Chapter 8

RELIABILITY OF THE ASSESSMENT RESULTS

In this chapter we summarize main results of the activity devoted to the model testing, verification of modeling results and evaluation of their uncertainty.

8.1. Model verification and sensitivity analysis

Advection scheme

Advection scheme used in the atmospheric module is based on widely applied and extensively tested Bott scheme adapted to the spherical co-ordinates (Section 3.2). To verify the scheme operation consistency in particular conditions of the spherical co-ordinates (especially in the vicinity of the pole) standard advection tests have been performed. Detailed description of the tests is presented in Annex B. The main conclusions of the tests are the advection scheme does not produce considerable distortions of transported substances (dispersion error) and has comparatively low artificial diffusion. Besides, the scheme is stable in strong deformational flows and does not produce observable time-splitting error.

Atmospheric transport

Simulation of a tracer airborne transport in real atmospheric conditions has been tested on the base of lead. It is commonly assumed that lead occurs in the atmosphere solely in solid phase as a part of aerosol particles. In the frame of the study, modeling results obtained by the hemispheric model were compared with available measurements and results of regional model of heavy metal atmospheric transport (MSCE-HM). The MSCE-HM model has been verified in a number of intercomparison campaigns with other regional models [*Sofiev et al.*, 1996; *Gusev et al.*, 2000; *Ryaboshapko et al.*, 2001] and has been qualified by means of sensitivity and uncertainty studies [*Travnikov*, 2000]. Thus, its results can be considered as quite reliable within European region. The verification procedure is described in detail in Annex B.

It was concluded that results of a tracer airborne transport modeling are in satisfactory agreement both with available measurements and with results of regional MSCE-HM model, and discrepancy does not exceed a factor of two in both cases. Thus, the developed atmospheric module can satisfactory simulate airborne transport of an inert tracer in the atmosphere.

Atmospheric chemistry

Chemical scheme of mercury transformation in the atmosphere was verified in comparison with other mercury transport models and with measurements during the models intercomparison study [*Ryaboshapko et al.*, 2002; *Ryaboshapko et al.*, in press]. The comparison has shown that all the models involved apply similar physical and chemical principles of mercury transformations and their

results are in reasonable agreement. Besides, newest findings of the most advanced scientific models were included to the model chemical scheme.

Sensitivity of the model chemical scheme to atmospheric parameters (air temperature, pH, liquid water content) and concentration of main chemical reactants (such as ozone, sulfur dioxide, etc.) was studied in [*Ryaboshapko et al.*, 2001]. The most important parameters for certain atmospheric conditions were determined and their description in the model scheme was refined.

Gas/particle partitioning

The application of the constant value of the specific aerosol surface to the calculation of gas/particle partitioning can lead to uncertainties of depositions and mean annual air concentrations ranging within about 20-30% for the Russian North. For other regions of the Northern Hemisphere the uncertainty can be higher. In further model development the spatial distribution of the specific aerosol surface should be taken into account (Annex F).

Degradation

Atmospheric degradation can be significant sink of low chlorinated PCBs, which present in the atmosphere mainly in gaseous phase. One of the most important processes of PCB destruction in the atmosphere is reaction with OH radical. The atmospheric concentrations of OH radical depend on a lot of factors (latitude, cloudiness, day time, season, etc.). At present in the model as a first approximation OH radical concentrations have no diurnal variations and depend only on a season. To assess the influence of this assumption rough calculation experiments are made (Annex F).

Oceanic transport and ice cover

Oceanic transport module describing behaviour of POPs in the marine environment was verified in comparison with available measurements of PCB in seawater [*Strukov et al.*, 2000]. Measurements from different depths of the Northern Atlantic were involved in the comparison. The results showed reasonable agreement between modeled and observed values.

An extensive analysis of the oceanic transport module sensitivity to some processes affecting POP transport and accumulation in the environment is presented in Annex E. In particular, influence of the partitioning between dissolved and adsorbed forms as well as ice cover effect on POP transport is considered. The most substantial details of the processes are outlined and appropriate parameterization is selected.

Soil accumulation

Sensitivity of the soil module, describing POP transformation and accumulation in the soil environment to such processes as transport with dissolved organic carbon and distribution between dissolved and adsorbed forms, is studied in Annex D. In particular, it is demonstrated that proper description of this processes can considerably improve the modeling of POP accumulation in soil and soil/atmosphere exchange processes.

8.2. Uncertainty of emission data

Emission data are among the most important input information drastically influencing the modeling results [*Travnikov*, 2000]. Therefore, assessment of emission uncertainty requires separate consideration.

Mercury

Uncertainty analysis of anthropogenic mercury emission estimates appropriate to the utilized emission data was published in [*Pacyna and Pacyna*, 2001]. As it was mentioned in this work uncertainty of the emission estimates can be evaluated per source categories as follows:

- Stationary fossil fuel combustion: ±25%
- Non-ferrous metal production: ±30%
- Iron and steel production: ±30%
- Cement production: ±30%
- Waste disposal: up to a factor of 5

Taking into account different contribution of the source categories to mercury emission from different continents the emission uncertainty can vary from 25% to more than 100% from continent to continent.

Estimates of natural mercury emission and re-emission contain higher uncertainty. As it follows from Table 5.2 the global estimates available from the literature (disregarding evidently overestimated values) varies almost twice. Besides, conventional character of the spatial distribution of emission fluxes contributes additional uncertainty. Thus, uncertainty of natural emission and re-emission of mercury potentially reaches a factor of two.

PCBs

Analysis of emission estimates uncertainties for PCB is presented in Section 4.2 of the report. The main sources of the uncertainty are identified as follows:

- The representativeness and accuracy of emission factors are the major source of uncertainties.
- The global movement of PCB-containing products and wastes between countries was not considered in detail.
- Potential “point sources” of PCB atmospheric emissions, incidental formation, and emissions of PCB from the combustion process (*de novo* synthesis) were not considered separately.

Besides, uncertainties of estimates in global consumption and emissions will grow with the increase of the specification level (e.g. more detailed usage and waste disposal categories).

γ-HCH

Uncertainties of γ-HCH emission estimates are analyzed in Section 4.3. It is concluded that:

- The main uncertainty is connected with the country-based usage of γ-HCH that may be uncertain themselves.
- Another source of uncertainties arises from distribution of estimated emission over cropland areas since HCH consumption for other purposes unconnected with agriculture was not considered.
- Substantial source of uncertainties originates from the rather rough description of seasonal variations of γ-HCH emissions used in the model

8.3. Modeling results vs. measurements

The most important analysis of modeling results accuracy is comparison of calculated values with measured ones. However, one should note that measuring data with appropriate spatial and temporal representativeness are often unavailable for statistically correct analysis.

Mercury

Comparison of mercury modeling results with available measurements is presented in Section 5.2. Nineteen monitoring station from Europe and North America are involved in the comparison. It is demonstrated that the model quite well reproduces annual air concentrations at these stations and the discrepancy does not exceed 40%. Modeled deposition fluxes satisfactorily conform to the measured ones. The discrepancy for all the stations does not exceed a **factor of two** with the correlation coefficient 0.54.

PCBs

Model results on PCB transport was verified by comparison computed concentrations in air and precipitation and deposition fluxes with available measurement data (Section 6.3). Measured data on PCB-28, 118, 153 and 180 from eleven sites for the period from 1989-96 were used in comparison. The comparison showed that most of computed air concentration values were within a **factor of four** with regard to measurements. Modeled concentrations of all considered PCB congeners correlate rather well with observed air concentrations. Computed concentrations of some congeners in precipitation also agreed quite well with measured ones, but for others distinction is significant.

γ-HCH

Comparison of calculated and observed γ-HCH concentrations in the ambient air and precipitation is based on monitoring and literature data (Section 7.2). Available measurements on γ-HCH air concentrations cover the Arctic, European and Baikal regions, whereas the data on concentrations in precipitation are mostly from the European region. The comparison showed that the model overestimates γ-HCH air concentrations on average 2.5 times with correlation between measured and calculated values about 0.5. Besides, more than 75% of compared values are within a **factor of four**. Reasonable agreement was obtained for measured and modeled concentrations of γ-HCH in precipitation: on average calculated concentrations 1.2 times overestimate measured ones with correlation coefficient 0.8.

8.4. Concluding remarks

Summarizing mentioned above we can conclude that models involved in the assessment are extensively tested and can be considered as sufficiently reliable within the confidence limits. Uncertainties of modeled air concentrations and deposition fluxes could be roughly estimated by a factor of two for mercury results and by a factor of four for PCB and γ-HCH. Uncertainties of the relative contributions of different sources to the total deposition to some region (source-receptor relationships) are assumed to be lower. More precise quantitative estimates of the model uncertainties require comprehensive sensitivity and uncertainty analysis of the models with respect to all the processes and input parameters.

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