Programme on Stage II of POP model intercomparison study

The programme of Stage II of POP model intercomparison study was discussed in detail at the second EMEP expert meeting on intercomparison of POP models in Moscow, December 2003 and was finally approved by the involved experts.

Stage II is aimed at the comparison of mass balance estimates (POPs masses in different environmental compartments; masses of POPs degraded in these compartments; mass fluxes of POPs transported in/out of 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). These 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, 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 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.

The output of this stage is to be presented in the second intermediate report and/or scientific paper.

Pollutants considered:

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

Base year for the calculations: 2000

Input data:

“Reference data sets” of physical-chemical properties and degradation rate constants: “Reference data sets” of the considered PCBs presented in the report on Stage I 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 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.

Emissions scenario: 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*. 2002] (see also 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 pollutants in media: Initial concentrations of the considered pollutants in media for calculations are prepared by MSC-E.

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.

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. For your reference, the table below presents the values of some of these parameters, which are not obligatory for use in calculations.

Media	Parameter	Dimension	Value
Atmosphere	Total Suspended Matter, *TSP*	$\mu g/m^3$	30
	Fraction of organic carbon content in the aerosol, *foc*	%	20
	Specific aerosol surface, θ	m^2/m^3	$1.5 \cdot 10^{-4}$
Soil	Bulk soil density, ρ	kg/m^3	$1.35 \cdot 10^3$
	Volumetric water content in soil	%	30
	Volumetric air content in soil	%	20
Vegetation	Specific surface area of vegetation, a_V	m^2/m^3	$8 \cdot 10^3$

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 for some precipitation episodes and comparison of their results with measurements.

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). Results will include*:

   – values of PCB mass in compartments (atmosphere, soil, water, vegetation);

   – mass of PCB degraded in these compartments;

   – mass flow of PCB transported in/out of 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 (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".

The detailed description of input data for computational experiments within Stage II together with a number of tabular templates on each experiments to be filled in by all participants are presented in the "Templates for Stage II".

Timetable.

The timetable of activities within Stage II adopted by the participants is presented in Table 1.

Table 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)	Knut Breivik and Sunling 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	Knut Breivik	May 2004	Experts
Experiment on wet deposition process	Gerhard Petersen	May 2004	Experts
Descriptions of mass balance approaches used in the participating models and output of computational experiments	Experts	June 2004	MSC-E
Processing of the results	MSC-E	July - August 2004	Experts
Preparation of the draft of intermediate report on Stage II	MSC-E/ Experts	August - October 2004	Experts
Third EMEP meeting on POP model intercomparison study	MSC-E	October 2004	Experts
Preparation of the final version of intermediate report on Stage II	MSC-E/ Experts	October - December 2004	Experts
Preparation of the draft of a joint scientific article	MSC-E/ Experts	November 2004- December 2004	Experts
Preparation of the final version of a joint scientific article and its submission to publication	MSC-E/ Experts	January 2005 – March 2005	Experts