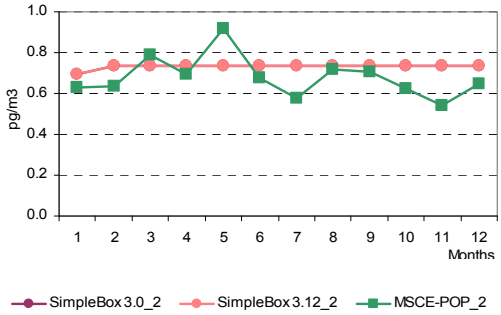


Fig. C.113b. *PCB-180 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 concentration in the atmosphere at its interface with ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.94.

Monthly values of PCB-180 concentration in the atmosphere at its interface with ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.114 a and b, respectively.

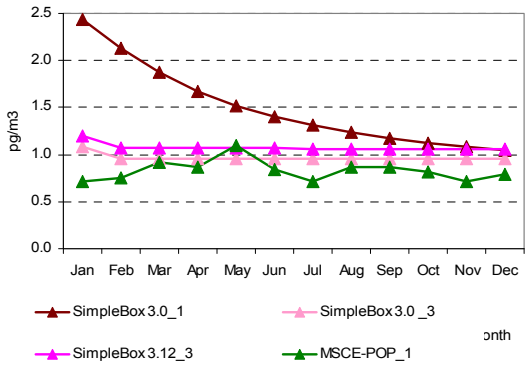


Fig. C.114a. *PCB-180 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

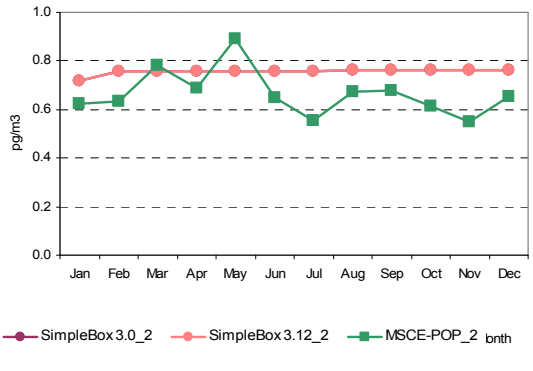


Fig. C.114b. *PCB-180 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.93. *Calculation results: PCB-180 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.21	0.70	0.88	0.94	*0.93*	*0.21*	Jan	0.70	0.70	0.63	*0.67*	*0.04*
Feb	1.07	0.72	0.76	0.83	*0.85*	*0.16*	Feb	0.73	0.73	0.64	*0.70*	*0.05*
Mar	1.00	0.89	0.76	0.83	*0.87*	*0.10*	Mar	0.73	0.73	0.79	*0.75*	*0.03*
Apr	0.95	0.83	0.76	0.83	*0.84*	*0.08*	Apr	0.73	0.73	0.70	*0.72*	*0.02*
May	0.91	1.07	0.76	0.82	*0.89*	*0.14*	May	0.73	0.73	0.92	*0.79*	*0.11*
Jun	0.88	0.83	0.76	0.82	*0.82*	*0.05*	Jun	0.73	0.73	0.68	*0.71*	*0.03*
Jul	0.85	0.71	0.76	0.82	*0.78*	*0.07*	Jul	0.73	0.73	0.58	*0.68*	*0.09*
Aug	0.84	0.87	0.76	0.82	*0.82*	*0.05*	Aug	0.73	0.73	0.72	*0.73*	*0.01*
Sep	0.82	0.85	0.76	0.82	*0.81*	*0.04*	Sep	0.73	0.73	0.70	*0.72*	*0.02*
Oct	0.81	0.77	0.76	0.82	*0.79*	*0.03*	Oct	0.73	0.73	0.62	*0.70*	*0.06*
Nov	0.80	0.67	0.75	0.82	*0.76*	*0.07*	Nov	0.73	0.73	0.54	*0.67*	*0.11*
Dec	0.79	0.74	0.75	0.82	*0.78*	*0.04*	Dec	0.73	0.73	0.65	*0.70*	*0.05*
Annual	**0.91**	**0.82**	**0.77**	**0.83**	***0.83***	***0.06***	**Annual**	**0.73**	**0.73**	**0.70**	***0.72***	***0.02***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table C.94. *Calculation results: PCB-180 concentration in the atmosphere at its interface with ocean (pg/m3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.44	0.72	1.09	1.19	*1.36*	*0.75*	Jan	0.72	0.72	0.63	*0.69*	*0.05*
Feb	2.13	0.75	0.96	1.07	*1.23*	*0.62*	Feb	0.76	0.76	0.64	*0.72*	*0.07*
Mar	1.87	0.92	0.96	1.07	*1.21*	*0.45*	Mar	0.76	0.76	0.78	*0.77*	*0.01*
Apr	1.67	0.86	0.96	1.07	*1.14*	*0.36*	Apr	0.76	0.76	0.69	*0.74*	*0.04*
May	1.52	1.10	0.96	1.07	*1.16*	*0.25*	May	0.76	0.76	0.89	*0.80*	*0.08*
Jun	1.40	0.84	0.96	1.07	*1.07*	*0.24*	Jun	0.76	0.76	0.65	*0.72*	*0.06*
Jul	1.31	0.72	0.95	1.06	*1.01*	*0.24*	Jul	0.76	0.76	0.55	*0.69*	*0.12*
Aug	1.23	0.87	0.95	1.06	*1.03*	*0.16*	Aug	0.76	0.76	0.68	*0.73*	*0.05*
Sep	1.18	0.87	0.95	1.06	*1.02*	*0.13*	Sep	0.76	0.76	0.68	*0.73*	*0.05*
Oct	1.13	0.81	0.95	1.06	*0.99*	*0.14*	Oct	0.76	0.76	0.62	*0.71*	*0.08*
Nov	1.09	0.72	0.95	1.06	*0.95*	*0.17*	Nov	0.76	0.76	0.55	*0.69*	*0.12*
Dec	1.05	0.79	0.95	1.06	*0.96*	*0.13*	Dec	0.76	0.76	0.65	*0.73*	*0.06*
Annual	**1.50**	**0.83**	**0.97**	**1.08**	***1.09***	***0.29***	**Annual**	**0.76**	**0.76**	**0.67**	***0.73***	***0.05***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.95.

Table C.95. *The percentage difference between calculation results on PCB-180 concentration in the atmosphere at its interface with ocean obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	102.0%	2.9%	2.9%	24.4%	26.7%	3.2%	-0.3%
Feb	98.1%	3.2%	3.2%	26.9%	29.5%	3.5%	-0.5%
Mar	86.4%	3.4%	3.4%	26.7%	29.4%	3.4%	-0.6%
Apr	76.0%	3.4%	3.4%	26.6%	29.4%	4.3%	-1.0%
May	67.1%	3.5%	3.5%	26.5%	29.3%	2.8%	-2.7%
Jun	59.6%	3.6%	3.6%	26.4%	29.3%	1.8%	-4.3%
Jul	53.2%	3.6%	3.6%	26.3%	29.2%	2.0%	-4.2%
Aug	47.7%	3.6%	3.6%	26.3%	29.2%	0.1%	-5.6%
Sep	43.1%	3.7%	3.7%	26.2%	29.2%	2.4%	-3.4%
Oct	39.1%	3.7%	3.7%	26.1%	29.2%	5.3%	-1.1%
Nov	35.7%	3.7%	3.7%	26.1%	29.2%	7.5%	1.1%
Dec	32.8%	3.8%	3.8%	26.0%	29.2%	5.6%	1.2%
Annual	**64.7%**	**3.5%**	**3.5%**	**26.2%**	**29.0%**	**0.9%**	**-4.3%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.5.3. Comparison of calculated values of PCB-180 concentration in the atmosphere at its interface with vegetation

Reference data set. Calculation results on PCB-180 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.96.

Monthly values of PCB-180 concentration in the atmosphere at its interface with vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.115 a and b, respectively.

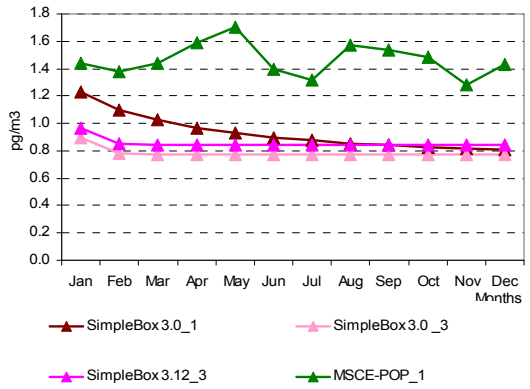


Fig. C.115a. *PCB-180 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

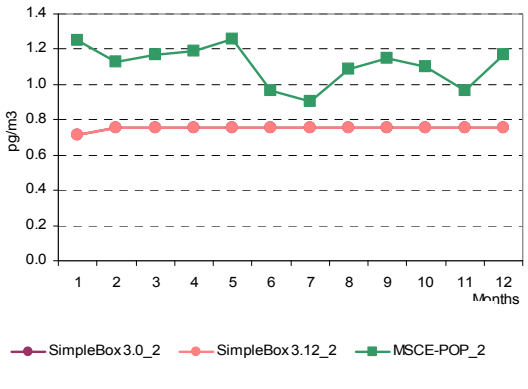


Fig. C.115b. *PCB-180 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 concentration in the atmosphere at its interface with vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.97.

Monthly values of PCB-180 concentration in the atmosphere at its interface with vegetation calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.116 a and b, respectively.

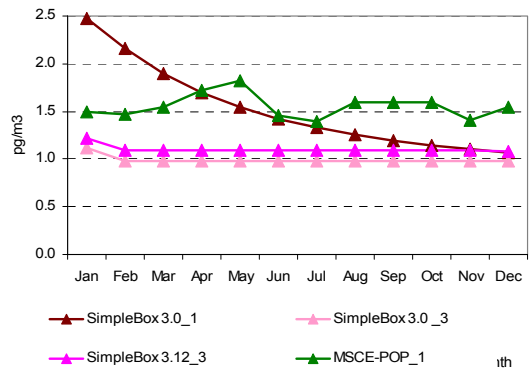


Fig. C.116a. *PCB-180 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

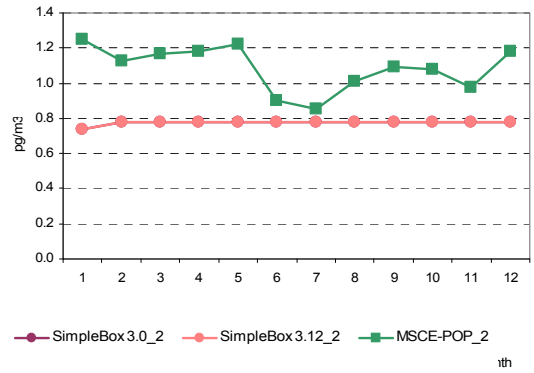


Fig. C.116b. *PCB-180 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.96. *Calculation results: PCB-180 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE- POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.23	1.44	0.90	0.96	*1.13*	*0.25*	Jan	0.71	0.71	1.25	*0.89*	*0.31*
Feb	1.10	1.38	0.78	0.85	*1.03*	*0.27*	Feb	0.75	0.75	1.13	*0.88*	*0.22*
Mar	1.02	1.44	0.78	0.85	*1.02*	*0.30*	Mar	0.75	0.75	1.17	*0.89*	*0.24*
Apr	0.97	1.59	0.78	0.85	*1.05*	*0.37*	Apr	0.75	0.75	1.19	*0.90*	*0.25*
May	0.93	1.70	0.78	0.84	*1.06*	*0.43*	May	0.75	0.75	1.26	*0.92*	*0.29*
Jun	0.90	1.40	0.78	0.84	*0.98*	*0.28*	Jun	0.75	0.75	0.97	*0.82*	*0.12*
Jul	0.87	1.32	0.78	0.84	*0.95*	*0.25*	Jul	0.75	0.75	0.90	*0.80*	*0.09*
Aug	0.86	1.57	0.77	0.84	*1.01*	*0.37*	Aug	0.75	0.75	1.09	*0.87*	*0.19*
Sep	0.84	1.54	0.77	0.84	*1.00*	*0.36*	Sep	0.75	0.75	1.15	*0.89*	*0.23*
Oct	0.83	1.48	0.77	0.84	*0.98*	*0.33*	Oct	0.75	0.75	1.10	*0.87*	*0.20*
Nov	0.82	1.28	0.77	0.84	*0.93*	*0.24*	Nov	0.75	0.75	0.97	*0.82*	*0.12*
Dec	0.81	1.43	0.77	0.84	*0.96*	*0.31*	Dec	0.75	0.75	1.17	*0.89*	*0.24*
Annual	**0.93**	**1.49**	**0.79**	**0.85**	***1.01***	***0.32***	**Annual**	**0.75**	**0.75**	**1.12**	***0.87***	***0.21***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table C.97. *Calculation results: PCB-180 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.48	1.50	1.12	1.22	*1.58*	*0.62*	Jan	0.73	0.73	1.25	*0.91*	*0.30*
Feb	2.16	1.47	0.99	1.10	*1.43*	*0.53*	Feb	0.78	0.78	1.13	*0.89*	*0.20*
Mar	1.90	1.54	0.98	1.10	*1.38*	*0.42*	Mar	0.78	0.78	1.17	*0.91*	*0.23*
Apr	1.70	1.72	0.98	1.09	*1.37*	*0.39*	Apr	0.78	0.78	1.18	*0.91*	*0.23*
May	1.54	1.82	0.98	1.09	*1.36*	*0.39*	May	0.78	0.78	1.22	*0.93*	*0.26*
Jun	1.43	1.46	0.98	1.09	*1.24*	*0.24*	Jun	0.78	0.78	0.90	*0.82*	*0.07*
Jul	1.33	1.40	0.98	1.09	*1.20*	*0.20*	Jul	0.78	0.78	0.86	*0.80*	*0.04*
Aug	1.26	1.60	0.98	1.09	*1.23*	*0.27*	Aug	0.78	0.78	1.01	*0.86*	*0.13*
Sep	1.20	1.60	0.98	1.09	*1.22*	*0.27*	Sep	0.78	0.78	1.09	*0.88*	*0.18*
Oct	1.15	1.59	0.98	1.09	*1.20*	*0.27*	Oct	0.78	0.78	1.08	*0.88*	*0.17*
Nov	1.11	1.41	0.98	1.09	*1.14*	*0.19*	Nov	0.78	0.78	0.98	*0.85*	*0.12*
Dec	1.07	1.54	0.97	1.09	*1.17*	*0.25*	Dec	0.78	0.78	1.18	*0.91*	*0.23*
Annual	**1.53**	**1.55**	**0.99**	**1.10**	***1.29***	***0.29***	**Annual**	**0.78**	**0.78**	**1.09**	***0.88***	***0.18***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.98.

Table C.98. *The percentage difference between calculation results on PCB-180 concentration in the atmosphere at interface with vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	101.3%	2.9%	2.9%	24.4%	26.8%	4.2%	0.0%
Feb	97.2%	3.2%	3.2%	26.8%	29.5%	6.5%	0.0%
Mar	85.6%	3.3%	3.3%	26.6%	29.4%	6.9%	0.0%
Apr	75.2%	3.4%	3.4%	26.5%	29.4%	8.2%	-0.8%
May	66.3%	3.5%	3.5%	26.4%	29.3%	7.1%	-3.2%
Jun	58.8%	3.5%	3.5%	26.3%	29.3%	4.3%	-6.8%
Jul	52.4%	3.6%	3.6%	26.2%	29.3%	6.1%	-5.2%
Aug	47.0%	3.6%	3.6%	26.2%	29.3%	1.9%	-7.3%
Sep	42.4%	3.7%	3.6%	26.1%	29.2%	3.9%	-5.2%
Oct	38.5%	3.7%	3.7%	26.0%	29.2%	7.4%	-1.8%
Nov	35.1%	3.7%	3.7%	26.0%	29.2%	10.2%	1.3%
Dec	32.2%	3.7%	3.7%	25.9%	29.2%	7.7%	0.9%
Annual	64.0%	3.5%	3.5%	26.1%	29.1%	4.6%	-3.0%

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.5.4. Comparison of calculated values of PCB-180 concentration in surface ocean layer

Reference data set. Calculation results on PCB-180 concentration in surface ocean layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.99.

Monthly values of PCB-180 concentration in surface ocean layer calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.117 a and b, respectively.

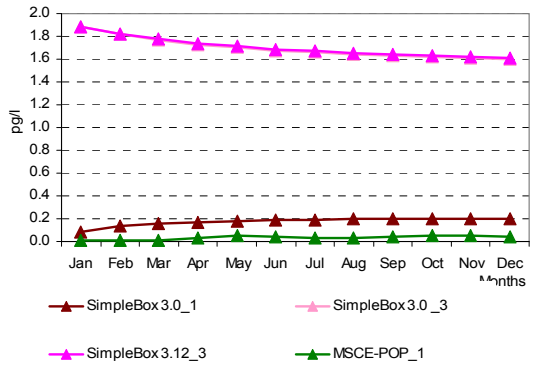


Fig. C.117a. *PCB-180 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

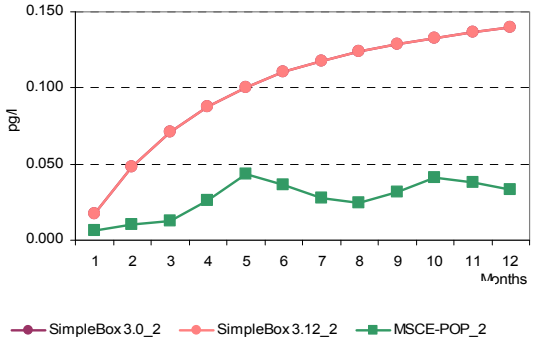


Fig. C.117b. *PCB-180 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 concentration in surface ocean layer calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.100.

Monthly values of PCB-180 concentration in surface ocean layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.118 a and b, respectively.

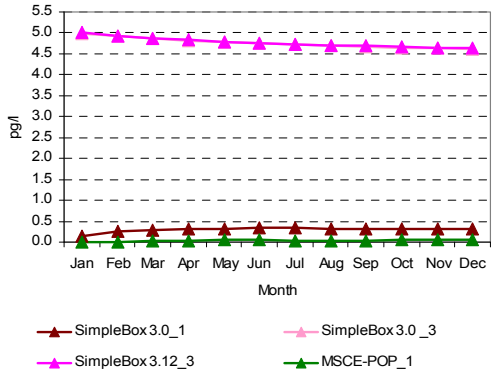


Fig. C.118a. *PCB-180 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

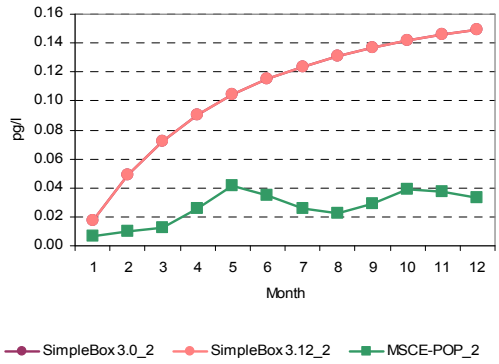


Fig. C.118b. *PCB-180 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.99. *Calculation results: PCB-180 concentration in surface ocean layer (pg/l) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.09	0.01	1.89	1.89	*0.97*	*1.06*	Jan	0.02	0.02	0.01	*0.01*	*0.01*
Feb	0.13	0.01	1.82	1.82	*0.95*	*1.01*	Feb	0.05	0.05	0.01	*0.04*	*0.02*
Mar	0.16	0.01	1.77	1.78	*0.93*	*0.98*	Mar	0.07	0.07	0.01	*0.05*	*0.03*
Apr	0.17	0.03	1.73	1.74	*0.92*	*0.94*	Apr	0.09	0.09	0.03	*0.07*	*0.04*
May	0.18	0.05	1.70	1.71	*0.91*	*0.92*	May	0.10	0.10	0.04	*0.08*	*0.03*
Jun	0.19	0.05	1.68	1.69	*0.90*	*0.91*	Jun	0.11	0.11	0.04	*0.09*	*0.04*
Jul	0.19	0.04	1.66	1.67	*0.89*	*0.90*	Jul	0.12	0.12	0.03	*0.09*	*0.05*
Aug	0.20	0.03	1.64	1.66	*0.88*	*0.89*	Aug	0.12	0.12	0.02	*0.09*	*0.06*
Sep	0.20	0.04	1.63	1.64	*0.88*	*0.88*	Sep	0.13	0.13	0.03	*0.10*	*0.06*
Oct	0.20	0.05	1.62	1.63	*0.88*	*0.87*	Oct	0.13	0.13	0.04	*0.10*	*0.05*
Nov	0.20	0.05	1.61	1.62	*0.87*	*0.86*	Nov	0.14	0.14	0.04	*0.10*	*0.06*
Dec	0.20	0.04	1.60	1.61	*0.86*	*0.86*	Dec	0.14	0.14	0.03	*0.10*	*0.06*
Annual	**0.18**	**0.03**	**1.70**	**1.71**	***0.90***	***0.92***	**Annual**	**0.10**	**0.10**	**0.03**	***0.08***	***0.04***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table C.100. *Calculation results: PCB-180 concentration in surface ocean layer (pg/l) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.15	0.01	5.00	5.00	*2.54*	*2.84*	Jan	0.02	0.02	0.01	*0.01*	*0.01*
Feb	0.24	0.01	4.92	4.93	*2.53*	*2.77*	Feb	0.05	0.05	0.01	*0.04*	*0.02*
Mar	0.29	0.02	4.86	4.87	*2.51*	*2.72*	Mar	0.07	0.07	0.01	*0.05*	*0.03*
Apr	0.32	0.03	4.81	4.83	*2.50*	*2.68*	Apr	0.09	0.09	0.03	*0.07*	*0.04*
May	0.33	0.05	4.78	4.79	*2.49*	*2.65*	May	0.10	0.10	0.04	*0.08*	*0.04*
Jun	0.33	0.05	4.74	4.76	*2.47*	*2.64*	Jun	0.12	0.12	0.03	*0.09*	*0.05*
Jul	0.33	0.04	4.72	4.73	*2.45*	*2.62*	Jul	0.12	0.12	0.03	*0.09*	*0.06*
Aug	0.33	0.03	4.69	4.71	*2.44*	*2.61*	Aug	0.13	0.13	0.02	*0.09*	*0.06*
Sep	0.32	0.04	4.67	4.69	*2.43*	*2.60*	Sep	0.14	0.14	0.03	*0.10*	*0.06*
Oct	0.32	0.06	4.65	4.67	*2.42*	*2.58*	Oct	0.14	0.14	0.04	*0.11*	*0.06*
Nov	0.31	0.05	4.63	4.65	*2.41*	*2.58*	Nov	0.15	0.15	0.04	*0.11*	*0.06*
Dec	0.31	0.04	4.61	4.63	*2.40*	*2.57*	Dec	0.15	0.15	0.03	*0.11*	*0.07*
Annual	**0.30**	**0.04**	**4.76**	**4.77**	***2.47***	***2.66***	**Annual**	**0.11**	**0.11**	**0.03**	***0.08***	***0.05***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.101.

Table C.101. *The percentage difference between calculation results on PCB-180 concentration in surface ocean layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	69.4%	-0.5%	-0.5%	164.8%	164.7%	5.3%	0.2%
Feb	85.3%	0.9%	0.9%	170.5%	170.2%	5.6%	0.0%
Mar	86.3%	2.1%	2.1%	174.9%	174.4%	4.8%	0.0%
Apr	84.1%	3.0%	3.0%	178.2%	177.6%	3.9%	-0.8%
May	80.4%	3.9%	3.9%	180.8%	180.0%	2.1%	-4.1%
Jun	76.2%	4.6%	4.6%	182.7%	181.8%	1.7%	-5.7%
Jul	71.8%	5.1%	5.1%	184.2%	183.3%	0.6%	-7.2%
Aug	67.3%	5.6%	5.6%	185.4%	184.4%	0.3%	-8.2%
Sep	63.1%	6.0%	6.0%	186.4%	185.3%	1.2%	-7.0%
Oct	59.2%	6.3%	6.3%	187.2%	186.1%	3.9%	-4.4%
Nov	55.7%	6.6%	6.6%	187.9%	186.8%	5.5%	-2.4%
Dec	52.4%	6.8%	6.8%	188.5%	187.4%	5.7%	-1.2%
Annual	**70.0%**	**5.0%**	**5.0%**	**180.6%**	**179.8%**	**9.9%**	**1.9%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.5.5. Comparison of calculated values of PCB-180 concentration in vegetation

Reference data set. Calculation results on PCB-180 concentration in vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.102.

Monthly values of PCB-180 concentration in vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.119 a and b, respectively.

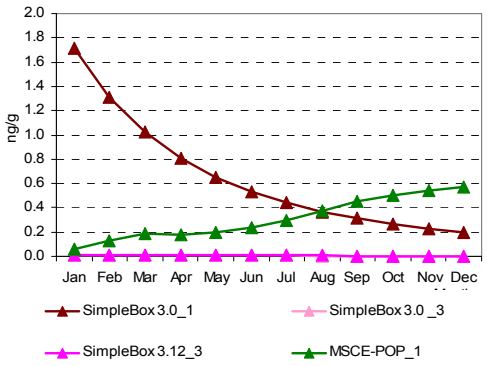


Fig. C.119a. *PCB-180 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

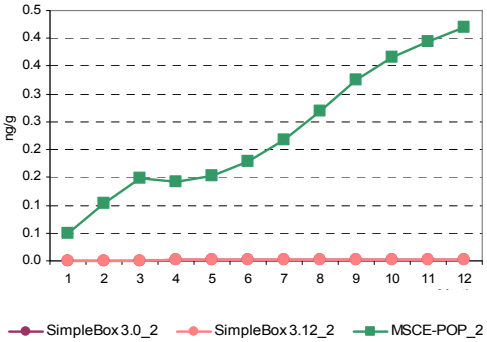


Fig. C.119b. *PCB-180 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 concentration in vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.103.

Monthly values of PCB-180 concentration in vegetation calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.121 a and b, respectively.

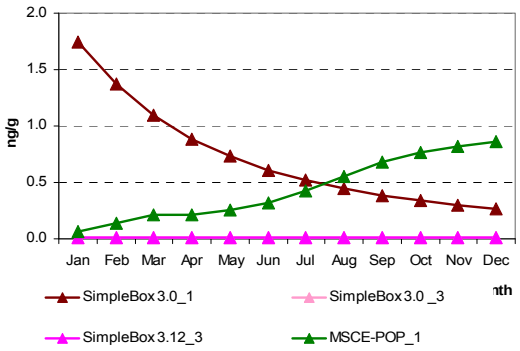


Fig. C.120a. *PCB-180 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

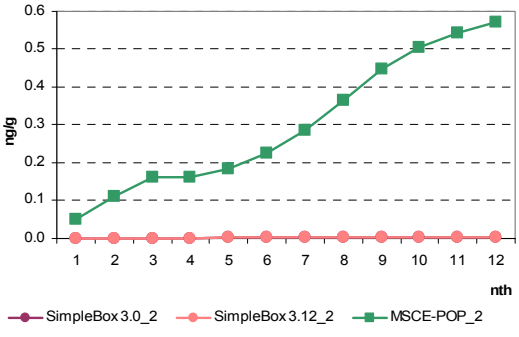


Fig. C.120b. *PCB-180 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.102. *Calculation results: PCB-180 concentration in vegetation (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.72	0.06	0.01	0.01	*0.45*	*0.85*	Jan	0.0002	0.0002	0.05	*0.02*	*0.03*
Feb	1.31	0.13	0.01	0.01	*0.36*	*0.64*	Feb	0.001	0.001	0.10	*0.03*	*0.06*
Mar	1.02	0.18	0.01	0.01	*0.31*	*0.49*	Mar	0.001	0.001	0.15	*0.05*	*0.09*
Apr	0.81	0.18	0.01	0.01	*0.25*	*0.38*	Apr	0.001	0.001	0.14	*0.05*	*0.08*
May	0.65	0.19	0.01	0.01	*0.21*	*0.30*	May	0.001	0.001	0.15	*0.05*	*0.09*
Jun	0.53	0.23	0.01	0.01	*0.19*	*0.25*	Jun	0.002	0.002	0.18	*0.06*	*0.10*
Jul	0.44	0.29	0.01	0.01	*0.19*	*0.22*	Jul	0.002	0.002	0.22	*0.07*	*0.12*
Aug	0.37	0.37	0.00	0.00	*0.19*	*0.21*	Aug	0.002	0.002	0.27	*0.09*	*0.15*
Sep	0.31	0.45	0.00	0.00	*0.19*	*0.22*	Sep	0.002	0.002	0.33	*0.11*	*0.19*
Oct	0.27	0.50	0.00	0.00	*0.19*	*0.24*	Oct	0.002	0.002	0.37	*0.12*	*0.21*
Nov	0.23	0.54	0.00	0.00	*0.19*	*0.25*	Nov	0.002	0.002	0.39	*0.13*	*0.23*
Dec	0.20	0.57	0.00	0.00	*0.19*	*0.27*	Dec	0.002	0.002	0.42	*0.14*	*0.24*
Annual	**0.66**	**0.26**	**0.01**	**0.01**	***0.23***	***0.31***	**Annual**	**0.002**	**0.002**	**0.20**	***0.07***	***0.11***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table C.103. *Calculation results: PCB-180 concentration in vegetation (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	1.74	0.06	0.01	0.01	*0.45*	*0.86*	Jan	0.0003	0.0003	0.05	*0.02*	*0.03*
Feb	1.37	0.14	0.01	0.01	*0.38*	*0.66*	Feb	0.001	0.001	0.11	*0.04*	*0.06*
Mar	1.10	0.21	0.01	0.01	*0.33*	*0.52*	Mar	0.001	0.001	0.16	*0.05*	*0.09*
Apr	0.89	0.22	0.01	0.01	*0.28*	*0.42*	Apr	0.002	0.002	0.16	*0.06*	*0.09*
May	0.73	0.25	0.01	0.01	*0.25*	*0.34*	May	0.002	0.002	0.18	*0.06*	*0.11*
Jun	0.61	0.32	0.01	0.01	*0.24*	*0.29*	Jun	0.002	0.002	0.23	*0.08*	*0.13*
Jul	0.52	0.43	0.01	0.01	*0.24*	*0.27*	Jul	0.002	0.002	0.29	*0.10*	*0.16*
Aug	0.44	0.56	0.01	0.01	*0.25*	*0.29*	Aug	0.002	0.002	0.36	*0.12*	*0.21*
Sep	0.38	0.68	0.01	0.01	*0.27*	*0.33*	Sep	0.003	0.003	0.45	*0.15*	*0.26*
Oct	0.34	0.77	0.01	0.01	*0.28*	*0.36*	Oct	0.003	0.003	0.50	*0.17*	*0.29*
Nov	0.30	0.82	0.01	0.01	*0.28*	*0.38*	Nov	0.003	0.003	0.54	*0.18*	*0.31*
Dec	0.26	0.86	0.01	0.01	*0.28*	*0.40*	Dec	0.003	0.003	0.57	*0.19*	*0.33*
Annual	**0.63**	**0.44**	**0.01**	**0.01**	***0.27***	***0.32***	**Annual**	**0.002**	**0.002**	**0.30**	***0.10***	***0.17***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.104.

Table C.104. *The percentage difference between calculation results on PCB-180 concentration in vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	1.4%	22.7%	22.7%	-14.6%	-14.4%	8.5%	2.9%
Feb	4.2%	24.2%	24.2%	-9.8%	-9.1%	13.6%	6.8%
Mar	6.9%	25.5%	25.5%	-4.9%	-3.7%	15.8%	8.7%
Apr	9.6%	26.7%	26.7%	0.1%	1.7%	21.3%	14.0%
May	12.3%	27.9%	27.9%	5.1%	7.1%	30.6%	20.3%
Jun	14.9%	28.9%	28.9%	10.1%	12.4%	39.2%	26.4%
Jul	17.4%	29.9%	29.9%	14.9%	17.6%	46.4%	32.3%
Aug	20.0%	30.8%	30.8%	19.7%	22.6%	50.4%	35.3%
Sep	22.6%	31.7%	31.7%	24.2%	27.3%	51.9%	37.1%
Oct	25.2%	32.5%	32.5%	28.5%	31.8%	52.4%	37.3%
Nov	27.8%	33.3%	33.3%	32.6%	36.0%	51.9%	37.6%
Dec	30.4%	34.0%	34.0%	36.4%	39.9%	50.6%	36.4%
Annual	**-3.9%**	**30.5%**	**30.5%**	**11.3%**	**13.7%**	**71.4%**	**54.0%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.5.6. Comparison of calculated values of PCB-180 concentration in surface soil layer

Reference data set. Calculation results on PCB-180 concentration in surface soil layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table C.105.

Monthly values of PCB-180 concentration in surface soil layer calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.121 a and b, respectively.

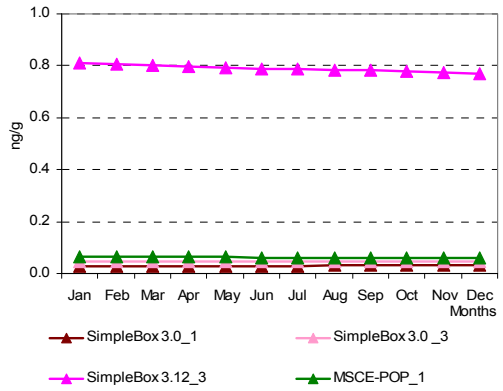


Fig.3.121a. *PCB-180 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

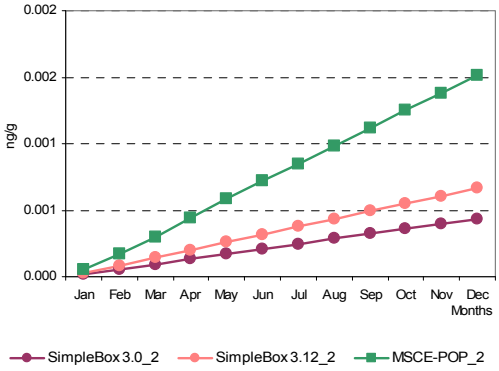


Fig.3.121b. *PCB-180 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-180 concentration in surface soil layer calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table C.106.

Monthly values of PCB-180 concentration in surface soil layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. C.122a and b, respectively.

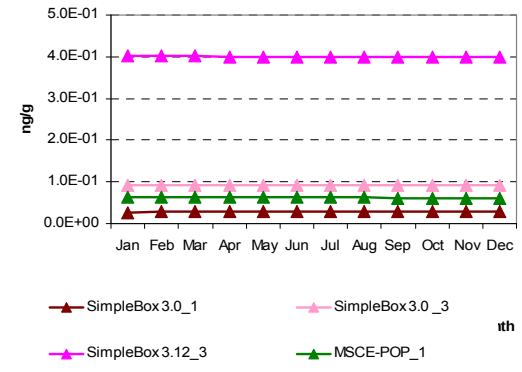


Fig. C.122a. *PCB-180 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

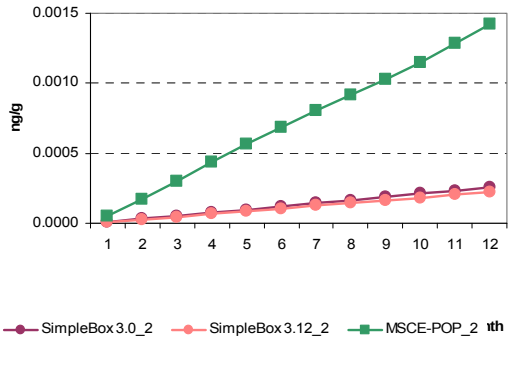


Fig. C.122b. *PCB-180 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table C.105. *Calculation results: PCB-180 concentration in surface soil layer (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.72E-02	6.38E-02	4.83E-02	8.11E-01	*2.38E-01*	*3.83E-01*	Jan	1.77E-05	2.71E-05	5.20E-05	*3.23E-05*	*1.77E-05*
Feb	2.81E-02	6.34E-02	4.81E-02	8.08E-01	*2.37E-01*	*3.81E-01*	Feb	5.53E-05	8.45E-05	1.70E-04	*1.03E-04*	*5.96E-05*
Mar	2.87E-02	6.30E-02	4.79E-02	8.04E-01	*2.36E-01*	*3.79E-01*	Mar	9.30E-05	1.42E-04	2.98E-04	*1.78E-04*	*1.07E-04*
Apr	2.92E-02	6.26E-02	4.77E-02	7.96E-01	*2.34E-01*	*3.75E-01*	Apr	1.31E-04	2.01E-04	4.43E-04	*2.58E-04*	*1.64E-04*
May	2.95E-02	6.23E-02	4.75E-02	7.93E-01	*2.33E-01*	*3.73E-01*	May	1.70E-04	2.59E-04	5.82E-04	*3.37E-04*	*2.17E-04*
Jun	2.97E-02	6.19E-02	4.73E-02	7.89E-01	*2.32E-01*	*3.71E-01*	Jun	2.08E-04	3.17E-04	7.18E-04	*4.14E-04*	*2.69E-04*
Jul	2.99E-02	6.15E-02	4.71E-02	7.89E-01	*2.32E-01*	*3.72E-01*	Jul	2.46E-04	3.75E-04	8.51E-04	*4.91E-04*	*3.19E-04*
Aug	3.00E-02	6.11E-02	4.69E-02	7.85E-01	*2.31E-01*	*3.70E-01*	Aug	2.84E-04	4.34E-04	9.83E-04	*5.67E-04*	*3.68E-04*
Sep	3.01E-02	6.08E-02	4.67E-02	7.81E-01	*2.30E-01*	*3.68E-01*	Sep	3.22E-04	4.92E-04	1.12E-03	*6.45E-04*	*4.20E-04*
Oct	3.01E-02	6.04E-02	4.65E-02	7.78E-01	*2.29E-01*	*3.66E-01*	Oct	3.60E-04	5.49E-04	1.25E-03	*7.20E-04*	*4.69E-04*
Nov	3.01E-02	6.01E-02	4.63E-02	7.74E-01	*2.28E-01*	*3.64E-01*	Nov	3.97E-04	6.06E-04	1.38E-03	*7.95E-04*	*5.18E-04*
Dec	3.01E-02	5.98E-02	4.62E-02	7.70E-01	*2.27E-01*	*3.63E-01*	Dec	4.34E-04	6.62E-04	1.51E-03	*8.69E-04*	*5.67E-04*
Annual	**2.94E-02**	**6.21E-02**	**4.71E-02**	**7.91E-01**	***2.32E-01***	***3.73E-01***	**Annual**	**2.45E-04**	**3.46E-04**	**6.47E-04**	***4.13E-04***	***2.09E-04***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table C.106. *Calculation results: PCB-180 concentration in surface soil layer (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data		Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.70E-02	6.39E-02	9.21E-02	4.01E-01	*1.46E-01*	*1.72E-01*	Jan	1.01E-05	8.81E-06	5.19E-05	*2.36E-05*	*2.45E-05*
Feb	2.76E-02	6.36E-02	9.20E-02	4.01E-01	*1.46E-01*	*1.72E-01*	Feb	3.17E-05	2.76E-05	1.69E-04	*7.61E-05*	*8.05E-05*
Mar	2.80E-02	6.33E-02	9.20E-02	4.01E-01	*1.46E-01*	*1.72E-01*	Mar	5.34E-05	4.67E-05	2.96E-04	*1.32E-04*	*1.42E-04*
Apr	2.84E-02	6.31E-02	9.19E-02	4.00E-01	*1.46E-01*	*1.72E-01*	Apr	7.57E-05	6.61E-05	4.38E-04	*1.93E-04*	*2.12E-04*
May	2.87E-02	6.28E-02	9.19E-02	4.00E-01	*1.46E-01*	*1.71E-01*	May	9.80E-05	8.56E-05	5.70E-04	*2.51E-04*	*2.76E-04*
Jun	2.89E-02	6.25E-02	9.18E-02	4.00E-01	*1.46E-01*	*1.71E-01*	Jun	1.20E-04	1.05E-04	6.90E-04	*3.05E-04*	*3.33E-04*
Jul	2.91E-02	6.22E-02	9.17E-02	4.00E-01	*1.46E-01*	*1.71E-01*	Jul	1.43E-04	1.25E-04	8.02E-04	*3.57E-04*	*3.86E-04*
Aug	2.92E-02	6.18E-02	9.17E-02	4.00E-01	*1.46E-01*	*1.71E-01*	Aug	1.66E-04	1.45E-04	9.13E-04	*4.08E-04*	*4.38E-04*
Sep	2.93E-02	6.15E-02	9.16E-02	3.99E-01	*1.45E-01*	*1.71E-01*	Sep	1.88E-04	1.64E-04	1.03E-03	*4.61E-04*	*4.93E-04*
Oct	2.94E-02	6.13E-02	9.16E-02	3.99E-01	*1.45E-01*	*1.71E-01*	Oct	2.11E-04	1.84E-04	1.15E-03	*5.15E-04*	*5.50E-04*
Nov	2.95E-02	6.10E-02	9.15E-02	3.99E-01	*1.45E-01*	*1.71E-01*	Nov	2.34E-04	2.04E-04	1.29E-03	*5.76E-04*	*6.19E-04*
Dec	2.96E-02	6.08E-02	9.15E-02	3.98E-01	*1.45E-01*	*1.71E-01*	Dec	2.56E-04	2.23E-04	1.42E-03	*6.33E-04*	*6.82E-04*
Annual	**2.89E-02**	**6.23E-02**	**9.17E-02**	**4.00E-01**	***1.46E-01***	***1.71E-01***	**Annual**	**1.43E-04**	**1.15E-04**	**7.35E-04**	***3.31E-04***	***3.50E-04***

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table C.107.

Table C.107. *The percentage difference between calculation results on PCB-180 concentration in surface soil layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Jan	-0.8%	-42.9%	-67.4%	90.7%	-50.5%	0.2%	-0.2%
Feb	-1.8%	-42.7%	-67.3%	91.4%	-50.3%	0.3%	-0.6%
Mar	-2.4%	-42.5%	-67.2%	92.0%	-50.1%	0.5%	-0.7%
Apr	-2.7%	-42.4%	-67.1%	92.7%	-49.7%	0.8%	-1.1%
May	-2.9%	-42.2%	-67.0%	93.4%	-49.5%	0.8%	-2.1%
Jun	-2.9%	-42.0%	-66.9%	94.1%	-49.3%	1.0%	-3.9%
Jul	-2.8%	-41.8%	-66.8%	94.7%	-49.3%	1.1%	-5.8%
Aug	-2.6%	-41.7%	-66.7%	95.4%	-49.1%	1.1%	-7.1%
Sep	-2.4%	-41.5%	-66.6%	96.1%	-48.9%	1.2%	-8.0%
Oct	-2.2%	-41.3%	-66.5%	96.8%	-48.7%	1.5%	-8.0%
Nov	-1.9%	-41.2%	-66.4%	97.5%	-48.5%	1.5%	-6.5%
Dec	-1.6%	-41.0%	-66.3%	98.1%	-48.3%	1.7%	-6.0%
Annual	**-1.7%**	**-41.6%**	**-66.6%**	**94.7%**	**-49.4%**	**0.4%**	**13.7%**

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;
MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;
SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;
SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;
SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

C.5.7. Comparison of PCB-180 intermedia mass flows and concentrations at the interfaces of main environmental media

A preliminary analysis of model results on intermedia mass flows and on concentrations in the main environmental media formed at their interfaces is presented in this section. In the comparison the calculated values of PCB-180 mass flows from the atmosphere to soil, to water, to vegetation and from vegetation to soil (see Sections 3.4.1-3.4.4 above) and values of PCB-180 concentrations in the atmosphere at its interface with underlying surfaces (soil, ocean and vegetation); in the surface layer of soil, ocean and vegetation (see Sections 3.5.1–3.5.6 above) are considered.

The comparison of PCB-180 mass flows transported from one compartment to another presented in Sections 3.4.1-3.4.4 includes results of one-year calculation with zero initial concentrations obtained by CliMoChem, MSCE-POP, SimpleBox models and with initial concentrations in media given as input data calculated by CAN/POPs, MSCE-POP and SimpleBox models; as well as results of long-term calculations for 20-year period with zero initial data with historical emissions carried out by CliMoChem and SimpleBox models. Results of CliMoChem, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of the estimates on intermedia mass flows to the variations in the input data.

The comparison of calculated concentrations presented in Sections 3.5.1–3.5.6 includes results of one-year calculations made on the basis of initial conditions (MSCE-POP, SimpleBox) and zero initial

concentrations (MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (SimpleBox 3.0 and 3.12). The results on concentrations in the main environmental media are obtained with the use of two different physical-chemical data sets by MSCE-POP and SimpleBox models.

In the section below the analysis of mass flows and concentrations in the media is presented for model results obtained on the basis of initial conditions and historical emissions. Calculated values of PCB intermedia mass flows and concentrations in the main media are presented in this section for four following interfaces: atmosphere-soil; vegetation – soil; atmosphere - seawater and atmosphere – vegetation.

Atmosphere-soil. Annual values of net exchange flow between atmosphere and soil calculated on the basis of two data sets of physical-chemical properties are compared between different models in Fig. C.123. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions). The blue line in the plots shows the value of the corresponding parameter averaged between models.

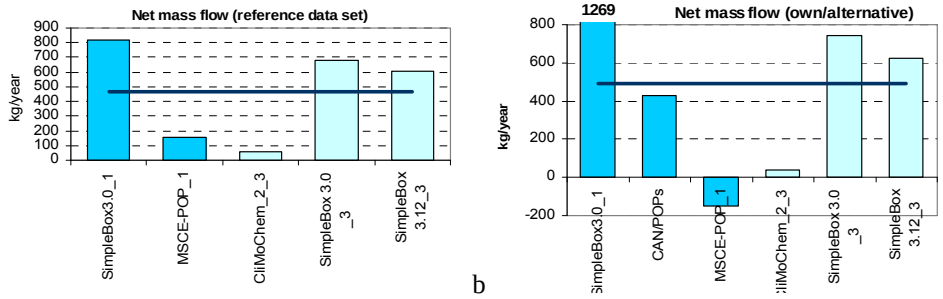


Fig.3.123. *Comparison of PCB-180 annual values of net exchange flow between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Since the net exchange flow is a sum of different types of exchange flows, below the latter are considered separately. Comparison of annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by models on the basis of two physical-chemical data sets is presented in Fig. C.124.

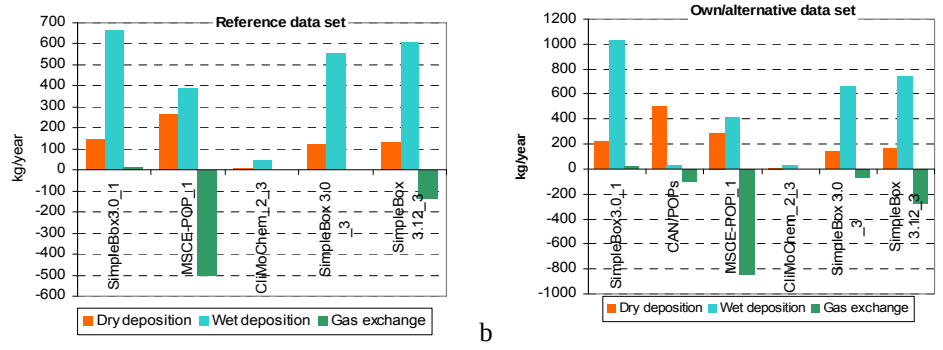
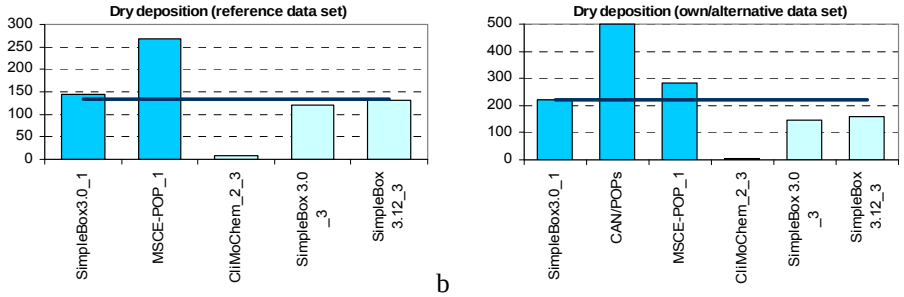


Fig.3.124. *Comparison of PCB-180 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

To reveal differences in calculated values obtained on “reference” and “own/alternative” data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

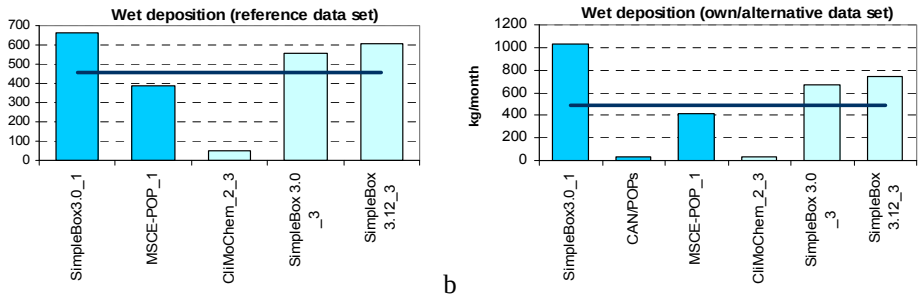
Comparison of annual values of PCB-180 dry deposition from the atmosphere to soil calculated by the models on the basis of “**reference”** and “**own or alternative”** data sets is presented in Fig. C.125. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.125. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to soil: dry deposition (kg/year) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

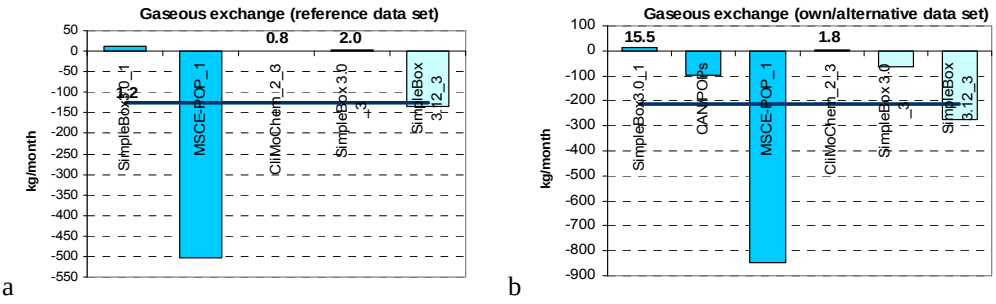
Comparison of annual values of PCB-180 wet deposition mass flows from the atmosphere to soil calculated by the models on the basis of “**reference**” and “**own or alternative**” data sets is presented in Fig.3.126. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.126. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to soil: wet deposition (kg/year) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

A comparison of annual values of PCB-180 gaseous exchange between the atmosphere and soil calculated by the models on the basis of “**reference**” and “**own or alternative”** data sets is presented in Fig.3.127. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

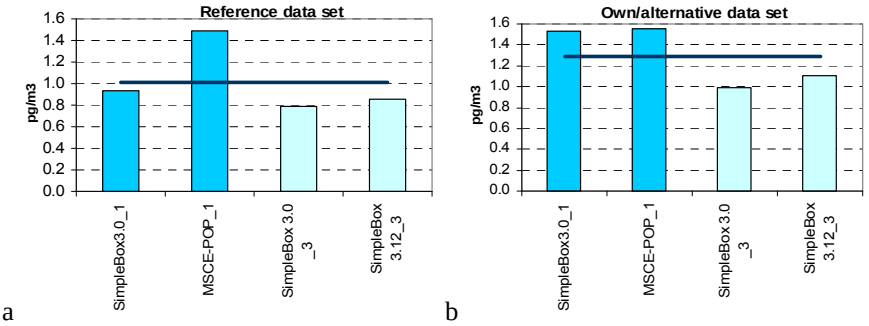


a b

Fig.3.127. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to soil: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

Model results on concentrations of PCB-180 in the atmosphere at its interface with soil and in the surface soil layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

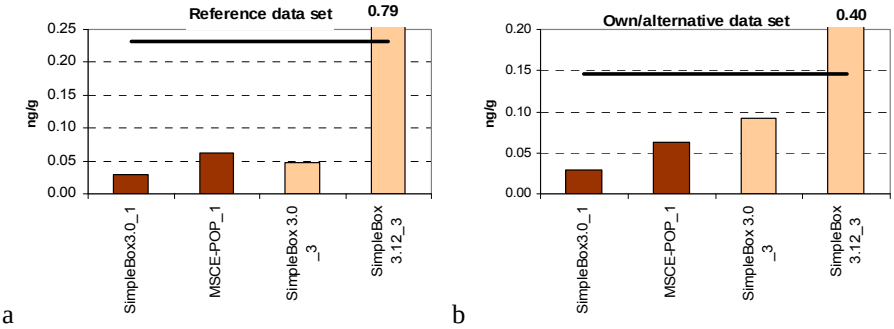
Comparison of annual values of PCB-180 concentration in the atmosphere at its interface with soil calculated by the models on the basis of "reference" and "own or alternative" data set is presented in Fig.3.128. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.128. *Comparison of annual values of PCB-180 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

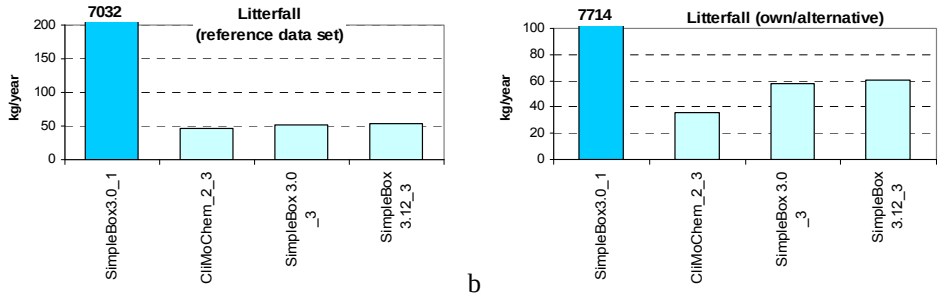
Comparison of annual values of PCB-180 concentration in surface soil layer calculated by the models on the basis of "reference" and "own/alternative" data sets is presented in Fig.3.129. The black line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.129. *Comparison of annual values of PCB-180 concentration in surface soil layer (ng/g) calculated by different models on the basis of "reference" (a) and "own or alternative" (b) data sets.*

Vegetation – soil. Comparison of annual values of PCB-180 mass flows from vegetation to soil calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.130. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).



a b

Fig.3.130. *Comparison of annual values of PCB-180 mass flows transported from vegetation to soil (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" data sets (b)*

Comparison of annual values of litterfall mass flows calculated by models on the basis of two physical-chemical data sets is presented in Fig. C.131 (see also Table C.70 given in Section 3.4.2).

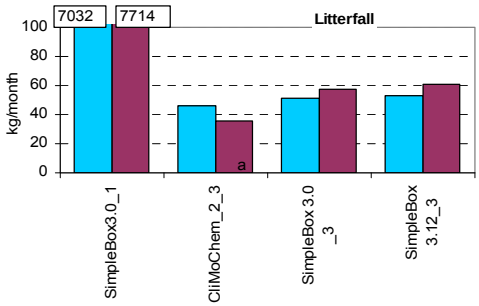
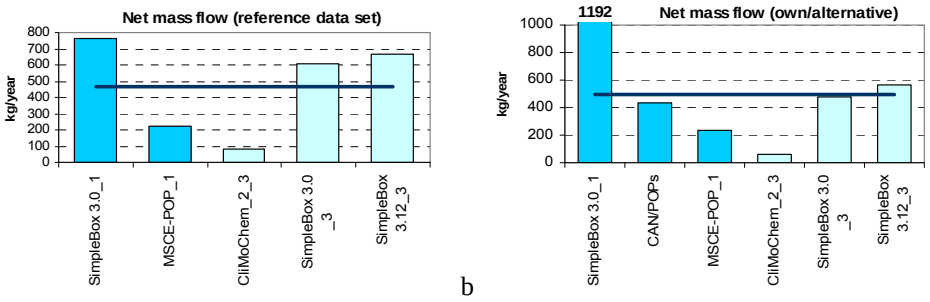


Fig.3.131. *Comparison of PCB-180 annual values of mass flows between vegetation and soil calculated by different models on the basis of two data sets*

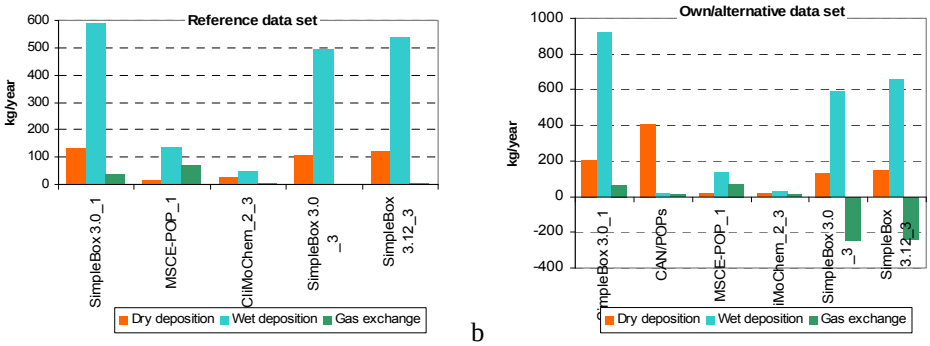
Atmosphere - seawater. Annual values of net exchange flow between atmosphere and seawater calculated on the basis of two data sets are compared between different models in Fig. C.132. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.132. *Comparison of PCB-180 annual values of net exchange flow between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Annual absolute values of dry and wet deposition and gaseous exchange flows, which formed the considered net exchange flows between the atmosphere and seawater, are compared below. Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and seawater calculated by models on the basis of two physical-chemical data sets is presented in Fig. C.133.

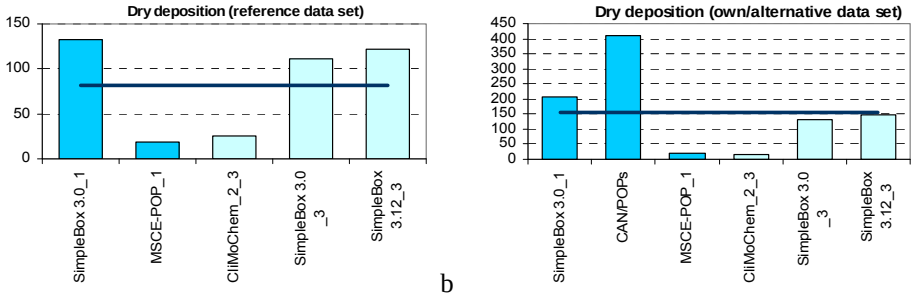


a b

Fig.3.133. *Comparison of PCB-180 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

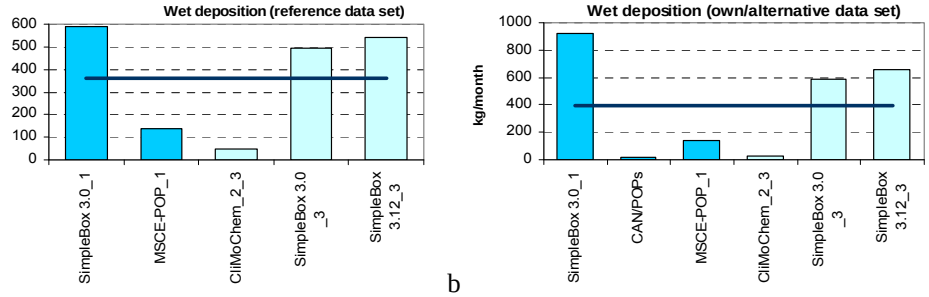
Comparison of annual values of PCB-180 dry deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.134. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.134. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to water: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

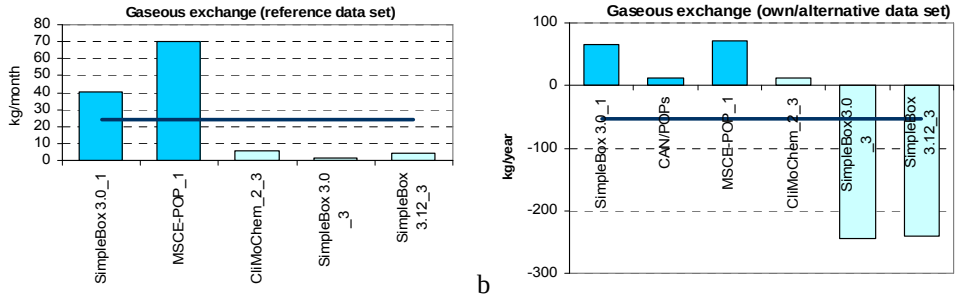
Comparison of annual values of PCB-180 wet deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.135. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.135. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to water: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Comparison of annual values of PCB-180 gaseous exchange mass flows between the atmosphere and water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.136. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

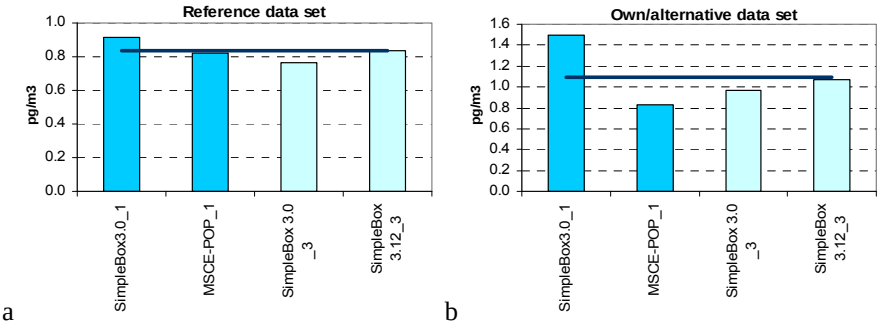


a b

Fig.3.136. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to water: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Model results on concentrations of PCB-180 in the atmosphere at its interface with ocean and in the surface water layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

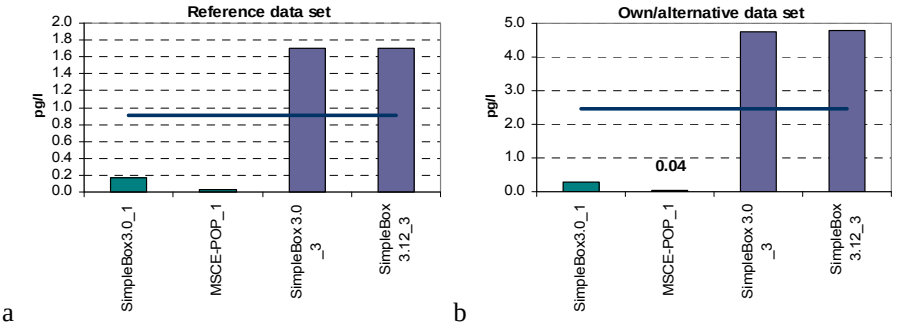
Comparison of annual values of PCB-180 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" and "own/alternative" data sets is presented in Fig.3.137. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.137. *Comparison of annual values of PCB-180 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

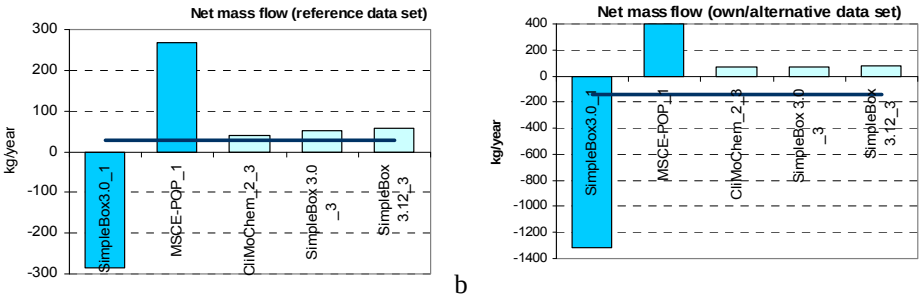
Comparison of annual values of PCB-180 concentration in surface ocean layer calculated by the models on the basis of "reference" and "own/alternative" data sets is presented in Fig.3.138. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.138. *Comparison of annual values of PCB-180 concentration in surface ocean layer (pg/l) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

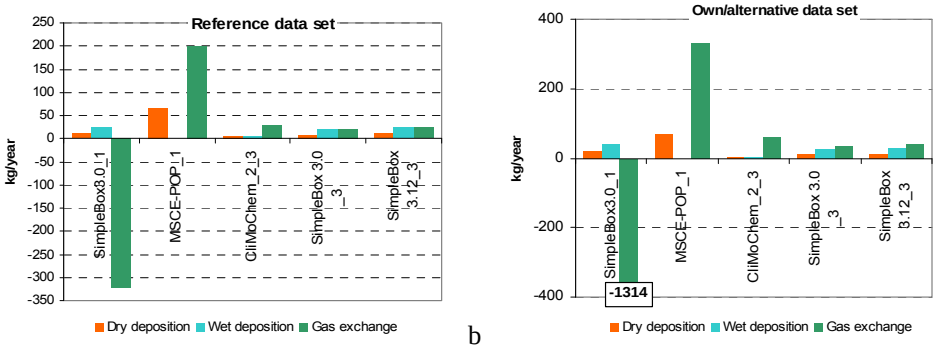
Atmosphere – vegetation. Annual values of net exchange flow between atmosphere and vegetation calculated on the basis of two data sets ("reference" and "own/alternative") are compared between different models in Fig. C.139. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.139. *Comparison of PCB-180 annual values of net exchange flow between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and vegetation calculated by models on the basis of two physical-chemical data sets is presented in Fig. C.140.

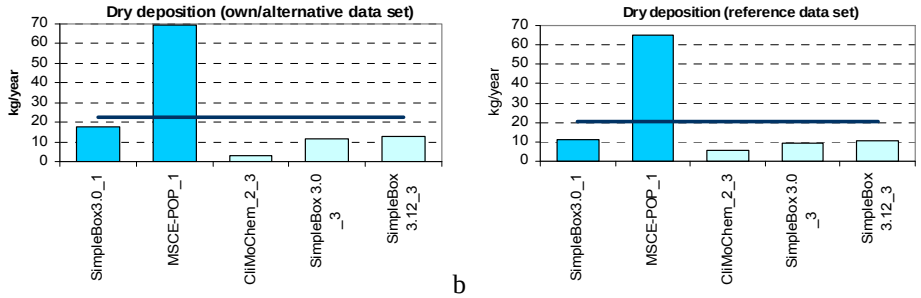


a b

Fig.3.140. *Comparison of PCB-180 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

To reveal differences in calculated values obtained on "reference" and "own/alternative" data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

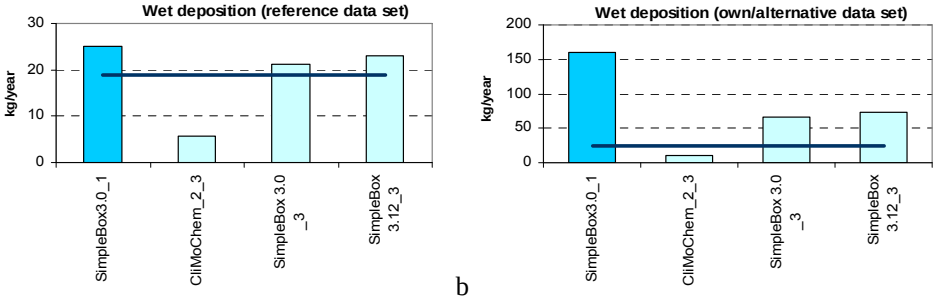
Comparison of annual values of PCB-180 dry deposition mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.142. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.141. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to vegetation: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

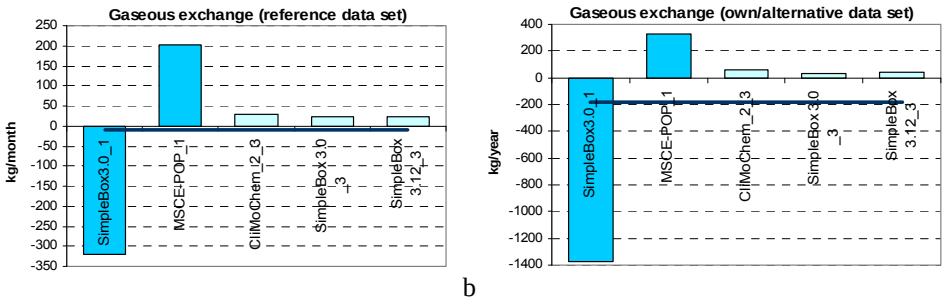
Comparison of annual values of PCB-180 wet deposition mass flows transported from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.142. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.142. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to vegetation: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Comparison of annual values of PCB-180 gaseous exchange mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.143. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

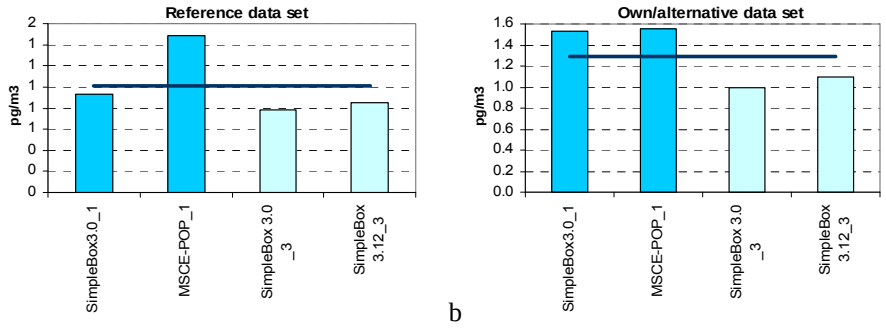


a b

Fig.3.143. *Comparison of annual values of PCB-180 mass flows transported from the atmosphere to vegetation: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Model results on concentrations of PCB-180 in the atmosphere at its interface with vegetation and in vegetation, which are conditioned by the considered above intermedia flows calculated with “reference” and “own/alternative” data sets are considered below.

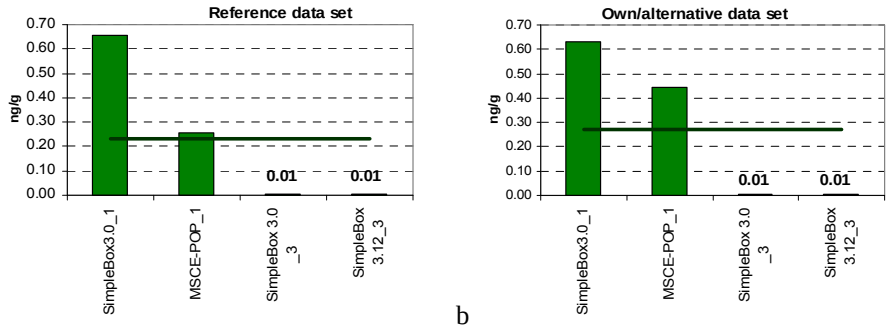
Comparison of annual values of PCB-180 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of “reference” and ‘own/alternative” data sets (see Tables 3.97 and 3.98 in Section 3.5.3) is presented in Fig.3.144. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.144. *Comparison of annual values of PCB-180 concentration in the atmosphere at its interface with vegetation (pg/m3) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

Comparison of annual values of PCB-180 concentration in vegetation calculated by the models on the basis of “reference” and ‘own/alternative” data sets (see Tables 3.103 and 3.104 in Section 3.5.5) is presented in Fig.3.145. The green line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.145. *Comparison of annual values of PCB-180 concentration in vegetation (ng/g) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

C.6. Spatial distribution of depositions and concentrations in different compartments (optional)

Four models present results on spatial distribution of depositions and concentrations of PCB-180 in different environmental compartments: DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox.

Calculated fields of PCB-180 concentrations in the atmosphere, soil, water and vegetation and net deposition fluxes in 2000 obtained by the participating models with the use of two different data sets ("reference" and "own or alternative") are compared below. The results on spatial distribution of PCB-180 deposition and concentrations in the main environmental media are obtained with the use of the two physical-chemical data sets by DEHM-POP, MSCE-POP and different versions of SimpleBox model.

The comparison of calculated deposition and concentration fields presented in Sections C.6.1 and C.6.2 below includes results of one-year calculations made on the basis of initial conditions (DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP, SimpleBox), zero initial concentrations (DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (EVN-BETR and UK-MODEL, SimpleBox 3.0 and 3.12) (See Table C.109). The model results obtained taking into account initial concentrations of pollutants in media and historical emissions, and on the basis of zero initial concentrations in the environmental media are compared in two different groups.

Table C.109. *Results on spatial distribution of PCB-180 depositions and concentrations in different compartments presented by the models*

Maps	Data set used	DEHM-POP_1	DEHM-POP_2	EVN-BETR _1[a]	EVN-BETR _2[a]	EVN-BETR _3[a]	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0 _3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Surface atmospheric concentrations, pg/m^3	ref	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt	+	+				+	+	+	+	+	+	+
Surface soil concentration, ng/g	ref	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt	+	+				+	+	+	+	+	+	+
Surface water concentration, pg/l	ref	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt	+	+				+	+	+	+	+	+	+
Concentration in vegetation, ng/g (optional)	ref			+	+	+	+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+
Net deposition flux, mg/m^2/hour	ref						+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+
Wet deposition of gaseous phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Wet deposition of particle phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Wet deposition total, mg/m^2/hour	ref						+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+
Dry deposition of gaseous phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Dry deposition of particle phase, mg/m^2/hour	ref											+	+
	own or alt											+	+
Dry deposition total, mg/m^2/hour	ref						+	+	+	+	+	+	+
	own or alt						+	+	+	+	+	+	+

EVN-BETR _1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data, the only exception was that the initial conditions for the vegetation were set to zero;

EVN-BETR _2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;

EVN-BETR _3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;

DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;

DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

[a] - EVN-BETR and UK-MODEL results were calculated with the help of a spatially resolved version of the model;

[b] – SimpleBox: results were calculated on the basis of initial concentrations given as input data. The concentrations calculated are the bulk concentrations in the compartments. Maps of concentrations are obtained on the basis of annual values of concentrations at regional and continental levels.

C.6.1. Comparison of results on spatial distribution of PCB-180 depositions and concentrations in different compartments obtained on the basis of "reference" data set

In this section a comparison of spatial distributions of PCB-180 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models with the use of "reference" data set on the basis of initial PCB-180 concentrations in the media, historical emissions and zero initial conditions is presented.

Concentration in the atmosphere. The calculated fields of PCB-180 annual concentrations in the atmosphere of the European calculation domain presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. C.147.

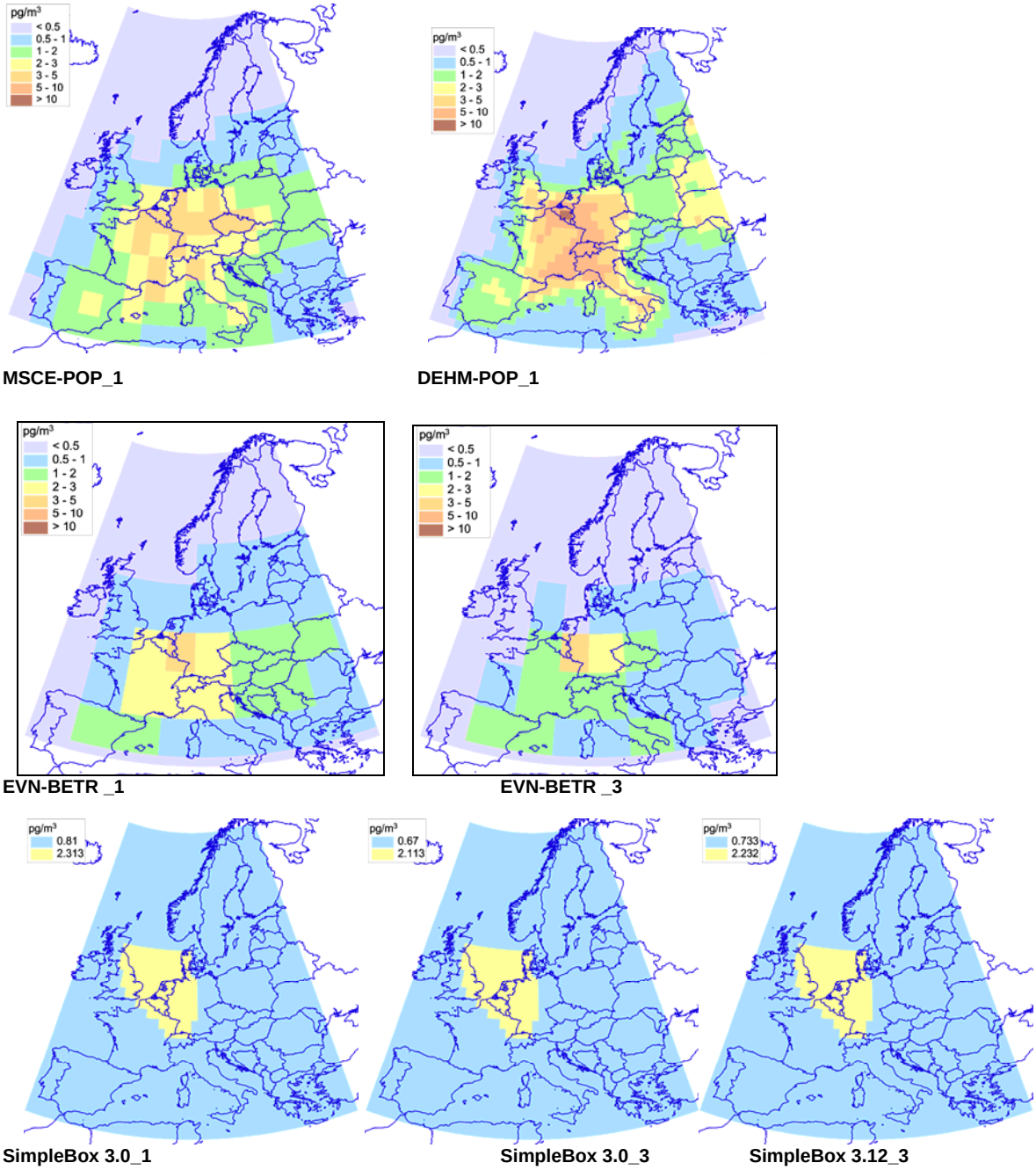


Fig. C.147. *Spatial distribution of PCB-180 concentrations in the atmosphere calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

Soil concentration. The spatial distributions of PCB-180 concentration in soil of the European region presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.148.

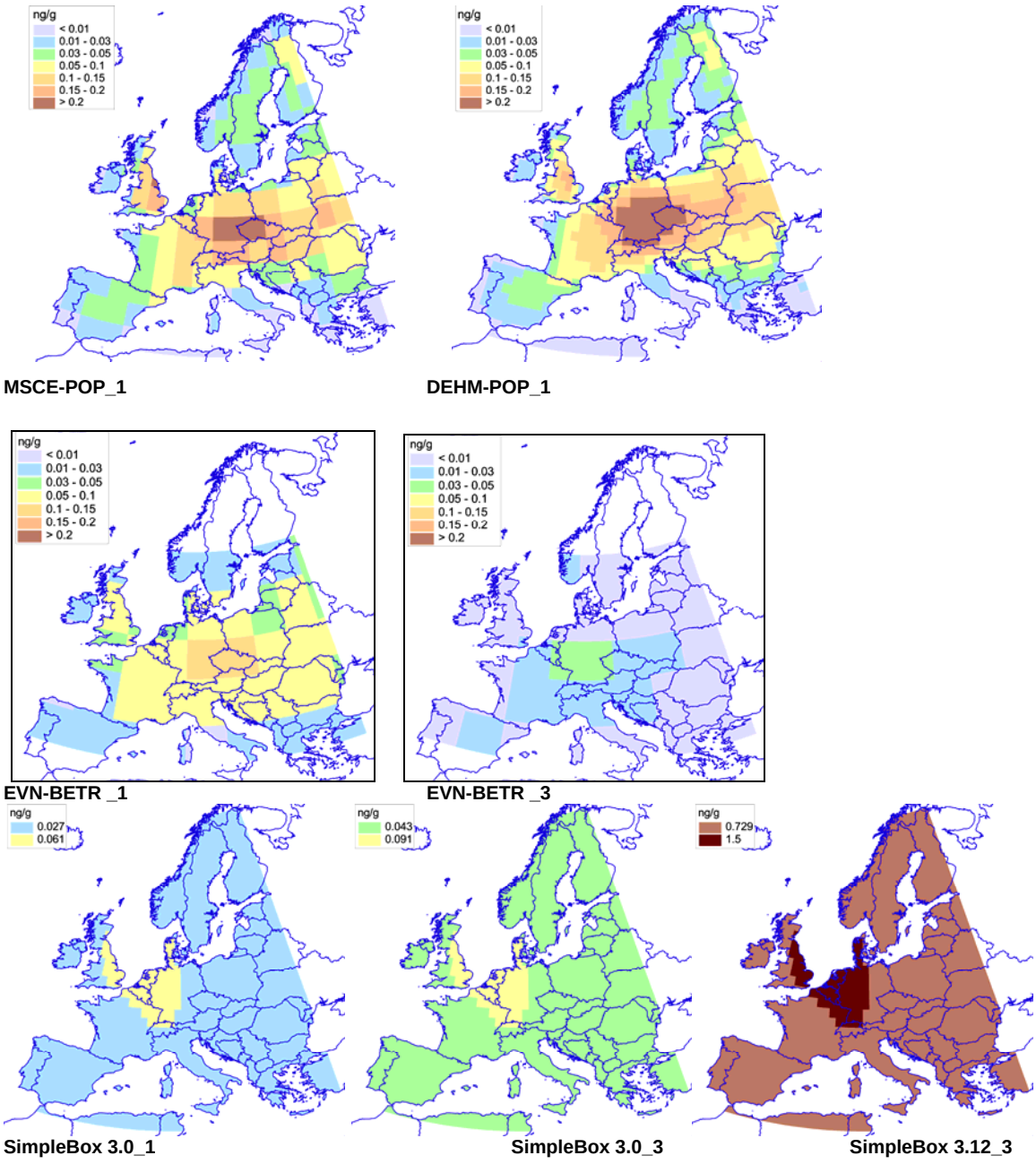


Fig. C.148. *Spatial distribution of PCB-180 concentrations in soil calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Water concentration. The calculated fields of PCB-180 annual concentrations in water of the European calculation domain in 2000 presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. C.149.

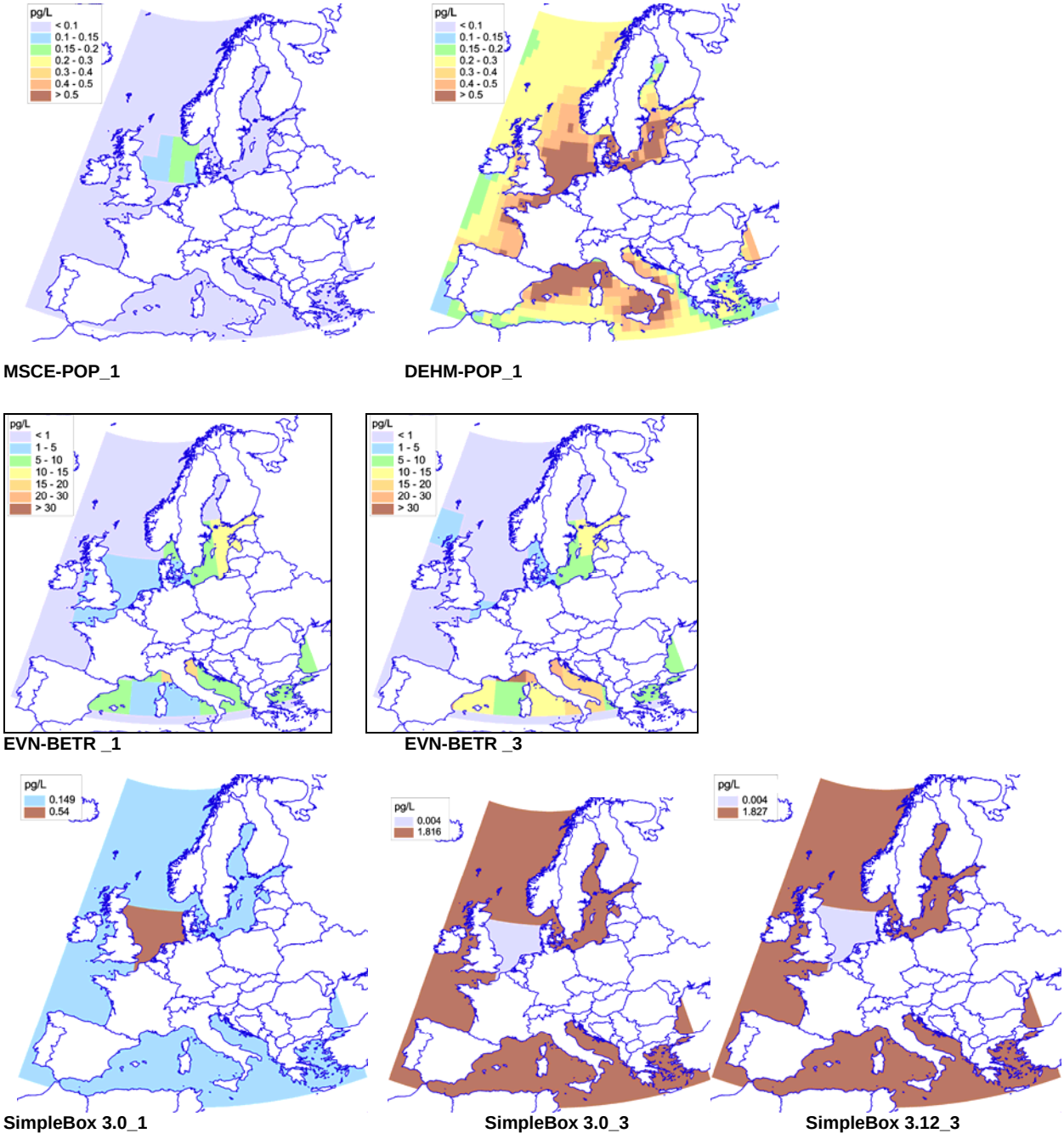


Fig. C.149. *Spatial distribution of PCB-180 concentrations in water calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Concentration in vegetation. The spatial distributions of PCB-180 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.3.150.

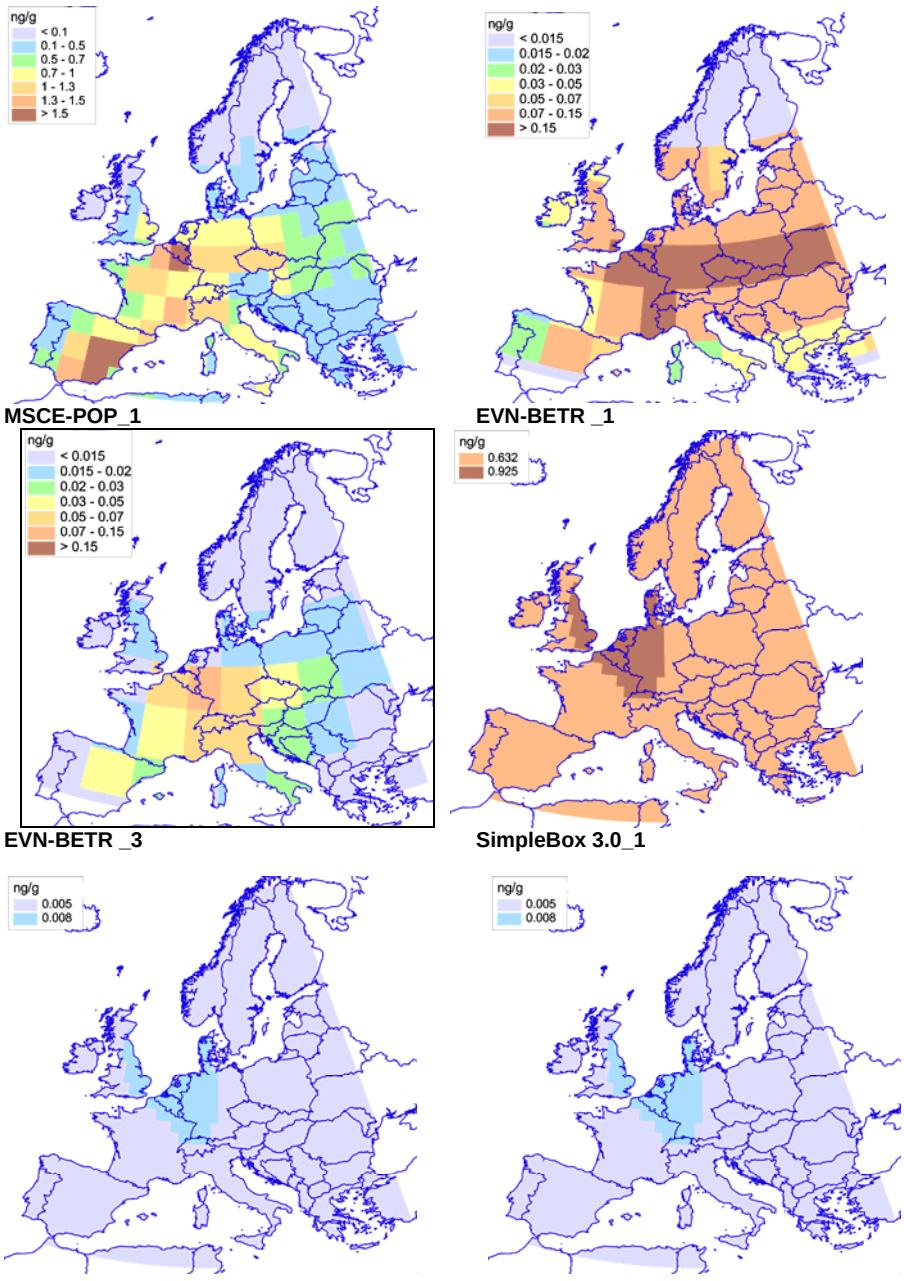


Fig. C.150. *Spatial distribution of PCB-180 concentrations in vegetation calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.*

Net deposition flux. Spatial distributions of PCB-180 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.151. The values of net deposition flux include dry and wet depositions and gaseous exchange. Of note, the spatial variability of SimpleBox results in this case is higher than that in the presented above results on concentrations in the media since the deposition values in this model are dependent on the different types of underlying surfaces, which were taken into account in their calculations.

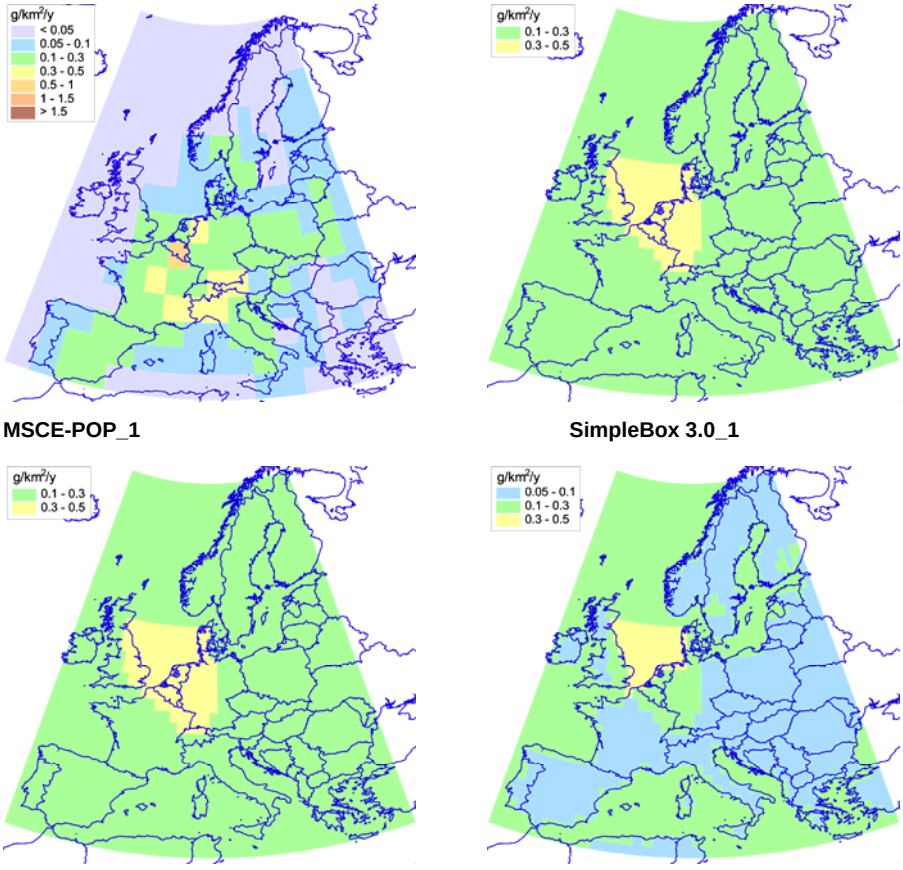


Fig. C.151. *Spatial distribution of PCB-180 net depositions calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions*

Below the comparison of model results obtained on the basis of zero initial concentrations in the environmental media is presented.

Concentration in the atmosphere. The calculated fields of PCB-180 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models for 2000 are compared in Fig. C.152.

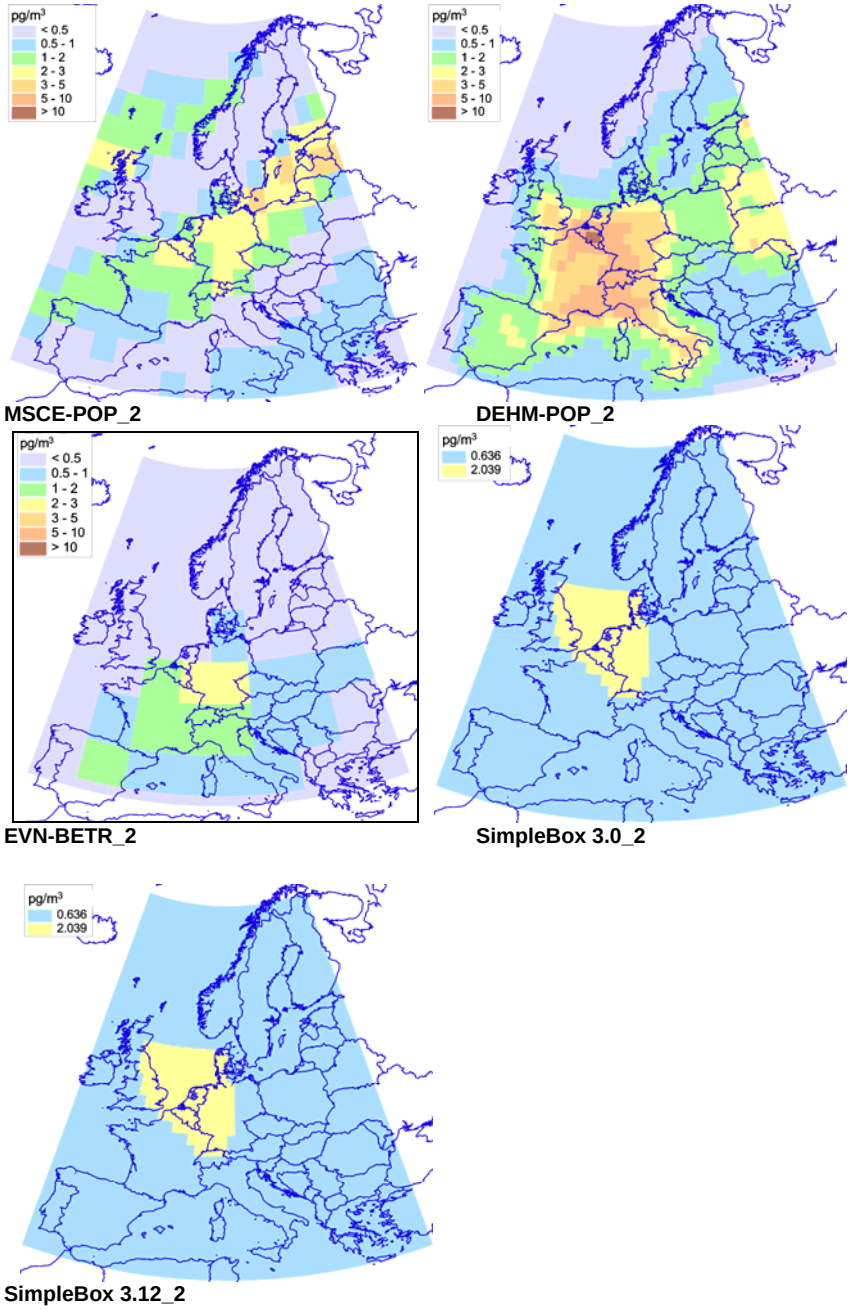
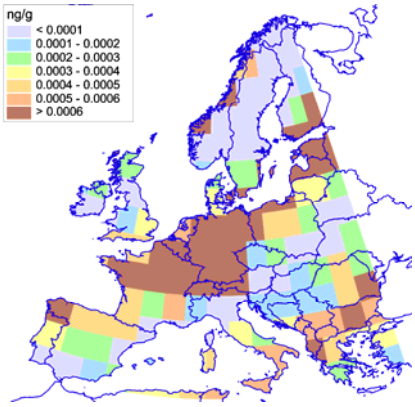
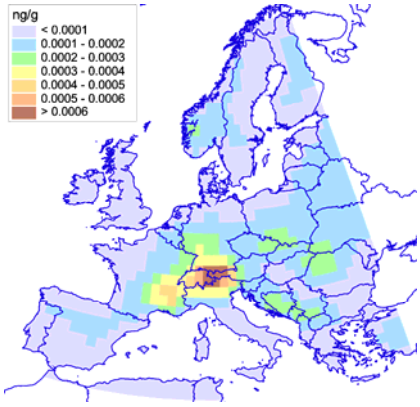


Fig. C.152. *Spatial distribution of PCB-180 concentrations in the atmosphere calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

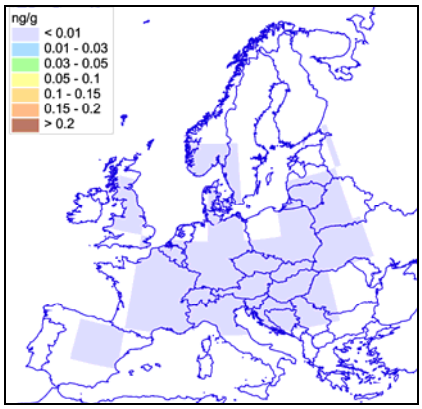
Soil concentration. The spatial distributions of PCB-180 concentration in soil of the European region presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are illustrated in Fig.3.153.



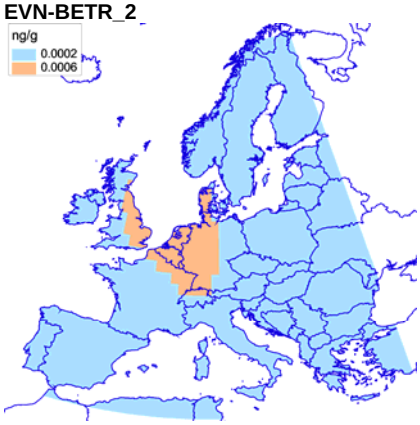
MSCE-POP_2



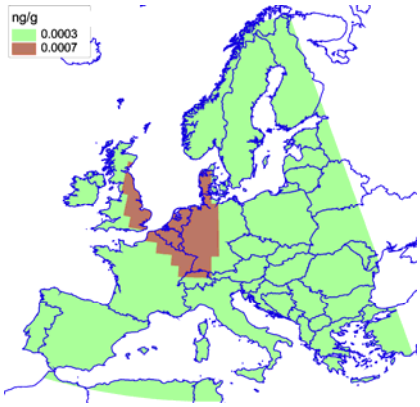
DEHM-POP_2



EVN-BETR_2



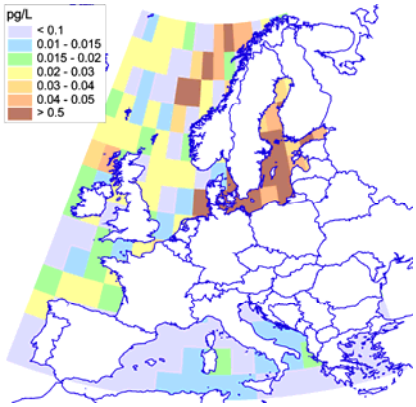
SimpleBox 3.0_2



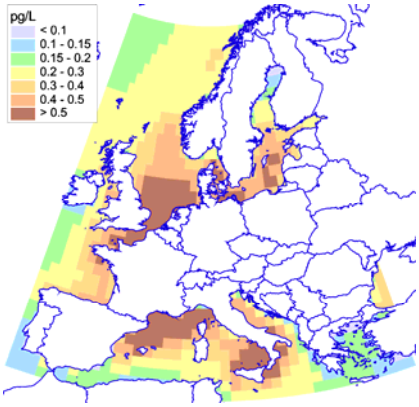
SimpleBox 3.12_2

Fig. C.153. *Spatial distribution of PCB-180 concentrations in soil calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

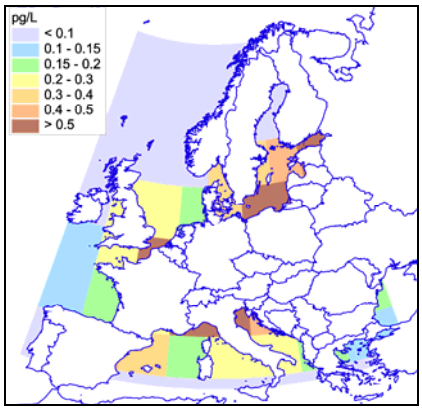
Water concentration. The calculated fields of PCB-180 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig. C.154.



MSCE-POP_2



DEHM-POP_2



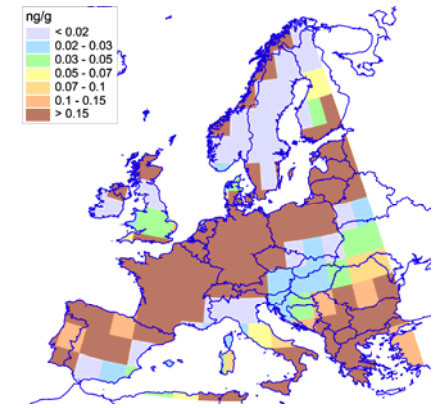
EVN-BETR_2

SimpleBox 3.0_2

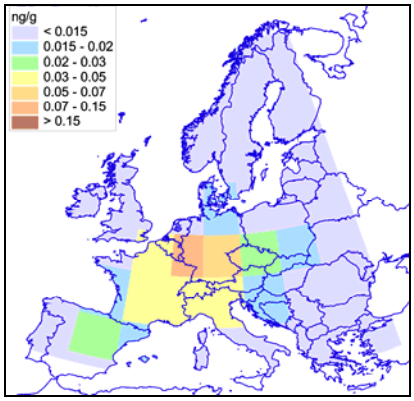
SimpleBox 3.12_2

Fig. C.154. *Spatial distribution of PCB-180 concentrations in water calculated by the participating models on the basis of "reference" data set and zero initial concentrations.*

Concentration in vegetation. The spatial distributions of PCB-180 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.3.155.

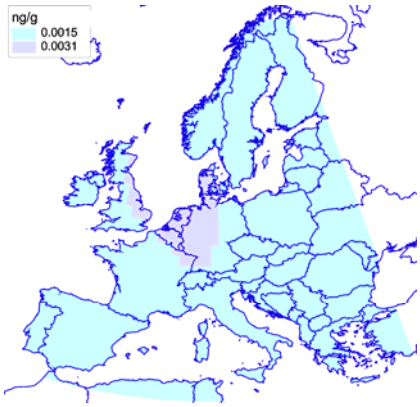


MSCE-POP_2



EVN-BETR_2

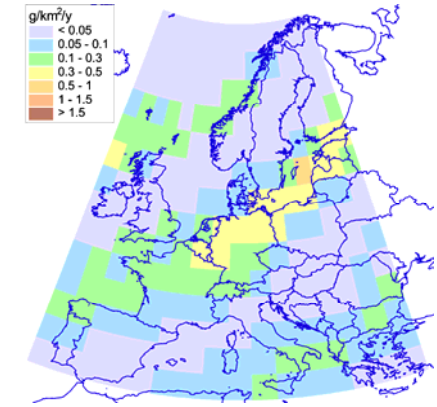
SimpleBox 3.0_2



SimpleBox 3.12_2

Fig. C.155. *Spatial distribution of PCB-180 concentrations in vegetation calculated by the participating models on the basis of "reference" data set and zero initial concentrations.*

Net deposition flux. Spatial distributions of PCB-180 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.156. The values of net deposition flux include dry and wet depositions and gaseous exchange.



MSCE-POP_2

SimpleBox 3.0_2

SimpleBox 3.12_2

Fig. C.156. *Spatial distribution of PCB-180 net depositions calculated by the participating models on the basis of "reference" data set and zero initial concentrations*

C.6.2. Comparison of results on spatial distribution of PCB-180 depositions and concentrations in different compartments obtained on the basis of "own or alternative" data sets

In this section a comparison of spatial distributions of PCB-180 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models "own or alternative" data sets on the basis of initial concentrations of pollutants in media, historical emissions and zero initial conditions is presented.

Concentration in the atmosphere. The calculated fields of PCB-180 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. C.157.

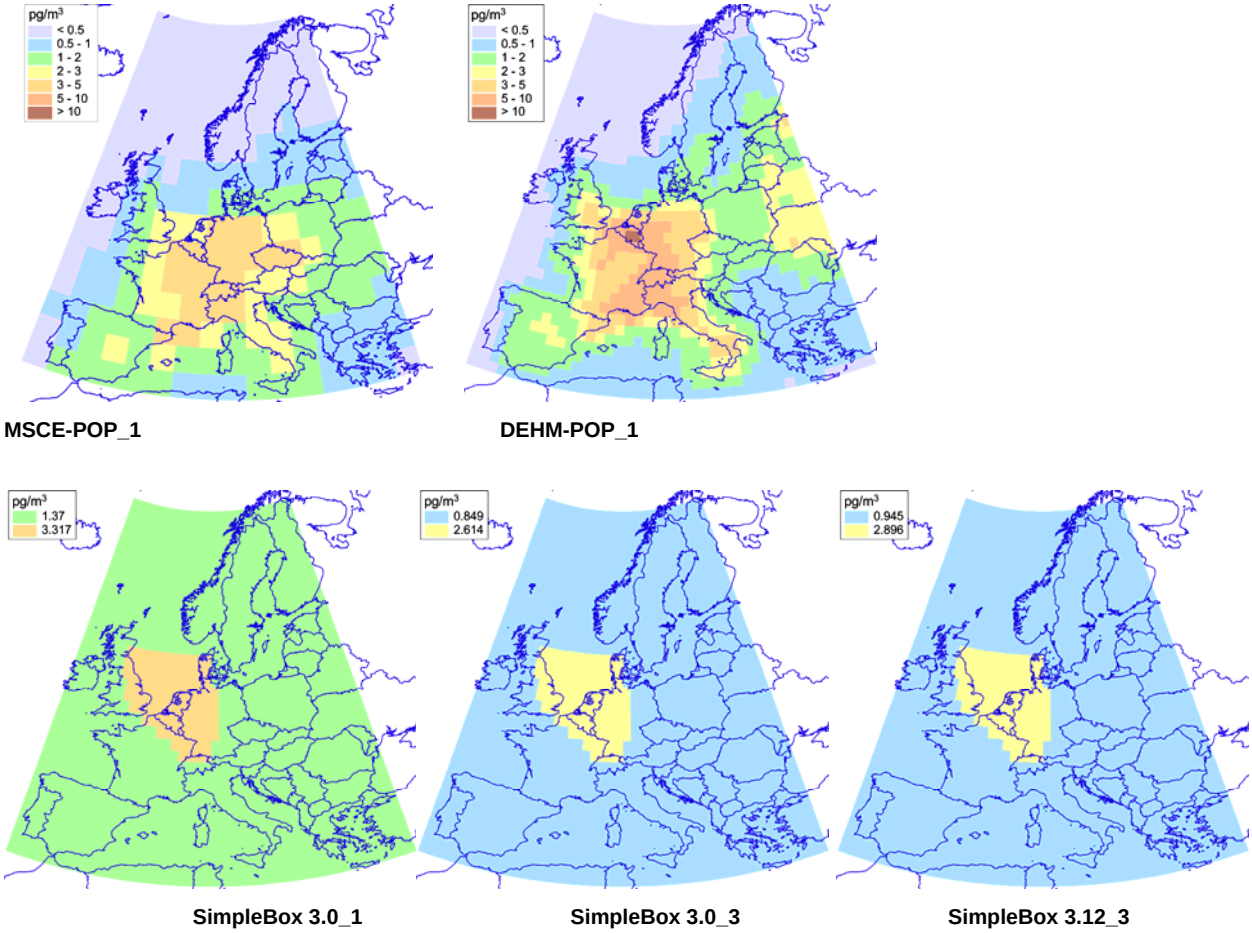
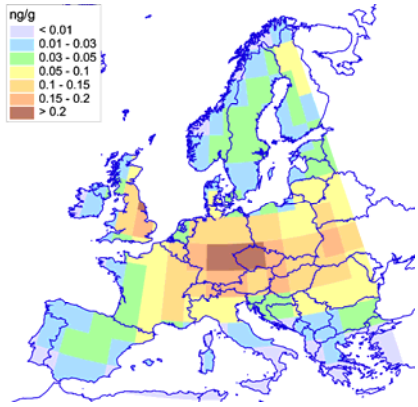
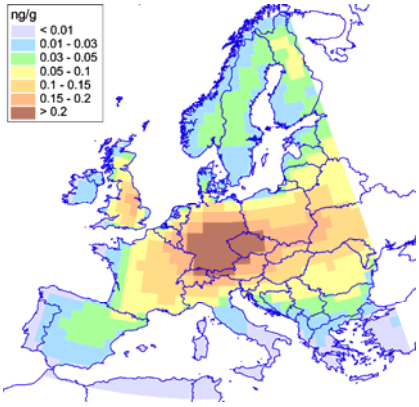


Fig. C.157. *Spatial distribution of PCB-180 concentrations in the atmosphere calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*

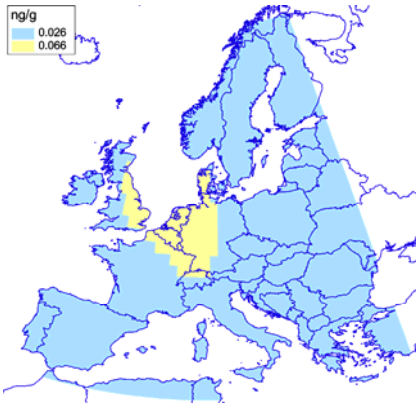
Soil concentration. The spatial distributions of PCB-180 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.158.



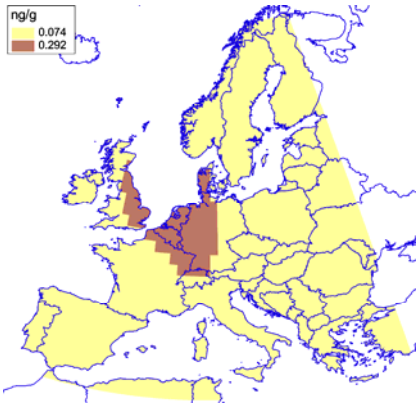
MSCE-POP_1



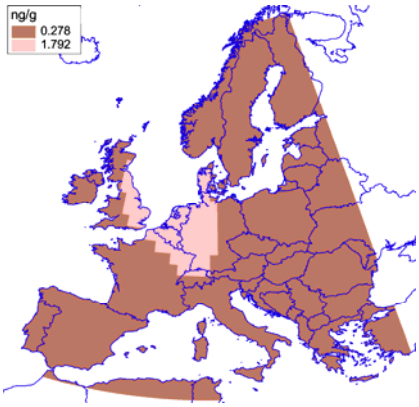
DEHM-POP_1



SimpleBox 3.0_1



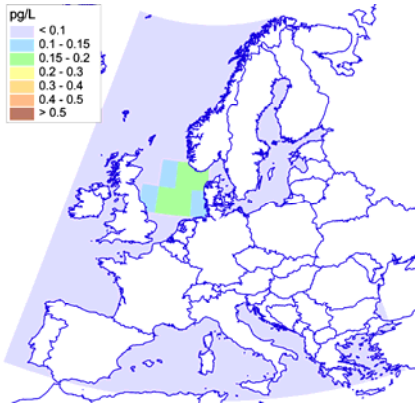
SimpleBox 3.0_3



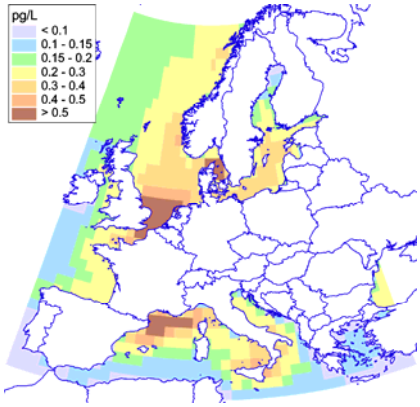
SimpleBox 3.12_3

Fig. C.158. *Spatial distribution of PCB-180 concentrations in soil calculated by the participating models on the basis of "own or alternative" data set taking into account initial concentrations of pollutants in media or historical emissions*

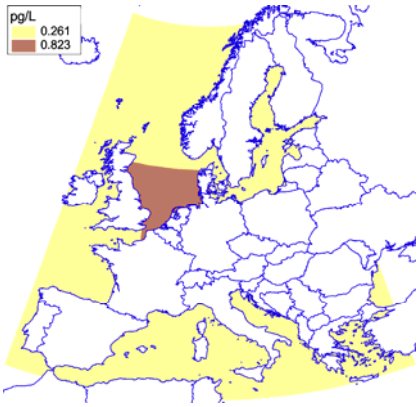
Water concentration. The calculated fields of PCB-180 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. C.159.



MSCE-POP_1



DEHM-POP_1



SimpleBox 3.0_1

SimpleBox 3.0_3

SimpleBox 3.12_3

Fig. C.159. *Spatial distribution of PCB-180 concentrations in water calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*

Concentration in vegetation. The spatial distributions of PCB-180 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.3.160.

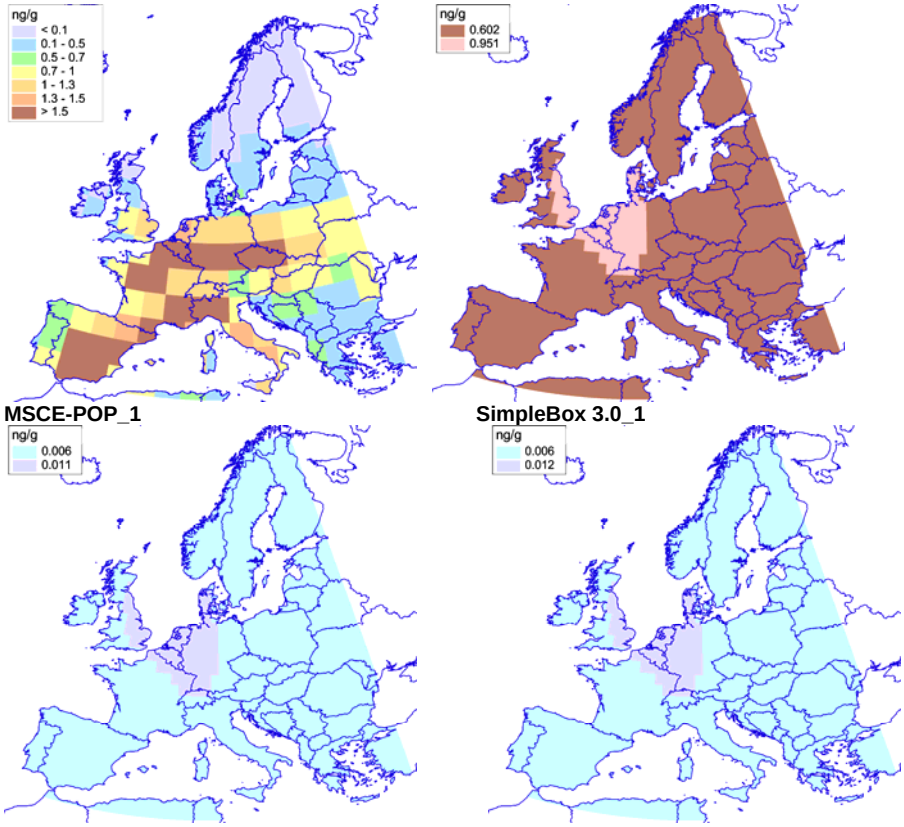


Fig. C.160. *Spatial distribution of PCB-180 concentrations in vegetation calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions***.**

Net deposition flux. Spatial distributions of PCB-180 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.161. The values of net deposition flux include dry and wet depositions and gaseous exchange.

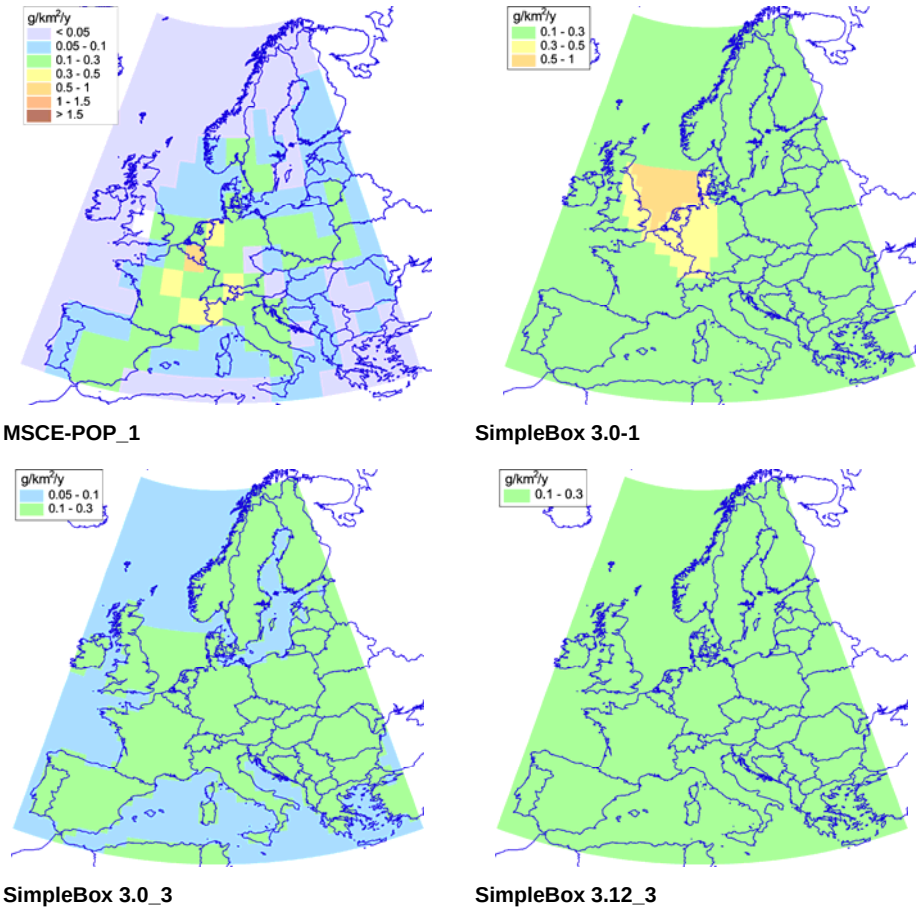


Fig. C.161. *Spatial distribution of PCB-180 net depositions calculated by the participating models on the basis of "own or alternative" data sets taking into account initial concentrations of pollutants in media or historical emissions*.

The model results obtained on the basis of zero initial concentrations in the environmental media are compared below.

Concentration in the atmosphere. The calculated fields of PCB-180 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. C.162.

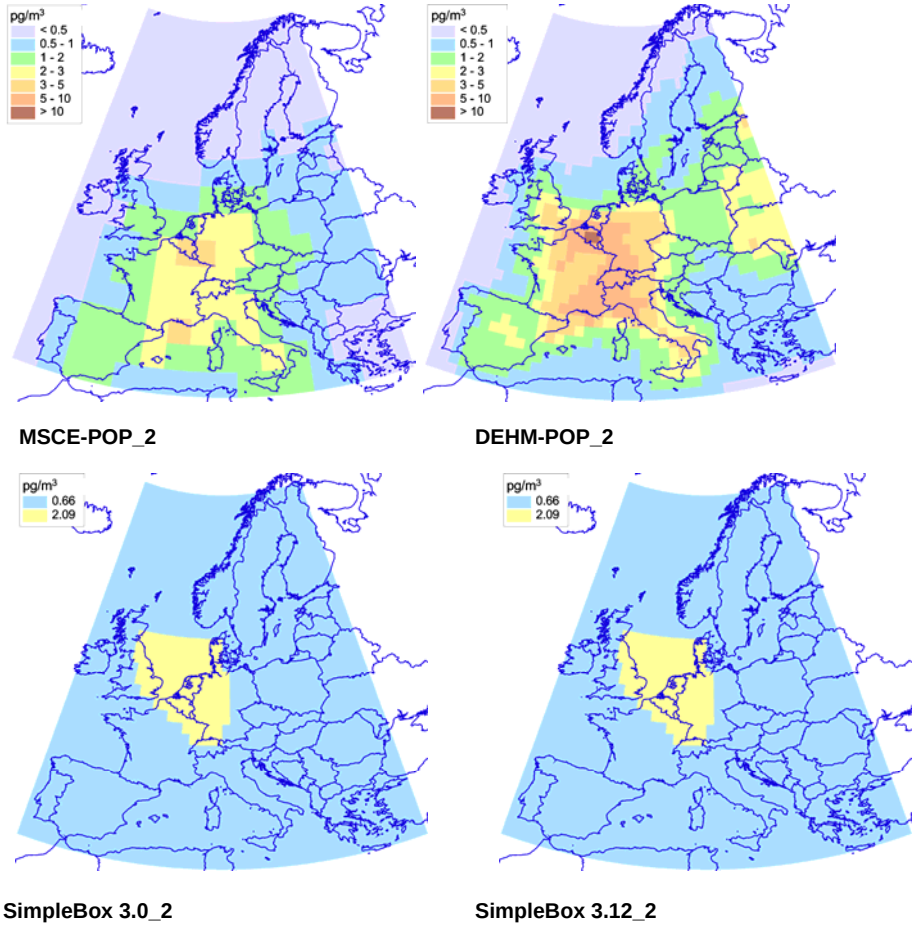


Fig. C.162. *Spatial distribution of PCB-180 concentrations in the atmosphere calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations.*

Soil concentration. The spatial distributions of PCB-180 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.163.

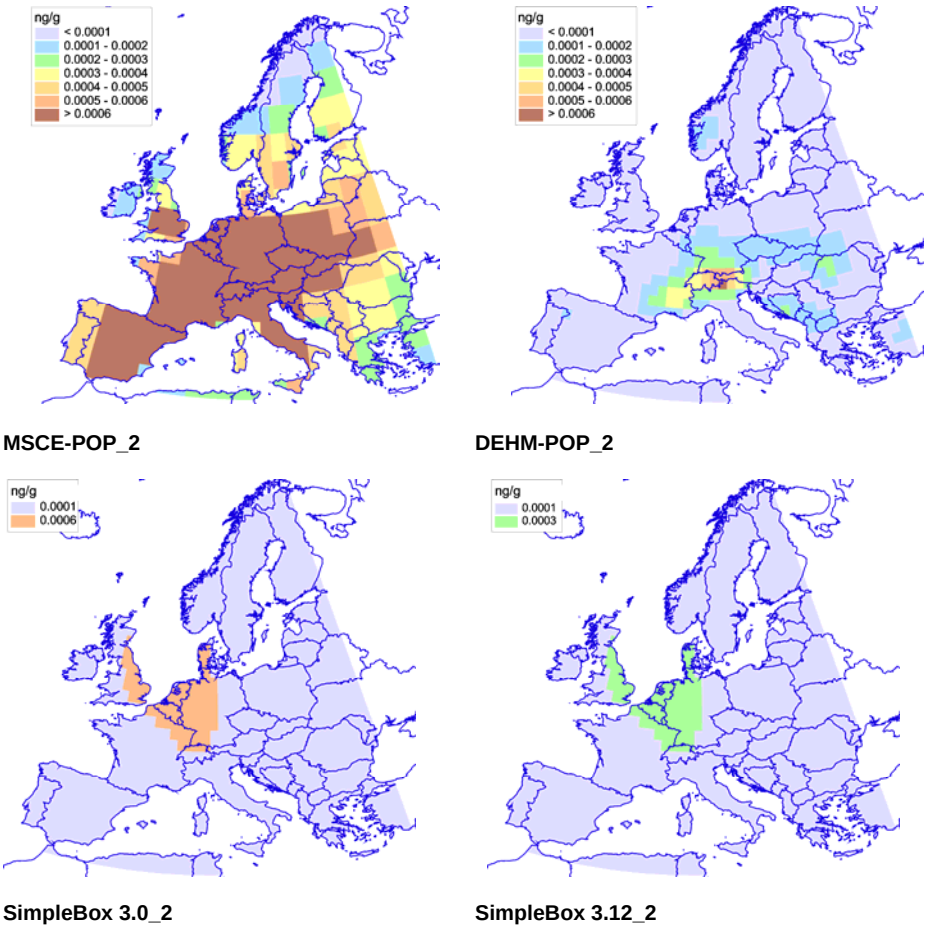


Fig. C.163. *Spatial distribution of PCB-180 concentrations in soil calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*.

Water concentration. The calculated fields of PCB-180 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. C.188.

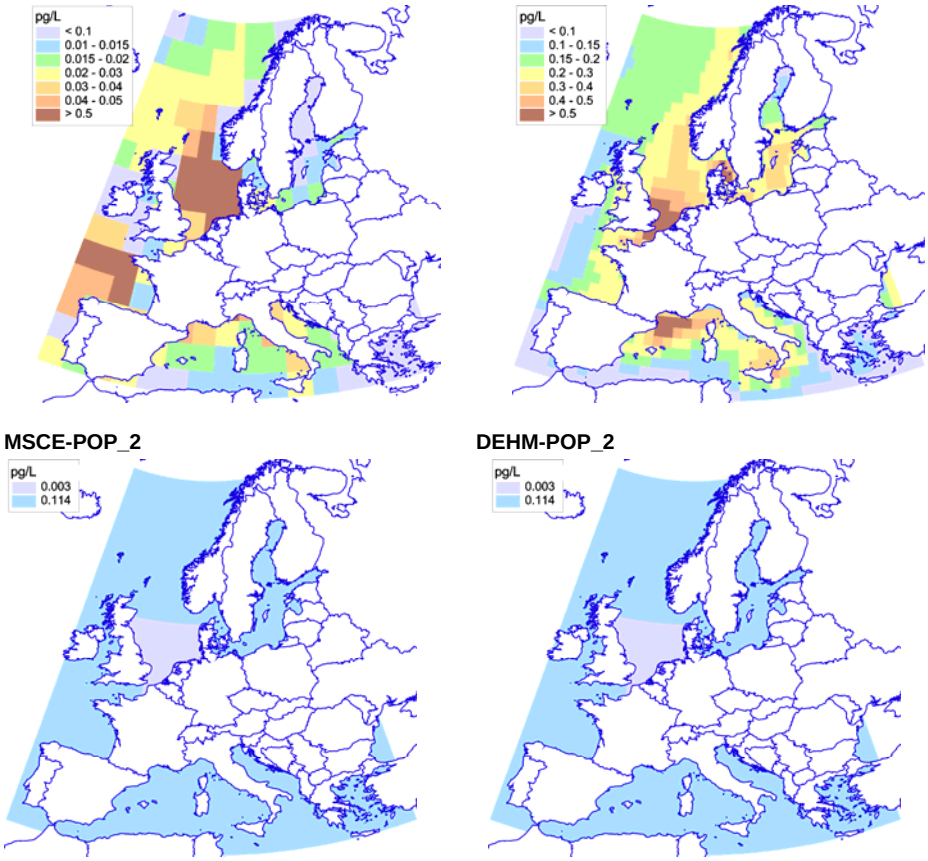
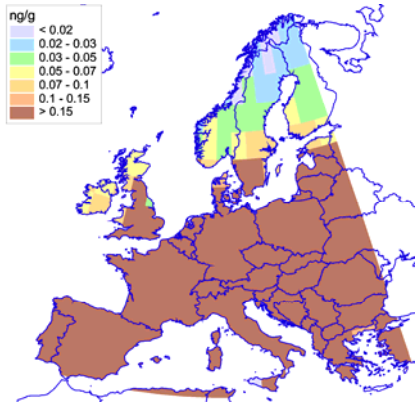
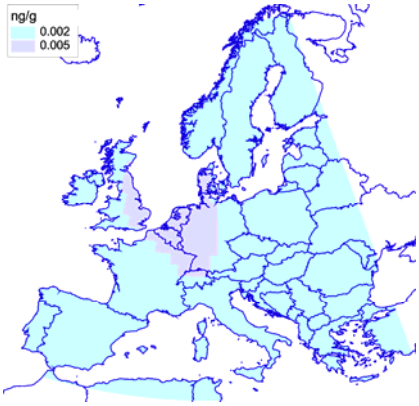


Fig. C.164. *Spatial distribution of PCB-180 concentrations in water calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

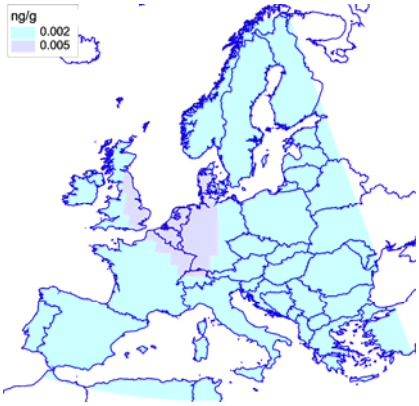
Concentration in vegetation. The spatial distributions of PCB-180 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.3.165.



MSCE-POP_2



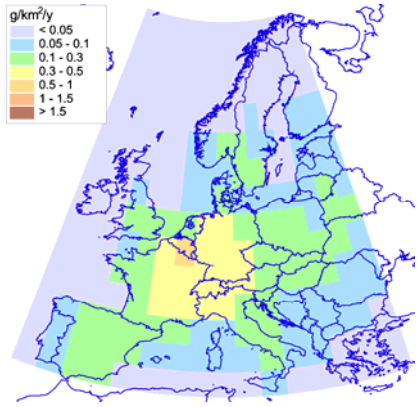
SimpleBox 3.0_2



SimpleBox 3.12_2

Fig. C.165. *Spatial distribution of PCB-180 concentrations in vegetation calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

Net deposition flux. Spatial distributions of PCB-180 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.166. The values of net deposition flux include dry and wet depositions and gaseous exchange.



MSCE-POP_2

SimpleBox 3.0_2

SimpleBox 3.12_2

Fig. C.166. *Spatial distribution of PCB-180 net depositions calculated by the participating models on the basis of "own or alternative" data sets and zero initial concentrations*

Annex D

SENSITIVITY STUDY WITH RESPECT TO SUBSTANCE-SPECIFIC PROPERTIES USED IN THE DESCRIPTION OF BASIC PROCESSES FOR PCB-28

D.1. Gas/particle partitioning

Reference data set. Calculation results for PCB-28 together with m_φ and σ_φ are presented in Table D.1.

Table D.1. *Calculation results: fractions of particulate phase of PCB-28 calculated by models and statistical parameters used for evaluation ("reference" data set)*

Exp.No	T (°C)	DEHM-POP	CliMoChem	SimpleBox*	m_φ	σ_φ
1	-12	0.044	0.011	0.256	**0.104**	**0.133**
2	-5	0.018	0.009	0.123	**0.050**	**0.064**
3	0	0.009	0.008	0.071	**0.029**	**0.036**
4	6	0.004	0.007	0.036	**0.016**	**0.018**
5	10	0.003	0.006	0.023	**0.011**	**0.011**
6	15	0.002	0.006	0.014	**0.007**	**0.006**
7	20	0.001	0.005	0.008	**0.005**	**0.004**
8	25	0.001	0.008		**0.004**	**0.005**
9	25	0.001	0.005		**0.003**	**0.003**
10	26	0.001	0.008	0.004	**0.004**	**0.003**
11	32	0.001	0.009	0.002	**0.004**	**0.005**

* - only 9 experiments for Simple Box

The plot of dependence of φ on T calculated by participating models is presented in Fig. D.1.

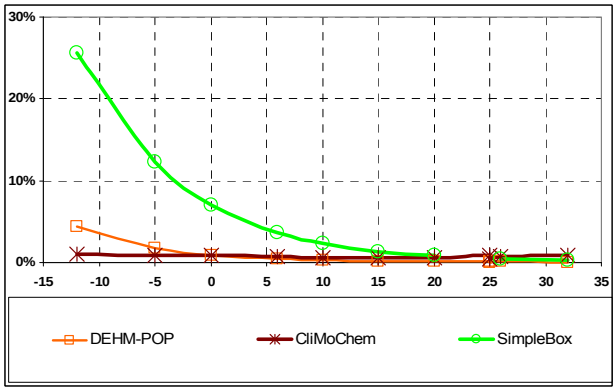


Fig. D.1. *Calculation results of the participating models (gas-particle partitioning) obtained with reference data set*

Calculated correlation coefficients between the results of participating models are given in Table D.2.

Table D.2. *Correlation coefficients* r_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.70	1.00
CliMoChem	–	0.75

* - by 9 experiments only

The values of regression coefficients α and β calculated for all pairs of models are shown in Table D.3.

Table D.3. *Coefficients of regression dependence between the models (α / β)*

	CliMoChem	SimpleBox*
DEHM-POP	0.10 / 0.01	5.80 / 0.01
CliMoChem	–	35.44 / - 0.21

* - by 9 experiments only

Results of the calculation of pairwise residual square deviation σ are given in Table D.4.

Table D.4. *Residual square deviation,* σ^{res}_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.004	0.022
CliMoChem	–	0.156

* - by 9 experiments only

Own/altenative data set. Calculation results for PCB-28 together with m_φ and $\sigma_{,\varphi}$ are presented in Table D.5. The data set used in calculations by each model is indicated in the first row.

Table D.5. *Calculation results: fractions of particulate phase of PCB-28 calculated by models and statistical parameters used for evaluation (own/alternative data set)*

Exp.No	*T* (°C)	EVN-BETR and UK-MODEL	DEHM-POP	MSCE-POP_1	MSCE-POP_2	CliMoChem	SimpleBox	m_φ	σ_φ
Data set		own	own	own	own	own	alt		
1	-12	0.190	0.061	0.061	0.054	0.028	0.058	**0.075**	**0.058**
2	-5	0.083	0.025	0.025	0.023	0.017	0.034	**0.034**	**0.024**
3	0	0.045	0.014	0.013	0.013	0.012	0.023	**0.020**	**0.013**
4	6	0.022	0.007	0.006	0.007	0.008	0.015	**0.011**	**0.006**
5	10	0.014	0.004	0.004	0.004	0.007	0.011	**0.007**	**0.004**
6	15	0.008	0.002	0.002	0.002	0.005	0.008	**0.005**	**0.003**
7	20	0.004	0.001	0.001	0.001	0.004	0.006	**0.003**	**0.002**
8	25	0.004	0.001	0.001	0.001	0.005	0.006	**0.002**	**0.002**
9	25	0.003	0.001	0.001	0.001	0.003	0.004	**0.002**	**0.001**
10	26	0.004	0.001	0.001	0.001	0.004	0.006	**0.003**	**0.002**
11	32	0.003	0.001	0.0004	0.001	0.004	0.006	**0.003**	**0.002**

The plot of dependence of φ on *T* calculated by participating models with “own or alternative” data set is presented in Fig. D.2.

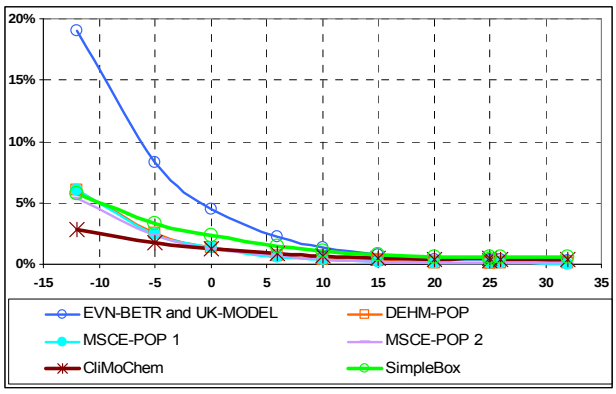


Fig. D.2. *Calculation results of the participating models (gas-particle partitioning) obtained with “own/alternative” data set*

Calculated correlation coefficients between the results of participating models are given in Table D.6.

Table D.6. *Correlation coefficients* r_{12}

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	1.00	1.00	1.00	0.98	0.99
DEHM-POP	–	1.00	1.00	0.98	0.99
MSCE-POP 1	–	–	1.00	0.98	0.98
MSCE-POP 2	–	–	–	0.98	0.99
CliMoChem	–	–	–	–	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table D.7.

Table D.7. *Coefficients of regression dependence between the models* (α / β)

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.317 / - 0.0001	0.318 / -0.0004	0.283 / 0.00003	0.135 / 0.004	0.287 / 0.006
DEHM-POP	–	1.0021 / -0.0003	0.893 / 0.0002	0.423 / 0.004	0.901 / 0.006
MSCE-POP 1	–	–	0.890 / 0.0004	0.420 / 0.004	0.896 / 0.007
MSCE-POP 2	–	–	–	0.475 /0.004	1.011 / 0.006
CliMoChem	–	–	–	–	2.118 / -0.003

Results of calculations of pairwise residual square deviation σ are given in Table D.8.

Table D.8. *Residual square deviation,* σ^{res}_{12}

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.001	0.002	0.001	0.004	0.008
DEHM-POP	–	0.001	0.001	0.005	0.009
MSCE-POP 1	–	–	0.002	0.005	0.009
MSCE-POP 2	–	–	–	0.004	0.008
CliMoChem	–	–	–	–	0.002

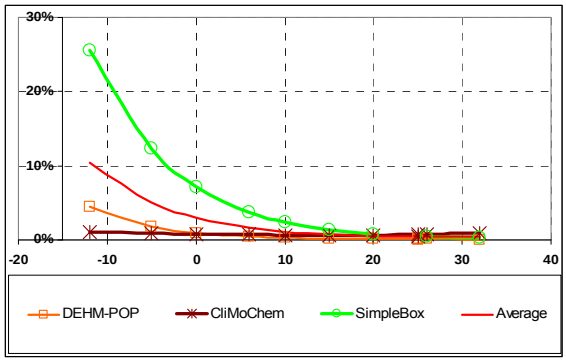
Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table D.9.

Table D.9. *Difference between calculations with two data sets*

Exp.No	*T* (°C)	DEHM-POP	CliMoChem	SimpleBox
1	-12	37%	162%	-77%
2	-5	43%	91%	-73%
3	0	47%	53%	-68%
4	6	52%	19%	-59%
5	10	54%	1%	-52%
6	15	58%	-18%	-42%
7	20	61%	-32%	-30%
8	25	64%	-44%	
9	25	64%	-44%	
10	26	65%	-46%	42%
11	32	69%	-56%	136%

This difference is visualized in Fig. D.3.

a



b

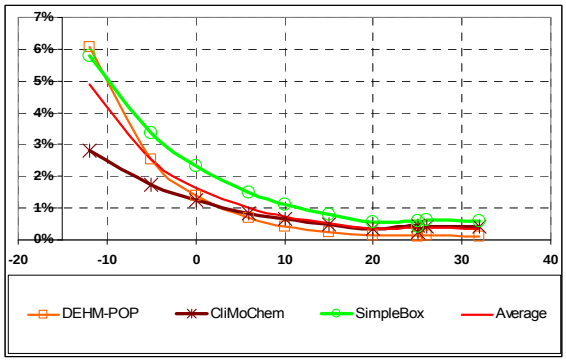


Fig. D.3. *Calculation results of the participating models obtained with "reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

4.2. Wet deposition

Reference data set. Calculation results for PCB-28 together with *m* and σ are presented in Tables 4. 4.10 and 4.11.

Table D.10. *Calculation results: concentrations in precipitation (pg/L) ("reference" data set)*

Exp. No	*T* (°C)	CliMoChem	SimpleBox	*m*	σ
1	-1	176	612	**394**	**308**
2	3	311	1077	**694**	**542**
3	10	28	202	**115**	**123**
4	-1	18	612	**315**	**420**
5	3	31	1077	**554**	**740**
6	10	3	202	**103**	**141**

Table D.11. *Calculation results: wet deposition flux, ng/m^2/hour ("reference" data set)*

Exp. No	*T* (°C)	CliMoChem	SimpleBox	*m*	σ
1	-1	0.176	0.612	**0.394**	**0.308**
2	3	0.311	1.077	**0.694**	**0.542**
3	10	0.028	0.202	**0.115**	**0.123**
4	-1	0.176	6.119	**3.147**	**4.202**
5	3	0.311	10.773	**5.542**	**7.398**
6	10	0.028	2.022	**1.025**	**1.410**

The comparison of calculated values of concentrations in precipitation is displayed in Fig. D.4.

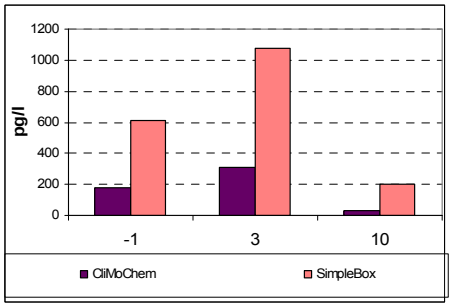


Fig. D.4. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (reference data set)*

Calculated correlation coefficients between the results of participating models are given in Table D.12.

Table D.12. *Correlation coefficients* r_{12}

	SimpleBox
CliMoChem	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table D.13.

Table D.13. *Coefficients of regression dependence between the models* (α / β)

	SimpleBox
CliMoChem	3.09 / 100.33

Pairwise residual square deviation σ are shown in Table D.14.

Table D.14. *Residual square deviation,* σ^{res}_{12}

	SimpleBox
CliMoChem	39.84

Own/alternative data set. Calculation results for PCB-28 together with *m* and σ are presented in Tables 4. 4.15 and 4.16.

Table D.15. *Calculation results: concentrations in precipitation (pg/L) (own/alternative data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1	24	456	176	603	**315**	**263**
2	3	30	803	310	1065	**552**	**468**
3	10	166	99	26	109	**100**	**58**
4	-1	–	456	18	603	**359**	**305**
5	3	–	803	31	1065	**633**	**538**
6	10	–	99	3	109	**70**	**59**

Table D.16. *Calculation results: wet deposition flux, ng/m*^{2}*/hour (own/alternative data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1	0.024	0.456	0.176	0.603	**0.315**	**0.263**
2	3	0.030	0.803	0.310	1.065	**0.552**	**0.468**
3	10	0.166	0.099	0.026	0.109	**0.100**	**0.058**
4	-1	–	4.560	0.176	6.029	**3.588**	**3.045**
5	3	–	8.030	0.310	10.651	**6.330**	**5.376**
6	10	–	0.990	0.026	1.090	**0.702**	**0.588**

The comparison of calculated values of concentrations in precipitation is displayed in Fig. D.5.

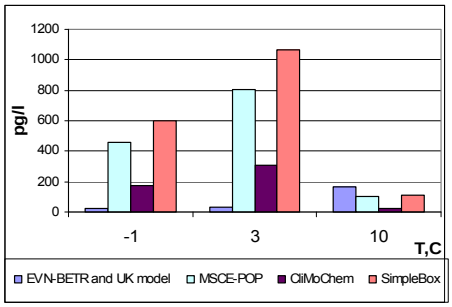


Fig. D.5. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (own/alternative data set)*

Calculated correlation coefficients between the results of participating models are given in Table D.17.

Table D.17. *Correlation coefficients* r_{12}

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	-0.85	-0.86	-0.86
MSCE-POP	–	1.00	1.00
CliMoChem	–	–	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table D.18.

Table D.18. *Coefficients of regression dependence between the models* (α / β)

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	-3.73 / 726.24	-1.53 / 282.69	-5.10 / 966.39
MSCE-POP	–	0.40 / -12.32	1.36 / -22.48
CliMoChem	–	–	3.36 / 19.10

Finally, pairwise residual square deviation σ are shown in Table D.19.

Table D.19. *Residual square deviation,* σ^{res}_{12}

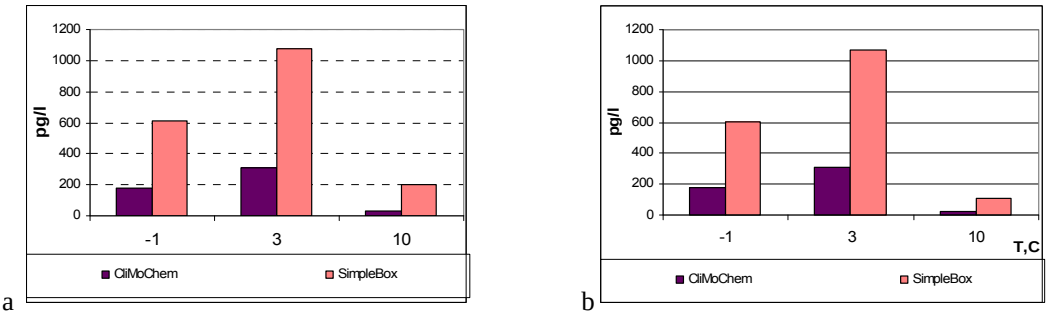
	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	261.38	101.63	348.77
MSCE-POP	–	4.68	7.33
CliMoChem	–	–	8.38

Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table D.20.

Table D.20. *Difference between calculations with two data sets*

Exp. No	*T* (°C)	CliMoChem	SimpleBox
1	-1	-0.1%	-1.5%
2	3	-0.1%	-1.1%
3	10	-7.7%	-46.1%

These results are visualized in Fig. D.6.



a b

Fig. D.6. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

4.3. Gaseous exchange between atmosphere and soil

Here we present numerical results of calculations of soil concentrations and net gaseous flux to soil obtained by the participating models and their analysis for PCB-28 with "reference" and "own/alternative" data sets.

Fig. D.7 illustrates air concentration trend used in calculations for Experiment 1.

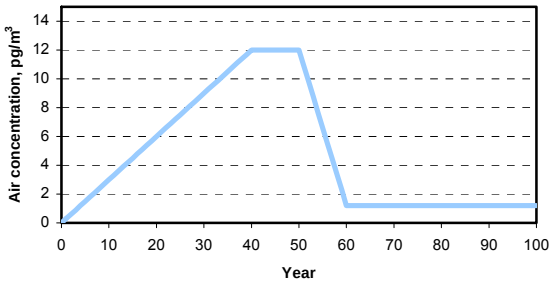


Fig. D.7. *Air concentration trend used for calculations for MSCE-POP model (MSCE-POP 2) for Experiment 1*

Reference data set. Calculation results for soil concentrations together with m and σ calculated with "reference" data set of PCB-28 properties are presented in Table D.21. Net gaseous fluxes to soil of PCB-28 calculated by the models and statistical parameters used for its evaluation are given in Table D.22.

Table D.21. *Calculation results: soil concentrations of PCB-28 (ng/g) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	DEHM-POP	CliMoChem	SimpleBox	m	σ
1	1.2	0.137	0.001	0.0001	**0.046**	**0.079**
2	5.6	0.043	0.003	0.001	**0.016**	**0.024**
3	4.2	0.020	0.003	0.001	**0.008**	**0.011**
4	1.8	0.004	0.001	0.0001	**0.002**	**0.002**

Table D.22. *Calculation results: net gaseous flux to soil, of PCB-28 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	CliMoChem	SimpleBox	m	σ
1	1.2	0.02	0.07	**0.05**	**0.04**
2	5.6	0.09	0.40	**0.25**	**0.22**
3	4.2	0.07	0.25	**0.16**	**0.13**
4	1.8	0.03	0.08	**0.05**	**0.04**

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Pairwise regression analysis is performed only for values of soil concentrations and deposition fluxes calculated by models using steady state and dynamic approaches. In spite of the fact that numerical values of soil concentrations are highly different, the variations of the corresponding numerical values

caused by change of environmental conditions between different experiments are similarly described by most of models. This can be seen from values of pairwise correlation coefficients (Table D.23).

Table D.23. *Correlation coefficients for soil concentrations of PCB-28 ("reference" data set)*

	CliMoChem	SimpleBox
DEHM-POP	-0.39	-0.26
CliMoChem	–	0.95

Correlation coefficients for net gaseous flux are presented in Table D.24.

Table D.24. *Correlation coefficients for net gaseous flux to soil of PCB-28 ("reference" data set)*

	SimpleBox
CliMoChem	0.03

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Tables 4.25 and 4.26, respectively.

Table D.25. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-28 ("reference" data set)*

	CliMoChem	SimpleBox
DEHM-POP	-0.008 /0.0021	-0.002 /0.0006
CliMoChem	–	0.342 / -0.0001

Table D.26. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-28 ("reference" data set)*

	SimpleBox
CliMoChem	4.287 / -0.022

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table D.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-28 ("reference" data set)*

	CliMoChem	SimpleBox
DEHM-POP	0.002	0.001
CliMoChem	–	0.0002

Table D.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-28 ("reference" data set)*

	SimpleBox
CliMoChem	0.16

Own/alternative data set. Calculation results soil concentrations together with m and σ calculated with "own/alternative" data set of PCB-28 properties are presented in Table D.29. Net gaseous fluxes to soil of PCB-28 calculated by the models and statistical parameters used for its evaluation are given

in Table D.30. Table D.29 contains also the information of the data set used for calculations for each model.

Table D.29. *Calculation results: soil concentrations of PCB-28 (ng/g) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	*m*	σ
				1	2				
		own	own	own		own	alt		
1	1.2	0.0001	0.018	0.010	0.051	0.0005	0.003	**0.014**	**0.020**
2	5.6	0.0005	0.196	0.076	0.421	0.002	0.026	**0.120**	**0.165**
3	4.2	0.0004	0.089	0.045	0.241	0.002	0.016	**0.066**	**0.092**
4	1.8	0.0001	0.019	0.007	0.036	0.0004	0.003	**0.011**	**0.014**

Table D.30. *Calculation results: net gaseous flux to soil, of PCB-28 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*[*]

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	*m*	σ
				1	2				
1	1.2	0.001	–	-0.029	-0.152	0.019	0.044	**-0.023**	**0.077**
2	5.6	0.005	–	-0.031	-0.617	0.094	0.282	**-0.053**	**0.338**
3	4.2	0.004	–	-0.096	-0.509	0.068	0.158	**-0.075**	**0.260**
4	1.8	0.002	–	-0.071	-0.205	0.024	0.046	**-0.041**	**0.102**

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Pairwise correlation coefficients are given in Table D.31.

Table D.31. *Correlation coefficients for soil concentrations of PCB-28 ("own/alternative" data set)*

		DEHM-POP	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.93	0.97	0.97	1.00	0.98
DEHM-POP		–	0.99	0.99	0.94	0.98
MSCE-POP	1	–	–	1.00	0.98	1.00
	2	–	–	–	0.97	1.00
CliMoChem		–	–	–	–	0.99

Correlation coefficients for net gaseous flux are presented in Table D.32.

Table D.32. *Correlation coefficients for net gaseous flux to soil of PCB-28 ("own/alternative" data set)*

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
EVN-BETR and UK MODEL		-0.08	-1.00	1.00	0.97
MSCE-POP	1	–	-0.13	-0.02	0.14
	2	–	–	-0.99	-0.96
CliMoChem		–	–	–	0.99

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Table D.33 and 34, respectively.

Table D.33. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-28 ("own/alternative" data set)*

		DEHM-POP	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		398 / -0.026	164 / -0.010	903 / -0.056	5.4 / -0.0001	57.2 / -0.003
DEHM-POP		–	0.39 / 0.003	2.15 / 0.014	0.01 / 0.0004	0.13 / 0.001
MSCE-POP	1	–	–	5.55 / -0.004	0.03 / 0.0003	0.35 / 0.00004
	2	–	–	–	0.01 / 0.0003	0.06 / 0.0003
CliMoChem		–	–	–	–	10.62 / -0.002

Table D.34. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-28 ("own/alternative" data set)*

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
EVN-BETR and UK MODEL		-1.38/ -0.05	-120.5 / -0.01	19.21 / -0.01	58.68 / -0.04
MSCE-POP	1	–	0.90 / -0.32	-0.02 / 0.05	0.50 / 0.16
	2	–	–	-0.16 / -0.01	-0.48 / -0.04
CliMoChem		–	–	–	3.08 / -0.03

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table D.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-28 ("own/alternative" data set)*

		DEHM-POP	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.055	0.013	0.081	0.0001	0.004
DEHM-POP		–	0.009	0.043	0.0006	0.004
MSCE-POP	1	–	–	0.0074	0.0004	0.0008
	2	–	–	–	0.0004	0.0012
CliMoChem		–	–	–	–	0.003

Table D.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-28 ("own/alternative" data set)*

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
EVN-BETR and UK MODEL		0.056	0.031	0.004	0.044
MSCE-POP	1	–	0.390	0.063	0.194
	2	–	–	0.007	0.055
CliMoChem		–	–	–	0.034

Comparison between two data sets. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table D.29. The corresponding differences between calculated values of net flux to soil were not calculated since near the equilibrium small changes in pollutant properties can lead to essential changes of fluxes (in relative values).

Table D.29. *Difference between calculations with two data sets*

No	Air conc, pg/m^3	DEHM-POP	CliMoChem	SimpleBox
1	1.2	-87%	-11%	2089%
2	5.6	352%	-14%	2365%
3	4.2	342%	-23%	2547%
4	1.8	338%	-30%	2599%

Accumulation/clearance dynamics of PCBs in soil.

Fig. D.8 shows the results of the experiment obtained by CliMoChem and SimpleBox models with the use of "reference" data set.

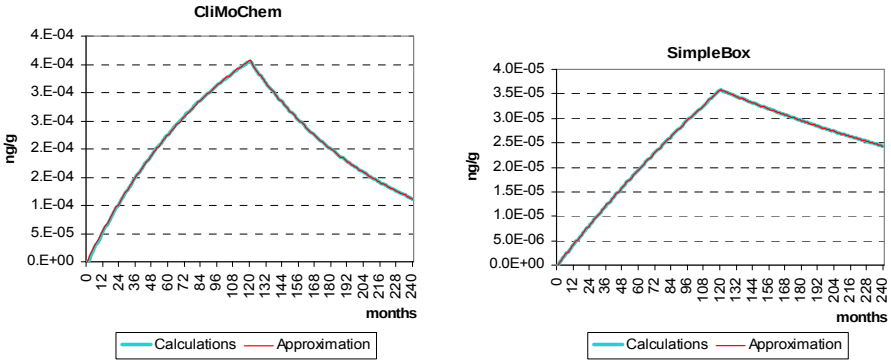


Fig. D.8. *Long-term trends of accumulation and clearance obtained by participating models ("reference" data set)*

The results obtained by CliMoChem, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models with the use of "own/alternative" data sets are presented in Fig. D.9.

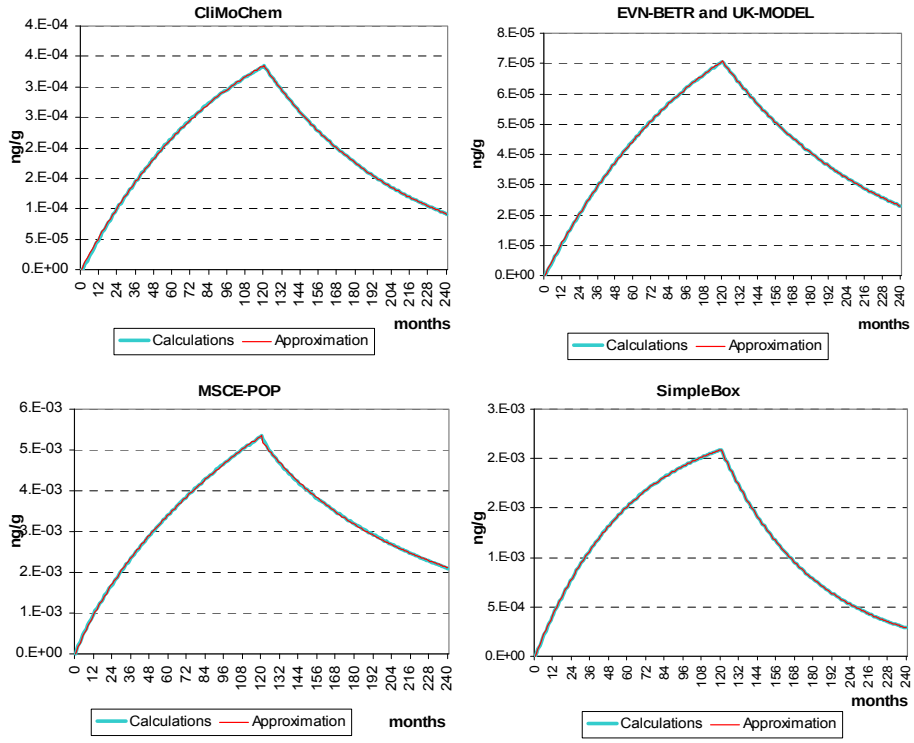


Fig. D.9. *Long-term trends of accumulation and clearance obtained by participating models ("own/alternative" data set)*

The values of characteristic times obtained by the approximation are shown in Table D.30.

Table D.30. *Parameters of multi-exponential approximation*

	CliMoChem		EVN-BETR and UK model		MSCE-POP		SimpleBox	
	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast
"Reference" data set								
Accumulation phase	6.4	6.4	–	–	–	–	18.7	18.7
Clearance phase	6.0	6.0	–	–	–	–	17.8	17.8
"Own/alternative" data set								
Accumulation phase	5.7	5.7	6.5	6.5	10.3	1.2	3.5	3.5
Clearance phase	5.3	5.4	6.2	6.0	10.7	2.9	3.5	3.5

The difference between results obtained with “reference” and “own/alternative” data sets (for those models which have performed both calculations) is illustrated by Fig. D.10.

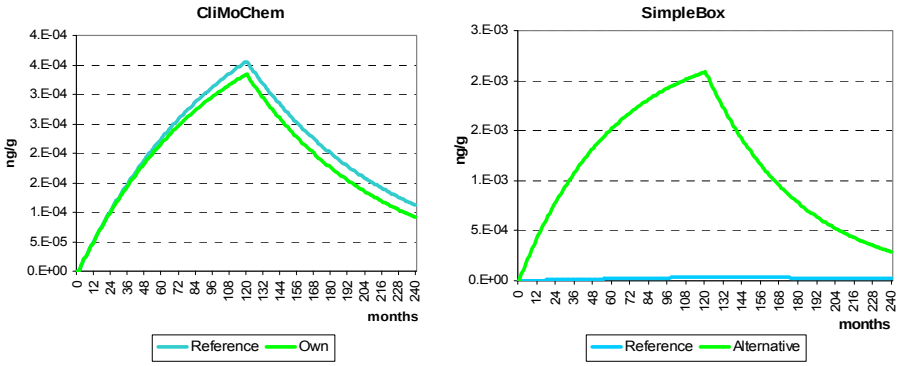


Fig. D.10. *Difference in long-term trends due to usage of different sets of PCB properties*

4.4. Gaseous exchange between atmosphere and water

Reference data set. Calculation results for water concentrations together with m and σ calculated with “reference” data set of PCB-28 properties are presented in Table D.31.

Table D.31. *Calculation results: water concentrations of PCB-28 (pg/L) calculated by all participating models and statistical parameters used for evaluation (“reference” data set)*

N	DEHM-POP	CliMoChem	SimpleBox	m	σ
1	7.03	4.86	19.61	**10.50**	**7.96**
2	15.74	10.90	54.87	**27.17**	**24.11**
3	33.45	17.55	103.76	**51.59**	**45.88**
4	9.38	5.46	26.06	**13.63**	**10.94**

Fig. D.11 displays the result on water concentrations of PCB-28 calculated by the participating models with the use of “reference” data set.

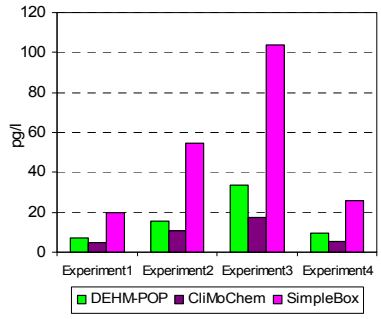


Fig. D.11. *Calculation results of the participating models (water concentrations) obtained with “reference” data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-28 calculated by the participating models are given in Table D.32.

Table D.32. *Calculation results: fluxes of PCB-28 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation (“reference” data set)*

N	CliMoChem	SimpleBox	*m*	σ
Gaseous flux to water				
1	2.61	5.92	**4.27**	**2.34**
2	5.85	26.28	**16.07**	**14.44**
3	6.90	31.32	**19.11**	**17.27**
4	2.38	6.64	**4.51**	**3.01**
Gaseous flux from water				
1	1.66	3.54	**2.60**	**1.33**
2	3.73	19.61	**11.67**	**11.23**
3	3.48	21.81	**12.64**	**12.96**
4	1.31	4.08	**2.70**	**1.96**
Net gaseous flux				
1	0.95	2.38	**1.67**	**1.01**
2	2.13	6.67	**4.40**	**3.21**
3	3.43	9.51	**6.47**	**4.30**
4	1.07	2.56	**1.81**	**1.06**

Below we present parwise comparison of modelling results for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table D.32.

Table D.32. *Correlation coefficients for water concentrations ("reference" data set)*

	CliMoChem	SimpleBox
DEHM-POP	0.98	0.99
CliMoChem	-	1.00

Correlation coefficients for net gaseous flux are demonstrated in Table D.33.

Table D.33. *Correlation coefficients for net gaseous flux ("reference" data set)*

	SimpleBox
CliMoChem	0.99

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4.34 and s.35, respectively.

Table D.34. *Coefficients of regression dependence between the models (α / β) for water concentrations ("reference" data set)*

	CliMoChem	SimpleBox
DEHM-POP	0.49 / 1.72	3.19 / -1.26
CliMoChem	–	6.48 / -11.70

Table D.35. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("reference" data set)*

	SimpleBox
CliMoChem	2.96 / -0.33

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.36 and 4.37.

Table D.36. *Residual square deviation, σ for water concentrations ("reference" data set)*

	CliMoChem	SimpleBox
DEHM-POP	1.80	6.84
CliMoChem	-	5.01

Table D.37. *Residual square deviation, σ for net gaseous flux ("reference" data set)*

	SimpleBox
CliMoChem	0.82

Own/alternative data set. Calculation results for water concentrations together with *m* and σ calculated with "own/alternative" data set of PCB-28 properties are presented in Table D.38. Here data set of PCB-28 properties used for calculations by each model is indicated (second row).

Table D.38*. Calculation results: water concentrations of PCB-28 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own	own	own	alt	own		
1	4.74	290.37	1.02	13.29	7.46	**63.38**	**126.97**
2	10.43	83.90	2.30	39.02	16.77	**30.48**	**32.83**
3	17.00	67.16	4.62	39.70	39.43	**33.58**	**24.05**
4	5.32	150.45	1.34	11.44	10.72	**35.85**	**64.19**

Fig. D.12 displays the result on water concentrations of PCB-28 calculated by the participating models with the use of "own / alternative" data set.

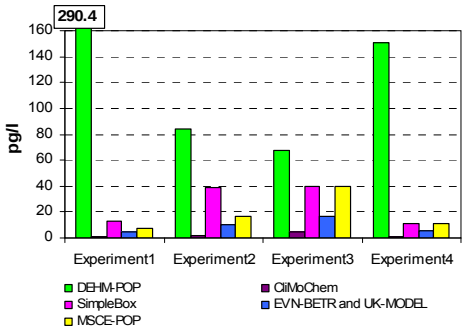


Fig. D.12. *Calculation results of the participating models (water concentrations) obtained with "own/alternative" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-28 calculated by the models are given in Table D.39.

Table D.39*. Calculation results: fluxes of PCB-28 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to water						
1	4.29	2.55	4.97	7.81	**4.90**	**2.19**
2	9.44	5.71	22.37	21.08	**14.65**	**8.33**
3	15.82	6.61	19.20	20.17	**15.45**	**6.18**
4	4.89	2.28	4.27	6.75	**4.55**	**1.84**
Gaseous flux from water						
1	1.91	0.38	2.53	7.63	**3.11**	**3.14**
2	4.19	0.85	14.92	20.67	**10.16**	**9.23**
3	4.48	1.01	11.99	19.21	**9.17**	**8.11**
4	1.64	0.35	2.23	6.49	**2.68**	**2.66**
Net gaseous flux						
1	2.38	2.17	2.44	0.18	**1.79**	**1.08**
2	5.25	4.87	7.44	0.41	**4.49**	**2.95**
3	11.34	5.60	7.21	0.96	**6.28**	**4.29**
4	3.25	1.93	2.04	0.26	**1.87**	**1.23**

The parwise comparison of modelling results is done for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table D.40.

Table D.40. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	-0.78	0.99	0.89	0.98
DEHM-POP	-	-0.75	-0.80	-0.72
CliMoChem	-	-	0.81	1.00
SimpleBox	-	-	-	0.77

Correlation coefficients for net gaseous flux are demonstrated in Table D.41.

Table D.41. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.87	0.76	1.00
CliMoChem	-	0.98	0.85
SimpleBox	-	-	0.73

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4. 4.42 and 4.43, respectively.

Table D.42. *Coefficients of regression dependence between the models (α / β) for water concentrations ("own/alternative" data set)*

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	-13.93 / 278.54	0.28 / -0.33	2.43 / 3.09	2.47 / -4.60
DEHM-POP	–	-0.01/ 4.10	-0.12 / 43.98	-0.10 / 33.77
CliMoChem	–	–	7.80 / 7.76	8.83 / -1.91
SimpleBox	–	–	–	0.71 / 0.26

Table D.43. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.40 / 1.42	0.55 / 1.72	0.09/ -0.03
CliMoChem	–	1.55 / -0.86	0.16 / -0.13
SimpleBox	–	–	0.09 / 0.03

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.44 and 4.45.

Table D.44. *Residual square deviation, σ for water concentrations ("own/alternative" data set)*

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	109.82	0.39	12.52	5.32
DEHM-POP	-	1.87	16.33	17.26
CliMoChem	-	-	15.73	1.87
SimpleBox	-	-	-	16.01

Table D.45. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

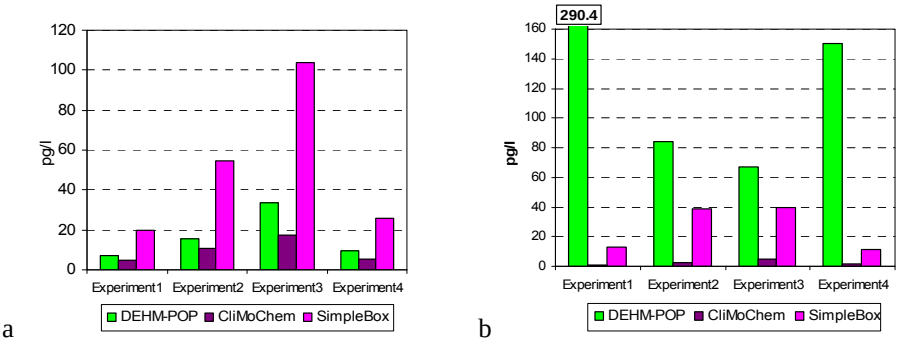
	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	1.61	3.33	0.02
CliMoChem	-	0.99	0.32
SimpleBox	-	-	0.41

Comparison between two data sets. The difference between calculated values of concentrations in water and gaseous fluxes to/from water obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.46 and 4.47, respectively.

Table D.46. *Difference between calculations with two data sets (water concentrations)*

N	DEHM-POP	CliMoChem	SimpleBox
1	4031%	-79%	-32%
2	433%	-79%	-29%
3	101%	-74%	-62%
4	1504%	-75%	-56%

This difference is visualized in Fig. D.13.



a b

Fig. D.13. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

Table D.47. *Difference between calculations with two data sets (net gaseous flux)*

N	CliMoChem	SimpleBox
1	52%	115%
2	300%	5%
3	245%	-12%
4	70%	59%

4.5. Gaseous exchange between atmosphere and vegetation

Reference data set. Calculation results for concentrations in vegetation together with *m* and σ calculated with "reference" data set of PCB-28 properties are presented in Table D.48. Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-28 calculated by the models are given in Table D.49.

Table D.48*. Calculation results: concentrations of PCB-28 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CliMoChem	SimpleBox	*m*	σ
1	0.180	0.067	**0.12**	**0.08**
2	0.299	0.057	**0.18**	**0.17**
3	0.242	0.073	**0.16**	**0.12**
4	0.142	0.034	**0.09**	**0.08**

Table D.49. *Calculation results: fluxes of PCB-28 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CliMoChem	SimpleBox	*m*	σ
Gaseous flux to vegetation				
1	0.59	30.33	**15.46**	**21.03**
2	2.07	106.14	**54.11**	**73.59**
3	1.01	51.55	**26.28**	**35.74**
4	0.77	39.42	**20.10**	**27.33**
Gaseous flux from vegetation				
1	0.59	28.00	**14.29**	**19.38**
2	2.07	102.72	**52.40**	**71.17**
3	1.01	48.68	**24.84**	**33.71**
4	0.77	37.81	**19.29**	**26.19**
Net gaseous flux				
1	0	2.33	-	-
2	0	3.42	-	-
3	0	2.88	-	-
4	0	1.61	-	-

Below we present pairwise comparison of modelling results for concentrations in vegetation and net gaseous flux. Correlation coefficients for concentrations in vegetation are shown in Table D.50.

Table D.50. *Correlation coefficients for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	0.51

Values of regression coefficients α and β for concentrations in vegetation calculated for all pairs of models are given in Table D.51.

Table D.51. *Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	2.06 / 0.10

Regression coefficients α and β between SimpleBox and MSCE-POP models equal 0.94 and –0.02, respectively. This testifies good agreement of net flux calculated by these two models.

Finally, values of residual square deviation for concentrations in vegetation are collected in Table D.52.

Table D.52. *Residual square deviation, σ for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	0.10

Own/alternative data set. Calculation results for concentrations in vegetation together with *m* and σ calculated with "own/alternative" data set of PCB-28 properties are presented in Table D.53. Here data set of PCB-28 properties used for calculations by each model is indicated (second row).

Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-28 calculated by the models are given in Table D.54.

***Table D.53**. Calculation results: concentrations of PCB-28 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own	own	alt	own		
1	0.010	0.083	0.026	0.126	**0.06**	**0.05**
2	0.004	0.084	0.057	0.150	**0.07**	**0.06**
3	0.008	0.104	0.038	0.171	**0.08**	**0.07**
4	0.003	0.052	0.025	0.089	**0.04**	**0.04**

***Table D.54**. Calculation results: fluxes of PCB-28 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to vegetation						
1	8.69	0.59	0.86	–	**3.38**	**4.60**
2	30.58	2.07	3.02	–	**11.89**	**16.19**
3	14.52	1.01	1.47	–	**5.66**	**7.67**
4	11.31	0.77	1.12	–	**4.40**	**5.99**
Gaseous flux from vegetation						
1	8.60	0.18	0.81	–	**3.20**	**4.69**
2	30.55	1.65	2.91	–	**11.70**	**16.33**
3	14.45	0.46	1.39	–	**5.44**	**7.82**
4	11.28	0.49	1.07	–	**4.28**	**6.07**
Net gaseous flux						
1	0.09	0.41	0.05	0.41	**0.24**	**0.19**
2	0.03	0.42	0.11	0.48	**0.26**	**0.22**
3	0.07	0.54	0.07	0.55	**0.31**	**0.27**
4	0.03	0.28	0.05	0.29	**0.16**	**0.14**

The parwise comparison of modelling results is done for concentrations in vegetation and net gaseous flux to vegetation. Correlation coefficients for concentrations in vegetation are shown in Table D.55.

***Table D.55.** Correlation coefficients for water concentrations ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-0.33	0.42	0.63
SimpleBox	-	0.62	0.43
CliMoChem	-	-	0.97

Correlation coefficients for net gaseous flux are demonstrated in Table D.56.

***Table D.56.** Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-0.43	0.32	0.51
SimpleBox	-	0.62	0.40
CliMoChem	-	-	0.97

Values of regression coefficients α and β for concentrations in vegetation and net gaseous flux calculated for all pairs of models are given in Tables 4.57 and 4.58, respectively.

***Table D.57.** Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and	-1.45 / 0.05	4.25 / 0.11	3.95 / 0.06

UK MODEL			
SimpleBox	–	1.43/ 0.08	0.61 / 0.06
CliMoChem	–	–	0.60 / 0.0001

Table D.58. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-0.44 / 0.10	1.20 / 0.36	1.84 / 0.31
SimpleBox	–	2.29 / 0.27	1.45 / 0.31
CliMoChem	–	–	0.95 / 0.004

Finally, values of residual square deviation for concentrations in vegetation and net gaseous flux are collected in Tables 4.59 and 4.60.

Table D.59. *Residual square deviation, σ for concentrations in vegetation ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.02	0.05	0.03
SimpleBox	-	0.05	0.03
CliMoChem	-	-	0.01

Table D.60. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.05	0.18	0.16
SimpleBox	-	0.15	0.17
CliMoChem	-	-	0.05

Comparison between two data sets. The difference between calculated values of water concentrations and net gaseous flux obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.61 – 4.64.

Table D.61. *Difference between calculations with two data sets (concentrations in vegetation)*

N	CliMoChem	SimpleBox
1	-54%	-61%
2	-72%	-0.2%
3	-57%	-48%
4	-64%	-28%

Table D.62. *Difference between calculations with two data sets (gaseous flux to vegetation)*

N	CliMoChem	SimpleBox
1	0%	-97%
2	0%	-97%
3	0%	-97%
4	0%	-97%

Table D.63. *Difference between calculations with two data sets (gaseous flux from vegetation)*

N	CliMoChem	SimpleBox
1	-69%	-97%
2	-20%	-97%
3	-54%	-97%
4	-36%	-97%

Table D.64. *Difference between calculations with two data sets (net gaseous flux)*[*]

N	SimpleBox
1	-98%
2	-97%
3	-97%
4	-97%

* The difference between values of net gaseous flux calculated by CliMoChem model is not calculated because for "reference" data set this flux is reported to be zero

Annex E

SENSITIVITY STUDY WITH RESPECT TO SUBSTANCE-SPECIFIC PROPERTIES USED IN THE DESCRIPTION OF BASIC PROCESSES FOR PCB-180

4.1. Gas/particle partitioning

Reference data set. Calculation results for PCB-180 together with m_φ and σ_φ are presented in Table E.1.

Table E.1. *Calculation results: fractions of particulate phase of PCB-180 calculated by models and statistical parameters used for evaluation ("reference" data set)*

Exp.No	T (°C)	DEHM-POP	CliMoChem	SimpleBox*	m_φ	σ_φ
1	-12	0.96	0.24	1.00	**0.73**	**0.43**
2	-5	0.88	0.20	0.99	**0.69**	**0.43**
3	0	0.79	0.20		**0.50**	**0.42**
4	3	0.69	0.17		**0.43**	**0.37**
5	5	0.49	0.10		**0.29**	**0.28**
6	8	0.46	0.12		**0.29**	**0.24**
7	10	0.44	0.14	0.92	**0.50**	**0.40**
8	12	0.37	0.13	0.90	**0.25**	**0.17**
9	15	0.35	0.16		**0.25**	**0.13**
10	17	0.25	0.13		**0.19**	**0.09**
11	20	0.19	0.12		**0.15**	**0.05**
12	25	0.10	0.09		**0.10**	**0.00**

* - only 4 experiments for Simple Box

The plot of dependence of φ on T calculated by participating models is presented in Fig. E.1.

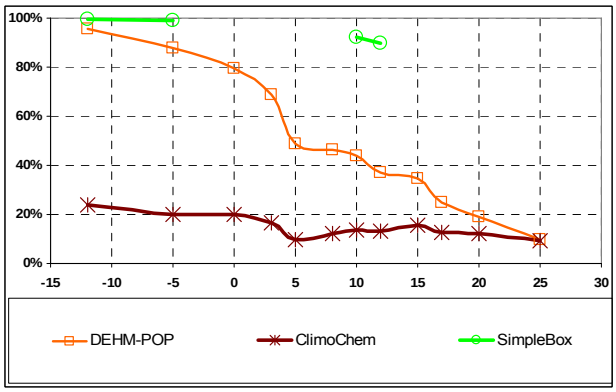


Fig. E.1. *Calculation results of the participating models (gas-particle partitioning) obtained with reference data set*

Calculated correlation coefficients between the results of participating models are given in Table E.2.

Table E.2. *Correlation coefficients* r_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.88	0.99
CliMoChem	-	0.96

* - by 4 experiments only

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.3.

Table E.3. *Coefficients of regression dependence between the models (α / β)*

	CliMoChem	SimpleBox*
DEHM-POP	0.14 / 0.08	0.16 / 0.84
CliMoChem	–	0.91 / 0.79

* - by 9 experiments only

Results of the calculation of pairwise residual square deviation σ are given in Table E.4.

Table E.4. *Residual square deviation,* σ^{res}_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.069	0.009
CliMoChem	-	0.024

* - by 9 experiments only

Own/altenative data set. Calculation results for PCB-180 together with m_φ and $\sigma_{.\varphi}$ are presented in Table E.5. The data set used in calculations by each model is indicated in the first row.

Table E.5. *Calculation results: fractions of particulate phase of PCB-180 calculated by models and statistical parameters used for evaluation (own/alternative data set)*

Exp.No	T (°C)	EVN-BETR and UK-MODEL	DEHM-POP	CAN/ POPs	MSCE-POP_1	MSCE-POP_2	CliMoChem	SimpleBox	m_φ	σ_φ
Data set		own	own	own	own	own	own	alt		
1	-12	0.98	0.93	0.99	0.98	0.97	0.22	0.99	**0.87**	**0.29**
2	-5	0.95	0.84	0.97	0.94	0.92	0.14	0.98	**0.82**	**0.30**
3	0	0.92	0.75	0.95	0.87	0.87	0.12	0.96	**0.75**	**0.32**
4	3	0.86	0.64	0.92	0.81	0.80	0.09	0.94	**0.69**	**0.31**
5	5	0.73	0.45	0.82	0.76	0.64	0.05	0.88	**0.62**	**0.29**
6	8	0.71	0.44	0.81	0.67	0.62	0.05	0.88	**0.60**	**0.28**
7	10	0.69	0.42	0.79	0.60	0.60	0.05	0.88	**0.58**	**0.27**
8	12	0.63	0.36	0.74	0.53	0.54	0.05	0.85	**0.47**	**0.24**
9	15	0.60	0.34	0.71	0.43	0.52	0.05	0.85	**0.44**	**0.23**
10	17	0.49	0.25	0.60	0.36	0.41	0.04	0.79	**0.36**	**0.20**
11	20	0.40	0.20	0.51	0.27	0.33	0.03	0.73	**0.29**	**0.17**
12	25	0.23	0.11	0.31	0.16	0.19	0.02	0.60	**0.17**	**0.10**

The plot of dependence of φ on T calculated by participating models with “own or alternative” data set is presented in Fig. E.2.

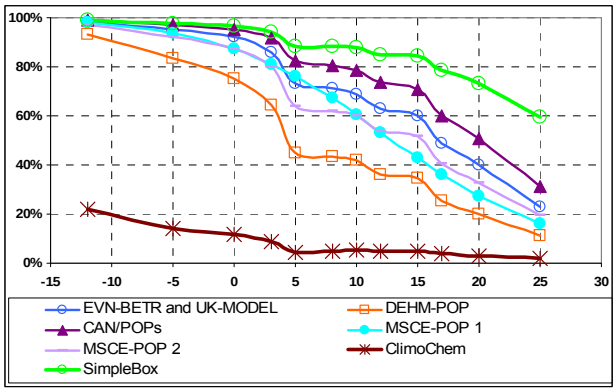


Fig. E.2. *Calculation results of the participating models (gas-particle partitioning) obtained with "own/alternative" data set*

Calculated correlation coefficients between the results of participating models are given in Table E.6.

Table E.6. *Correlation coefficients* r_{12}

	DEHM-POP	CAN/POPs	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.96	0.99	0.98	0.99	0.81	0.99
DEHM-POP	-	0.92	0.96	0.98	0.93	0.91
CAN/POPs	-	-	0.97	0.97	0.75	1.00
MSCE-POP 1	-	-	-	0.98	0.80	0.95
MSCE-POP 2	-	-	-	-	0.86	0.96
CliMoChem	-	-	-	-	-	0.74

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.7.

Table E.7. *Coefficients of regression dependence between the models* (α / β)

	DEHM-POP	CAN/POPs	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	1.08 / - 0.0001	0.88 /	1.15 / -0.17	1.04 / -0.09	0.20 / -0.06	0.48 / 0.53
DEHM-POP	–	0.72 /	0.99 / 0.14	0.92 / 0.18	0.21 / -0.02	0.39 / 0.67
CAN/POPs			1.28 / -0.35	1.15 / -0.26	0.21 / -0.09	0.55 / 0.44
MSCE-POP 1	–		–	0.88 / 0.07	0.17 / -0.03	0.40 / 0.62
MSCE-POP 2	–		–	–	0.21/ -0.05	0.45 / 0.58
CliMoChem	–		–	–	–	1.44 / 0.75

Results of calculations of pairwise residual square deviation σ are given in Table E.8.

Table E.8. *Residual square deviation,* σ^{res}_{12}

	DEHM-POP	CAN/POPs	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.25	0.08	0.16	0.09	0.11	0.06
DEHM-POP	-	0.27	0.26	0.15	0.07	0.16
CAN/POPs	-	-	0.22	0.18	0.13	0.03
MSCE-POP 1	-	-	-	0.15	0.11	0.12
MSCE-POP 2	-	-	-	-	0.10	0.10
CliMoChem	-	-	-	-	-	0.25

Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table E.9.

Table E.9. *Difference between calculations with two data sets*

Exp.No	*T* (°C)	DEHM-POP	CliMoChem	SimpleBox
1	-12	-2%	-8%	-1%
2	-5	-5%	-29%	-1%
3	0	-5%	-42%	
4	3	-6%	-49%	
5	5	-8%	-54%	
6	8	-6%	-59%	
7	10	-5%	-61%	-5%
8	12	-3%	-64%	-5%
9	15	0%	-67%	
10	17	2%	-70%	
11	20	6%	-74%	
12	25	13%	-78%	

This difference is visualized in Fig. E.3.

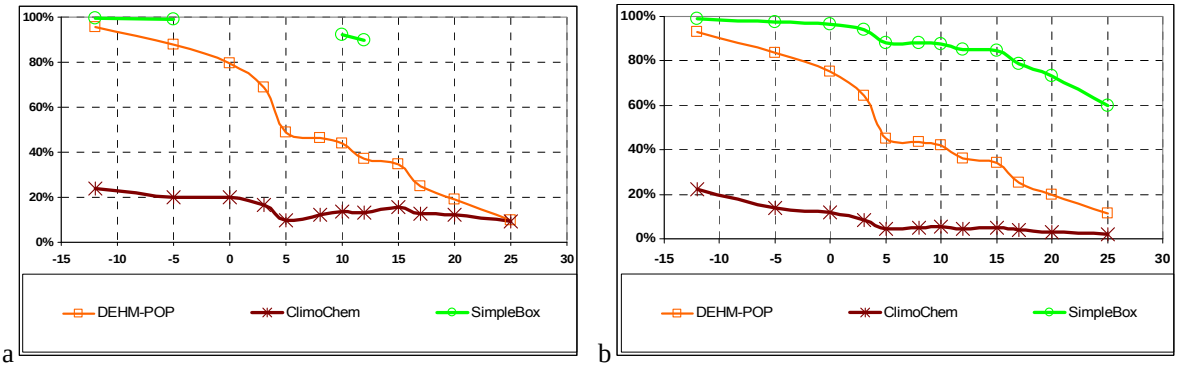


Fig. E.3. *Calculation results of the participating models obtained with "reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

4.2. Wet deposition

Reference data set. Calculation results for PCB-180 together with *m* and σ are presented in Tables 4. 4.10 and 4.11.

Table E.10. *Calculation results: concentrations in precipitation (pg/L) ("reference" data set)*

Exp. No	*T* (°C)	CliMoChem	SimpleBox	*m*	σ
1	-1	273	929	**601**	**464**
2	3	81	277	**179**	**139**
3	10	121	410	**265**	**204**
4	15	33	113	**73**	**56**
5	-1	27	929	**478**	**638**
6	3	8	277	**143**	**190**
7	10	12	410	**211**	**281**
8	15	3	113	**58**	**77**

Table E.11. *Calculation results: wet deposition flux, ng/m^2/hour ("reference" data set)*

Exp. No	*T* (°C)	CliMoChem	SimpleBox	*m*	σ
1	-1	0.273	0.929	**0.601**	**0.464**
2	3	0.081	0.277	**0.179**	**0.139**
3	10	0.121	0.410	**0.265**	**0.204**
4	15	0.033	0.113	**0.073**	**0.056**
5	-1	0.273	9.293	**4.783**	**6.379**
6	3	0.081	2.770	**1.426**	**1.901**
7	10	0.121	4.099	**2.110**	**2.813**
8	15	0.033	1.126	**0.579**	**0.773**

The comparison of calculated values of concentrations in precipitation is displayed in Fig. E.4.

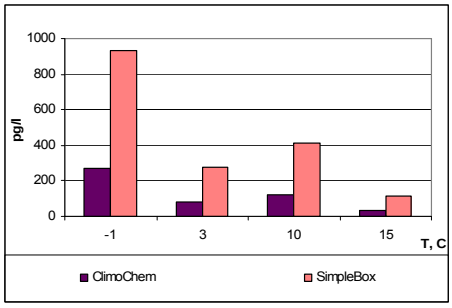


Fig. E.4. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (reference data set)*

Calculated correlation coefficients between the results of participating models are given in Table E.12.

Table E.12. *Correlation coefficients* r_{12}

	SimpleBox
CliMoChem	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.13.

Table E.13. *Coefficients of regression dependence between the models* (α / β)

	SimpleBox
CliMoChem	3.41 / -0.305

Pairwise residual square deviation σ are shown in Table E.14.

Table E.14. *Residual square deviation,* σ^{res}_{12}

	SimpleBox
CliMoChem	2.76

Own/alternative data set. Calculation results for PCB-180 together with m and σ are presented in Tables 4. 4.15 and 4.16.

Table E.15. *Calculation results: concentrations in precipitation (pg/L) (own/alternative data set)*

Exp. No	T (°C)	EVN-BETR and UK-MODEL	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	m	σ
1	-1	138	5720	663	254	882	**1531**	**2361**
2	3	609	1403	199	76	266	**511**	**537**
3	10	3900	9110	250	91	341	**2738**	**3901**
4	15	570	1048	78	30	105	**366**	**439**
5	-1	–	–	663	25	882	**523**	**445**
6	3	–	–	199	8	266	**157**	**134**
7	10	–	–	250	9	341	**200**	**172**
8	15	–	–	78	3	105	**62**	**53**

Table E.16. *Calculation results: wet deposition flux, ng/m*^{2}*/hour (own/alternative data set)*

Exp. No	T (°C)	EVN-BETR and UK-MODEL	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	m	σ
1	-1	0.138	5.720	0.663	0.254	0.882	**1.531**	**2.361**
2	3	0.609	1.403	0.199	0.076	0.266	**0.511**	**0.537**
3	10	3.900	9.110	0.250	0.091	0.341	**2.738**	**3.901**
4	15	0.570	1.048	0.078	0.030	0.105	**0.366**	**0.439**
5	-1	–	–	6.630	0.254	8.821	**5.235**	**4.451**
6	3	–	–	1.990	0.076	2.658	**1.575**	**1.340**

7	10	–	–	2.500	0.091	3.413	**2.001**	**1.716**
8	15	–	–	0.780	0.030	1.051	**0.620**	**0.529**

The comparison of calculated values of concentrations in precipitation is displayed in Fig. E.5.

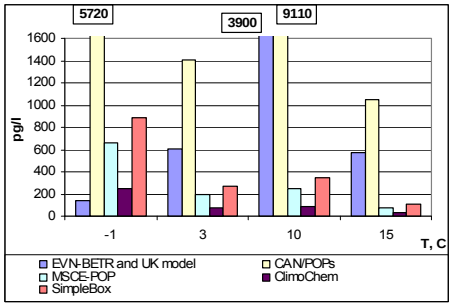


Fig. E.5. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (own/alternative data set)*

Calculated correlation coefficients between the results of participating models are given in Table E.17.

Table E.17. *Correlation coefficients* r_{12}

	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	0.76	-0.24	-0.26	-0.23
CAN/POPs	-	0.44	0.42	0.45
MSCE-POP	-	-	1.00	1.00
CliMoChem	-	-	-	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.18.

Table E.18. *Coefficients of regression dependence between the models* (α / β)

	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	1.67 / 2143	-0.04 / 343.3	-0.01 / 131.8	-0.04 / 456.5
CAN/POPs		0.03 / 171.2	0.01 / 66.41	0.04 / 227.1
MSCE-POP		–	0.38 / -1.43	1.33 / 3.96
CliMoChem		–	–	3.45 / 9.18

Finally, pairwise residual square deviation σ are shown in Table E.19.

Table E.19. *Residual square deviation,* σ^{res}_{12}

	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	4322	427	163	568
CAN/POPs	-	395	153	521
MSCE-POP	-	-	4	7
CliMoChem	-	-	-	19

Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table E.20.

Table E.20. *Difference between calculations with two data sets*

Exp. No	*T* (°C)	CliMoChem	SimpleBox
1	-1	-7%	-5%
2	3	-6%	-4%
3	10	-25%	-17%
4	15	-10%	-7%

5	-1	-7%	-5%
6	3	-6%	-4%
7	10	-25%	-17%
8	15	-10%	-7%

These results are visualized in Fig. E.6.

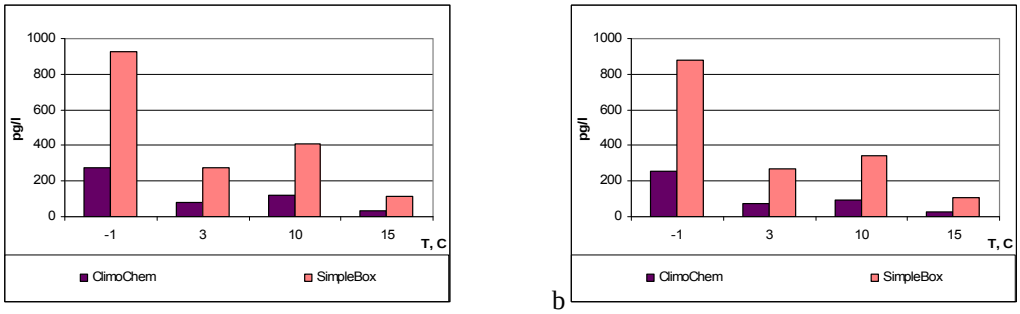


Fig. E.6. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

4.3. Gaseous exchange between atmosphere and soil

Here we present numerical results of calculations of soil concentrations and net gaseous flux to soil obtained by the participating models and their analysis for PCB-180 with "reference" and "own/alternative" data sets.

Fig. E.7 illustrates air concentration trend used in calculations for Experiment 1.

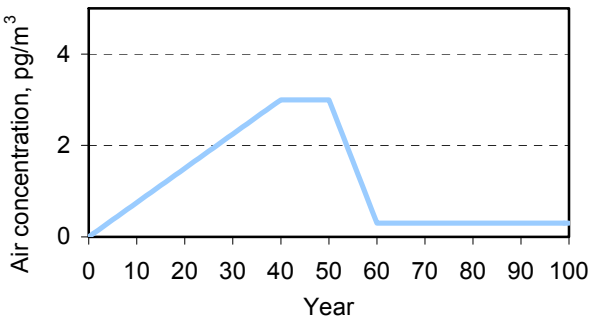


Fig. E.7. *Air concentration trend used for calculations for MSCE-POP model (MSCE-POP 2) for Experiment 1*

Reference data set. Calculation results for soil concentrations together with m and σ calculated with "reference" data set of PCB-180 properties are presented in Table E.21. Net gaseous fluxes to soil of PCB-180 calculated by the models and statistical parameters used for its evaluation are given in Table E.22.

Table E.21. *Calculation results: soil concentrations of PCB-180 (ng/g) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	DEHM-POP	CAN/POPs	CliMoChem	SimpleBox	m	σ
1	0.3	0.240	0.368	0.0001	0.0001	**0.15**	**0.18**
2	1.3	0.071	3.317	0.0007	0.0003	**0.85**	**1.65**

3	2.4	0.083	4.119	0.0016	0.0005	**1.05**	**2.05**
4	0.7	0.013	0.390	0.0003	0.0001	**0.10**	**0.19**

Table E.22. *Calculation results: net gaseous flux to soil, of PCB-180 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	CAN/POPs	CliMoChem	SimpleBox	*m*	σ
1	0.3	1.75E-13	5.40E-03	2.71E-02	**1.083E-02**	**1.434E-02**
2	1.3	2.33E-12	2.34E-02	1.18E-01	**4.698E-02**	**6.221E-02**
3	2.4	1.92E-12	4.32E-02	2.17E-01	**8.662E-02**	**1.147E-01**
4	0.7	1.97E-13	1.26E-02	6.31E-02	**2.522E-02**	**3.337E-02**

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Values of pairwise correlation coefficients are presented in Table E.23.

Table E.23. *Correlation coefficients for soil concentrations of PCB-180 ("reference" data set)*

	CAN/POPs	CliMoChem	SimpleBox
DEHM-POP	-0.28	-0.31	-0.29
CAN/POPs	-	0.91	0.97
CliMoChem	-	-	0.98

Correlation coefficients for net gaseous flux are presented in Table E.24.

Table E.24. *Correlation coefficients for net gaseous flux to soil of PCB-180 ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.77	0.77
CliMoChem	-	1.00

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Tables 4.25 and 4.26, respectively.

Table E.25. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-180 ("reference" data set)*

	CAN/POPs	CliMoChem	SimpleBox
DEHM-POP	-5.700 / 2.629	-0.002 /0.0009	-0.001 /0.0003
CAN/POPs		0.0003 / 0.0001	0.0001 / 0.00001
CliMoChem		–	0.338 / 0.00001

Table E.26. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-180 ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	1.12E+10 / 0.008	5.64E+10 / 0.041
CliMoChem	-	5.019 / -0.00001

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table E.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-180 ("reference" data set)*

	CAN/POPs	CliMoChem	SimpleBox
DEHM-POP	3.2485	0.0011	0.0004
CAN/POPs	-	0.0005	0.0001
CliMoChem	-	-	0.0001

Table E.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-180 ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.018	0.091
CliMoChem	-	0.0002

Own/alternative data set. Calculation results soil concentrations together with *m* and σ calculated with "own/alternative" data set of PCB-180 properties are presented in Table E.29. Net gaseous fluxes to soil of PCB-180 calculated by the models and statistical parameters used for its evaluation are given in Table E.30. Table E.29 contains also the information of the data set used for calculations for each model.

Table E.29. *Calculation results: soil concentrations of PCB-180 (ng/g) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	CAN/ POPs	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	*m*	σ
					1	2				
		own		own	own		own	alt		
1	0.3	0.004	0.355	0.638	0.013	0.075	0.002	0.602	**0.241**	**0.287**
2	1.3	0.019	3.742	6.604	0.064	0.363	0.008	3.667	**2.067**	**2.624**
3	2.4	0.034	4.808	7.203	0.139	0.792	0.016	5.680	**2.668**	**3.112**
4	0.7	0.006	0.768	0.710	0.027	0.154	0.003	0.747	**0.345**	**0.375**

Table E.30. *Calculation results: net gaseous flux to soil, of PCB-180 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*[*]

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	CAN/ POPs	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	*m*	σ
					1	2				
1	0.3	3.59E-04	3.51E-13	–	6.75E-03	3.62E-03	5.28E-03	-4.42E-02	**-4.69E-03**	**1.95E-02**
2	1.3	1.62E-03	3.27E-12	–	3.15E-02	2.50E-02	2.31E-02	-7.09E-02	**1.72E-03**	**3.78E-02**
3	2.4	2.89E-03	3.84E-12	–	5.40E-02	2.94E-02	4.24E-02	-2.69E-01	**-2.33E-02**	**1.22E-01**
4	0.7	8.47E-04	3.94E-13	–	1.26E-02	-4.37E-03	1.20E-02	-1.45E-01	**-2.06E-02**	**6.13E-02**

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Pairwise correlation coefficients are given in Table E.31.

Table E.31. *Correlation coefficients for soil concentrations of PCB-180 ("own/alternative" data set)*

		DEHM-POP	CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
				1	2		
EVN-BETR and UK MODEL		0.97	0.93	0.99	0.99	1.00	0.99
DEHM-POP		-	0.99	0.93	0.93	0.94	0.99
CAN/POPs		-	-	0.87	0.87	0.89	0.96
MSCE-POP	1	-	-	-	1.00	1.00	0.97
	2	-	–	–	1.00	1.00	0.97
CliMoChem		-	–	–	–	–	0.98

Correlation coefficients for net gaseous flux are presented in Table E.32.

Table E.32. *Correlation coefficients for net gaseous flux to soil of PCB-180 ("own/alternative" data set)*

		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.92	1.00	0.86	1.00	-0.82
CAN/POPs		–	0.94	0.98	0.91	-0.53
MSCE-POP	1	–	–	0.90	1.00	-0.78
	2	–	–	–	0.85	-0.43
CliMoChem		–	–	–	–	-0.83

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Table E.33 and 34, respectively.

Table E.33. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-180 ("own/alternative" data set)*

		DEHM-POP	CAN/POPS	MSCE-POP		CliMoChem	SimpleBox
				1	2		
EVN-BETR and UK MODEL		152.1 / -0.01	239 / 0.02	4.00 / -0.003	22.8 / -0.02	0.46 / -0.0003	175 / -0.11
DEHM-POP		–	1.62 / -0.14	0.02 / 0.003	0.14 / 0.02	0.003 / 0.0003	1.10 / 0.003
CAN/POPs				0.01 / 0.01	0.08 / 0.05	0.002 / 0.001	0.65 / 0.19
MSCE-POP	1		–	–	5.70 / -0.004	0.11 / 0.0001	42.18 / 0.11
	2		–	–	–	0.02 / 0.0001	7.39 / 0.11
CliMoChem		–		–	–	–	373 / 0.07

Table E.34. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-180 ("own/alternative" data set)*

		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		1.54E+09 / -2.40E-13	19.26 / -0.001	12.69 / -0.005	14.72 / -0.0004	-75.04 / -0.02
CAN/POPs		–	1.09E+10 / 0.005	8.62E+09 / -0.004	8.01E+09 / 0.005	-2.89E+10 / -0.08
MSCE-POP	1	–	–	0.69 / -0.005	0.76 / 0.0008	-3.67 / -0.04
	2	–	–	–	0.85 / 0.009	-2.63 / -0.10
CliMoChem		–	–	–	–	-5.13 / -0.03

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table E.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-180 ("own/alternative" data set)*

		DEHM-POP	CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
				1	2		
EVN-BETR and UK MODEL		0.96	2.36	0.01	0.08	0.001	0.48
DEHM-POP		-	0.93	0.04	0.21	0.004	0.64
CAN/POPs		-	-	0.05	0.28	0.005	1.15
MSCE-POP	1	-	-	-	0.001	0.001	1.04
	2	-	–	–		0.001	1.04
CliMoChem		-	–	–	–	–	0.85

Table E.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-180 ("own/alternative" data set)*

		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		1.27E-12	0.003	0.015	0.001	0.099
CAN/POPs		-	0.012	0.006	0.011	0.147
MSCE-POP	1	–	–	0.012	0.003	0.109
	2	–	–	–	0.015	0.157
CliMoChem		–	–	–	–	0.097

Comparison between two data sets. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table E.29. The corresponding differences between calculated values of net flux to soil were not calculated since near the equilibrium small changes in pollutant properties can lead to essential changes of fluxes (in relative values).

Table E.29. *Difference between calculations with two data sets*

No	Air conc, pg/m^3	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox
1	0.3	73%	48%	1014%	1192427%
2	1.3	99%	5158%	979%	1182447%
3	2.4	75%	5667%	884%	1072561%
4	0.7	82%	5938%	812%	988515%

Accumulation/clearance dynamics of PCBs in soil.

Fig. E.8 shows the results of the experiment obtained by CAN/POPs, CliMoChem and SimpleBox models with the use of “reference” data set.

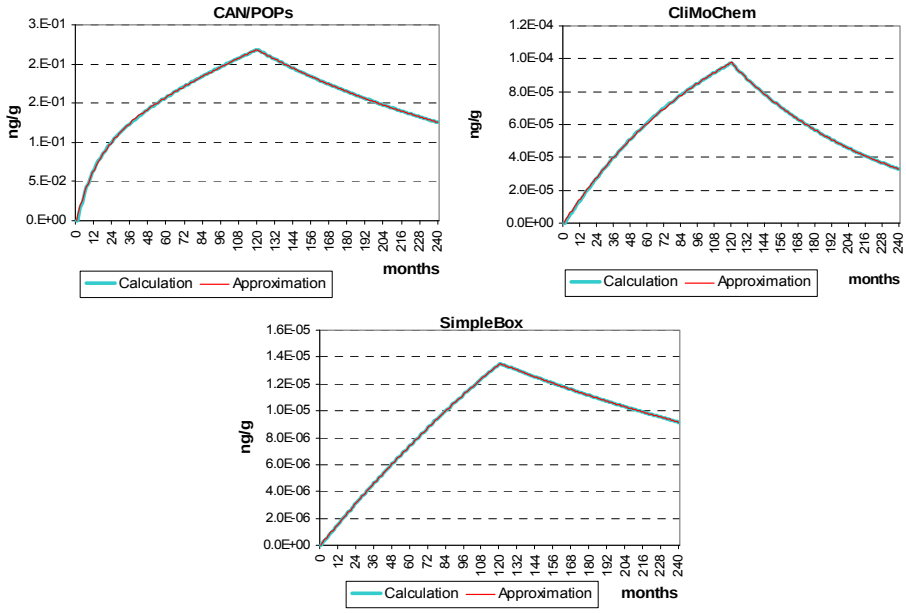


Fig. E.8. *Long-term trends of accumulation and clearance obtained by participating models (“reference” data set)*

The results obtained by CliMoChem, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models with the use of “own/alternative” data sets are presented in Fig. E.9.

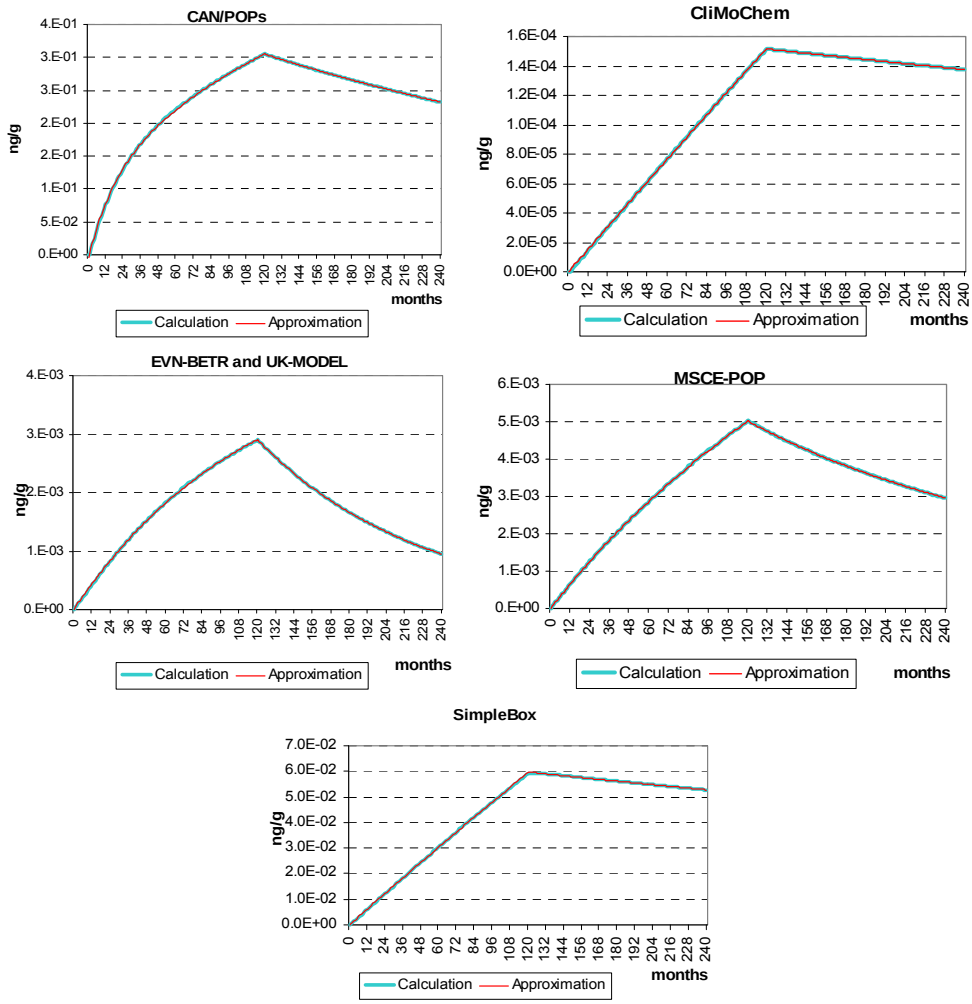


Fig. E.9. *Long-term trends of accumulation and clearance obtained by participating models ("own/alternative" data set)*

The values of characteristic times obtained by the approximation are shown in Table E.30.

Table E.30. *Parameters of multi-exponential approximation*

	CAN/POPs		CliMoChem		EVN-BETR and UK model		MSCE-POP		SimpleBox	
	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast
"Reference" data set										
Accumulation phase	15.0	0.8	6.9	6.9	–	–	–	–	17.9	17.9
Clearance phase	23.1	9.3	6.4	6.4	–	–	–	–	17.8	17.8
"Own/alternative" data set										
Accumulation phase	10.5	1.0	172.4	172.1	6.7	6.7	18.8	3.3	84.4	84.6
Clearance phase	30.5	11.6	70.8	71.0	6.3	6.2	17.7	5.8	55.8	55.8

The difference between results obtained with "reference" and "own/alternative" data sets (for those models which have performed both calculations) is illustrated by Fig. E.10.

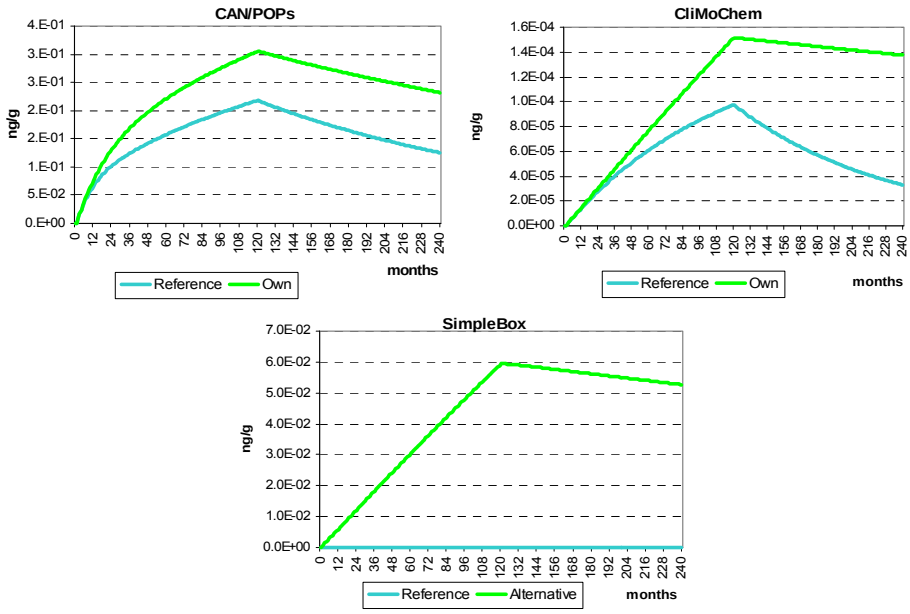


Fig. E.10. *Difference in long-term trends due to usage of different sets of PCB properties*

4.4. Gaseous exchange between atmosphere and water

Reference data set. Calculation results for water concentrations together with m and σ calculated with "reference" data set of PCB-180 properties are presented in Table E.31.

Table E.31*. Calculation results: water concentrations of PCB-180 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	m	σ
1	1.70	1.20	2.71	2.10	**1.92**	**0.64**
2	5.20	1.23	2.79	3.72	**3.23**	**1.66**
3	23.10	4.87	4.07	7.07	**9.78**	**8.97**
4	50.00	11.52	13.26	14.94	**22.43**	**18.43**

Fig. E.11 displays the result on water concentrations of PCB-180 calculated by the participating models with the use of "reference" data set.

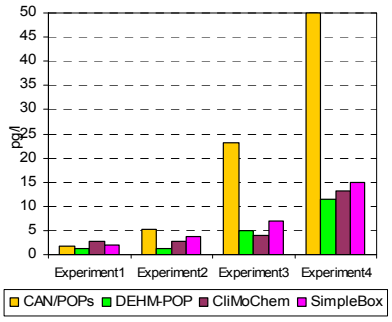


Fig. E.11. *Calculation results of the participating models (water concentrations) obtained with "reference" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-180 calculated by the participating models are given in Table E.32.

***Table E.32**. Calculation results: fluxes of PCB-180 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CAN/POPs	CliMoChem	SimpleBox	*m*	σ
Gaseous flux to water					
1	-	0.22	0.63	**0.43**	**0.29**
2	-	0.23	1.15	**0.69**	**0.65**
3	-	0.29	1.57	**0.93**	**0.90**
4	-	0.98	3.57	**2.27**	**1.83**
Gaseous flux from water					
1	0.11	0.06	0.02	**0.06**	**0.05**
2	1.57	0.06	0.05	**0.56**	**0.87**
3	2.31	0.04	0.03	**0.79**	**1.31**
4	4.63	0.18	0.07	**1.62**	**2.60**
Net gaseous flux					
1	0.11	0.16	0.62	**0.30**	**0.28**
2	1.57	0.17	1.10	**0.95**	**0.71**
3	2.31	0.25	1.54	**1.36**	**1.04**
4	4.63	0.80	3.50	**2.98**	**1.97**

Below we present parwise comparison of modelling results for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table E.32.

***Table E.32.** Correlation coefficients for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	SimpleBox
CAN/POPs	1.00	0.95	1.00
DEHM-POP	-	0.97	0.99
CliMoChem	-	-	0.97

Correlation coefficients for net gaseous flux are demonstrated in Table E.33.

***Table E.33.** Correlation coefficients for net gaseous flux ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.92	0.98
CliMoChem	-	0.98

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4.34 and s.35, respectively.

***Table E.34.** Coefficients of regression dependence between the models (α / β) for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	SimpleBox
CAN/POPs	0.22 /0.32	0.22 / 1.34	0.26 / 1.81
DEHM-POP	-	1.01 / 0.93	1.17 / 1.46
CliMoChem	-	–	1.09 / 0.74

***Table E.35.** Coefficients of regression dependence between the models (α / β) for net gaseous flux ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.15 / 0.02	0.66 / 0.28
CliMoChem	- CliMoChem	4.04 / 0.30

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.36 and 4.37.

Table E.36. *Residual square deviation, σ for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	SimpleBox
CAN/POPs	0.79	2.73	0.94
DEHM-POP	-	2.08	1.12
CliMoChem	-	-	2.49

Table E.37. *Residual square deviation, σ for net gaseous flux ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.21	0.47
CliMoChem	-	0.44

Own/alternative data set. Calculation results for water concentrations together with *m* and σ calculated with "own/alternative" data set of PCB-180 properties are presented in Table E.38. Here data set of PCB-180 properties used for calculations by each model is indicated (second row).

Table E.38*. Calculation results: water concentrations of PCB-180 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own		own	own	alt	own		
1	0.96	1.70	2.24	0.80	19.17	0.89	**4.29**	**7.31**
2	0.96	5.20	4.99	0.82	20.03	0.91	**5.49**	**7.41**
3	5.16	23.10	0.45	3.79	93.35	3.87	**21.62**	**36.05**
4	12.50	50.00	0.47	8.63	208.43	8.98	**48.17**	**80.42**

Fig. E.12 displays the result on water concentrations of PCB-180 calculated by the participating models with the use of "own / alternative" data set.

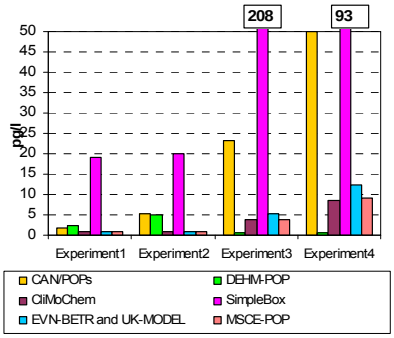


Fig. E.12. *Calculation results of the participating models (water concentrations) obtained with "own/alternative" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-180 calculated by the models are given in Table E.39.

Table E.39*. Calculation results: fluxes of PCB-180 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to water							
1	0.47	0.32	0.14	0.44	0.43	**0.36**	**0.14**
2	0.47	0.35	0.14	0.84	0.50	**0.46**	**0.26**
3	1.03	0.29	0.25	1.30	0.67	**0.71**	**0.46**

4	3.47	0.76	0.79	2.73	2.14	**1.98**	**1.19**
Gaseous flux from water							
1	0.02	-	0.13	0.35	0.42	**0.23**	**0.19**
2	0.02	-	0.13	0.68	0.49	**0.33**	**0.31**
3	0.04	-	0.22	1.55	0.64	**0.61**	**0.67**
4	0.14	-	0.71	2.86	2.08	**1.45**	**1.25**
Net gaseous flux							
1	0.45	0.32	0.01	0.09	0.01	**0.17**	**0.20**
2	0.45	0.35	0.01	0.16	0.01	**0.19**	**0.20**
3	0.99	0.29	0.03	-0.25	0.03	**0.22**	**0.47**
4	3.33	0.76	0.07	-0.14	0.07	**0.82**	**1.44**

The parwise comparison of modelling results is done for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table E.40.

Table E.40. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	1.00	-0.71	1.00	1.00	1.00
CAN/POPs	-	-0.70	1.00	1.00	1.00
DEHM-POP	-	-	-0.72	-0.72	-0.71
CliMoChem	-	-	-	1.00	1.00
SimpleBox	-	-	-	-	1.00

Correlation coefficients for net gaseous flux are demonstrated in Table E.41.

Table E.41. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.96	1.00	-0.53	0.98
CAN/POPs	-	0.93	-0.26	0.89
CliMoChem	-	-	-0.59	0.99
SimpleBox	-	-	-	-0.67

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4. 4.42 and 4.43, respectively.

Table E.42. *Coefficients of regression dependence between the models (α / β) for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	4.04 / 0.22	-0.28 / 3.40	0.68 / 0.19	16.38 / 5.07	0.70 / 0.23
CAN/POPs	-	-0.07 / 3.40	0.17 / 0.18	4.03 / 4.68	0.17 / 0.22
DEHM-POP	-	-	-1.24 / 6.03	-30.02 / 146.4	-1.26 / 6.23
CliMoChem	-	-	-	24.15 / 0.49	1.03 / 0.04
SimpleBox	-	-	-	-	0.04 / 0.02

Table E.43. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.16 / 0.23	0.02 / 0.002	-0.07 / 0.06	0.02 / 0.01
CAN/POPs	-	0.13 / -0.02	-0.22 / 0.06	0.11 / -0.02
CliMoChem	-	-	-3.72 / 0.08	0.94 / -0.001
SimpleBox	-	-	-	-0.10 / 0.02

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.44 and 4.45.

Table E.44. *Residual square deviation, σ for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP

EVN-BETR and UK MODEL	3.409	2.612	0.113	4.393	0.029
CAN/POPs	-	2.641	0.486	10.70	0.559
DEHM-POP	-	-	4.463	107.1	4.652
CliMoChem	-	-	-	1.666	0.094
SimpleBox	-	-	-	-	0.165

Table E.45. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.113	0.004	0.282	0.009
CAN/POPs	-	0.019	0.320	0.023
CliMoChem	-	-	0.267	0.005
SimpleBox	-	-	-	0.037

Comparison between two data sets. The difference between calculated values of concentrations in water and gaseous fluxes to/from water obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.46 and 4.47, respectively.

Table E.46. *Difference between calculations with two data sets (water concentrations)*

N	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox
1	0.0%	87%	-71%	815%
2	0.0%	305%	-71%	439%
3	0.0%	-91%	-7%	1220%
4	0.0%	-96%	-35%	1295%

This difference is visualized in Fig. E.13.

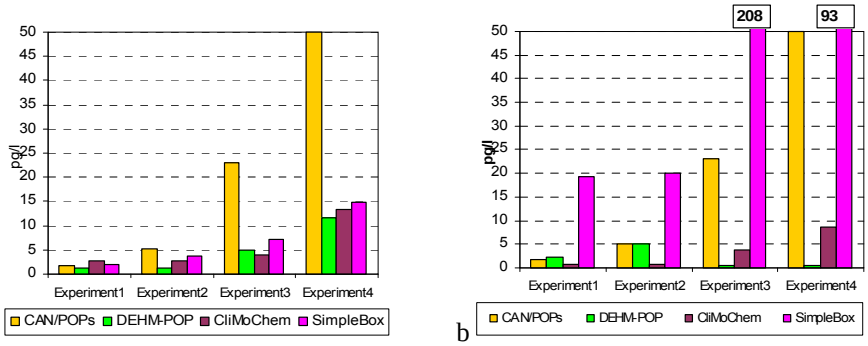


Fig. E.13. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

Table E.47. *Difference between calculations with two data sets (net gaseous flux)*

N	CAN/POPs	CliMoChem	SimpleBox
1	192%	-94%	-86%
2	-78%	-94%	-85%
3	-88%	-89%	-116%
4	-84%	-91%	-104%

4.5. Gaseous exchange between atmosphere and vegetation

Reference data set. Calculation results for concentrations in vegetation together with m and σ calculated with "reference" data set of PCB-180 properties are presented in Table E.48. Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-180 calculated by the models are given in Table E.49.

Table E.48*. Calculation results: concentrations of PCB-180 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CliMoChem	SimpleBox	m	σ
1	4.28	0.08	**2.18**	**2.97**
2	20.26	0.46	**10.36**	**14.00**
3	2.54	0.05	**1.30**	**1.76**
4	9.05	0.21	**4.63**	**6.25**

Table E.49*. Calculation results: fluxes of PCB-180 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CliMoChem	SimpleBox	m	σ
Gaseous flux to vegetation				
1	0.06	3.03	**1.55**	**2.10**
2	0.65	33.36	**17.00**	**23.13**
3	0.05	2.34	**1.19**	**1.62**
4	0.24	12.13	**6.18**	**8.41**
Gaseous flux from vegetation				
1	0.06	0.18	**0.12**	**0.09**
2	0.65	6.11	**3.38**	**3.86**
3	0.05	0.21	**0.13**	**0.12**
4	0.24	1.81	**1.02**	**1.11**
Net gaseous flux				
1	0	2.85	-	-
2	0	27.25	-	-
3	0	2.12	-	-
4	0	10.32	-	-

Below we present pairwise comparison of modelling results for concentrations in vegetation and net gaseous flux. Correlation coefficients for concentrations in vegetation are shown in Table E.50.

Table E.50. *Correlation coefficients for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	1.00

Values of regression coefficients α and β for concentrations in vegetation calculated for all pairs of models are given in Table E.51.

Table E.51. *Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	43.26 / 0.39

Regression coefficients α and β between SimpleBox and MSCE-POP models equal 0.94 and –0.02, respectively. This testifies good agreement of net flux calculated by these two models.

Finally, values of residual square deviation for concentrations in vegetation are collected in Table E.52.

Table E.52. *Residual square deviation, σ for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	0.50

Own/alternative data set. Calculation results for concentrations in vegetation together with *m* and σ calculated with "own/alternative" data set of PCB-180 properties are presented in Table E.53. Here data set of PCB-180 properties used for calculations by each model is indicated (second row). Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-180 calculated by the models are given in Table E.54.

Table E.53*. Calculation results: concentrations of PCB-180 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own	own	alt	own		
1	0.12	0.12	0.16	0.02	**0.10**	**0.06**
2	0.13	0.69	0.52	0.19	**0.38**	**0.27**
3	0.06	0.08	0.08	0.01	**0.06**	**0.03**
4	0.10	0.31	0.24	0.07	**0.18**	**0.11**

Table E.54*. Calculation results: fluxes of PCB-180 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to vegetation						
1	0.57	0.06	0.09	–	**0.24**	**0.29**
2	9.44	0.65	0.95	–	**3.68**	**4.99**
3	0.67	0.05	0.07	–	**0.26**	**0.35**
4	3.64	0.24	0.35	–	**1.41**	**1.93**
Gaseous flux from vegetation						
1	0.59	0.01	0.04	–	**0.21**	**0.33**
2	9.5	0.34	0.62	–	**3.48**	**5.21**
3	0.68	0.01	0.03	–	**0.24**	**0.38**
4	3.68	0.09	0.20	–	**1.32**	**2.04**
Net gaseous flux						
1	-0.02	0.05	0.04	0.06	**0.03**	**0.04**
2	-0.06	0.31	0.33	0.62	**0.30**	**0.28**
3	-0.01	0.04	0.03	0.04	**0.03**	**0.02**
4	-0.04	0.15	0.14	0.23	**0.12**	**0.11**

The parwise comparison of modelling results is done for concentrations in vegetation and net gaseous flux to vegetation. Correlation coefficients for concentrations in vegetation are shown in Table E.55.

Table E.55. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.73	0.63	0.65
SimpleBox	-	0.99	0.99
CliMoChem	-	-	1.00

Correlation coefficients for net gaseous flux are demonstrated in Table E.56.

Table E.56. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and	-0.97	-0.95	-0.98

UK MODEL			
SimpleBox	-	1.00	1.00
CliMoChem	-	-	1.00

Values of regression coefficients α and β for concentrations in vegetation and net gaseous flux calculated for all pairs of models are given in Tables 4.57 and 4.58, respectively.

Table E.57. *Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	4.55 / -0.22	1.69 / -0.10	5.94/ –0.31
SimpleBox	-	0.43 / -0.03	1.45 / -0.06
CliMoChem	-	-	3.36 / 0.05

Table E.58. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-6.04 / -0.06	-11.51 / -0.14	-5.61 / -0.04
SimpleBox		1.93 / -0.03	0.92 / 0.01
CliMoChem			0.47 / 0.03

Finally, values of residual square deviation for concentrations in vegetation and net gaseous flux are collected in Tables 4.59 and 4.60.

Table E.59. *Residual square deviation, σ for concentrations in vegetation ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.23	0.11	0.37
SimpleBox	-	0.02	0.05
CliMoChem	-	-	0.03

Table E.60. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.06	0.14	0.05
SimpleBox	-	0.02	0.01
CliMoChem	-	-	0.02

Comparison between two data sets. The difference between calculated values of water concentrations and net gaseous flux obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.61 – 4.64.

Table E.61. *Difference between calculations with two data sets (concentrations in vegetation)*

N	CliMoChem	SimpleBox
1	-97%	92%
2	-97%	13%
3	-97%	46%
4	-97%	18%

Table E.62. *Difference between calculations with two data sets (gaseous flux to vegetation)*

N	CliMoChem	SimpleBox
1	0%	-97%
2	0%	-97%

3	0%	-97%
4	0%	-97%

Table E.63. *Difference between calculations with two data sets (gaseous flux from vegetation)*

N	CliMoChem	SimpleBox
1	-90%	-77%
2	-48%	-90%
3	-82%	-84%
4	-64%	-89%

Table E.64. *Difference between calculations with two data sets (net gaseous flux)*[*]

N	SimpleBox
1	-98%
2	-99%
3	-98%
4	-99%

* The difference between values of net gaseous flux calculated by CliMoChem model is not calculated because for "reference" data set this flux is reported to be zero