

Table 3.109. Results on spatial distribution of PCB-153 depositions and concentrations in different compartments presented by the models

Maps	Data set used	ADEPT ^c	DEHM-POP_1	DEHM-POP_2	EVN-BETR_1 ^a	EVN-BETR_2 ^a	EVN-BETR_3 ^a	SimpleBox 3.0_1	SimpleBox 3.0_2	SimpleBox 3.12_2	SimpleBox 3.0_3	SimpleBox 3.12_3	MSCE-POP_1	MSCE-POP_2
Surface atmospheric concentrations, pg/m ³	ref	+	+	+	+	+	+	+	+	+	+	+	+	+
	own or alt		+	+				+	+	+	+	+	+	+
Surface soil concentration, ng/g	ref		+	+	+	+	+	+	+	+	+	+	+	+
	own or alt		+	+				+	+	+	+	+	+	+
Surface water concentration, pg/l	ref		+	+	+	+	+	+	+	+	+	+	+	+
	own or alt		+	+				+	+	+	+	+	+	+
Concentration in vegetation, ng/g (optional)	ref				+	+	+	+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+
Net deposition flux, mg/m ² /hour	ref	+						+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+
Wet deposition of gaseous phase, mg/m ² /hour	ref												+	+
	own or alt												+	+
Wet deposition of particle phase, mg/m ² /hour	ref												+	+
	own or alt												+	+
Wet deposition total, mg/m ² /hour	ref							+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+
Dry deposition of gaseous phase, mg/m ² /hour	ref												+	+
	own or alt												+	+
Dry deposition of particle phase, mg/m ² /hour	ref												+	+
	own or alt												+	+
Dry deposition total, mg/m ² /hour	ref							+	+	+	+	+	+	+
	own or alt							+	+	+	+	+	+	+

EVN-BETR_1 - EVN-BETR and UK-MODEL results calculated on the basis of initial concentrations given as input data, the only exception was that the initial conditions for the vegetation were set to zero;

EVN-BETR_2 - EVN-BETR and UK-MODEL results calculated on the basis of zero initial concentrations;

EVN-BETR_3 - EVN-BETR and UK-MODEL results calculated on the basis of historical emissions for 20-year period;

DEHM-POP_1 - DEHM-POP results calculated on the basis of initial concentrations given as input data;

DEHM-POP_2 - DEHM-POP results calculated on the basis of zero initial concentrations;

SimpleBox 3.0_1 - SimpleBox results of version 3.0 calculated on the basis of initial concentrations given as input data;

SimpleBox 3.0_2 and SimpleBox 3.12_2 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated on the basis of zero initial concentrations;

SimpleBox 3.0_3 and SimpleBox 3.12_3 – SimpleBox results of versions 3.0 and 3.12, respectively, calculated with historical emissions for 20-year period.

MSCE-POP_1 - MSCE-POP results calculated on the basis of initial concentrations given as input data;

MSCE-POP_2 - MSCE-POP results calculated on the basis of zero initial concentrations;

^a - EVN-BETR and UK-MODEL results were calculated with the help of a spatially resolved version of the model;

^b – SimpleBox: results were calculated on the basis of initial concentrations given as input data. The concentrations calculated are the bulk concentrations in the compartments. Maps of concentrations are obtained on the basis of annual values of concentrations at regional and continental levels;

^c - ADEPT results calculated on the basis of zero initial concentrations are winter averaged.

3.6.1. Comparison of results on spatial distribution of PCB-153 depositions and concentrations in different compartments obtained on the basis of “reference” data set

In this section a comparison of spatial distributions of PCB-153 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models with the use of “reference” data set on the basis of initial PCB-153 concentrations in the media, historical emissions and zero initial conditions is presented. A preliminary analysis of calculated deposition and concentration fields is made only for the model results obtained on the basis of non-zero initial conditions.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.147.

Due to different types and overall model approaches, the participating models provided calculated fields of PCB-153 air concentrations with different resolution. The finest resolution of the presented results is characteristic of DEHM-POP model. For SimpleBox model a spatial variability of results on concentration in the media is obtained by division of the cells of the calculation model domain into two types: regional and continental scales. However, it can be noted that in general all participating models describe spatial distributions of air pollution rather closely. In particular, the area of the most contaminated air with concentration equal approximately 10 pg/m^3 and higher is predicted to be over such countries as Belgium, France, Germany and Switzerland. The location of regions with relatively high, moderate and low PCB-153 concentrations in the atmosphere is similarly reproduced by EVN-BETR and UK-MODEL, DEHM-POP and MSCE-POP models. The difference between the lowest and the highest absolute values of air concentrations within the calculation domain calculated by all models is noticeable. Thus, for DEHM-POP air concentration levels in the considered region are in the range from 0.2 to 11.5 pg/m^3 ; for MSCE-POP – from 0.3 to 15.2 pg/m^3 ; for EVN-BETR and UK-MODEL (EVN-BETR_1 - initial concentrations) - from 0.0 to 15.8 pg/m^3 ; for EVN-BETR and UK-MODEL (EVN-BETR_3 - historical emissions) - from 0.0 to 14.3 pg/m^3 ; for SimpleBox 3.0 (initial concentrations) - from 5.4 to 12.8 pg/m^3 ; for SimpleBox 3.0 (historical emissions) - from 3.0 to 8.8 pg/m^3 ; for SimpleBox 3.12 (historical emissions) - from 3.4 to 9.5 pg/m^3 . The maximum average value of air concentration within this domain is characteristic of SimpleBox 3.0 results obtained on the basis of initial concentrations (6 pg/m^3) and the minimum average value – of DEHM-POP results also based on initial conditions (1.4 pg/m^3). According to the results of EVN-BETR and UK-MODEL (historical emissions and initial concentrations), MSCE-POP, SimpleBox 3.0 and 3.12 (historical emissions), the annual air concentration averaged for the calculation domain varies from 2.9 to 3.8 pg/m^3 .

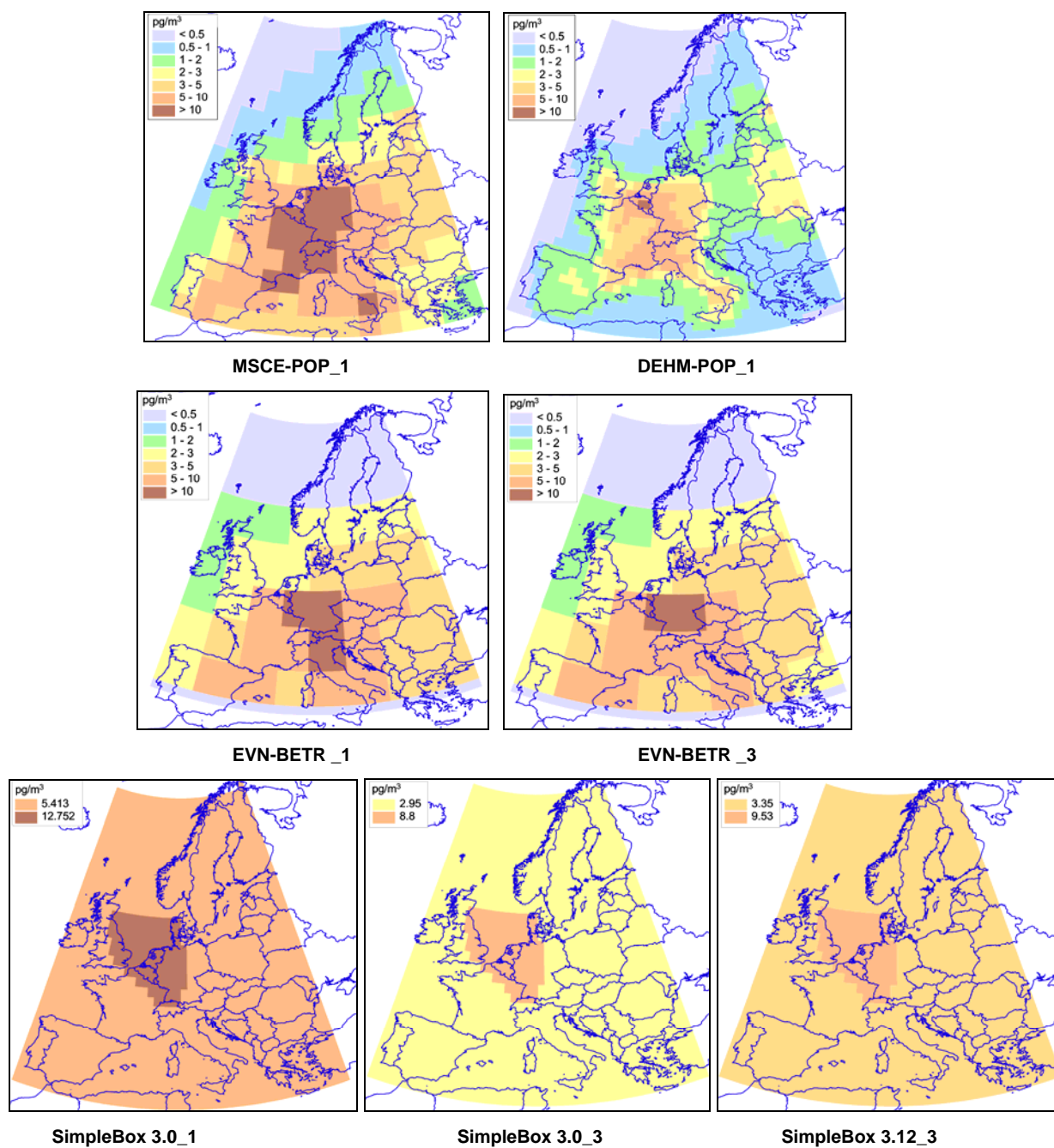


Fig. 3.147. Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of “reference” data set taking into account initial concentrations of pollutants in media or historical emissions

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.148.

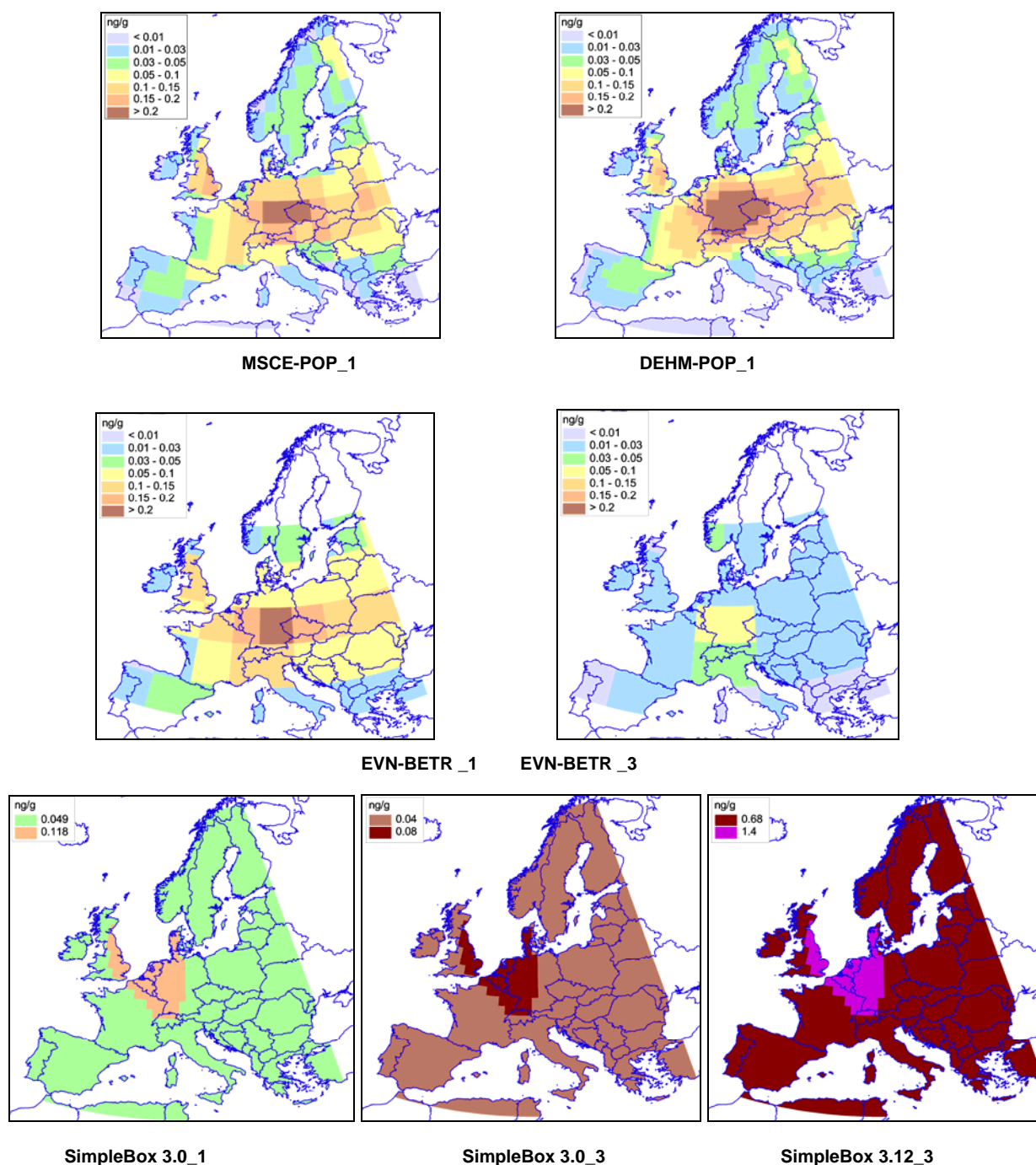


Fig. 3.148. Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of “reference” data set taking into account initial concentrations of pollutants in media or historical emissions.

As in the case with spatial distribution of air concentrations, the calculated fields of PCB-153 concentrations in soil calculated by the participating models on the basis of “reference” data set taking into account initial concentrations of pollutants in media or historical emissions are in reasonable agreement between each other. EVN-BETR and UK-MODEL (initial concentrations), DEHM-POP and

MSCE-POP models demonstrate very close results. Thus, according to these models results, considerably high PCB-153 soil concentrations (> 0.2 ng/g) in 2000 are typical for Central European countries (Germany, Austria, Poland, and the Czech Republic). In the results of different versions of SimpleBox model the region with the most contaminated soil covers not only some parts of Germany but also France, Belgium, the Netherlands and the UK. At that estimates of PCB-153 soil concentrations obtained by version 3.12 of SimpleBox model are considerably higher than those obtained by version 3.0. In general, concentrations of this pollutant in soil of Europe varied from 0.0 to 0.23 ng/g according to the results of EVN-BETR and UK-MODEL (initial concentrations); 0.0 to 0.05 ng/g according to the results of EVN-BETR and UK-MODEL (historical emissions); from $7.6 \cdot 10^{-9}$ to 0.27 ng/g according to the results of DEHM-POP model; from 0 to 0.44 ng/g according to the results of MSCE-POP; from 0.05 to 0.12 ng/g according to the results of SimpleBox 3.0 (initial concentrations); from 0.04 to 0.08 ng/g according to the results of SimpleBox 3.0 (historical emissions); and from 0.68 to 1.4 ng/g according to the results of SimpleBox 3.12 (historical emissions). The average value of soil concentration within the calculation domain obtained by the participating models is in the range from 0.01 to 0.74 ng/g.

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by EVN-BETR and UK-MODEL, DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. 3.149.

The difference in the spatial distribution of water concentrations of PCB-153 obtained by the participating models is more considerable than that in the results on concentrations in the atmosphere and soil. Thus, high values of PCB-153 seawater concentrations in the coastal waters of the North Sea vary from 1.0 to 10.0 pg/l according to the results of EVN-BETR and UK-MODEL obtained on the basis of initial concentrations and historical emissions, exceed 0.5 pg/l in the results of MSCE-POP and DEHM-POP models, and equal 0.03 and 0.87 pg/l in the results of SimpleBox 3.0 and 3.12 (historical emissions) and SimpleBox 3.0 (initial concentrations), respectively. The spatial distribution of PCB-153 water concentrations in the Mediterranean and Adriatic Seas are characterised by high values of water concentrations obtained by DEHM-POP (more than 0.5 pg/l) and EVN-BETR and UK-MODEL (more than 30.0 pg/l). The latter model predicts also the highest level of water pollution for the Baltic Sea. The average value of water concentration within the calculation domain provided by EVN-BETR and UK-MODEL (initial concentrations) is equal to 11.4 pg/l, by EVN-BETR and UK-MODEL (historical emissions) - to 6.5 pg/l, by MSCE-POP - to 0.1 pg/l, by DEHM-POP - to 0.15 pg/l, by SimpleBox 3.0 (initial concentrations) - to 1.0 pg/l, by SimpleBox 3.12 (historical emissions) - to 1.9 pg/l, by SimpleBox 3.0 (historical emissions) - to 1.95 pg/l.

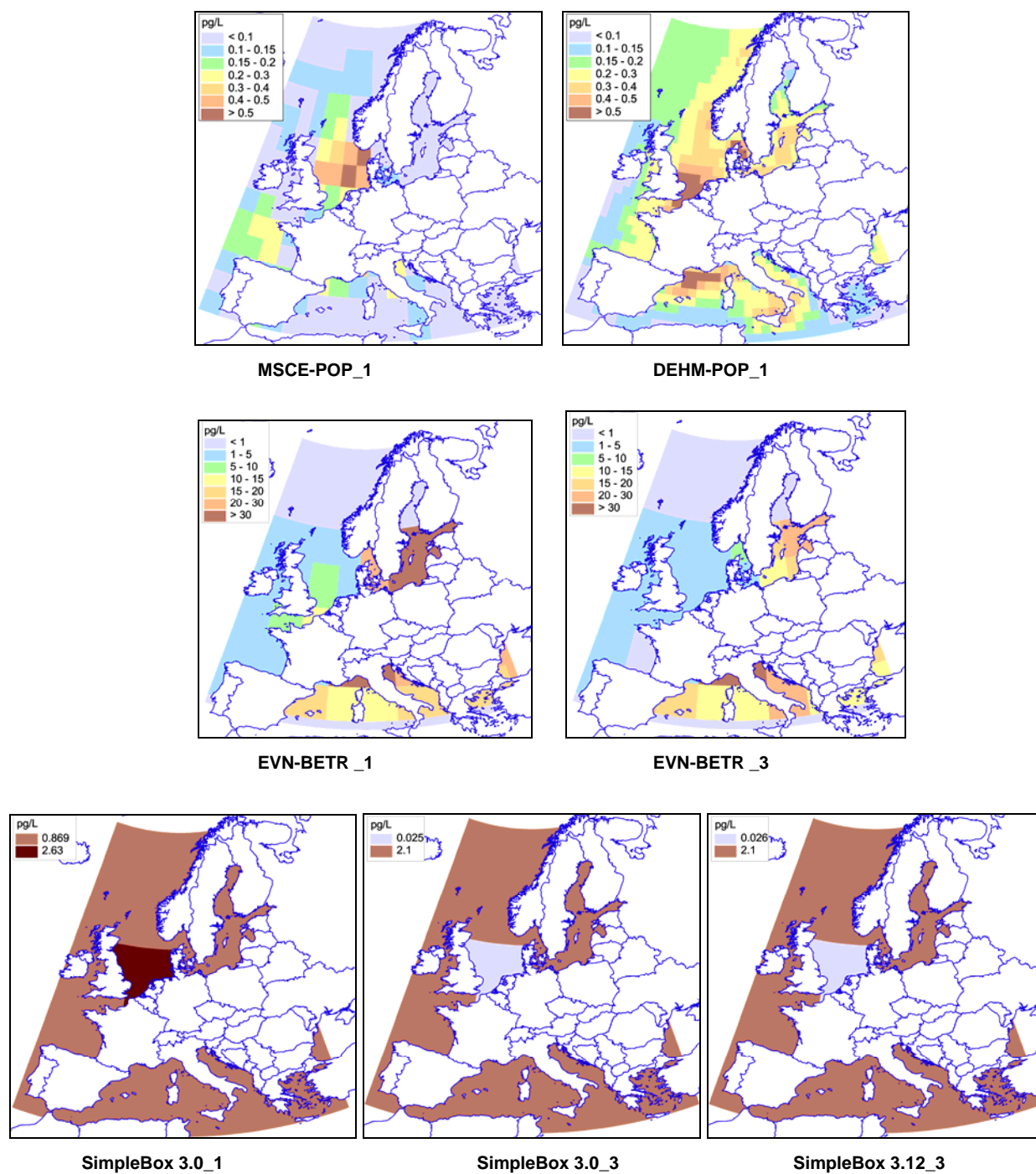


Fig. 3.149. Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of "reference" data set taking into account initial concentrations of pollutants in media or historical emissions.

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.3.150.

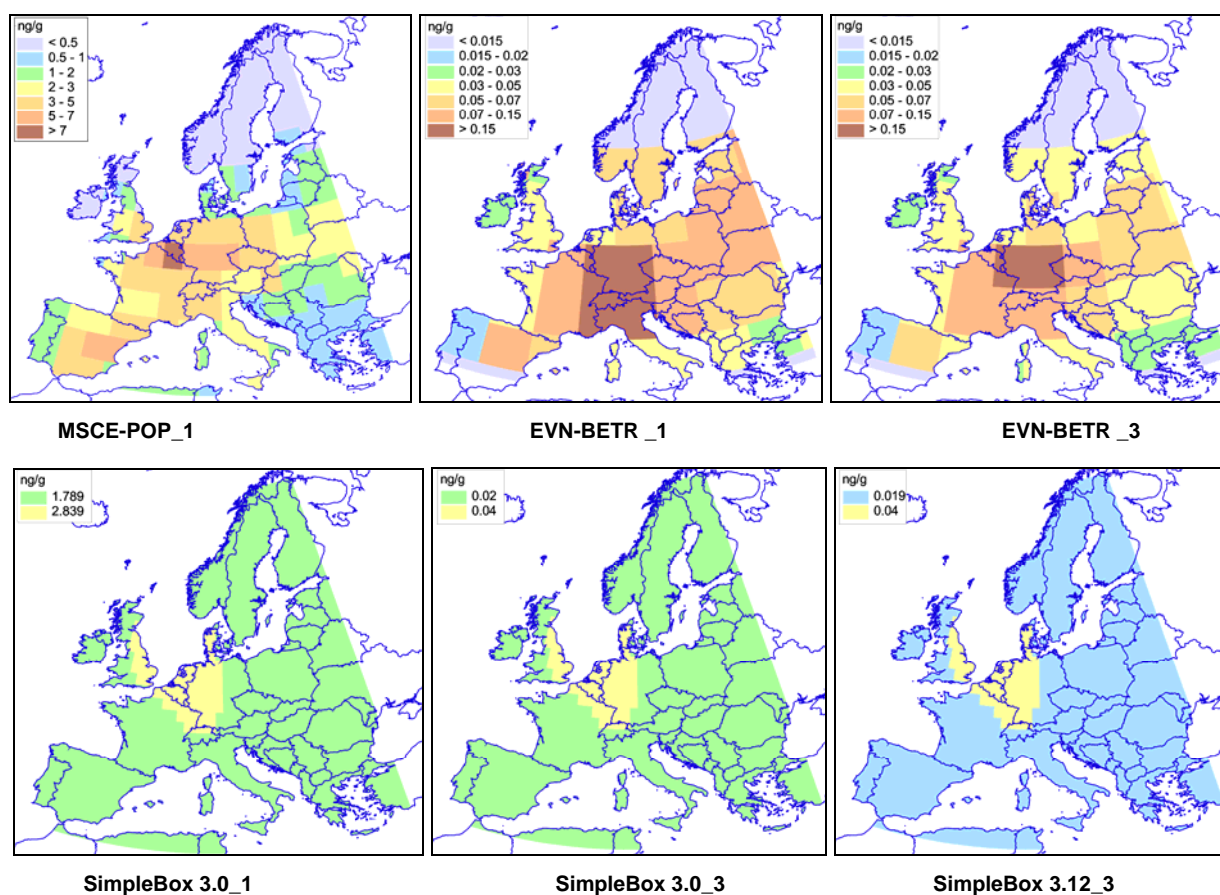


Fig. 3.150. Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of “reference” data set taking into account initial concentrations of pollutants in media or historical emissions

According to the results presented, the participating models predicted rather close spatial distribution of PCB-153 concentrations in vegetation. All models results show that the highest levels of concentrations in vegetation are observed in some regions of Belgium, France, Germany and the UK. At that estimates of PCB-153 concentrations obtained by MSCE-POP and SimpleBox 3.0 (initial concentrations) are considerably higher than others. Thus, in MSCE-POP results concentration levels in vegetation of the Europe are in the range from 0.0 to 9.6 ng/g; in EVN-BETR and UK-MODEL results (initial concentrations in all media except vegetation) - from 0.0 to 0.25 ng/g; in EVN-BETR and UK-MODEL results (historical emissions) - from 0.0 to 0.19 ng/g; in SimpleBox 3.0 results (initial concentrations) - from 1.79 to 2.84 ng/g; in SimpleBox 3.0 and 3.12 results (historical emissions) - from 0.02 to 0.04 ng/g.

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.151. The values of net deposition flux include dry and wet depositions and gaseous exchange. Of note, the spatial variability of SimpleBox results in this case is higher than that in the presented above results on concentrations in the media since the deposition values in this model are dependent on the different types of underlying surfaces, which were taken into account in their calculations.

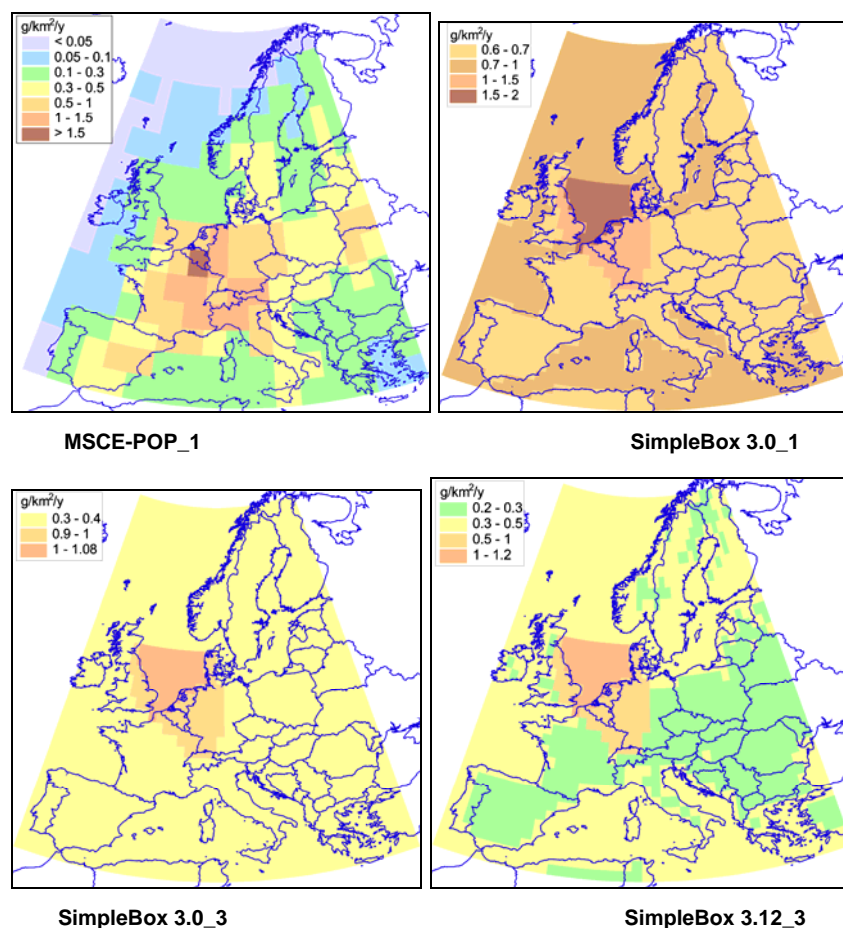


Fig. 3.151. Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of “reference” data set taking into account initial concentrations of pollutants in media or historical emissions

Spatial distribution of PCB-153 net depositions obtained both by MSCE-POP and SimpleBox models shows that relatively high values of this flux within the European domain are observed in some parts of Belgium, France, Germany, the Netherlands and coastal water of the North Sea. In the results of MSCE-POP model the highest net deposition flux is directed to the territories covered by soil, but the highest flux obtained by SimpleBox model is directed to the water. For SimpleBox 3.0 (initial concentrations) the levels of depositions over different parts of the calculation domain varied from 0.6 to 2.0 g/km²/y; for SimpleBox 3.0 (historical emissions) - from 0.3 to 1.1 g/km²/y; for SimpleBox 3.12 (historical emissions) - from 0.2 to 1.2 g/km²/y; and for MSCE-POP model - from 0.02 to 1.9 g/km²/y.

Below the comparison of model results obtained on the basis of zero initial concentrations in the environmental media is presented.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by ADEPT, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.152.

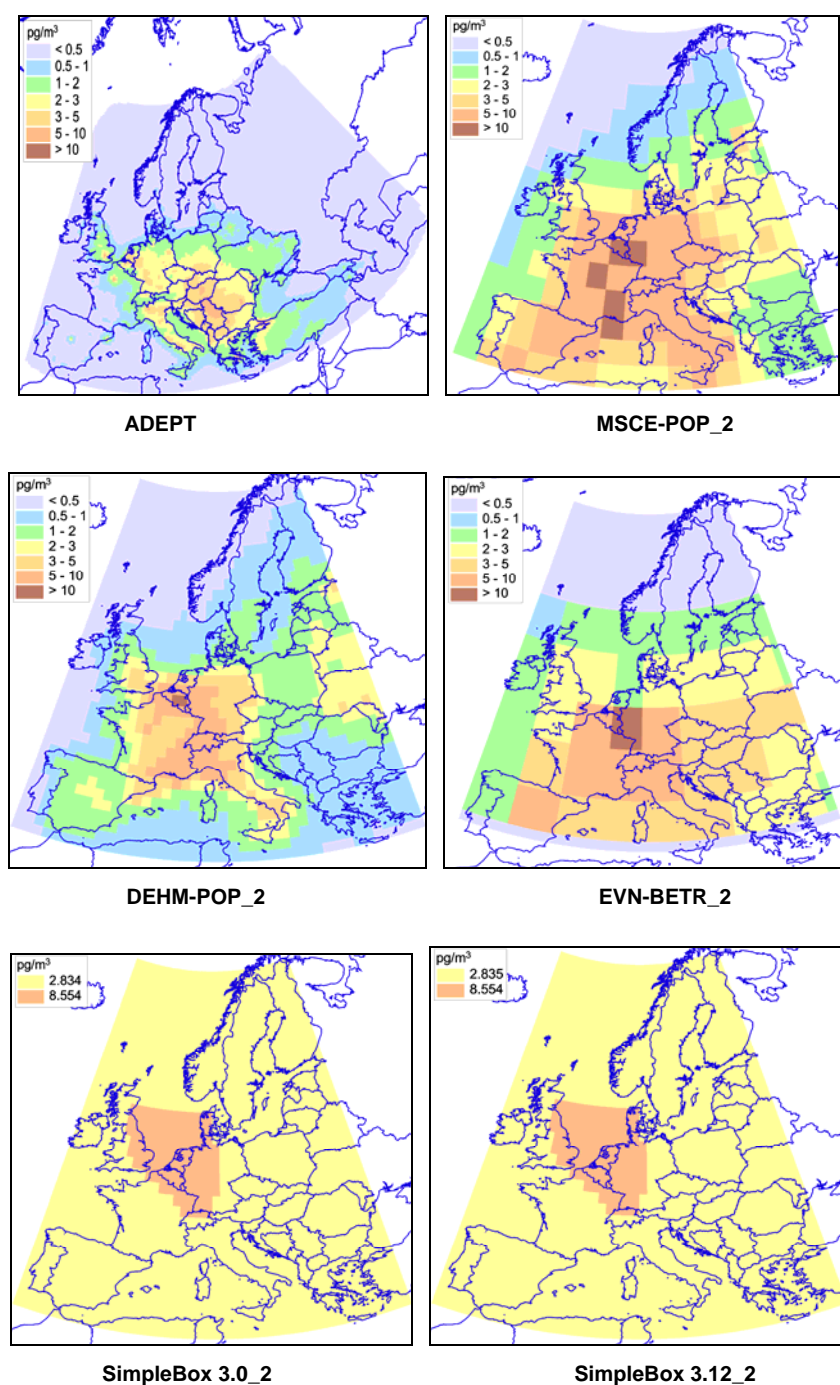


Fig. 3.152. Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of “reference” data set and zero initial concentrations

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are illustrated in Fig.3.153.

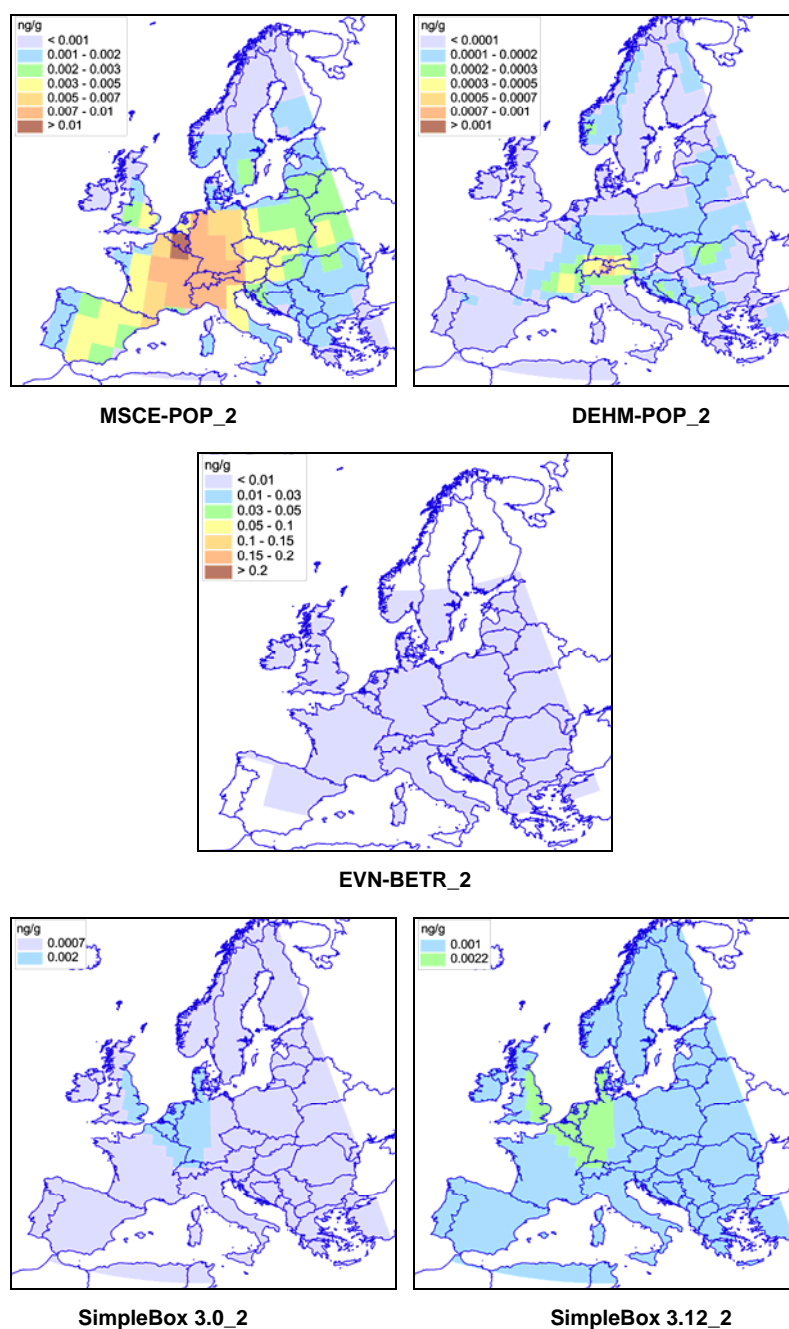


Fig. 3.153. Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of “reference” data set and zero initial concentrations

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig. 3.154.

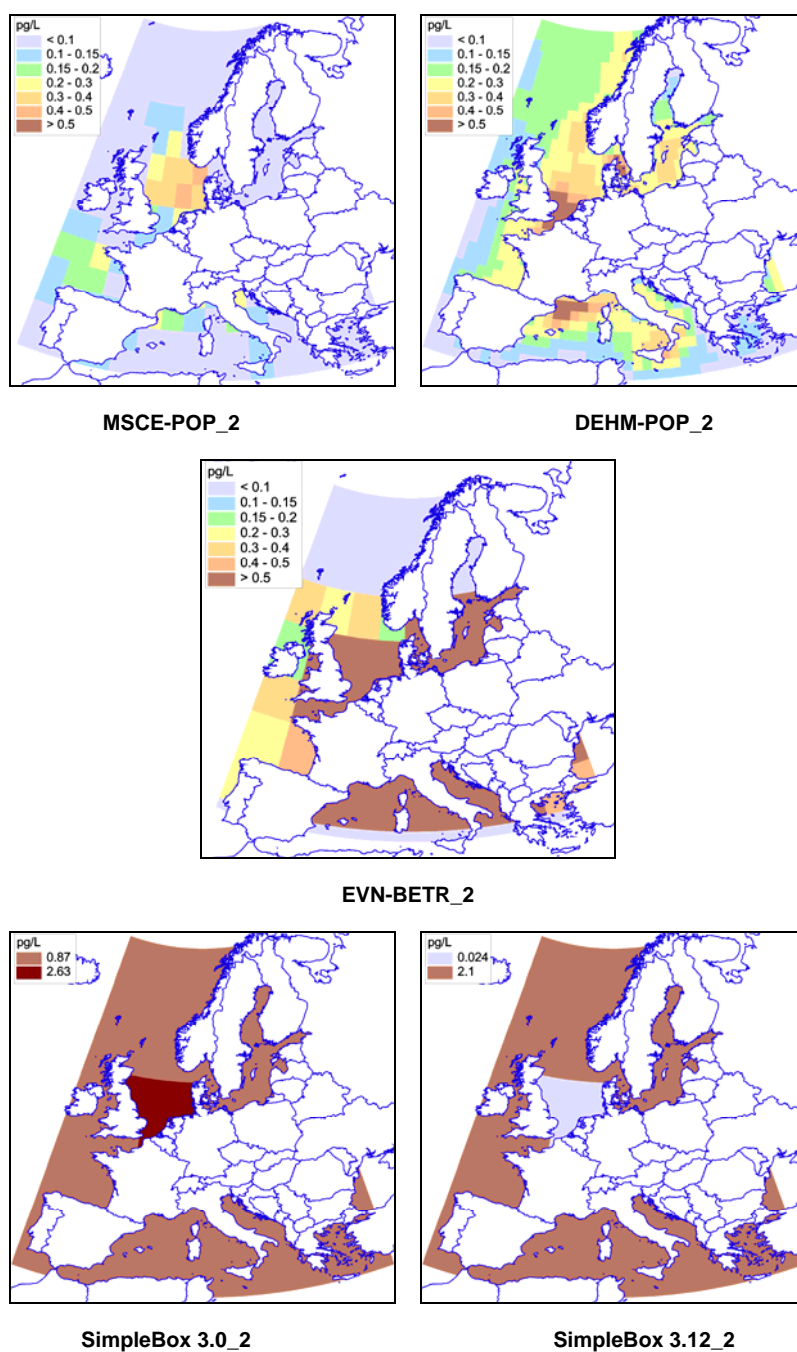


Fig. 3.154. Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of “reference” data set and zero initial concentrations.

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models are compared in Fig.3.155.

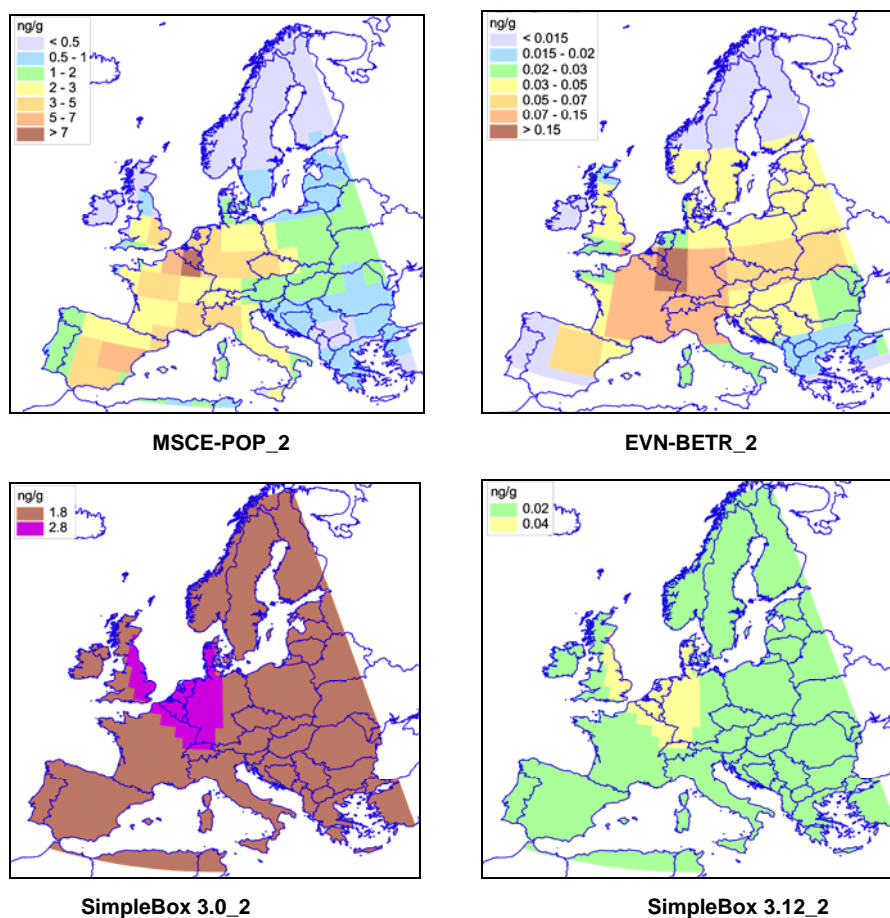


Fig. 3.155. Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of “reference” data set and zero initial concentrations.

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by ADEPT, MSCE-POP and SimpleBox models are shown in Fig.3.156. The values of net deposition flux include dry and wet depositions and gaseous exchange.

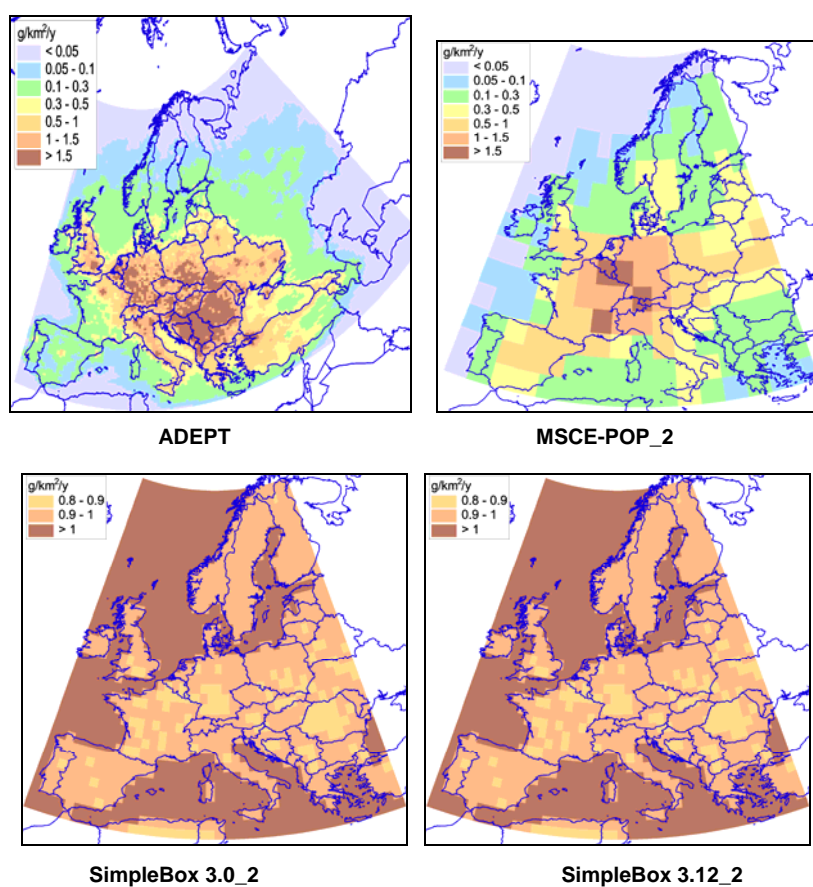


Fig. 3.156. Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of “reference” data set and zero initial concentrations

3.6.2. Comparison of results on spatial distribution of PCB-153 depositions and concentrations in different compartments obtained on the basis of “own or alternative” data sets

In this section a comparison of spatial distributions of PCB-153 depositions and concentrations in different environmental compartments for 2000 obtained by the participating models “own or alternative” data sets on the basis of initial concentrations of pollutants in media, historical emissions and zero initial conditions is presented.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.157.

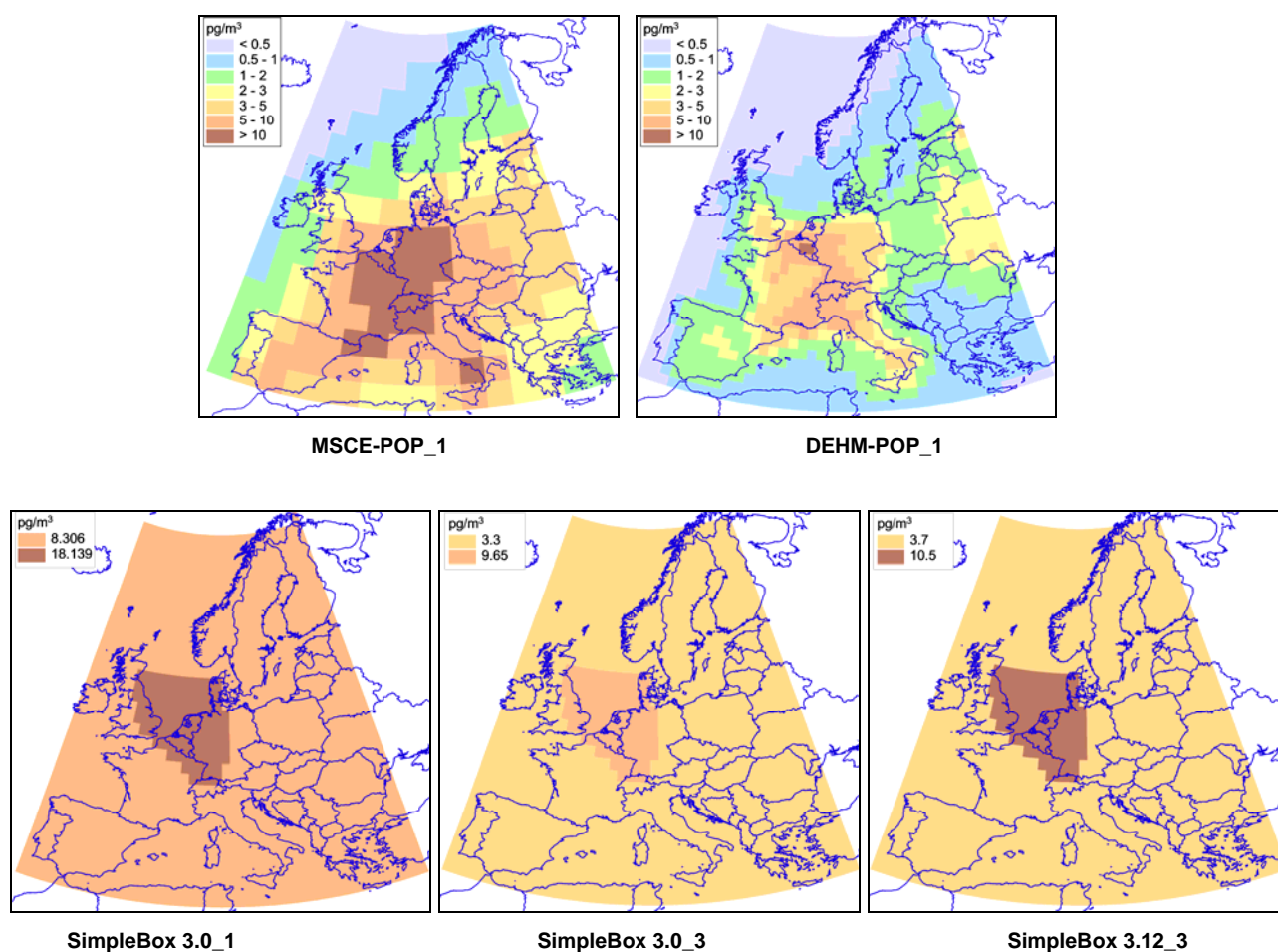


Fig. 3.157. Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of “own or alternative” data sets taking into account initial concentrations of pollutants in media or historical emissions

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.158.

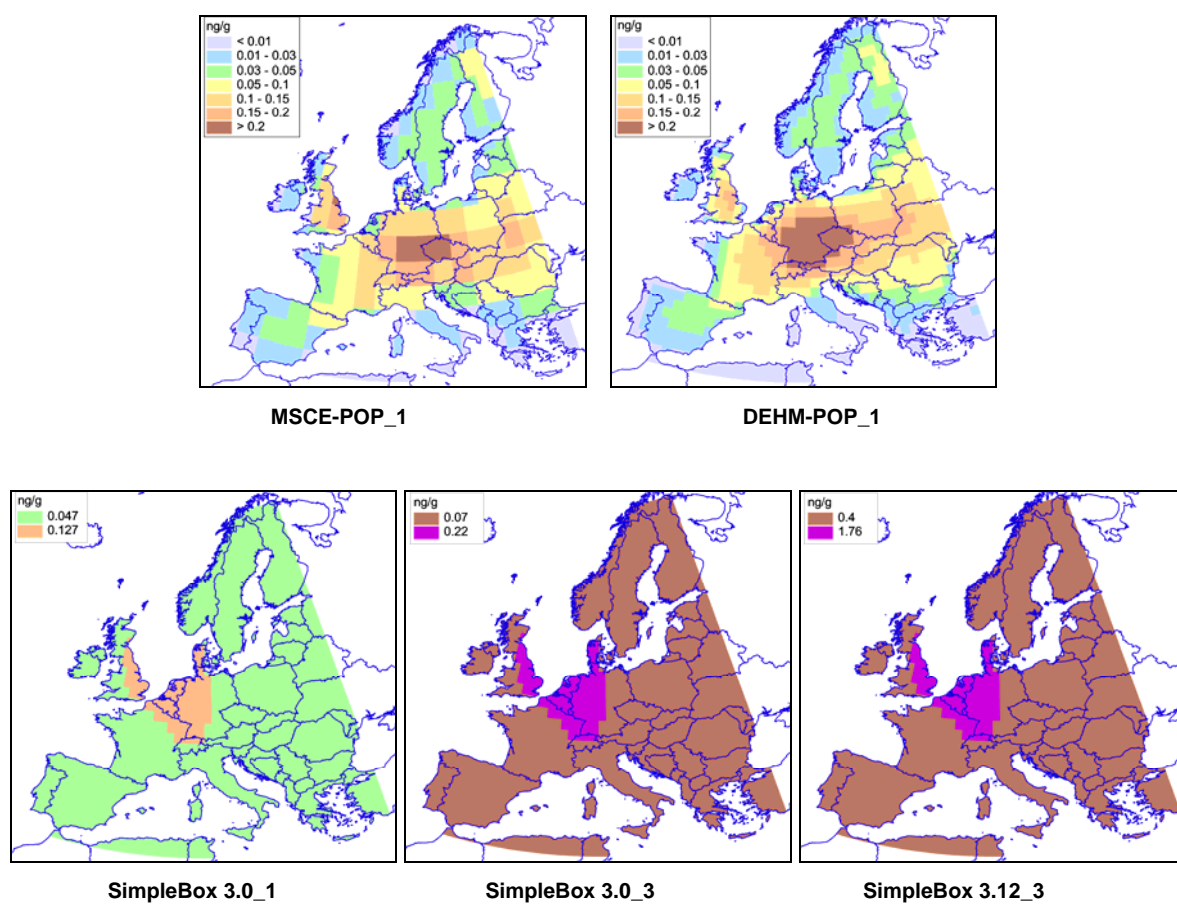


Fig. 3.158. Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of “own or alternative” data set taking into account initial concentrations of pollutants in media or historical emissions

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. 3.159.

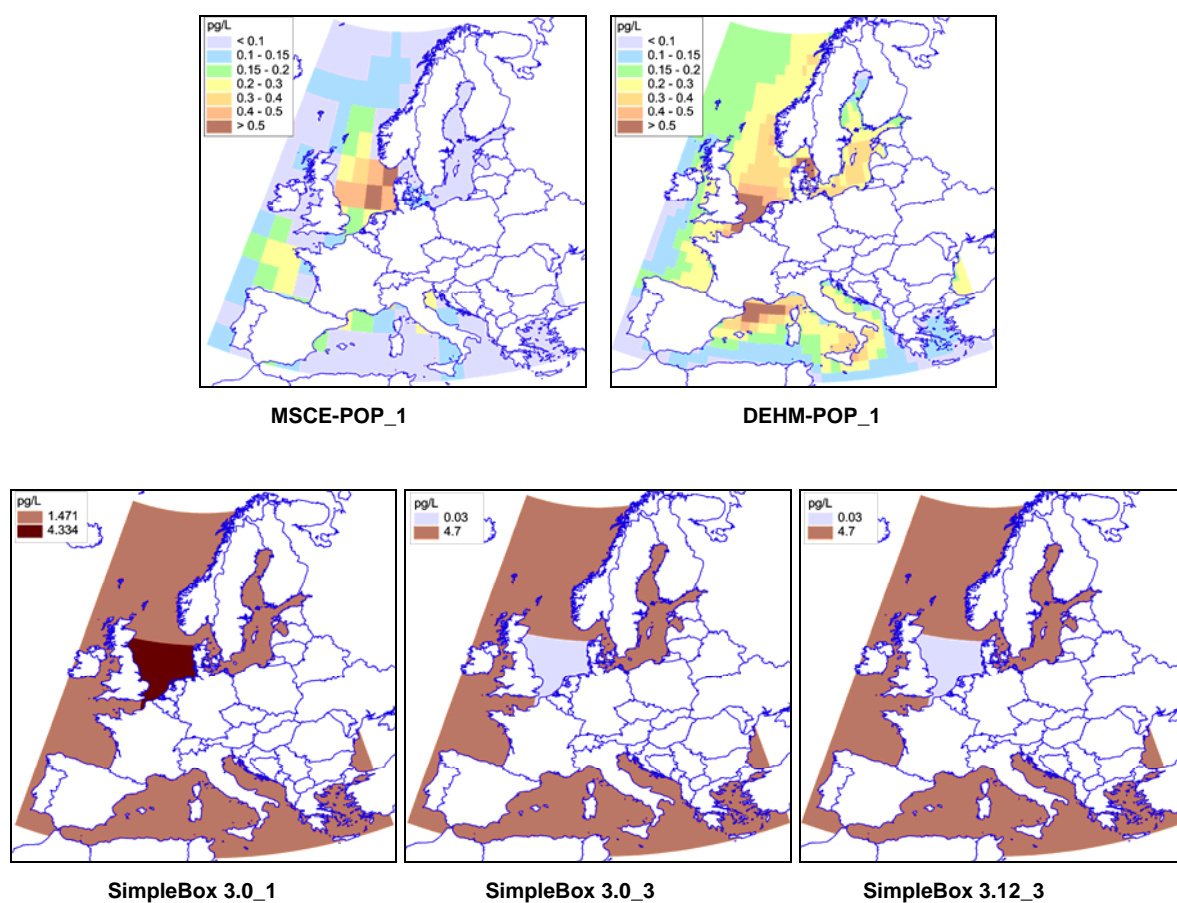


Fig. 3.159. Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of “own or alternative” data sets taking into account initial concentrations of pollutants in media or historical emissions

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.3.160.

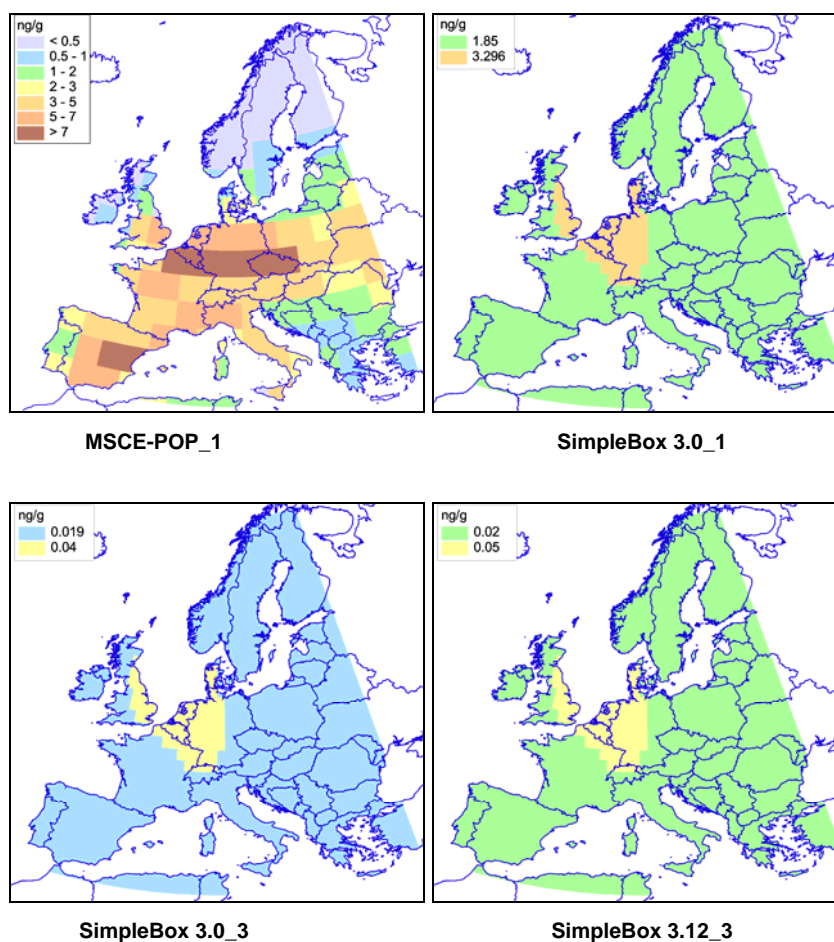


Fig. 3.160. Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of “own or alternative” data sets taking into account initial concentrations of pollutants in media or historical emissions.

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.161. The values of net deposition flux include dry and wet depositions and gaseous exchange.

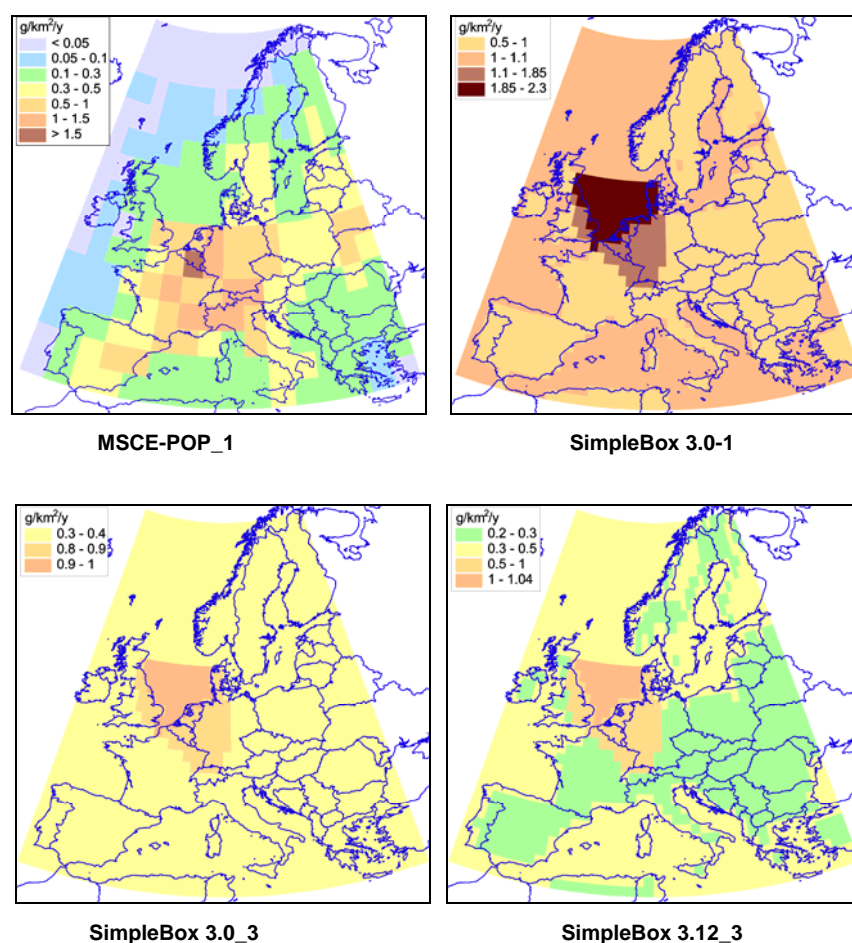


Fig. 3.161. Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of “own or alternative” data sets taking into account initial concentrations of pollutants in media or historical emissions.

The model results obtained on the basis of zero initial concentrations in the environmental media are compared below.

Concentration in the atmosphere. The calculated fields of PCB-153 annual concentrations in the atmosphere of the European calculation domain presented by DEHM-POP, MSCE-POP and SimpleBox models for 2000 are compared in Fig. 3.162.

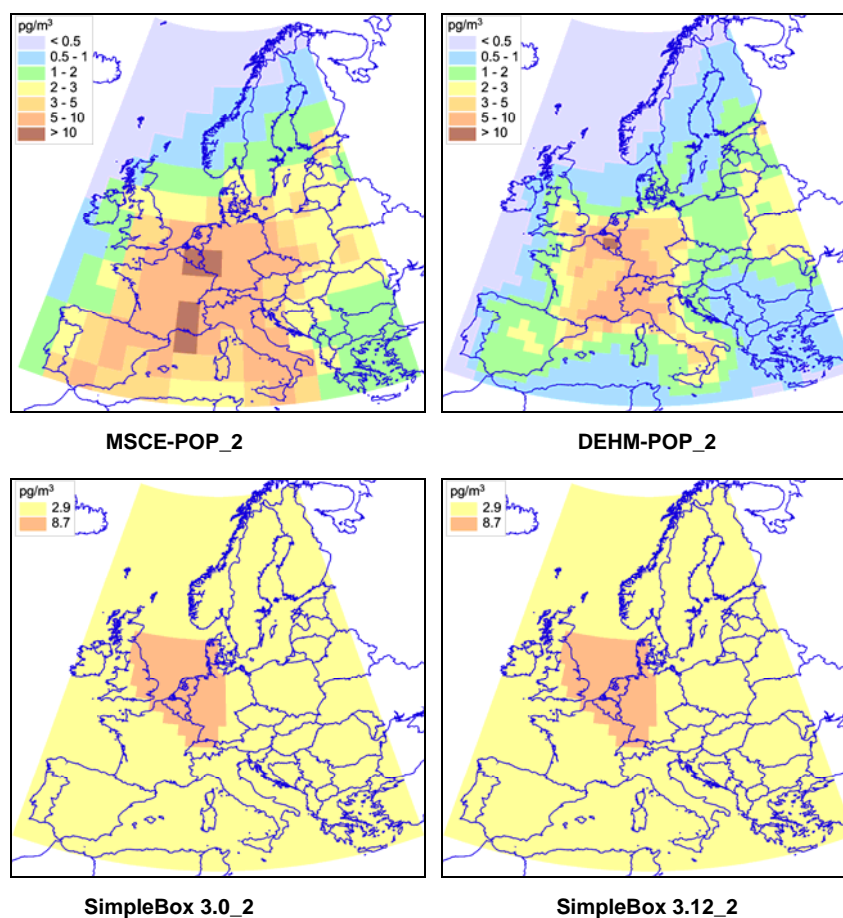


Fig. 3.162. Spatial distribution of PCB-153 concentrations in the atmosphere calculated by the participating models on the basis of “own or alternative” data sets and zero initial concentrations.

Soil concentration. The spatial distributions of PCB-153 concentration in soil of the European region presented by DEHM-POP, MSCE-POP and SimpleBox models are illustrated in Fig.3.163.

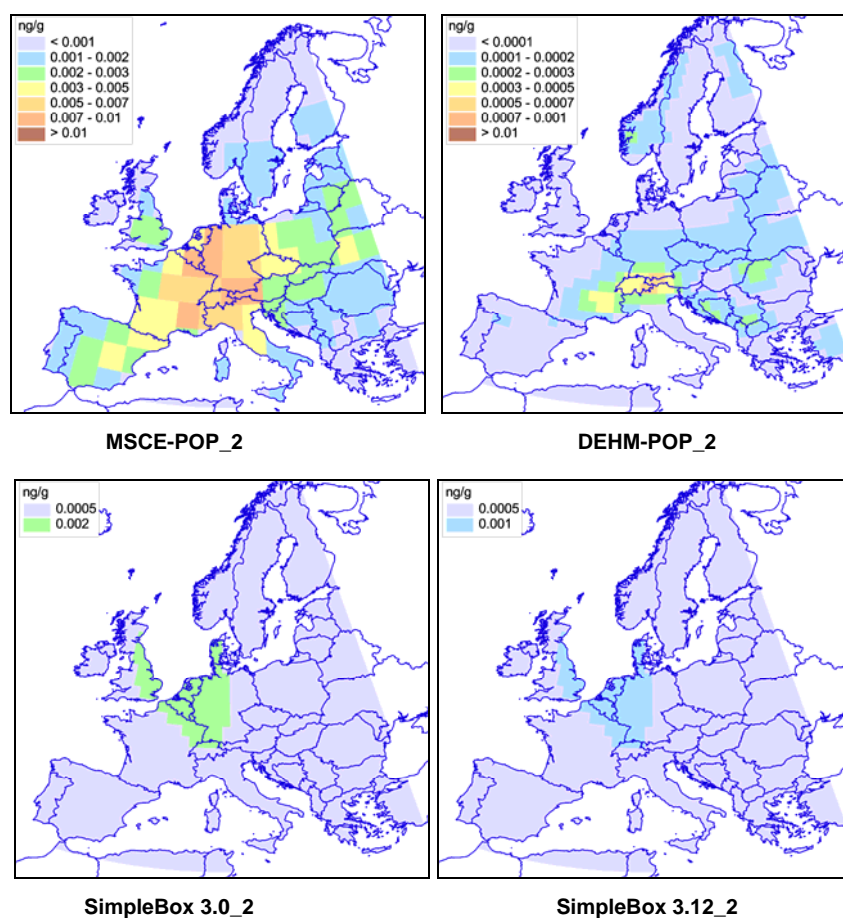


Fig. 3.163. Spatial distribution of PCB-153 concentrations in soil calculated by the participating models on the basis of “own or alternative” data sets and zero initial concentrations.

Water concentration. The calculated fields of PCB-153 annual concentrations in water of the European calculation domain in 2000 presented by DEHM-POP, MSCE-POP and SimpleBox models are compared in Fig. 3.188.

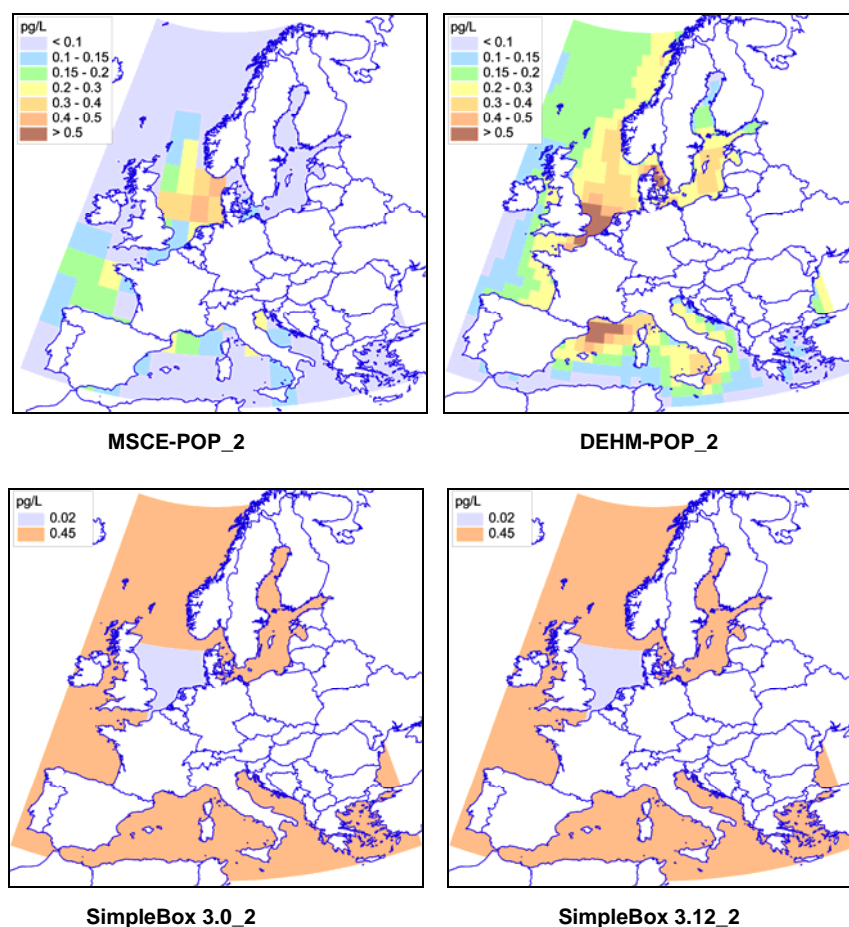


Fig. 3.164. Spatial distribution of PCB-153 concentrations in water calculated by the participating models on the basis of “own or alternative” data sets and zero initial concentrations

Concentration in vegetation. The spatial distributions of PCB-153 concentration in vegetation of the European region presented by MSCE-POP and SimpleBox models are compared in Fig.3.165.

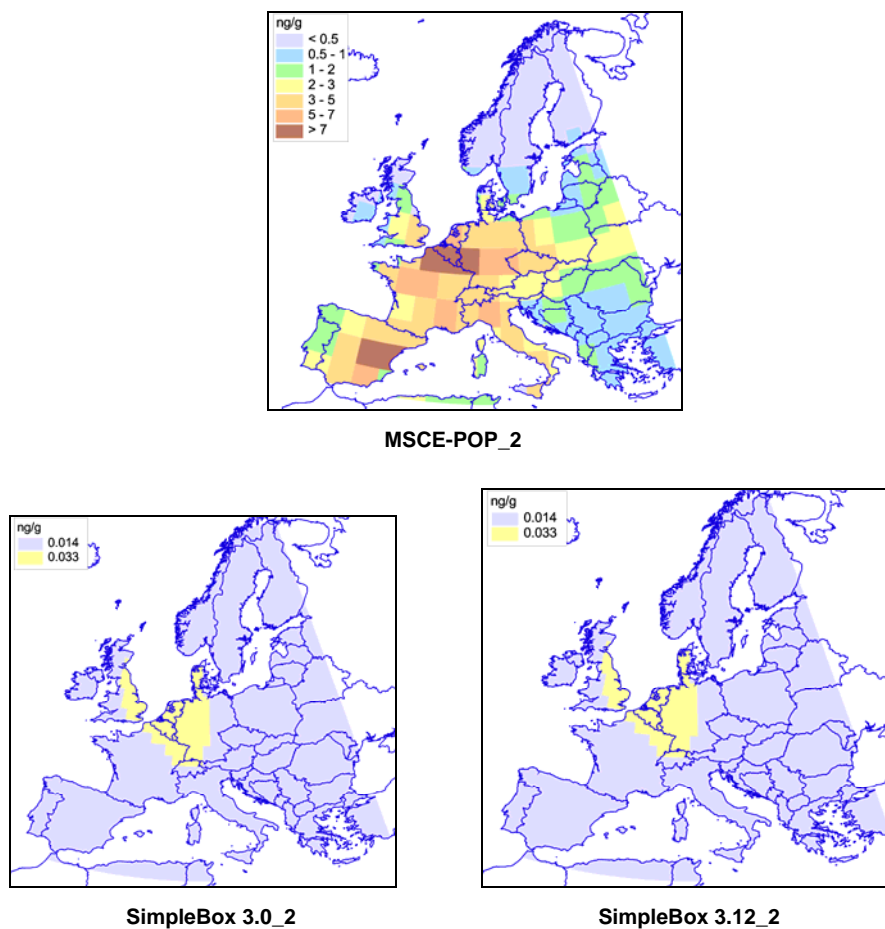


Fig. 3.165. Spatial distribution of PCB-153 concentrations in vegetation calculated by the participating models on the basis of “own or alternative” data sets and zero initial concentrations

Net deposition flux. Spatial distributions of PCB-153 net deposition flux in 2000 presented by MSCE-POP and SimpleBox models are shown in Fig.3.166. The values of net deposition flux include dry and wet depositions and gaseous exchange.

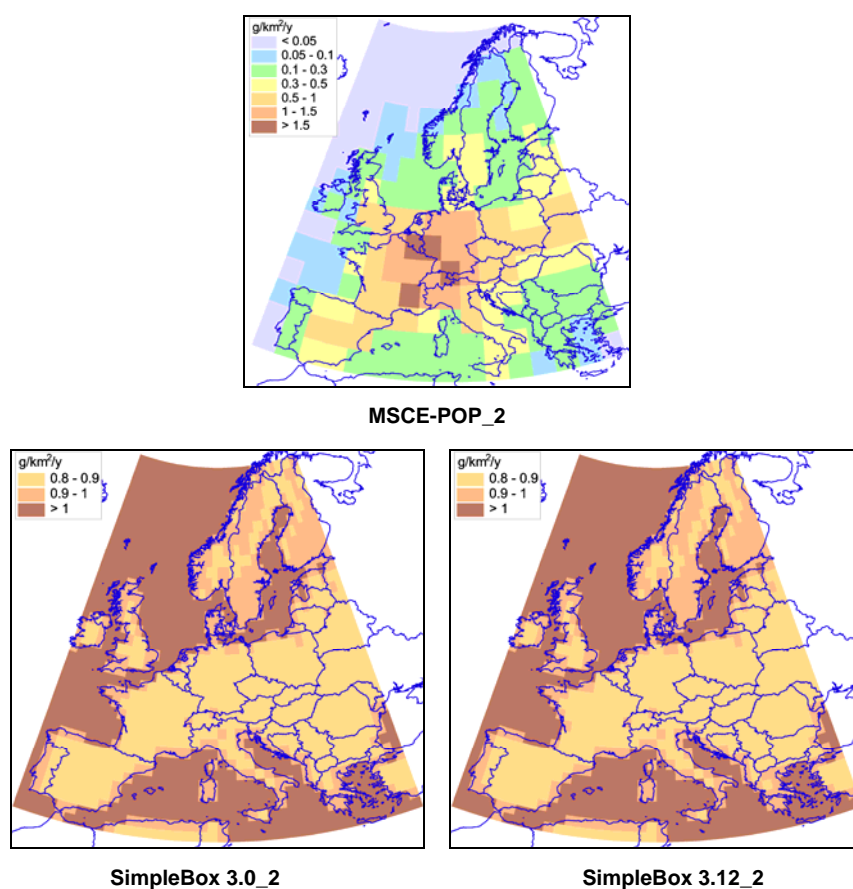


Fig. 3.166. Spatial distribution of PCB-153 net depositions calculated by the participating models on the basis of “own or alternative” data sets and zero initial concentrations

The comparison of calculated fields of depositions and concentrations in the main environmental media obtained on the basis of “reference” and “own/alternative” data sets presented in this Section demonstrates that the models of different type and resolution closely described the spatial distribution of PCB-153 pollution.

3.7. Comparison of model results with measurements

Comparison of modelling results with available measurements of PCB air concentrations and atmospheric depositions was carried out for 2000. Annual mean PCB concentrations obtained at 4 EMEP monitoring sites were selected: Kosetice (CZ3), Rörvik (SE2), Aspvreten (SE12), and Pallas (FI96). These sites are located (Fig. 3.167) within the modelling domain specified for the intercomparison study and reported in Berg et al. (2002). Air concentrations at all stations were sampled using conventional hi-volume air samplers, whilst atmospheric deposition at three stations (Rörvik, Aspvreten and Pallas), were sampled using bulk atmospheric deposition samplers. The samples were analyzed using conventional analytical techniques [Berg et al., 2002].

It is emphasized that the intercomparison between measured and modeled atmospheric depositions should be considered with some caution. That can be mostly explained by several discrepancies existing between what is implied as measured and simulated bulk deposition values. The bulk atmospheric deposition sampling is supposed to include wet deposition of gaseous and particulate phase of POPs and also some unknown part of dry deposition. In [Horstmann and McLachlan, 1997] it was found that the contribution of gaseous exchange to samples is small with respect to total depositions. According to [Guerzoni et al., 2004] the limitation of this sampling method is mainly possible underestimation of fluxes because of the limited collection of dry gases. In models atmospheric deposition of POPs is commonly described as a combination of various advective and diffusive processes. In this study for the comparison with measured bulk deposition values the sum of dry particle deposition and overall (gas+particle) wet deposition values usually calculated in models separately (so called direct deposition values) is used without taking into account diffusive fraction of dry deposition. Despite having been suggested that the diffusive process of gaseous exchange may be a key deposition/exchange mechanism for certain POPs between the atmosphere and the underlying surface [e.g. Wania et al. 19998 and references therein], direct measurements of the diffusive gaseous exchange flux are still rather limited. That is why for the sake of comparison the simulated values of gaseous exchange are not included into bulk deposition values obtained by the models in this intercomparison. For all these reasons, differences between predicted and observed bulk atmospheric deposition values are indeed expected.

Comparison with measurements was mostly done for the model results obtained with “own-alternative” data set of physical-chemical properties and defined initial conditions. Thus, results of DEHM-POP and MSCE-POP models calculated on the basis of initial concentrations given as input data (MSCE-POP_1 and DEHM-POP_1) are used for comparison with measurements. SimpleBox model provided three sets of model results obtained on the basis of “alternative” data set with the help of initial concentrations given as input data or with historical emissions for 20-year period (SimpleBox 3.0_1, SimpleBox 3.0_3 and SimpleBox 3.12_3). They are presented as SimpleBox1, SimpleBox2, and SimpleBox3 in figures below. Results of EVN-BETR and UK-MODEL calculated with the use of initial concentrations (EVN-BETR_1) and historical emissions (EVN-BETR_3) were obtained on the basis of “reference” data set.



Fig. 3.167. Location of selected monitoring sites