CONCLUSIONS

This report contains the main outcome of Stage II of the POP model intercomparison study. The following models participated in this stage: ADEPT, CAN/POPs, CliMoChem, DEHM-POP, EVN-BETR and UK-MODEL, G-CIEMS, SimpleBox, and MSCE-POP. The comparison of computed values of POP mass contained and degraded in the main environmental compartments (atmosphere, soil, water and vegetation), inflow and outflow for the specified domain, intermedia transport and spatial distribution of deposition and concentration fields in different environmental compartments is presented. Results of the sensitivity study with respect to physical-chemical parameter values used are presented. The comparison of model results on POP depositions and concentrations in the atmosphere with monitoring data is also given. In addition, the results on the sensitivity study with respect to physical-chemical parameter values used by the participating models in the description of gas/particles partitioning, wet deposition and gaseous exchange between the atmosphere and soil, water and vegetation are also considered.

The main body of this report provides a comparison of results of Stage II computational experiments for PCB-153 (first priority). The corresponding results for substances of the second priority (PCB-28 and PCB-180) are included in Annexes B, C, D and E. A preliminary analysis of the presented comparison is made for PCB-153 only.

A preliminary analysis of comparison of results for PCB-153 obtained by the participating models within Stage II shows the following:

- Most participating models provide reasonable agreement in description of mass distribution between the main environmental media. Thus, it can be concluded that:
    - The difference between the results of participating models on absolute values of PCB-153 mass contained in all considered layers of the atmosphere and soil, water and vegetation calculated on the basis of zero initial conditions (both for “reference” and “own/alternative” physical-chemical data sets) is considerably lower than that in results obtained on the basis of initial conditions. For the latter the values of PCB-153 mass contained in all considered layers of the atmosphere (except for 1 km results in “reference” data set) and 10 cm soil layer obtained by most models on the basis of both physical-chemical data sets are rather close. The difference in values of PCB-153 mass accumulated in 5cm layer of soil, 200m water layer and vegetation calculated with the use of initial conditions is more considerable than that in results obtained for the atmosphere.
    - According to the results presented by most models, PCB-153 is mainly accumulated in soil. PCB fractions in all other compartments are essentially lower and depend on type of calculations performed. The variability between PCB fractions in other environmental compartments is higher.
    - For most participating models the comparison of absolute and relative values of PCB-153 mass in the environmental media calculated with two different data sets show relatively weak sensitivity of mass balance values with respect to variations of pollutant-related parameters. Only in some cases the differences are essential.
- Model estimates of PCB-153 masses degraded in the main environmental media agree well for most models. In particular, it was noted that:
    - In calculations based on “reference” and “own/alternative” physical-chemical data sets most participating models provide rather close absolute values of PCB-153 mass degraded in the atmosphere. The difference in calculated absolute values of PCB-153 mass degraded in soil

and water is considerably higher. The limited number of models provided results on PCB-153 mass degraded in the vegetation compartment.

- Noticeable seasonal variations in computed absolute values are mostly characteristic of models that use temperature dependent degradation rates.
- The comparison of masses degraded in main environmental media calculated with “reference” and “own/alternative” data sets show that almost all models use higher degradation rates in the atmosphere in their “own or alternative” set of parameters compared with that in “reference” data set. Therefore the annual values of calculation results on PCB-153 masses degraded in the atmosphere obtained with the use of “own or alternative data sets” noticeably exceed those obtained with “reference data set”.
- Degradation rates in soil and water used by models are lower than that given in “reference” data set. Therefore, for all models’ results, the values of PCB-153 masses degraded in these media obtained with the use of “own or alternative data sets” are less than those obtained with “reference” data set.
- Analysis of relative fractions of PCB-153 mass degraded in the main environmental media that are ratios of the degraded mass and the mass contained in the considered compartment (taking into account also degraded mass) also show that most models closely describe distribution of PCB-153 mass in the environment due to degradation in the atmosphere and soil and water.

- Most models closely describe transport outside the calculation domain. Thus, it was revealed that:
  - According to the data presented for both “reference” and “own/alternative” data sets, in ADEPT, CAN/POPs and MSCE-POP model results the atmosphere is the main media of PCB-153 outside transport. Calculated fractions of overall outside transport through atmosphere considerably exceed those for other media in results of CliMoChem, G-CIEMS, and SimpleBox 3.0 and 3.12 (zero initial conditions) models. Results of SimpleBoxs 3.0 and 3.12 based on historical emissions are characterized by higher annual transport in the marine environment than in the atmosphere.
  - The most considerable contribution to the outside transport of PCB-153 due to the other considered media (sediment, soil and vegetation) than ocean and atmosphere is observed in the results of SimpleBox 3.0 model made on the basis of initial conditions.
- All model provide reasonable agreement in description of intermedia mass flows and concentrations in the main environmental media. Thus, it was obtained that:
  - Air concentrations as the most important output of the participating models are in good agreement for all models’ results. Several models predicted values of PCB-153 concentrations in the atmosphere at its interface with different underlying surfaces taking into account types of these surfaces.
  - The most part of participating models predicted close values of PCB-153 concentrations in soil, water and vegetation. However, variability of calculated concentrations in the environmental media other than the atmosphere is higher than that for the atmosphere. According to the results obtained within Stage II calculations, the bulk of overall PCB content in the environment is accumulated in soil. In this connection, it can be noted that the difference between the maximum and minimum values of calculated soil concentrations is higher than that for air concentrations but considerably less than that for the rest of media. Close absolute values of soil concentrations are characteristic of most models’ results.

- Most participating models provided reasonable agreement in description of net intermedia mass flows directed from the atmosphere to soil and to water. The scattering in results on net intermedia mass flows directed from the atmosphere to vegetation is higher. The similarity in description of dry and wet deposition processes from the atmosphere to different underlying surfaces implied in the model parameterisations is testified by close results of most models based on “reference” data set. Several models calculated dry deposition to different underlying surfaces taking into account types of these surfaces. Results on dry deposition flows from the atmosphere to all of the considered underlying surfaces, wet deposition flows from the atmosphere to soil and water obtained on the basis of “reference” data set, and wet depositions from the atmosphere to vegetation obtained on the basis of both data sets are in good agreement between all models. Scattering in values of gaseous exchange is more noticeable. Two models calculated re-emission gaseous flux from soil and one – from vegetation.
- For all considered media interfaces, agreement between different models’ results obtained on the basis of “reference” data set in most experiments performed is considerably better than that for results based on the “own/alternative” data set. Maximum difference between results of calculations of intermedia mass flows performed with both data sets of physical-chemical properties does not exceed 50% for dry and wet depositions, in calculations of gaseous exchange it is about 120%. The results of all models showed rather weak sensitivity of calculated values of air concentrations with respect to variations of pollutant-related parameters. The difference in concentrations in other media than the atmosphere is more noticeable (120% in maximum).

- The comparison of calculated fields of depositions and concentrations in the main environmental media demonstrates that the models of different type and resolution closely described the spatial distribution of PCB-153 pollution.
- The comparison of model results on PCB-153 depositions and concentrations in the atmosphere with monitoring data shows the following:
  - Participated models reasonably reproduced observed levels and trends of mean annual air concentrations. Comparison for other congeners has shown reasonable agreement for PCB-180 and larger differences for PCB-28.
  - All the models overestimate observed levels of PCB deposition fluxes.
  - The models reasonably reproduce PCB congener composition in air concentrations obtained by measurements. More discrepancies are found in the modeled and measured congener composition of PCB deposition fluxes.
- The sensitivity study with respect to physical-chemical parameter values used by the participating models in the description of gas/particles partitioning, wet deposition and gaseous exchange between the atmosphere and soil, water and vegetation performed on the basis of calculation experiments formulated at Stage I reveals that:
  - Most models describe similarly gas/particle partitioning. The results obtained with “own” set of pollutant-related data agree better between models than those based on “reference” data set. The difference in calculation of gas/particle partitioning caused by usage of “reference” and “own or alternative” data set of pollutant properties is moderate. Large differences are characteristic of high temperatures where values of fractions of particulate phase are small. The results obtained with “own or alternative” set of pollutant-related data agree better between models.

- The differences in absolute values of wet deposition flux and concentrations in precipitation calculated by models are essential. However, square deviation does not exceed the mean value of these parameters averaged between the participating models both in the results obtained on the basis of “reference” and “own/alternative” data sets. The difference in calculation results on wet deposition caused by the usage of “reference” and “own /alternative” data sets of pollutant properties is negligible. This process needs further investigation.
- Models describe gaseous flux between atmosphere and soil more closely than soil concentrations. The differences in concentrations are lower with “reference” data set than those with “own/alternative” data. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties (“reference” and “own/alternative”) is considerable for most models. Model descriptions of air/soil exchange and their parameterizations need further consideration.
- In general, most models closely describe processes of gaseous exchange between the atmosphere and water. The difference between calculated values of water concentrations and net gaseous flux from/to water obtained with two data sets of pollutant properties (“reference” and “own/alternative”) is essential for some models. The same applies to the description of gaseous exchange between atmosphere and vegetation.

A preliminary analysis of the main outcome of Stage II shows that in spite of the differences existing in the model descriptions and parameterisations, the reasonable agreement in the considered results on simulation of the basic processes of PCB behaviour in the environment is observed for most models. More detailed analysis of similarities and distinctions between different participating models in description of main processes is planned to be made in the framework of scientific publication.