

CONVENTION ON LONG-RANGE TRANSBOUNDARY AIR POLLUTION  
Cooperative Programme for Monitoring and Evaluation of the Long-Range Transmission of  
Air Pollutants in Europe (EMEP)

**THIRD EMEP EXPERT MEETING ON INTERCOMPARISON OF POP  
MODELS**

*Moscow, the Russian Federation, 10-11 February 2005*

**MINUTES**

**Introduction**

Following the recommendations of the Executive Body for the Convention on Long-Range Transboundary Air Pollution UN ECE [ECE/EB.AIR/75], POP model intercomparison study was initiated under EMEP. According to the EMEP work plans for 2004 and 2005 and the programme on intercomparison of POP models agreed at two previous expert meetings (Moscow, Russia, 2002; 2003), and noting the relevant ongoing activities of participants within Stage II of the intercomparison study, the third EMEP expert meeting was held in Moscow, Russia from 10 to 11 February 2005 (Agenda is attached).

The main objectives of the meeting are the following:

- Consideration of results on computational experiments performed by modelers in the framework of Stage II;
- Elaboration of an extended work programme and time-schedule of Stage III.

The meeting was attended by 15 experts from Canada, Germany, Japan, the Netherlands, Norway, Switzerland, the United Kingdom, the USA and EMEP/MSC-E (List of participants is attached).

Sergey Dutchak, Director of EMEP/MSC-E, opened the meeting stressing importance of the intercomparison study on POP models at scientific and political levels. On behalf of EMEP he welcomed participants to take part in the sixth meeting of the Task Force on Measurements and Modeling (TFMM), which will be partly devoted to the review of the EMEP models on heavy metals (HM) and persistent organic pollutants (POPs) (Zagreb, Croatia, April 4-7, 2005), and in the EMEP/TFMM Workshop on HM/POP model review (Moscow, Russia, October 13-14, 2005).

Victor Shatalov (EMEP/MSC-E), a chairman of the meeting, led the discussion on the comparison of results of Stage II; Gerhard Petersen (GKSS-Research Centre, Institute for Coastal Research System Analysis and Modelling, Germany), a co-chairman of the meeting, led the discussion on sensitivity study of wet deposition process; and Martin Scheringer (Institute for Chemical and Bioengineering, Swiss Federal Institute of Technology, Switzerland), a co-chairman of the meeting, led the discussion on the work programme of Stage III.

**Presentations**

Victor Shatalov (EMEP/MSC-E) informed participants about state of the art of Stage II of POP model intercomparison study.

Elena Mantseva (EMEP/MSC-E) gave an overview of results on mass balance estimates and their comparison between models. Analysis of sensitivity of participating models to variations in physical-chemical data set used in mass balance estimates was also presented.

Sunling Gong (Air Quality Research Branch, Meteorological Service of Canada) described current situation with CAM/POPs model calculations and his activities in the framework of Stage II.

Alexey Gusev (EMEP/MSC-E) reviewed results on spatial distribution of depositions and concentrations in main environmental media obtained by participating models. Comparison of model estimates of air concentrations and depositions with measurements was also presented.

Gerhard Petersen (GKSS-Research Centre, Institute for Coastal Research System Analysis and Modelling, Germany) summarized the main features of description of wet deposition process in ADOM-POP model, presented results obtained on wet deposition exercise for B[a]P and proposed to perform experiments on wet depositions of PCBs which can occur in the atmosphere both in particulate and gaseous phases.

Victor Shatalov (EMEP/MSC-E) described results of MSCE-POP model on wet deposition exercise and stressed the importance of further investigations on model simulations of POPs wet scavenging.

Victor Shatalov (EMEP/MSC-E) reviewed a comparison of results on sensitivity of participating models to variations of physical-chemical properties used in description of main processes.

Martin Scheringer (Institute for Chemical and Bioengineering, Swiss Federal Institute of Technology, Switzerland) reviewed main methods and experiences of the OECD model intercomparison study focusing on the question of how they can be transferred to the EMEP intercomparison study.

The meeting discussed in depth results on Stage II and an extended work-programme of Stage III. The experts agreed on the following conclusions:

## **Conclusions to Stage II**

In order to complete the comparison of mass balance estimates and sensitivity studies of these estimates and process descriptions with respect to physical-chemical parameters, additional data are decided to be submitted by the participants. Two following goals (short-term and long-term) can be respectively set apart for all participants:

### Short-term goals

1. to find masses of PCB-153 (of PCB-28 and PCB- 180 as optional) in specified sub-domains in air, soil and seawater compartments:
  - a. The atmosphere: layers of 1 km, 5 km and 10 km height.
  - b. Soil: 5 cm and 10 cm depth.
  - c. Sea: 200 m depth.

2. to find masses of PCB-153 (of PCB-28 and PCB- 180 as optional) degraded in specified sub-domains – for the same layers as in 1.
3. to submit the above-mentioned results to MSC-E by February 25, 2005.

#### Long-term goals

1. to perform calculations of mass balance estimates of PCB-153 (of PCB-28 and PCB-180 as optional) for one-year period (2000) with zero initial concentrations and with the use of two different data sets: “own or alternative” and “reference” (for models, which have not submitted these calculations yet). For mass contained and degraded in the environmental compartments the data on specified above sub-domains should be presented. Output parameters are:
  - values of PCB mass contained in the environmental compartments (atmosphere, soil, water, vegetation);
  - values of PCB mass degraded in these compartments;
  - mass flow of PCB transported in/out the specified domain (total) and through each transport media separately;
  - mass flow of PCB transported from one media to another in both directions (net and dry and wet deposition, gaseous exchange);
  - concentrations at each interface (pg/m<sup>3</sup>, pg/l, ng/g, for air, water and soil, respectively);
  - spatial distributions of deposition and concentrations in different compartments (optional).
2. to perform calculations of mass balance estimates of PCB-153 (of PCB-28 and PCB-180 as optional) for 20-year period (from 1981 to 2000) with zero initial data with historical emissions and with the use of “own or alternative” data sets for comparison with measurements (optional). Results will include all above-mentioned parameters.
3. to perform calculations of wet deposition exercises prepared for PCB-153 (for PCB-28 and PCB-180 as optional) by Gerhard Petersen (optional).
4. to submit all above-mentioned results to MSC-E by the middle of May, 2005.
5. to present more detailed description of processes on atmosphere/soil, atmosphere/seawater and atmosphere/vegetation gaseous exchange and wet deposition used in participating models and parameterization of these processes for the analysis of differences between models by the middle of May, 2005.
6. to make an analysis of differences in calculation results of Stage II obtained by participating modelers (mass balance estimates and in sensitivity studies of process description and mass balance estimates). In order to see in more detail why differences take place, to clarify what difference in model description and physical-chemical data sets leads to different results.
7. to submit the mentioned-above analysis to MSC-E by September, 2005.
8. to hold the intermediate EMEP meeting on additional results of Stage II in Moscow in October 2005.

Participants also offered:

- monthly and annual data are submitted by modelers (quarterly data as optional);
- in additional calculations emissions are continually distributed among the year;
- to analyze PCB mass distribution between environmental compartments on the basis of calculations made with zero initial concentrations; and for comparison of mass flows to use data obtained with non-zero initial concentrations. For comparison with measurements it is preferably to use results of optional calculations performed for 20-year period (from 1981 to 2000) with zero initial data with historical emissions (See point 2 above);
- to hold joint meeting of modelers and measurement community for the sake of comparison modeled results versus monitoring data.

At that MSC-E is responsible for the following:

1. specification of output protocols (a number of tabular templates on experiments on mass balance estimates to be filled in) for short- and long-term goals;
2. sending out the output protocols to all participants by February 18, 2005.
3. processing results obtained within short-term and long-term goals and distribution them between participants by the end of March and July, 2005, respectively;
4. organizing of intermediate and final meetings of the POP model intercomparison study.

## **Conclusions to report on Stage II**

The meeting decided that results of Stage II would be published in two parts. The first one is an Intermediate Technical Note on Stage II, which should be prepared by MSC-E on the basis of results considered at this meeting and additional data submitted by participants within the implementation of short-term goal by the end of May 2005. Final report on Stage II results (including the analysis of discrepancies) will be prepared as a part of final report on the whole POP model intercomparison study (?). Participants also offered:

- to save the existing order of results presentation: mass balance estimates, degradation, exchange processes (MSC-E);
- to make the following statistical processing of the data (MSC-E):
  - ✓ to use averages and square deviations between models for each parameter evaluated.
  - ✓ to make classification of models with respect to the obtained values.
  - ✓ in addition to absolute values to compare also fractions of PCB mass in environmental compartments. The same for degraded masses.
- to add new measurement data for comparison with model results (presented by Knut Breivik);
- to make a description of emission and measurement data used and their uncertainties (Knut Breivik);
- to include maps of initial concentrations in all considered media (MSC-E);
- to include trends of concentrations in media within 2000 (month by month) (MSC-E);

- to insert before the consideration of results on air/soil exchange process calculated with “own or alternative” and “reference” data sets, a comparison of parameters which take part in description of air/soil exchange process from both data sets.

**Table 1.** Time-schedule of Stage II (additional data submission).

<b>What</b>	<b>Who</b>	<b>When</b>	<b>To</b>
<i>Short-term goal</i>			
Specification of output protocols for short- and long-term goals and their distribution between participants	MSC-E	February 18, 2005	Experts
Submission of data on masses contained and degraded in specified sub-domains in air, soil and seawater compartments	Experts	February 25, 2005	MSC-E
Processing results obtained within short-term goal and distribution them between participants	MSC-E	End of March, 2005	Experts
Preparation of the final version of the Intermediate Technical Note on Stage II and its distribution between participants	MSC-E	End of May, 2005	Experts
<i>Long-term goal</i>			
Preparation of wet deposition exercises for PCBs (optional)	G. Petersen	?	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	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
Calculations of PCBs wet deposition exercises (optional) and their distribution between participants	Experts	Middle of May, 2005	MSC-E
Presentation of more detailed description of gaseous exchange and wet deposition processes used in participating models and parameterization of these processes for the analysis of differences between models	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
Making an analysis of differences in calculation results of Stage II obtained by participating modelers (mass balance estimates and in sensitivity studies of process description and mass balance estimates)	Experts	September, 2005	MSC-E
Intermediate EMEP meeting on additional results of Stage II	MSC-E/ Experts	October 2005	MSC-E/ Experts
Preparation of the draft of the final report on the intercomparison study	MSC-E/ Experts	May 2006	Experts

## Conclusions to Stage III Programme

Stage III of the POP model intercomparison study is aimed at the comparison of ranking a number of chemicals with respect to LRTP and  $P_{over}$  calculated by different models. Each model uses its own metrics. Ranking is performed according to absolute values. Proposals for calculation experiments for ranking substances with respect to LRTP and  $P_{over}$  will be prepared by MSC-E. An agreed set of pollutant-specific parameters for all pollutants is to be used for calculations by the models. A list of pollutants and agreed set of parameters is proposed to be prepared by Martin Scheringer. Final report on Stage III results will be prepared as a part of final report on the whole POP model intercomparison study (?). Data submission for Stage III is described in Table 2.

**Table 2.** Time-schedule of Stage III.

What	Who	When	To
Proposals for calculation experiments for ranking substances with respect to LRTP and $P_{over}$ and distribution between participants	MSC-E	February 28, 2005	Experts
Proposals on the list of substances and their properties (partitioning coefficients, vapor pressure with temperature dependence if possible, solubility, degradation rates) for evaluation of LRTP and $P_{over}$ and distribution between participants	M. Scheringer	February 28, 2005	Experts
Proposals from modelers on calculation experiments and list of chemicals for ranking pollutants.	Experts	March 11, 2005	MSC-E
Distribution of the final version of the description of approaches to ranking substances with respect to LRTP and $P_{over}$ .	M. Scheringer and MSC-E	End of March, 2005	Experts
Submission of description of own approach used for evaluation of LRTP and $P_{over}$	Experts	End of November, 2005	MSC-E
Submission of calculation results including explanation.	Experts	End of November, 2005	MSC-E
Processing of the results and their distribution	MSC-E	February 2006	Experts
Preparation of the draft of the final report on the intercomparison study	MSC-E/ Experts	May 2006	Experts

The participants also offered:

1. to define chemical with well studied characteristics of their behavior in the environment which can be use as benchmarks (e.g. B[a]P);
2. to include into calculations new chemicals which were considered by the Task Force on POPs (hexachlorobutadiene, pentachlorobenzene, pentachlorophenol,

polychlorinated naphthalenes, dicofol,  $\alpha$ - and  $\beta$ - endosulfans and polybrominated diphenyl ethers (BDE-47, BDE-99 and BDE-153);

3. to compare differences in ranking between models and try to explain reasons for that;
4. for spatially resolved models to provide additional information on spatial and temporal variation (optional).

It was agreed to held the forth EMEP meeting on POP model intercomparison study in Moscow in May 2006.