

## CONCLUSIONS

In accordance with the EMEP work-plan (ECE/EB.AIR/83/add2, item 2.7) and recommendations of the EMEP Task Force on Measurements and Modeling (TFMM) MSC-E has prepared a full set of documentation for the evaluation of MSCE-POP model. For the review of the model a detailed model description was prepared and model sensitivity study to variations of pollutant-specific and environmental parameters was performed. These results were presented and discussed at the 6<sup>th</sup> TFMM meeting in April 2005 in Zagreb (Croatia).

Following to the conclusions of 6<sup>th</sup> TFMM meeting, the review of MSCE-POP model will be continued at the forthcoming workshop in Moscow on 13-14 October 2005. It will be focused on the analysis of the outcome of **POP model intercomparison study** and **verification of MSCE-POP model results against measurements**.

This report summarizes the results of the work on the analysis of MSCE-POP model performance fulfilled on the basis of comparison with other modeling approaches and confronting its results with available measurement data on POPs.

### **POP model intercomparison study:**

In the course of model intercomparison study physical-chemical properties of selected POPs and the description of gas/particle partitioning and intermedia exchange processes were analyzed.

- To evaluate the influence of uncertainties of pollutant-related parameters on MSCE-POP model results the analysis of parameterizations used in participated POP models was carried out on the example of PCB-153. The scattering of pollutant-related parameters between models can be viewed as an estimate of uncertainties of these parameters. The maximum uncertainty of concentrations and depositions computed by MSCE-POP model due to estimated uncertainties of pollutant-related parameters is accounted for 20%.
- It was found that among the considered pollutant-related parameters the most significant contributions to the uncertainty of MSCE-POP model results are introduced by degradation rates and octanol-water partition coefficient. Degradation process can imply essential affect to the evaluation of long-range transport of various POPs. Thus, to improve MSCE-POP model results the refinement of model description of degradation process and the inclusion of temperature dependence for octanol-water partition coefficient is required.
- Reasonable agreement is obtained in simulation of gas-particle partitioning of PCB-153 for most of models, including MSCE-POP. Values of PCB-153 particulate phase fraction for the considered temperature interval calculated by most of models are rather close, in particular, the square deviation of the particulate fraction is about 60% of the mean value. For most of them high correlation (above 0.8) can be noted between computed variations of particulate phase fraction with temperature. The difference in model results can be explained by the difference in  $K_{oa}$  or  $p_{oi}$  values at reference temperature used by the models.
- Most of models, including MSCE-POP, reproduce closely air concentrations at interfaces with different types of underlying surface and show comparable results on concentrations in other environmental media. Computed PCB-153 concentrations in the atmosphere obtained by most of models agree within an accuracy of 50%. For other environment compartments the agreement of concentrations is within a factor of 2, with the exception of the concentrations in seawater, where the difference were more significant.

### ***Verification of MSCE-POP model results against measurement:***

Verification of MSCE-POP model results was carried out on the basis of the comparison of model calculations for PAHs, PCBs, and PCDD/Fs with available measurements. In particular, the following POP species were chosen: B[a]P as a representative of PAHs and PCB-153 and 2,3,4,7,8-PeCDF as a representatives of PCBs and PCDD/Fs. For the comparison of model results with measurements available data from EMEP monitoring network together with the data of national measurements and episodic campaigns were used. The emphasis is put to the comparison of model results with EMEP measurements. At the same time, to enlarge the basis of the comparison, the data of national measurements and episodic campaigns are taken into account. In particular, the comparison for PCDD/Fs is based entirely on the results such data.

- The comparison of computed and observed concentrations in air shows that about 60% of calculated values for B[a]P, 40% for PCB-153, and 50% for 2,3,4,7,8-PeCDF agree with measured values within a factor of 2. The model tends to underestimate measured levels of B[a]P and 2,3,4,7,8-PeCDF air concentrations and overestimate measured PCB-153 atmospheric levels.
- The comparison of spatial distribution of calculated B[a]P and PCB-153 air concentrations with measurements of EMEP sites shows that the model reasonably describes contamination levels in different parts of Europe. In particular, low levels of concentrations in remote areas, moderate levels in Northern Europe, and higher concentrations in Central Europe obtained by the model are generally consistent with the observed air concentrations. Some deviations in spatial distribution of computed and observed concentrations are mostly connected with the uncertainties of spatial distribution of B[a]P and PCB-153 emission.
- Reasonable agreement of measured and computed spatial variations of POP air concentrations for European region is also confirmed by the comparison with the distribution of atmospheric levels obtained during passive sampling study in Europe. Thus, spatial distribution of computed PCB-153 air concentrations for 2002 is consistent with the observed concentrations both in remote and contaminated regions.
- The comparison with long-term measurements reveals reasonable agreement between the computed and measured annual mean air concentrations. In particular, good agreement (within an accuracy of 50%) is found between computed and measured B[a]P air concentrations in the United Kingdom, Germany, and Poland.
- Temporal variations of PCB-153 computed air concentrations are rather close to long-term measurements of sites in Northern Europe in period 1997-2003. At the same time, decrease of PCB-153 air concentrations observed at CZ3 was not reproduced by the model, which could be caused by the uncertainties of temporal variation of emission in this region.
- Comparison of monthly mean PCB-153 air concentrations obtained by the model and observed at EMEP monitoring sites reveals that the model is capable to reproduce seasonal variations of air concentrations. In particular, reasonable agreement is found with measurement of the remote site FI96, located distantly from significant PCB emission sources, and at sites SE2, SE14, and SE12 in some periods. The deviations between computed and measured values are likely caused by the absence of seasonal variations in PCB emission data used for modeling.
- For B[a]P and 2,3,4,7,8-PeCDF model clearly underestimates seasonal variation of air concentrations. The disagreement can be connected with the underestimation of seasonal variations emissions and uncertainty of degradation process description in the model for B[a]P. To improve the agreement between calculated and measured seasonal variations of

air concentrations for these POPs data on seasonal variations of emissions are needed and refinement of the description of B[a]P degradation is required.

- Reasonable agreement is found between computed and observed B[a]P concentrations in precipitation (within an accuracy of 70%). For PCB-153 in precipitation the differences between the model results and measurements are more significant (within a factor of 2). At the same time, base of the comparison for concentrations in precipitation is considerably less than that for air concentrations. Existing discrepancies may be caused by the uncertainties in emission and measurement data, and differences between the precipitation amount used in the model and obtained at monitoring sites. Therefore, at the moment, the conclusions on agreement between calculated and measured concentrations in precipitation are of preliminary character.

### ***Final remarks***

POP model intercomparison study has shown that MSCE-POP model parameterization and the description of POP transport and exchange processes are in line with other participated models.

The comparison of model results with available measurements for selected POPs reveals that the MSCE-POP model reasonably reproduces spatial and temporal variations of observed atmospheric levels of pollution within the European region.

Further development of MSCE-POP model is required with respect to the description of atmospheric degradation and exchange processes with underlying surface, including the refinement of partition coefficients.

To improve MSCE-POP model results there is a need to refine official POP emission data, including emission totals, spatial distributions and seasonal variations. Parallel measurements of POPs in air and other environmental compartments and information on measurement data uncertainties are required.

