

## 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 [Karickhoff, 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<sup>3</sup>, 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
<b>Third EMEP expert meeting on POP model intercomparison study</b>	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
<b>Fourth EMEP expert meeting on intercomparison of POP models</b>	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
<b>Fifth EMEP expert meeting on intercomparison of POP models</b>	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.