Table 3.91. *Calculation results: PCB-153 concentration in the atmosphere at interface with soil (pg/m3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1	MSCE-POP_1	SimpleBox 3.0 _3	SimpleBox 3.12_3				G-CIEMS_2	SimpleBox 3.0_2	SimpleBox 3.12_2	MSCE-POP_2	ADEPT		
Jan	7.06	10.32	4.63	3.45	3.85	*5.86*	*2.86*	Jan	3.93	3.08	3.08	3.92	1.25	*3.05*	*1.09*
Feb	5.82	8.84	4.56	3.42	3.85	*5.30*	*2.18*	Feb	4.19	3.29	3.29	3.71	1.25	*3.15*	*1.12*
Mar	5.76	7.59	4.73	3.42	3.85	*5.07*	*1.67*	Mar	4.71	3.30	3.30	3.87	1.25	*3.29*	*1.28*
Apr	5.80	6.67	5.06	3.42	3.85	*4.96*	*1.35*	Apr	5.12	3.30	3.30	3.94	0.87	*3.31*	*1.55*
May	4.65	5.99	5.67	3.42	3.85	*4.72*	*1.12*	May	4.37	3.31	3.31	4.42	0.87	*3.26*	*1.44*
Jun	4.86	5.48	4.92	3.42	3.85	*4.51*	*0.85*	Jun	4.68	3.31	3.31	3.71	0.87	*3.18*	*1.40*
Jul	4.83	5.10	4.84	3.42	3.85	*4.41*	*0.73*	Jul	4.74	3.32	3.32	3.69	0.87	*3.19*	*1.42*
Aug	4.83	4.79	5.68	3.42	3.85	*4.51*	*0.89*	Aug	4.80	3.32	3.32	4.44	0.87	*3.35*	*1.54*
Sep	4.78	4.56	5.37	3.42	3.85	*4.39*	*0.77*	Sep	4.77	3.32	3.32	4.38	0.87	*3.33*	*1.52*
Oct	4.56	4.37	4.89	3.42	3.85	*4.22*	*0.58*	Oct	4.58	3.32	3.32	3.96	1.25	*3.29*	*1.25*
Nov	5.51	4.22	4.48	3.42	3.85	*4.29*	*0.79*	Nov	5.54	3.32	3.32	3.66	1.25	*3.42*	*1.52*
Dec	4.92	4.10	4.83	3.42	3.85	*4.22*	*0.64*	Dec	4.96	3.32	3.33	4.15	1.25	*3.40*	*1.38*
Annual	**5.28**	**6.00**	**4.97**	**3.42**	**3.85**	***4.71***	***1.06***	**Annual**	**4.70**	**3.29**	**3.29**	**3.99**	**1.06**	***3.27***	***1.36***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.92. *Calculation results: PCB-153 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.28	17.34	4.80	3.82	4.21	*7.29*	*5.70*	Jan	3.12	3.12	3.90	*3.38*	*0.45*
Feb	4.98	14.80	4.77	3.79	4.21	*6.51*	*4.66*	Feb	3.34	3.34	3.72	*3.47*	*0.22*
Mar	5.01	12.38	4.93	3.80	4.22	*6.07*	*3.56*	Mar	3.36	3.36	3.87	*3.53*	*0.29*
Apr	5.14	10.55	5.27	3.80	4.22	*5.80*	*2.73*	Apr	3.37	3.37	3.89	*3.54*	*0.30*
May	4.21	9.18	5.76	3.81	4.23	*5.44*	*2.22*	May	3.38	3.38	4.27	*3.68*	*0.51*
Jun	4.39	8.14	4.89	3.81	4.23	*5.09*	*1.75*	Jun	3.39	3.39	3.52	*3.43*	*0.08*
Jul	4.37	7.34	4.75	3.81	4.23	*4.90*	*1.41*	Jul	3.40	3.40	3.48	*3.42*	*0.05*
Aug	4.38	6.71	5.45	3.81	4.24	*4.92*	*1.17*	Aug	3.40	3.40	4.10	*3.63*	*0.40*
Sep	4.29	6.21	5.24	3.82	4.24	*4.76*	*0.96*	Sep	3.41	3.41	4.13	*3.65*	*0.42*
Oct	4.08	5.81	4.89	3.82	4.24	*4.57*	*0.80*	Oct	3.41	3.41	3.83	*3.55*	*0.24*
Nov	4.89	5.48	4.59	3.82	4.24	*4.60*	*0.63*	Nov	3.41	3.41	3.64	*3.49*	*0.13*
Dec	4.37	5.21	4.95	3.82	4.24	*4.52*	*0.56*	Dec	3.42	3.42	4.15	*3.66*	*0.42*
Annual	**4.70**	**9.10**	**5.02**	**3.81**	**4.23**	***5.37***	***2.13***	**Annual**	**3.37**	**3.37**	**3.88**	***3.54***	***0.29***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.93.

Table 3.93. *The percentage difference between calculation results on PCB-153 concentration in the atmosphere at its interface with soil obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	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
Jan	-11.1%	68.0%	1.2%	1.2%	10.8%	9.3%	3.7%	-0.5%
Feb	-14.4%	67.5%	1.6%	1.6%	11.0%	9.4%	4.6%	0.3%
Mar	-13.0%	63.0%	1.8%	1.8%	11.2%	9.6%	4.2%	0.0%
Apr	-11.3%	58.2%	2.0%	2.0%	11.3%	9.7%	4.2%	-1.3%
May	-9.5%	53.3%	2.2%	2.2%	11.4%	9.8%	1.6%	-3.4%
Jun	-9.6%	48.5%	2.3%	2.3%	11.5%	9.9%	-0.6%	-5.1%
Jul	-9.5%	44.0%	2.4%	2.4%	11.5%	10.0%	-1.9%	-5.7%
Aug	-9.4%	39.9%	2.5%	2.5%	11.6%	10.0%	-4.0%	-7.7%
Sep	-10.2%	36.2%	2.6%	2.6%	11.6%	10.0%	-2.4%	-5.7%
Oct	-10.5%	32.8%	2.7%	2.6%	11.7%	10.1%	0.0%	-3.3%
Nov	-11.3%	29.8%	2.7%	2.7%	11.7%	10.1%	2.5%	-0.5%
Dec	-11.1%	27.1%	2.8%	2.7%	11.7%	10.1%	2.5%	0.0%
Annual	**-11.0%**	**51.5%**	**2.2%**	**2.2%**	**11.4%**	**9.8%**	**1.1%**	**-2.8%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.

3.5.2. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with ocean

Reference data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.94.

Monthly values of PCB-153 concentration in the atmosphere at its interface with ocean calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.114 a and b, respectively.

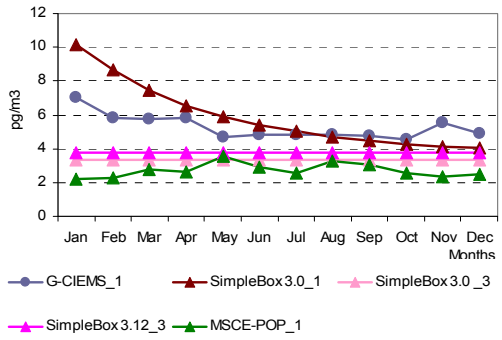


Fig. 3.114a. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

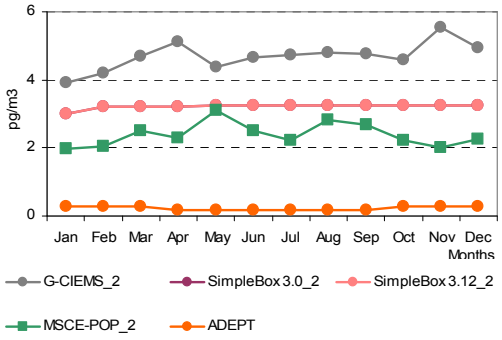


Fig. 3.114b. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with ocean calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.95.

Monthly values of PCB-153 concentration in the atmosphere at its interface with ocean calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.115 a and b, respectively.

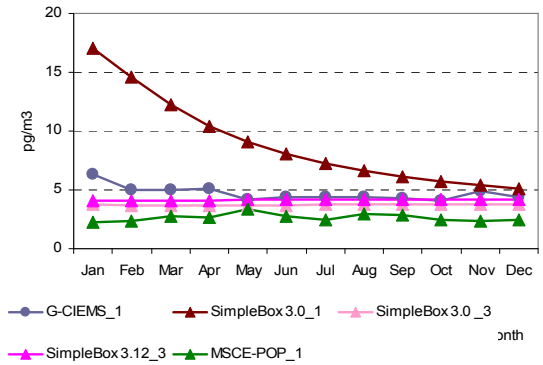


Fig. 3.115a. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

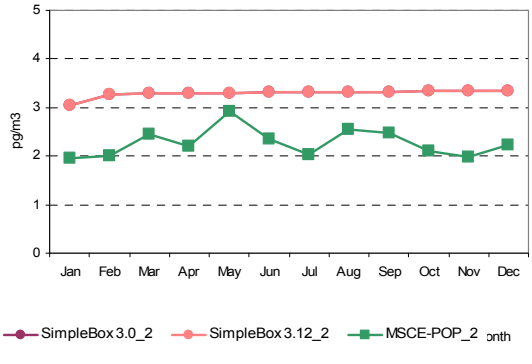


Fig. 3.115b. *PCB-153 concentration in the atmosphere at interface with ocean (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.94. *Calculation results: PCB-153 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations					*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2	ADEPT		
Jan	7.06	10.15	2.22	3.37	3.77	*5.31*	*3.25*	Jan	3.93	3.01	3.01	1.98	0.30	*2.45*	*1.38*
Feb	5.82	8.70	2.29	3.34	3.77	*4.78*	*2.54*	Feb	4.19	3.21	3.21	2.04	0.30	*2.59*	*1.49*
Mar	5.76	7.47	2.80	3.34	3.77	*4.63*	*1.94*	Mar	4.71	3.22	3.22	2.50	0.30	*2.79*	*1.61*
Apr	5.80	6.57	2.62	3.34	3.77	*4.42*	*1.68*	Apr	5.12	3.23	3.23	2.28	0.19	*2.81*	*1.79*
May	4.65	5.90	3.52	3.34	3.77	*4.24*	*1.06*	May	4.37	3.23	3.23	3.12	0.19	*2.83*	*1.56*
Jun	4.86	5.40	2.91	3.34	3.77	*4.05*	*1.04*	Jun	4.68	3.23	3.24	2.52	0.19	*2.77*	*1.64*
Jul	4.83	5.01	2.57	3.34	3.77	*3.90*	*1.03*	Jul	4.74	3.24	3.24	2.22	0.19	*2.73*	*1.68*
Aug	4.83	4.71	3.24	3.34	3.77	*3.98*	*0.75*	Aug	4.80	3.24	3.24	2.82	0.19	*2.86*	*1.67*
Sep	4.78	4.48	3.04	3.34	3.77	*3.88*	*0.74*	Sep	4.77	3.24	3.24	2.68	0.19	*2.83*	*1.67*
Oct	4.56	4.29	2.58	3.34	3.77	*3.71*	*0.79*	Oct	4.58	3.24	3.24	2.23	0.30	*2.72*	*1.59*
Nov	5.51	4.14	2.34	3.34	3.77	*3.82*	*1.16*	Nov	5.54	3.25	3.25	2.02	0.30	*2.87*	*1.92*
Dec	4.92	4.02	2.49	3.34	3.77	*3.71*	*0.89*	Dec	4.96	3.25	3.25	2.26	0.30	*2.80*	*1.70*
Annual	**5.28**	**5.90**	**2.72**	**3.34**	**3.77**	***4.20***	***1.34***	**Annual**	**4.70**	**3.22**	**3.22**	**2.39**	**0.25**	***2.75***	***1.63***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.95. *Calculation results: PCB-153 concentration in the atmosphere at its interface with ocean (pg/m3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.28	17.08	2.26	3.73	4.11	*6.69*	*5.98*	Jan	3.05	3.05	1.96	*2.68*	*0.63*
Feb	4.98	14.59	2.32	3.71	4.12	*5.94*	*4.93*	Feb	3.27	3.27	2.01	*2.85*	*0.73*
Mar	5.01	12.20	2.80	3.71	4.12	*5.57*	*3.79*	Mar	3.28	3.28	2.45	*3.00*	*0.48*
Apr	5.14	10.40	2.61	3.72	4.13	*5.20*	*3.05*	Apr	3.29	3.29	2.20	*2.93*	*0.63*
May	4.21	9.06	3.39	3.72	4.13	*4.90*	*2.35*	May	3.30	3.30	2.93	*3.18*	*0.21*
Jun	4.39	8.03	2.76	3.72	4.14	*4.61*	*2.01*	Jun	3.31	3.31	2.34	*2.99*	*0.56*
Jul	4.37	7.24	2.40	3.73	4.14	*4.38*	*1.77*	Jul	3.32	3.32	2.04	*2.89*	*0.74*
Aug	4.38	6.61	2.96	3.73	4.14	*4.36*	*1.37*	Aug	3.32	3.32	2.54	*3.06*	*0.45*
Sep	4.29	6.12	2.86	3.73	4.14	*4.23*	*1.19*	Sep	3.33	3.33	2.48	*3.04*	*0.49*
Oct	4.08	5.72	2.49	3.73	4.15	*4.03*	*1.15*	Oct	3.33	3.33	2.11	*2.92*	*0.71*
Nov	4.89	5.39	2.34	3.73	4.15	*4.10*	*1.17*	Nov	3.34	3.34	1.98	*2.88*	*0.78*
Dec	4.37	5.12	2.49	3.73	4.15	*3.97*	*0.97*	Dec	3.34	3.34	2.22	*2.97*	*0.65*
Annual	**4.70**	**8.96**	**2.64**	**3.72**	**4.14**	***4.83***	***2.43***	**Annual**	**3.29**	**3.29**	**2.27**	***2.95***	***0.59***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.96.

Table 3.96. *The percentage difference between calculation results on PCB-153 concentration in the atmosphere at its interface with ocean obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	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
Jan	-11.1%	68.2%	1.2%	1.2%	10.8%	9.2%	1.8%	-1.0%
Feb	-14.4%	67.8%	1.6%	1.6%	11.1%	9.3%	1.3%	-1.5%
Mar	-13.0%	63.3%	1.8%	1.8%	11.2%	9.5%	0.0%	-2.0%
Apr	-11.3%	58.4%	2.0%	2.0%	11.4%	9.7%	-0.4%	-3.5%
May	-9.5%	53.6%	2.2%	2.2%	11.5%	9.8%	-3.7%	-6.1%
Jun	-9.6%	48.8%	2.3%	2.3%	11.5%	9.9%	-5.2%	-7.1%
Jul	-9.5%	44.4%	2.4%	2.4%	11.6%	9.9%	-6.6%	-8.1%
Aug	-9.4%	40.2%	2.5%	2.5%	11.6%	10.0%	-8.6%	-9.9%
Sep	-10.2%	36.5%	2.6%	2.6%	11.7%	10.0%	-5.9%	-7.5%
Oct	-10.5%	33.2%	2.7%	2.7%	11.7%	10.1%	-3.5%	-5.4%
Nov	-11.3%	30.1%	2.8%	2.7%	11.7%	10.1%	0.0%	-2.0%
Dec	-11.1%	27.5%	2.8%	2.8%	11.8%	10.1%	0.0%	-1.8%
Annual	**-11.0%**	**51.8%**	**2.3%**	**2.3%**	**11.5%**	**9.8%**	**-2.9%**	**-4.9%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.

3.5.3. Comparison of calculated values of PCB-153 concentration in the atmosphere at its interface with vegetation

Reference data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.97.

Monthly values of PCB-153 concentration in the atmosphere at its interface with vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.116 a and b, respectively.

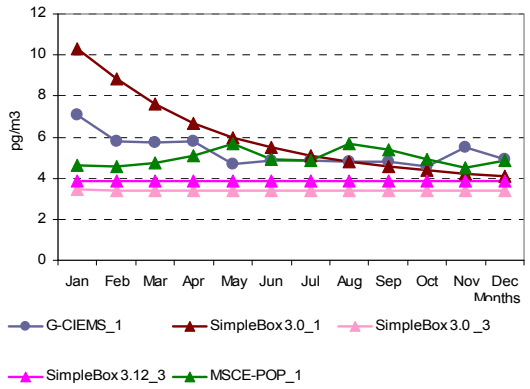


Fig. 3.116a. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

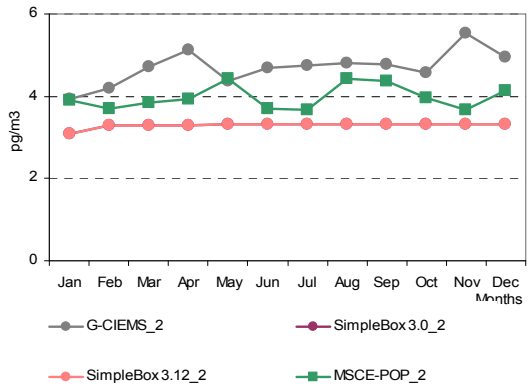


Fig. 3.116b. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m3) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in the atmosphere at its interface with vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.98.

Monthly values of PCB-153 concentration in the atmosphere at its interface with vegetation calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.117 a and b, respectively.

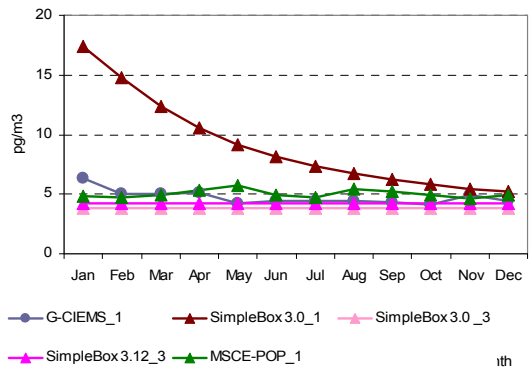


Fig. 3.117a. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

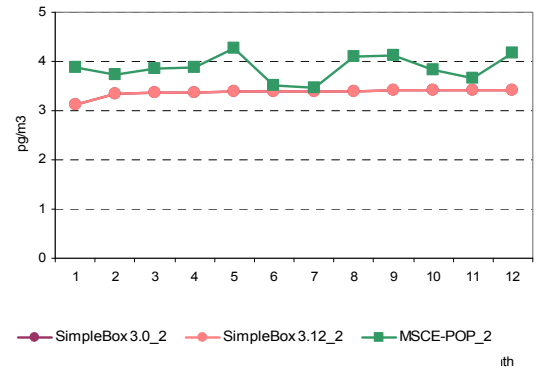


Fig. 3.117b. *PCB-153 concentration in the atmosphere at interface with vegetation (pg/m^3) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.97. *Calculation results: PCB-153 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE- POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	7.06	10.32	4.62	3.45	3.85	*5.86*	*2.86*	Jan	3.93	3.08	3.08	3.91	*3.50*	*0.48*
Feb	5.82	8.84	4.56	3.42	3.85	*5.30*	*2.18*	Feb	4.19	3.29	3.29	3.71	*3.62*	*0.43*
Mar	5.76	7.59	4.72	3.42	3.85	*5.07*	*1.67*	Mar	4.71	3.30	3.30	3.85	*3.79*	*0.67*
Apr	5.80	6.67	5.07	3.42	3.85	*4.96*	*1.35*	Apr	5.12	3.30	3.30	3.94	*3.92*	*0.86*
May	4.65	5.99	5.66	3.42	3.85	*4.71*	*1.11*	May	4.37	3.31	3.31	4.42	*3.85*	*0.63*
Jun	4.86	5.48	4.91	3.42	3.85	*4.50*	*0.85*	Jun	4.68	3.31	3.31	3.70	*3.75*	*0.64*
Jul	4.83	5.10	4.83	3.42	3.85	*4.41*	*0.73*	Jul	4.74	3.32	3.32	3.68	*3.76*	*0.68*
Aug	4.83	4.79	5.68	3.42	3.85	*4.51*	*0.89*	Aug	4.80	3.32	3.32	4.43	*3.97*	*0.76*
Sep	4.78	4.56	5.36	3.42	3.85	*4.39*	*0.77*	Sep	4.77	3.32	3.32	4.37	*3.95*	*0.74*
Oct	4.56	4.37	4.89	3.42	3.85	*4.22*	*0.58*	Oct	4.58	3.32	3.32	3.96	*3.80*	*0.60*
Nov	5.51	4.22	4.48	3.42	3.85	*4.29*	*0.79*	Nov	5.54	3.32	3.32	3.66	*3.96*	*1.07*
Dec	4.92	4.10	4.84	3.42	3.85	*4.22*	*0.65*	Dec	4.96	3.32	3.33	4.15	*3.94*	*0.78*
Annual	**5.28**	**6.00**	**4.97**	**3.42**	**3.85**	***4.70***	***1.06***	**Annual**	**4.70**	**3.29**	**3.29**	**3.98**	***3.82***	***0.67***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.98. *Calculation results: PCB-153 concentration in the atmosphere at its interface with vegetation (pg/m^3) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation.*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.28	17.34	4.80	3.82	4.21	*7.29*	*5.70*	Jan	3.12	3.12	3.89	*3.38*	*0.44*
Feb	4.98	14.80	4.77	3.79	4.21	*6.51*	*4.66*	Feb	3.34	3.34	3.72	*3.47*	*0.22*
Mar	5.01	12.38	4.92	3.80	4.22	*6.06*	*3.56*	Mar	3.36	3.36	3.85	*3.52*	*0.28*
Apr	5.14	10.55	5.28	3.80	4.22	*5.80*	*2.73*	Apr	3.37	3.37	3.89	*3.54*	*0.30*
May	4.21	9.18	5.75	3.81	4.23	*5.44*	*2.22*	May	3.38	3.38	4.26	*3.67*	*0.51*
Jun	4.39	8.14	4.89	3.81	4.23	*5.09*	*1.75*	Jun	3.39	3.39	3.51	*3.43*	*0.07*
Jul	4.37	7.34	4.75	3.81	4.23	*4.90*	*1.41*	Jul	3.40	3.40	3.47	*3.42*	*0.04*
Aug	4.38	6.71	5.44	3.81	4.24	*4.91*	*1.17*	Aug	3.40	3.40	4.09	*3.63*	*0.40*
Sep	4.29	6.21	5.23	3.82	4.24	*4.76*	*0.96*	Sep	3.41	3.41	4.12	*3.64*	*0.41*
Oct	4.08	5.81	4.89	3.82	4.24	*4.57*	*0.80*	Oct	3.41	3.41	3.83	*3.55*	*0.24*
Nov	4.89	5.48	4.60	3.82	4.24	*4.60*	*0.63*	Nov	3.41	3.41	3.65	*3.49*	*0.14*
Dec	4.37	5.21	4.96	3.82	4.24	*4.52*	*0.56*	Dec	3.42	3.42	4.16	*3.66*	*0.43*
Annual	**4.70**	**9.10**	**5.02**	**3.81**	**4.23**	***5.37***	***2.13***	**Annual**	**3.37**	**3.37**	**3.87**	***3.53***	***0.29***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.99.

Table 3.99. *The percentage difference between calculation results on PCB-153 concentration in the atmosphere at interface with vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	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
Jan	-11.1%	68.0%	1.2%	1.2%	10.8%	9.3%	3.9%	-0.5%
Feb	-14.4%	67.5%	1.6%	1.6%	11.0%	9.4%	4.6%	0.3%
Mar	-13.0%	63.0%	1.8%	1.8%	11.2%	9.6%	4.2%	0.0%
Apr	-11.3%	58.2%	2.0%	2.0%	11.3%	9.7%	4.1%	-1.3%
May	-9.5%	53.3%	2.2%	2.2%	11.4%	9.8%	1.6%	-3.6%
Jun	-9.6%	48.5%	2.3%	2.3%	11.5%	9.9%	-0.4%	-5.1%
Jul	-9.5%	44.0%	2.4%	2.4%	11.5%	10.0%	-1.7%	-5.7%
Aug	-9.4%	39.9%	2.5%	2.5%	11.6%	10.0%	-4.2%	-7.7%
Sep	-10.2%	36.2%	2.6%	2.6%	11.6%	10.0%	-2.4%	-5.7%
Oct	-10.5%	32.8%	2.7%	2.6%	11.7%	10.1%	0.0%	-3.3%
Nov	-11.3%	29.8%	2.7%	2.7%	11.7%	10.1%	2.7%	-0.3%
Dec	-11.1%	27.1%	2.8%	2.7%	11.7%	10.1%	2.5%	0.2%
Annual	**-11.0%**	**51.5%**	**2.2%**	**2.2%**	**11.4%**	**9.8%**	**1.1%**	**-2.8%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.

3.5.4. Comparison of calculated values of PCB-153 concentration in surface ocean layer

Reference data set. Calculation results on PCB-153 concentration in surface ocean layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.100.

Monthly values of PCB-153 concentration in surface ocean layer calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.118 a and b, respectively.

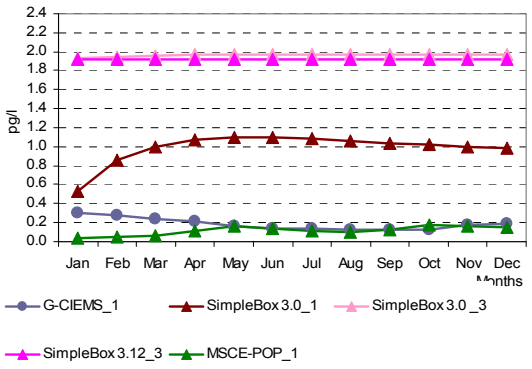


Fig. 3.118a. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

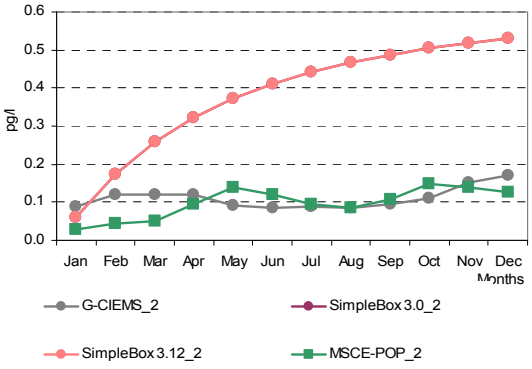


Fig. 3.118b. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in surface ocean layer calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.101.

Monthly values of PCB-153 concentration in surface ocean layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.119 a and b, respectively.

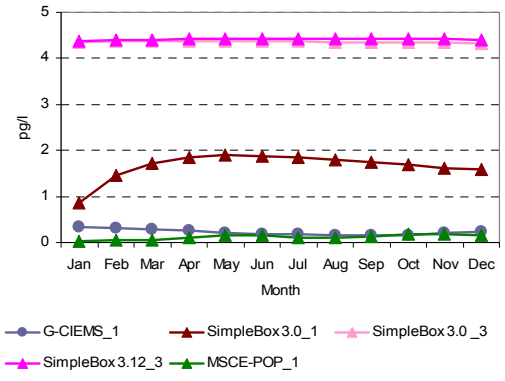


Fig. 3.119a. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

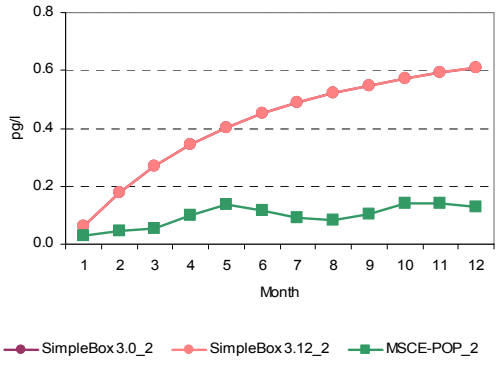


Fig. 3.119b. *PCB-153 concentration in surface ocean layer (pg/l) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.100. *Calculation results: PCB-153 concentration in surface ocean layer (pg/l) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.30	0.54	0.03	1.94	1.93	*0.95*	*0.92*	Jan	0.09	0.06	0.06	0.03	*0.06*	*0.02*
Feb	0.28	0.85	0.05	1.95	1.93	*1.01*	*0.89*	Feb	0.12	0.17	0.17	0.04	*0.13*	*0.06*
Mar	0.24	1.00	0.06	1.96	1.93	*1.04*	*0.90*	Mar	0.12	0.26	0.26	0.05	*0.17*	*0.10*
Apr	0.21	1.07	0.11	1.96	1.93	*1.06*	*0.89*	Apr	0.12	0.32	0.32	0.10	*0.22*	*0.13*
May	0.16	1.10	0.16	1.97	1.93	*1.06*	*0.89*	May	0.09	0.37	0.37	0.14	*0.24*	*0.15*
Jun	0.14	1.10	0.14	1.97	1.93	*1.06*	*0.90*	Jun	0.09	0.41	0.41	0.12	*0.26*	*0.18*
Jul	0.13	1.08	0.11	1.97	1.93	*1.05*	*0.91*	Jul	0.09	0.44	0.44	0.09	*0.27*	*0.20*
Aug	0.12	1.06	0.10	1.97	1.93	*1.04*	*0.92*	Aug	0.08	0.47	0.47	0.08	*0.28*	*0.22*
Sep	0.12	1.04	0.13	1.97	1.93	*1.04*	*0.91*	Sep	0.09	0.49	0.49	0.11	*0.29*	*0.22*
Oct	0.13	1.02	0.18	1.97	1.93	*1.05*	*0.90*	Oct	0.11	0.50	0.50	0.15	*0.32*	*0.22*
Nov	0.17	1.00	0.17	1.97	1.93	*1.05*	*0.89*	Nov	0.15	0.52	0.52	0.14	*0.33*	*0.22*
Dec	0.19	0.99	0.15	1.97	1.93	*1.04*	*0.89*	Dec	0.17	0.53	0.53	0.13	*0.34*	*0.22*
Annual	**0.18**	**0.99**	**0.12**	**1.97**	**1.93**	***1.04***	***0.90***	**Annual**	**0.11**	**0.38**	**0.38**	**0.10**	***0.24***	***0.16***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
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;
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.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.101. *Calculation results: PCB-153 concentration in surface ocean layer (pg/l) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	0.34	0.86	0.04	4.36	4.37	*1.99*	*2.18*	Jan	0.06	0.06	0.03	*0.05*	*0.02*
Feb	0.31	1.45	0.06	4.37	4.39	*2.12*	*2.13*	Feb	0.18	0.18	0.05	*0.13*	*0.08*
Mar	0.28	1.72	0.06	4.37	4.41	*2.17*	*2.13*	Mar	0.27	0.27	0.05	*0.20*	*0.13*
Apr	0.25	1.85	0.12	4.37	4.42	*2.20*	*2.11*	Apr	0.35	0.35	0.10	*0.26*	*0.14*
May	0.20	1.90	0.17	4.37	4.42	*2.21*	*2.12*	May	0.40	0.40	0.14	*0.32*	*0.15*
Jun	0.18	1.89	0.15	4.37	4.43	*2.20*	*2.12*	Jun	0.45	0.45	0.12	*0.34*	*0.19*
Jul	0.17	1.85	0.12	4.36	4.43	*2.19*	*2.14*	Jul	0.49	0.49	0.09	*0.36*	*0.23*
Aug	0.15	1.80	0.10	4.36	4.43	*2.17*	*2.14*	Aug	0.52	0.52	0.08	*0.37*	*0.25*
Sep	0.16	1.74	0.13	4.35	4.42	*2.16*	*2.14*	Sep	0.55	0.55	0.10	*0.40*	*0.26*
Oct	0.17	1.68	0.18	4.35	4.42	*2.16*	*2.12*	Oct	0.57	0.57	0.14	*0.43*	*0.25*
Nov	0.21	1.63	0.17	4.34	4.42	*2.15*	*2.11*	Nov	0.59	0.59	0.14	*0.44*	*0.26*
Dec	0.23	1.58	0.16	4.33	4.41	*2.14*	*2.11*	Dec	0.61	0.61	0.13	*0.45*	*0.28*
Annual	**0.22**	**1.66**	**0.12**	**4.36**	**4.41**	***2.16***	***2.13***	**Annual**	**0.42**	**0.42**	**0.10**	***0.31***	***0.19***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.102.

Table 3.102. *The percentage difference between calculation results on PCB-153 concentration in surface ocean layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	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
Jan	13.2%	60.4%	0.6%	0.6%	125.3%	126.8%	8.9%	4.7%
Feb	13.6%	70.1%	2.8%	2.8%	124.1%	128.0%	8.9%	5.4%
Mar	16.5%	72.0%	4.9%	4.9%	123.3%	128.9%	7.7%	4.6%
Apr	19.8%	72.8%	6.7%	6.7%	122.6%	129.4%	5.5%	2.9%
May	23.7%	72.8%	8.3%	8.3%	122.1%	129.7%	1.2%	-1.4%
Jun	25.0%	72.2%	9.7%	9.7%	121.6%	129.9%	2.8%	-0.8%
Jul	26.3%	71.0%	10.9%	10.9%	121.3%	130.0%	1.8%	-1.4%
Aug	26.8%	69.3%	11.9%	11.9%	120.9%	129.8%	-1.0%	-3.6%
Sep	26.5%	67.2%	12.7%	12.7%	120.6%	129.7%	-0.8%	-3.7%
Oct	26.3%	65.0%	13.4%	13.4%	120.3%	129.5%	0.6%	-2.7%
Nov	22.9%	62.6%	14.0%	13.9%	120.0%	129.3%	3.0%	0.0%
Dec	21.9%	60.2%	14.4%	14.4%	119.8%	129.0%	4.7%	2.4%
Annual	**20.4%**	**68.4%**	**10.8%**	**10.8%**	**121.8%**	**129.2%**	**2.6%**	**-0.3%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.

3.5.5. Comparison of calculated values of PCB-153 concentration in vegetation

Reference data set. Calculation results on PCB-153 concentration in vegetation calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.103.

Monthly values of PCB-153 concentration in vegetation calculated by participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.120 a and b, respectively.

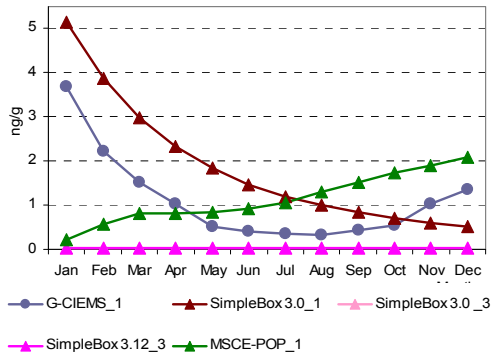


Fig. 3.120a. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions*

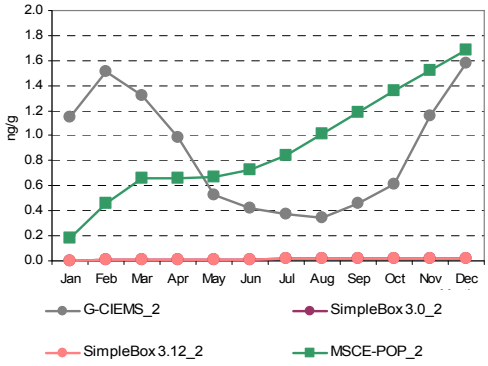


Fig. 3.120b. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in vegetation calculated by models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.104.

Monthly values of PCB-153 concentration in vegetation calculated by participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.121 a and b, respectively.

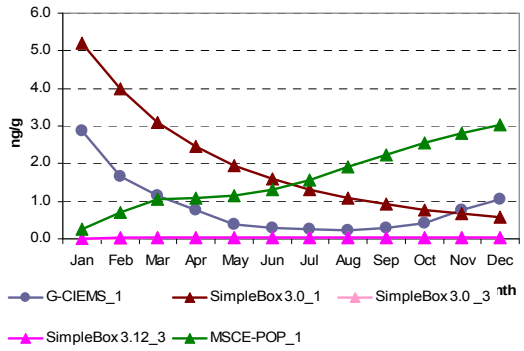


Fig. 3.121a. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions*

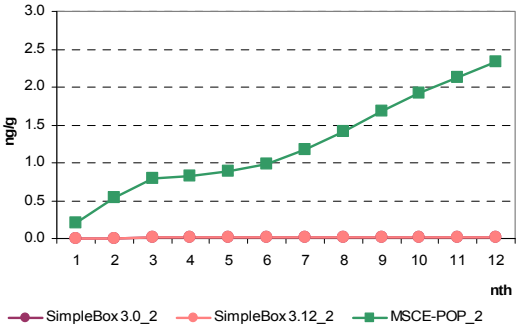


Fig. 3.121b. *PCB-153 concentration in vegetation (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.103. *Calculation results: PCB-153 concentration in vegetation (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	3.69	5.15	0.23	0.02	0.02	*1.82*	*2.43*	Jan	1.15	0.002	0.002	0.19	*0.34*	*0.55*
Feb	2.21	3.88	0.57	0.02	0.02	*1.34*	*1.68*	Feb	1.51	0.01	0.01	0.46	*0.50*	*0.71*
Mar	1.51	2.98	0.82	0.02	0.02	*1.07*	*1.24*	Mar	1.32	0.01	0.01	0.66	*0.50*	*0.63*
Apr	1.02	2.32	0.82	0.02	0.02	*0.84*	*0.94*	Apr	0.99	0.01	0.01	0.66	*0.42*	*0.49*
May	0.51	1.84	0.84	0.02	0.02	*0.65*	*0.75*	May	0.53	0.01	0.01	0.67	*0.31*	*0.34*
Jun	0.40	1.48	0.91	0.02	0.02	*0.57*	*0.63*	Jun	0.42	0.01	0.01	0.73	*0.29*	*0.35*
Jul	0.35	1.20	1.07	0.02	0.02	*0.53*	*0.57*	Jul	0.37	0.02	0.02	0.85	*0.31*	*0.39*
Aug	0.32	0.99	1.29	0.02	0.02	*0.53*	*0.58*	Aug	0.34	0.02	0.02	1.01	*0.35*	*0.47*
Sep	0.42	0.83	1.52	0.02	0.02	*0.56*	*0.63*	Sep	0.46	0.02	0.02	1.19	*0.42*	*0.55*
Oct	0.55	0.70	1.73	0.02	0.02	*0.60*	*0.70*	Oct	0.61	0.02	0.02	1.36	*0.50*	*0.64*
Nov	1.02	0.59	1.91	0.02	0.02	*0.71*	*0.79*	Nov	1.16	0.02	0.02	1.52	*0.68*	*0.78*
Dec	1.36	0.51	2.09	0.02	0.02	*0.80*	*0.91*	Dec	1.58	0.02	0.02	1.68	*0.82*	*0.93*
Annual	**1.11**	**1.87**	**1.15**	**0.02**	**0.02**	***0.84***	***0.80***	**Annual**	**0.87**	**0.01**	**0.01**	**0.91**	***0.45***	***0.51***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
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;
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.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.104. *Calculation results: PCB-153 concentration in vegetation (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS-1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	2.89	5.20	0.26	0.01	0.01	*1.67*	*2.31*	Jan	0.002	0.002	0.20	*0.07*	*0.12*
Feb	1.67	3.98	0.70	0.02	0.02	*1.28*	*1.66*	Feb	0.01	0.01	0.54	*0.18*	*0.31*
Mar	1.16	3.10	1.04	0.02	0.02	*1.07*	*1.26*	Mar	0.01	0.01	0.79	*0.27*	*0.45*
Apr	0.78	2.44	1.08	0.02	0.02	*0.87*	*1.00*	Apr	0.01	0.01	0.83	*0.28*	*0.47*
May	0.38	1.95	1.16	0.02	0.02	*0.71*	*0.84*	May	0.01	0.01	0.89	*0.30*	*0.50*
Jun	0.29	1.59	1.31	0.02	0.02	*0.65*	*0.75*	Jun	0.02	0.02	0.99	*0.34*	*0.56*
Jul	0.25	1.31	1.56	0.02	0.02	*0.63*	*0.74*	Jul	0.02	0.02	1.17	*0.40*	*0.67*
Aug	0.23	1.09	1.90	0.02	0.03	*0.65*	*0.82*	Aug	0.02	0.02	1.42	*0.49*	*0.81*
Sep	0.30	0.92	2.24	0.02	0.03	*0.70*	*0.93*	Sep	0.02	0.02	1.68	*0.57*	*0.96*
Oct	0.40	0.78	2.54	0.02	0.03	*0.75*	*1.05*	Oct	0.02	0.02	1.92	*0.65*	*1.10*
Nov	0.78	0.67	2.80	0.02	0.03	*0.86*	*1.14*	Nov	0.02	0.02	2.13	*0.72*	*1.22*
Dec	1.07	0.58	3.03	0.03	0.03	*0.95*	*1.24*	Dec	0.02	0.02	2.33	*0.79*	*1.33*
Annual	**0.85**	**1.97**	**1.64**	**0.02**	**0.02**	***0.90***	***0.90***	**Annual**	**0.01**	**0.01**	**1.24**	***0.42***	***0.71***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.105.

Table 3.105. *The percentage difference between calculation results on PCB-153 concentration in vegetation obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	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
Jan	-21.7%	0.8%	4.2%	4.2%	-37.1%	-35.3%	14.4%	9.7%
Feb	-24.3%	2.4%	5.1%	5.1%	-27.0%	-21.5%	23.6%	17.5%
Mar	-22.9%	3.9%	5.9%	5.9%	-19.0%	-10.4%	26.7%	20.9%
Apr	-23.7%	5.3%	6.5%	6.5%	-12.5%	-1.0%	32.0%	26.5%
May	-26.7%	6.5%	7.1%	7.1%	-7.3%	6.8%	38.8%	31.8%
Jun	-27.7%	7.7%	7.6%	7.6%	-3.0%	13.3%	43.5%	36.1%
Jul	-27.5%	8.7%	8.1%	8.1%	0.5%	18.8%	45.8%	38.5%
Aug	-27.9%	9.7%	8.5%	8.5%	3.5%	23.6%	47.3%	40.6%
Sep	-28.5%	10.7%	8.9%	8.9%	6.0%	27.6%	47.4%	41.2%
Oct	-27.2%	11.6%	9.2%	9.2%	8.2%	31.0%	46.8%	41.2%
Nov	-23.8%	12.4%	9.5%	9.5%	10.0%	34.0%	46.6%	40.1%
Dec	-21.7%	13.3%	9.8%	9.7%	11.5%	36.5%	45.0%	38.7%
Annual	**-23.7%**	**5.0%**	**8.2%**	**8.2%**	**-5.1%**	**10.3%**	**42.3%**	**35.9%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.

3.5.6. Comparison of calculated values of PCB-153 concentration in surface soil layer

Reference data set. Calculation results on PCB-153 concentration in surface soil layer calculated by the models on the basis of "reference" data set together with statistical parameters used for evaluation are presented in Table 3.106.

Monthly values of PCB-153 concentration in surface soil layer calculated by all participating models on the basis of "reference" data set and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.122 a and b, respectively.

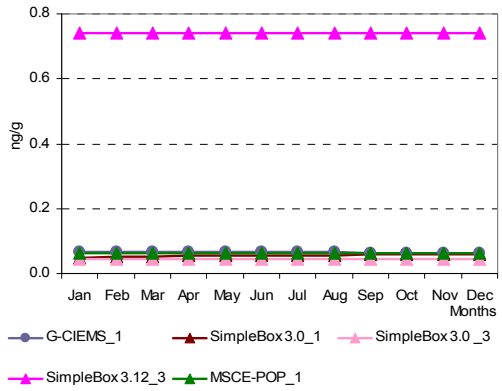


Fig.3.122a. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and non-zero initial conditions (all models)*

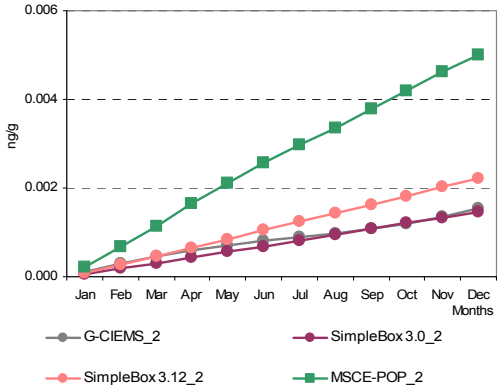


Fig.3.122b. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "reference" data set and zero-initial conditions*

Own/alternative data set. Calculation results on PCB-153 concentration in surface soil layer calculated by the models on the basis of "own or alternative" data sets together with statistical parameters used for evaluation are presented in Table 3.107.

Monthly values of PCB-153 concentration in surface soil layer calculated by all participating models on the basis of "own or alternative" data sets and taking into account non-zero (initial concentrations in media or historical emissions) and zero initial conditions are compared in Fig. 3.123a and b, respectively.

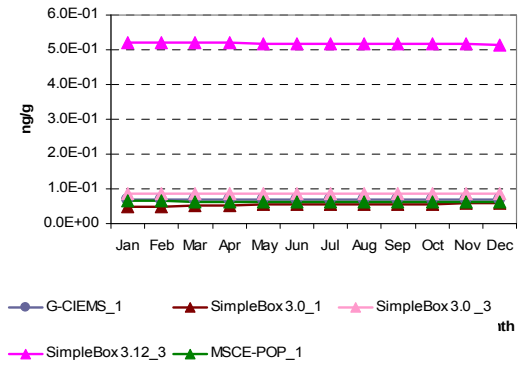


Fig. 3.123a. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and non-zero initial conditions (all models)*

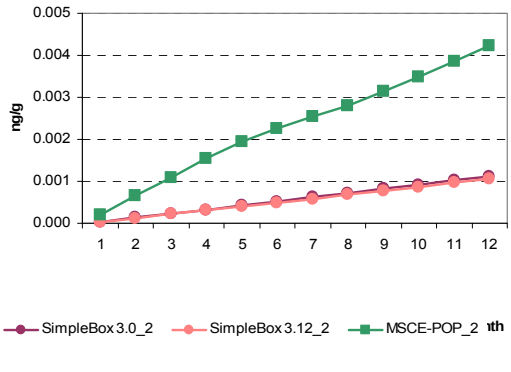


Fig. 3.123b. *PCB-153 concentration in surface soil layer (ng/g) calculated by the participating models on the basis of "own or alternative" data sets and zero-initial conditions*

Table 3.106. *Calculation results: PCB-153 concentration in surface soil layer (ng/g) calculated by models on the basis of "reference" data set and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations				*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0_3[a]	SimpleBox 3.12_3[a]				G-CIEMS_2	SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.82E-02	4.70E-02	6.39E-02	4.50E-02	7.41E-01	*1.93E-01*	*3.06E-01*	Jan	1.20E-04	5.59E-05	8.54E-05	2.18E-04	*1.20E-04*	*7.05E-05*
Feb	6.78E-02	5.00E-02	6.37E-02	4.49E-02	7.41E-01	*1.93E-01*	*3.06E-01*	Feb	3.04E-04	1.78E-04	2.72E-04	6.70E-04	*3.56E-04*	*2.16E-04*
Mar	6.74E-02	5.22E-02	6.36E-02	4.48E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Mar	4.59E-04	3.03E-04	4.61E-04	1.14E-03	*5.91E-04*	*3.74E-04*
Apr	6.69E-02	5.38E-02	6.34E-02	4.47E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Apr	6.02E-04	4.31E-04	6.55E-04	1.64E-03	*8.32E-04*	*5.47E-04*
May	6.64E-02	5.50E-02	6.33E-02	4.47E-02	7.41E-01	*1.94E-01*	*3.06E-01*	May	7.08E-04	5.59E-04	8.49E-04	2.12E-03	*1.06E-03*	*7.17E-04*
Jun	6.59E-02	5.59E-02	6.31E-02	4.46E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Jun	7.99E-04	6.88E-04	1.04E-03	2.56E-03	*1.27E-03*	*8.71E-04*
Jul	6.54E-02	5.65E-02	6.28E-02	4.45E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Jul	8.93E-04	8.17E-04	1.24E-03	2.96E-03	*1.48E-03*	*1.01E-03*
Aug	6.49E-02	5.70E-02	6.26E-02	4.44E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Aug	9.77E-04	9.48E-04	1.43E-03	3.36E-03	*1.68E-03*	*1.14E-03*
Sep	6.44E-02	5.73E-02	6.24E-02	4.43E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Sep	1.07E-03	1.08E-03	1.63E-03	3.79E-03	*1.89E-03*	*1.29E-03*
Oct	6.39E-02	5.76E-02	6.23E-02	4.42E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Oct	1.19E-03	1.21E-03	1.82E-03	4.20E-03	*2.10E-03*	*1.43E-03*
Nov	6.35E-02	5.78E-02	6.21E-02	4.42E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Nov	1.35E-03	1.33E-03	2.01E-03	4.61E-03	*2.33E-03*	*1.55E-03*
Dec	6.30E-02	5.79E-02	6.20E-02	4.41E-02	7.41E-01	*1.94E-01*	*3.06E-01*	Dec	1.54E-03	1.46E-03	2.20E-03	4.99E-03	*2.55E-03*	*1.66E-03*
Annual	**6.56E-02**	**5.48E-02**	**6.29E-02**	**4.45E-02**	**7.41E-01**	***1.94E-01***	***3.06E-01***	**Annual**	**8.35E-04**	**7.55E-04**	**1.14E-03**	**2.69E-03**	***1.35E-03***	***9.04E-04***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
G-CIEMS_2 - G-CIEMS results calculated on the basis of zero initial concentrations;
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;
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.
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Table 3.107. *Calculation results: PCB-153 concentration in surface soil layer (ng/g) calculated by models on the basis of "own or alternative" data sets and statistical parameters used for evaluation*

Month	Results obtained on the basis of initial concentrations given as input data			Results obtained on the basis of historical emissions		*m*	σ	Month	Results obtained on the basis of zero initial concentrations			*m*	σ
	G-CIEMS_1	SimpleBox 3.0_1[a]	MSCE-POP_1	SimpleBox 3.0 _3[a]	SimpleBox 3.12_3[a]				SimpleBox 3.0_2[a]	SimpleBox 3.12_2[a]	MSCE-POP_2		
Jan	6.86E-02	4.66E-02	6.40E-02	8.53E-02	5.22E-01	*1.57E-01*	*2.04E-01*	Jan	4.15E-05	3.96E-05	2.13E-04	*9.80E-05*	*9.96E-05*
Feb	6.88E-02	4.92E-02	6.38E-02	8.53E-02	5.22E-01	*1.58E-01*	*2.04E-01*	Feb	1.33E-04	1.27E-04	6.43E-04	*3.01E-04*	*2.96E-04*
Mar	6.89E-02	5.11E-02	6.37E-02	8.53E-02	5.21E-01	*1.58E-01*	*2.03E-01*	Mar	2.26E-04	2.15E-04	1.08E-03	*5.07E-04*	*4.96E-04*
Apr	6.89E-02	5.26E-02	6.36E-02	8.53E-02	5.20E-01	*1.58E-01*	*2.02E-01*	Apr	3.23E-04	3.07E-04	1.54E-03	*7.23E-04*	*7.07E-04*
May	6.88E-02	5.38E-02	6.34E-02	8.53E-02	5.19E-01	*1.58E-01*	*2.02E-01*	May	4.20E-04	3.99E-04	1.94E-03	*9.20E-04*	*8.84E-04*
Jun	6.88E-02	5.47E-02	6.30E-02	8.53E-02	5.18E-01	*1.58E-01*	*2.02E-01*	Jun	5.18E-04	4.92E-04	2.26E-03	*1.09E-03*	*1.01E-03*
Jul	6.87E-02	5.54E-02	6.26E-02	8.53E-02	5.18E-01	*1.58E-01*	*2.02E-01*	Jul	6.18E-04	5.85E-04	2.53E-03	*1.24E-03*	*1.11E-03*
Aug	6.86E-02	5.60E-02	6.23E-02	8.52E-02	5.18E-01	*1.58E-01*	*2.01E-01*	Aug	7.19E-04	6.81E-04	2.81E-03	*1.40E-03*	*1.22E-03*
Sep	6.86E-02	5.64E-02	6.20E-02	8.52E-02	5.17E-01	*1.58E-01*	*2.01E-01*	Sep	8.19E-04	7.75E-04	3.13E-03	*1.57E-03*	*1.35E-03*
Oct	6.86E-02	5.68E-02	6.19E-02	8.52E-02	5.16E-01	*1.58E-01*	*2.01E-01*	Oct	9.19E-04	8.69E-04	3.48E-03	*1.76E-03*	*1.49E-03*
Nov	6.86E-02	5.72E-02	6.17E-02	8.52E-02	5.16E-01	*1.58E-01*	*2.00E-01*	Nov	1.02E-03	9.64E-04	3.86E-03	*1.95E-03*	*1.66E-03*
Dec	6.86E-02	5.74E-02	6.16E-02	8.52E-02	5.15E-01	*1.58E-01*	*2.00E-01*	Dec	1.12E-03	1.06E-03	4.23E-03	*2.14E-03*	*1.81E-03*
Annual	**6.87E-02**	**5.39E-02**	**6.28E-02**	**8.53E-02**	**5.18E-01**	***1.58E-01***	***2.02E-01***	**Annual**	**5.73E-04**	**5.43E-04**	**2.31E-03**	***1.14E-03***	***1.01E-03***

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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;
a – In SimpleBox results, the concentrations calculated are the bulk concentrations in the compartments. Total concentrations are averages of those over regional and continental cells.

Comparison between results obtained on the basis of two data sets. The percentage difference between calculation results obtained with two data sets of physical-chemical properties (for those models who provided calculations for both these sets) is shown in Table 3.108.

Table 3.108. *The percentage difference between calculation results on PCB-153 concentration in surface soil layer obtained by models on the basis of two data sets: "reference" and "own or alternative" data sets*

Month	G-CIEMS_1	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
Jan	0.7%	-0.8%	-25.8%	-53.6%	89.7%	-29.5%	0.2%	-2.3%
Feb	1.4%	-1.6%	-25.6%	-53.5%	90.0%	-29.6%	0.2%	-4.0%
Mar	2.1%	-2.1%	-25.4%	-53.3%	90.4%	-29.7%	0.2%	-5.3%
Apr	2.9%	-2.2%	-25.1%	-53.1%	90.7%	-29.9%	0.3%	-6.1%
May	3.6%	-2.2%	-24.9%	-53.0%	91.0%	-30.0%	0.2%	-8.5%
Jun	4.3%	-2.2%	-24.6%	-52.8%	91.3%	-30.1%	-0.2%	-11.7%
Jul	5.1%	-2.0%	-24.4%	-52.7%	91.6%	-30.1%	-0.3%	-14.5%
Aug	5.8%	-1.8%	-24.2%	-52.5%	92.0%	-30.2%	-0.5%	-16.4%
Sep	6.6%	-1.6%	-24.0%	-52.4%	92.3%	-30.2%	-0.6%	-17.4%
Oct	7.3%	-1.3%	-23.8%	-52.3%	92.6%	-30.3%	-0.6%	-17.1%
Nov	8.1%	-1.1%	-23.6%	-52.2%	92.9%	-30.4%	-0.6%	-16.3%
Dec	8.8%	-0.8%	-23.4%	-52.0%	93.2%	-30.5%	-0.6%	-15.2%
Annual	**4.7%**	**-1.6%**	**-24.1%**	**-52.5%**	**91.5%**	**-30.0%**	**-0.2%**	**-14.1%**

G-CIEMS_1 - G-CIEMS results calculated on the basis of initial concentrations given as input data;
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;
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.

3.5.7. Comparison of PCB-153 intermedia mass flows and concentrations at the interfaces of main environmental media

A preliminary analysis of model results on intermedia mass flows and on concentrations in the main environmental media formed at their interfaces is presented in this section. In the comparison the calculated values of PCB-153 mass flows from the atmosphere to soil, to water, to vegetation and from vegetation to soil (see Sections 3.4.1-3.4.4 above) and values of PCB-153 concentrations in the atmosphere at its interface with underlying surfaces (soil, ocean and vegetation); in the surface layer of soil, ocean and vegetation (see Sections 3.5.1–3.5.6 above) are considered.

The comparison of PCB-153 mass flows transported from one compartment to another presented in Sections 3.4.1-3.4.4 includes results of one-year calculation with zero initial concentrations obtained by ADEPT, CliMoChem, G-CIEMS, MSCE-POP, SimpleBox models and with initial concentrations in media given as input data calculated by CAN/POPs, G-CIEMS, MSCE-POP and SimpleBox models; as well as results of long-term calculations for 20-year period with zero initial data with historical emissions carried out by CliMoChem and SimpleBox models. Results of CliMoChem, G-CIEMS, MSCE-POP, and SimpleBox models obtained on the basis of two different physical-chemical data sets allow us to reveal sensitivity of the estimates on intermedia mass flows to the variations in the input data.

The comparison of calculated concentrations presented in Sections 3.5.1–3.5.6 includes results of one-year calculations made on the basis of initial conditions (G-CIEMS, MSCE-POP, SimpleBox) and zero initial concentrations (ADEPT, G-CIEMS, MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (SimpleBox 3.0 and 3.12). The results on concentrations in the main environmental media are obtained with the use of two different physical-chemical data sets by G-CIEMS, MSCE-POP and SimpleBox models. SimpleBox and MSCE-POP predicted different values of PCB-153 concentrations in the atmosphere at its interface with different underlying surfaces. Variations in MSCE-POP air concentrations are more considerable than those in SimpleBox results.

In the section below the analysis of mass flows and concentrations in the media is presented for model results obtained on the basis of initial conditions and historical emissions. Calculated values of PCB intermedia mass flows and concentrations in the main media are presented in this section for four following interfaces: atmosphere-soil; vegetation – soil; atmosphere - seawater and atmosphere – vegetation.

Atmosphere-soil. Comparison of annual values of net exchange flow between the atmosphere and soil, which is a sum of dry and wet deposition and gaseous exchange flows, obtained on the basis of "reference" data set is presented in Table 3.67 (see Section 3.4.1). The scattering of absolute annual and monthly values between models using for calculations initial conditions and historical emissions is not large; square deviation σ_φ does not exceed the mean value of this parameter averaged between the participating models.

Annual values of net exchange flow between atmosphere and soil calculated on the basis of two data sets of physical-chemical properties are compared between different models in Fig. 3.124. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

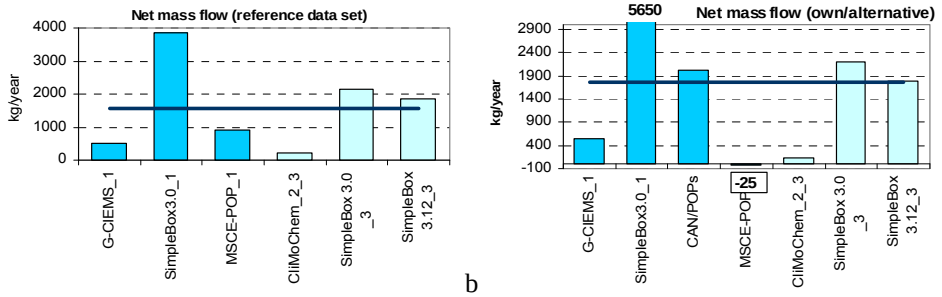


Fig.3.124. *Comparison of PCB-153 annual values of net exchange flow between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The blue line in the plots shows the value of the corresponding parameter averaged between models. For calculations performed on the basis of "reference" data set, the scattering of absolute annual values between models is not large (*m* = 1582 kg/year; σ = 1348 kg/year*)*. Square deviation σ does not exceed the mean value of this parameter averaged between the participating models. In the case of results obtained with the use of "own/alternative" data sets, the difference in absolute annual values between different models' calculations is more considerable (*m* = 1760 kg/year; σ = 1946 kg/year*)*. According to the data presented, for all models' results this flow is directed from the atmosphere to soil and only in the case of MSCE-POP calculations made on the basis of initial conditions with the use of "own/alternative" data sets it is practically compensated. The highest values in both sets of calculations are characteristic of SimpleBox 3.0 results based on initial concentrations given as input data. Two groups of the participating models in terms of close results can be distinguished further: with relatively low absolute values (CliMoChem, G-CIEMS and MSCE-

POP results) and with medium values, which are close to the averaged value (CAN/POPs, and all of the rest results of SimpleBox).

Since the net exchange flow is a sum of different types of exchange flows, below the latter are considered separately. Comparison of annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.125.

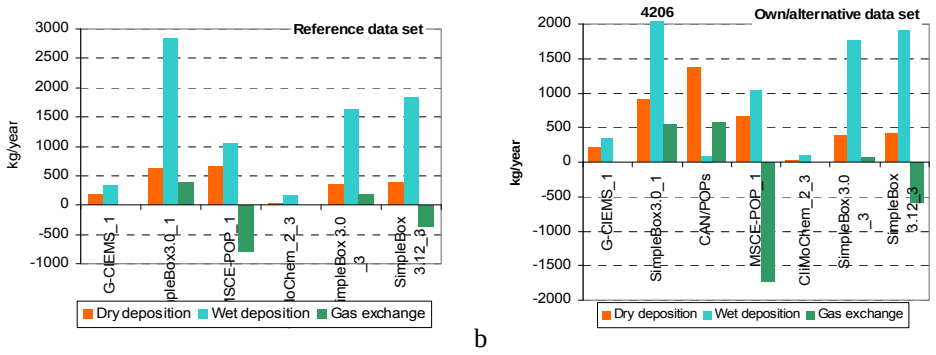
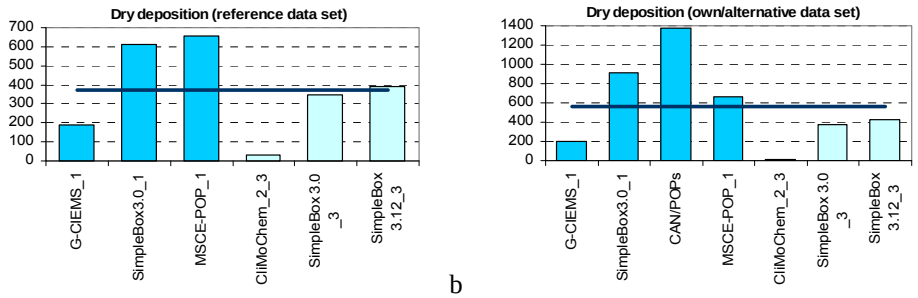


Fig.3.125. *Comparison of PCB-153 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and soil calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

The absolute values of dry deposition flows from the atmosphere to soil are the most close for all models among other flows. More noticeable difference between model results is observed in absolute values of wet deposition and gaseous exchange. The maximum value of dry deposition flow among all others is obtained in CAN/POPs calculations based on initial conditions and "own/alternative" data set. The highest values of wet deposition in both sets of results are characteristic of SimpleBox 3.0 calculations performed with the use of initial conditions. G-CIEMS model provided the lowest values of gaseous exchange flows. In the case of MSCE-POP results obtained on the basis of initial conditions and SimpleBox 3.12 results based on historical emissions the gaseous flow is a re-emission flow whereas in calculations of all other models it is directed from the atmosphere to soil. The relatively low values of all considered flows are characteristic of CliMoChem model in calculations performed with "reference" and "own/alternative" data sets. Difference between results of calculations with both physical-chemical data sets is not very large for most models.

To reveal differences in calculated values obtained on "reference" and "own/alternative" data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

According to the results on dry deposition of PCB-153 from the atmosphere to soil calculated on the basis of "reference" and "own/alternative" data sets (in "reference" set of results m = 372 kg/year, σ = 242 kg/year; in "own/alternative" set of results m = 565 kg/year, σ = 458 kg/year), most models give rather close values in terms of annual and monthly absolute values (see Tables 3.58 and 3.59 in Section 3.4.1). Square deviation σ does not exceed the mean values of this parameter averaged between the participating models. Comparison of annual values of PCB-153 dry deposition from the atmosphere to soil calculated by the models on the basis of "**reference"** and "**own or alternative"** data sets is presented in Fig. 3.126. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

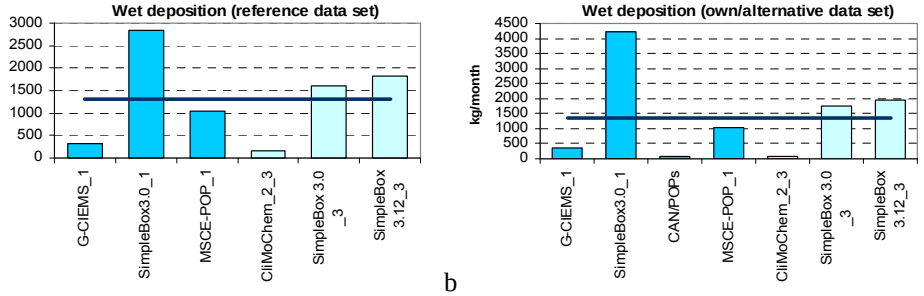


a b

Fig.3.126. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to soil: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the data presented, the difference between two sets of model results varies from 0.3 to 48% depending on a model (see Table 3.60 in Section 3.4.1). The largest difference in the values obtained with "reference" and "own/alternative" data sets is characteristic of SimpleBox 3.0 results based on initial conditions. There is a negligible difference between values obtained on both data sets and presented in the results of MSCE-POP obtained with the use of initial conditions. For G-CIEMS, SimpleBox 3.0 (initial conditions) and SimpleBox 3.0 and 3.12 results based on historical emissions, the annual values of PCB-153 dry deposition mass flows transported from the atmosphere to soil obtained with the use of "own or alternative" data sets are higher than those obtained with "reference" data set; and vice versa for the rest of model results.

The scattering between different models' results on PCB-153 wet deposition mass flows from the atmosphere to soil is more considerable than that on dry depositions (Tables 3.61 and 3.62 in Section 3.4.1). However, according to the results presented (in "reference" set of results m = 1303 kg/year, σ = 1006 kg/year; in "own/alternative" set of results m = 1356 kg/year, σ = 1468 kg/year), for annual values obtained on the basis of "reference" data set square deviation is less than the averaged value. Comparison of annual values of PCB-153 wet deposition mass flows from the atmosphere to soil calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.127. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.127. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to soil: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The difference between calculated annual values of PCB-153 wet deposition mass flows obtained by participating models with two data sets of physical-chemical properties lies in the range from 0.2 to 48% (Table 3.63 in Section 3.4.1). In results of G-CIEMS, SimpleBox 3.0 (initial conditions); SimpleBox (historical

emissions) and MSCE-POP (initial conditions), the annual values of calculation results obtained with the use of "own or alternative" data sets exceed those obtained with "reference" data set; and vice versa for CliMoChem results. The results of MSCE-POP model based on initial conditions show rather weak sensitivity of calculated values with respect to variations of pollutant-related parameters. Considerable difference in the results obtained with two data sets (48%) is characteristic of SimpleBox 3.0 results (initial conditions).

For two sets of results obtained, the differences in annual values of PCB-153 gaseous exchange flows between the atmosphere and soil calculated by the participating models are large (see Tables 3.64 and 3.65 given in Section 3.4.1). Square deviation of these values is considerably higher than mean values averaged between all models results (in "reference" set of results m = -93 kg/year, σ = 428 kg/year; in "own/alternative" set of results m = -162 kg/year, σ = 794 kg/year). A comparison of annual values of PCB-153 gaseous exchange between the atmosphere and soil calculated by the models on the basis of "**reference**" and "**own or alternative"** data sets is presented in Fig.3.128. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different colour of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

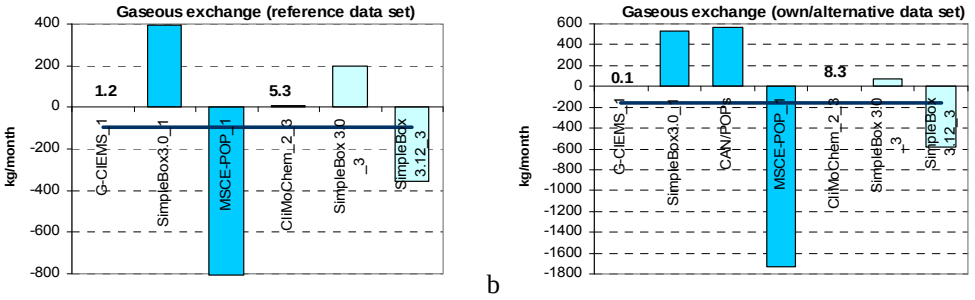


Fig.3.128. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to soil: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets.*

Considerable difference between absolute values obtained on the basis of two different data sets is characteristic of MSCE-POP calculations made on the basis of initial concentrations (more than 115%) and of SimpleBox 3.0 and 3.12 calculations performed with the use of initial conditions and historical emissions (36 – 65%). At that in all these results, the calculated absolute values based on "own/alternative" data set are higher than those based on "reference" data set.

Thus, according to the results presented above, most participating models provide reasonable agreement in description of net intermedia mass flows from the atmosphere to soil. The results obtained on the basis of "reference" data set of pollutant-related parameters are somewhat closer than those obtained with "own or alternative" data set. The absolute values of dry deposition flows from the atmosphere to soil agree better between all models than those calculated for other types of exchange flows contributing to the net flow considered above. More noticeable difference between model results is observed in absolute values of wet deposition; the highest dispersion is characteristic of values of gaseous exchange flows. Two models calculate considerable re-emission gaseous flux from soil. Difference between results of calculations performed with the use of "reference" and "own/alternative" data sets is not very large for most models. For dry and wet depositions it does not exceed 50%, in calculations of gaseous exchange it totals approximately to 100%.

Model results on concentrations of PCB-153 in the atmosphere at its interface with soil and in the surface soil layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with soil calculated by the models on the basis of "reference" and "own or alternative" data set (see Tables 3.91 and 3.92 in Section 3.5.1) is presented in Fig.3.129. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

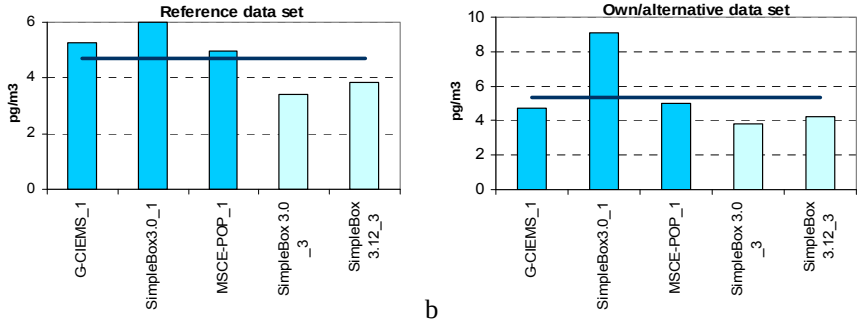
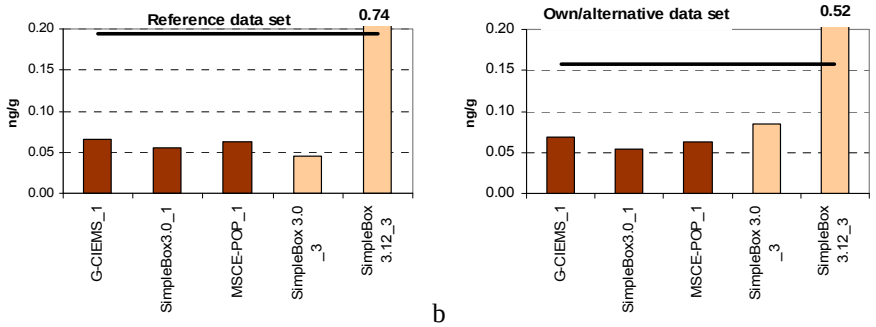


Fig.3.129. *Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with soil (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

It can be seen that air concentrations values obtained on "reference" and "own/alternative" data sets are very close for all models (in "reference" set of results m = 4.71 pg/m^3, σ = 1.06 pg/m^3; in "own/alternative" set of results m = 2.13 pg/m^3, σ = 0.20 pg/m^3). Square deviation of annual values presented by different participating models does not exceed the averaged value in both cases. The difference between results obtained with two different data sets of physical-chemical properties is rather small (see Table 3.93 in Section 3.5.1). For the calculation results of G-CIEMS, the annual values of PCB-153 concentration in the atmosphere at its interface with soil obtained with the use of "own or alternative" data sets are smaller than those obtained with "reference" data set; and vice versa for SimpleBox and MSCE-POP models' results. The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.0 calculations performed on the basis of initial conditions.

Comparison of annual values of PCB-153 concentration in surface soil layer calculated by the models on the basis of "reference" and "own/alternative" data sets (Tables 3.106 and Tables 3.107 given in Section 3.5.6) is presented in Fig.3.130. The black line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

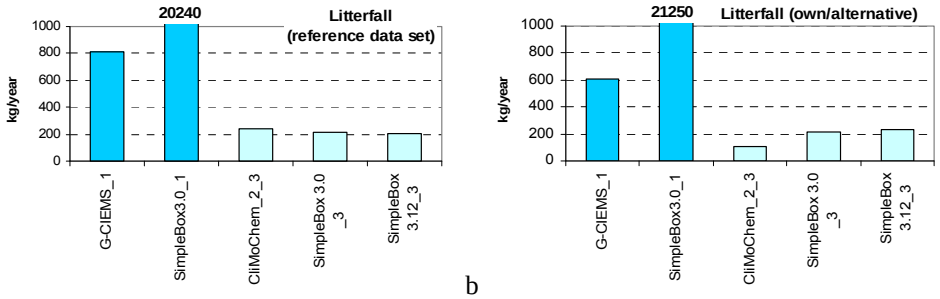
Fig.3.130. *Comparison of annual values of PCB-153 concentration in surface soil layer (ng/g) calculated by different models on the basis of "reference" (a) and "own or alternative" (b) data sets.*

According to the data presented, most models similarly describe soil concentrations. Results on PCB-153 concentration in surface soil layer calculated on the basis of "reference" and "own or alternative" data sets demonstrate reasonable agreement between most models' calculations except for results of version 3.12 of SimpleBox model. For annual values of PCB-153 concentration in surface soil layer (in "reference" set of results m = 0.19 ng/g, σ = 0.31 ng/g; in "own/alternative" set of results m = 0.16 ng/g, σ = 0.20 ng/g), square deviation is higher than the averaged value. Difference between the models' results obtained on the basis of two physical-chemical data sets varies from 0.2 to 92% (see Table 3.108 given in Section 3.5.6). For the calculation results of all models except G-CIEMS and SimpleBox 3.0 (based on historical emissions), the values of PCB-153 concentration in surface soil layer obtained with the use of "own or alternative" data sets are less than those obtained with "reference" data set. The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.12 results obtained on the basis of historical emissions. MSCE-POP results are characterised by the lowest sensitivity to the variations in physical-chemical data used.

Thus, the most part of participating models predicted close values of PCB-153 concentrations in the atmosphere at its interface with soil and in the surface soil layer taking into account the obtained estimates of intermediate flows. The high scattering in calculated values of mass flows conditioned by the gaseous exchange does not affect considerably calculated concentrations in comparison with contributions of dry and wet depositions. The difference between the maximum and minimum values of soil concentrations is higher than that for air concentrations. The difference between results obtained on the basis of "reference" and "own/alternative" physical-chemical data sets is rather small for air concentrations (50% in maximum). For soil concentrations it is about 90%.

Vegetation – soil. According to the calculation results on PCB-153 mass flows due litterfall from vegetation to soil calculated by models on the basis of both data sets of physical-chemical properties (Tables 3.68 and Tables 3.69 given in Section 3.4.2), the scattering between the maximum and minimum values obtained by different models is very high exceeding two orders of magnitude. Square deviation σ_φ between different model results in both cases considerably exceeds the averaged value (in "reference" set of results m = 4344 kg/year, σ = 9911 kg/year; in "own/alternative" set of results m = 4481 kg/year, σ = 9376 kg/year).

Comparison of annual values of PCB-153 mass flows from vegetation to soil calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.131. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; then long-tem calculations with historical emissions).



a b

Fig.3.131. *Comparison of annual values of PCB-153 mass flows transported from vegetation to soil (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" data sets (b)*

For both set of calculation results, the maximum absolute values of PCB-153 mass flows from vegetation to soil are obtained by SimpleBox 3.0 model on the basis of initial conditions. At that the value calculated by G-CIEMS model on the basis of initial conditions is much lower than results of SimpleBox mentioned above but considerably higher than the rest of other models' results, which are relatively close to each other. Comparison of annual values of litterfall mass flows calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.132 (see also Table 3.70 given in Section 3.4.2).

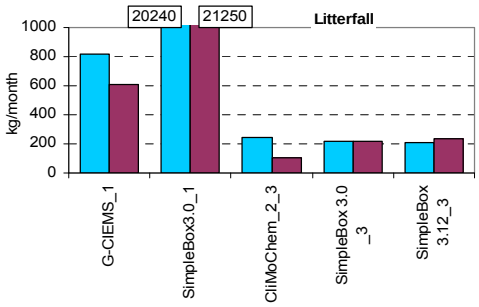


Fig.3.132. *Comparison of PCB-153 annual values of mass flows between vegetation and soil calculated by different models on the basis of two data sets*

For CliMoChem, G-CIEMS and SimpleBox 3.0 (historical emissions) results, the calculated values of PCB-153 mass flows transported from vegetation to soil obtained by the models on the basis of "reference" data set exceed those obtained with "own or alternative" data sets. According to the data presented in Table 3.70 (Section 3.4.2), the percentage difference between different models is in the range from 2 to 57%. The largest difference in the results obtained with two data sets is characteristic of CliMoChem model.

Atmosphere - seawater. Comparison of annual values of net exchange flow between the atmosphere and seawater obtained on the basis of "reference" data set is presented in Table 3.80 (see Section 3.4.3). The difference in absolute annual and monthly values obtained by the participating models is not considerable (in "reference" set of results m = 1831 kg/year, σ = 1292 kg/year; in "own/alternative" set of results m = 2298 kg/year, σ = 1922 kg/year). Square deviation σ does not exceed the mean value of this parameter averaged between the participating models in both cases.

Annual values of net exchange flow between atmosphere and seawater calculated on the basis of two data sets are compared between different models in Fig. 3.133. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

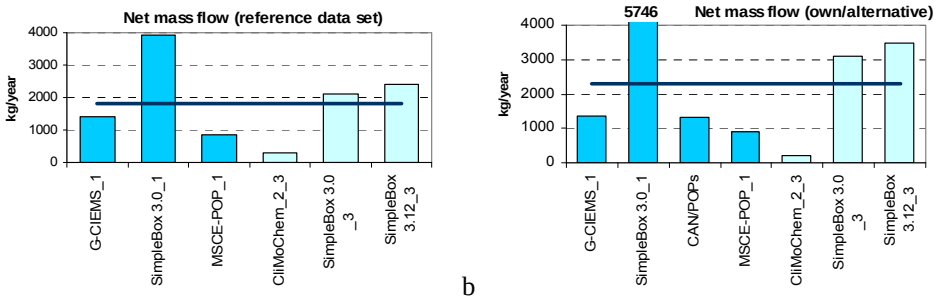


Fig.3.133. *Comparison of PCB-153 annual values of net exchange flow between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the results presented, all models obtained net flows directed from the atmosphere to water. There are three groups of close models' results, which can be isolated depending on magnitude of absolute values. First group of models with relatively low values includes CliMoChem, CAN/POPs, G-CIEMS and MSCE-POP models. Higher flows are calculated by SimpleBox 3.0 and 3.12 on the basis of historical emissions. Third group of results obtained on the basis of initial conditions by SimpleBox 3.0 models is characterized by the highest absolute value among others. Difference between results based on both physical-chemical data sets is rather small for all models except for SimpleBox.

Annual absolute values of dry and wet deposition and gaseous exchange flows, which formed the considered net exchange flows between the atmosphere and seawater, are compared below. Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and seawater calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.134.

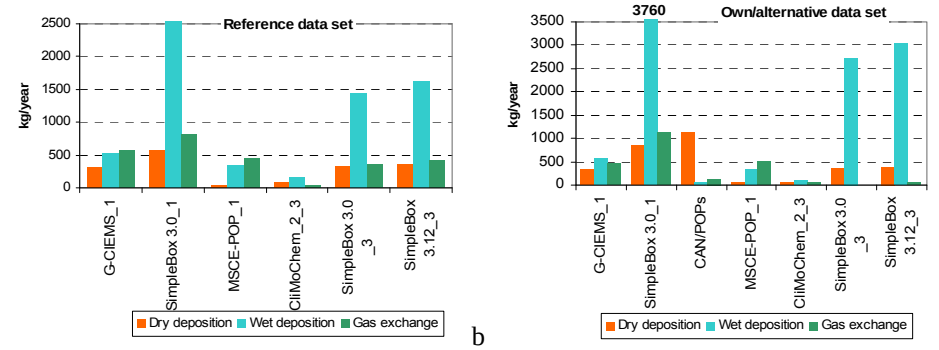
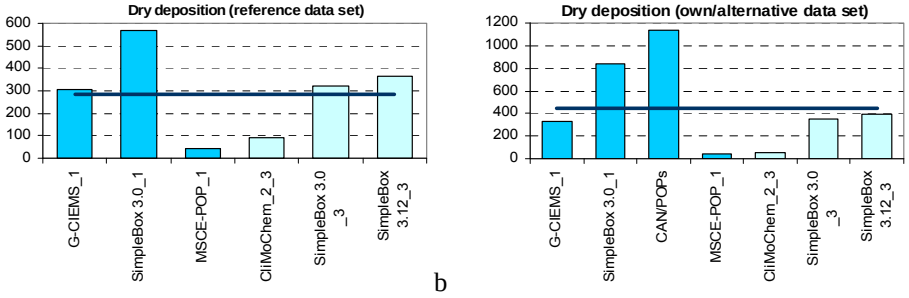


Fig.3.134. *Comparison of PCB-153 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and seawater calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The results on dry and wet deposition and gaseous exchange flows between these media obtained on both data sets ("reference" and "own/alternative") show that scattering of absolute values of wet deposition flows is the most noticeable in comparison with other flows. Similar to the results for atmosphere-soil interface, CAN/POPs calculations based on initial conditions and "own/alternative" data set predicted the maximum value of dry deposition flow among all others. The lowest values of dry depositions from the atmosphere to water are obtained by MSCE-POP model. The highest values of wet deposition in both sets of results are characteristic of Simple Box 3.0 calculations based on initial conditions. This model provided also the maximum values of gaseous exchange flows. Of note, most models show noticeable gaseous flows directed from the atmosphere to water. Difference between results of calculations with "reference" and "own/alternative" data sets is the most considerable for SimpleBox model.

Model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

The annual and monthly values of dry deposition of PCB-153 from the atmosphere to water calculated on the basis of "reference" and "own/alternative" data sets are in reasonable agreement for most models (see Tables 3.71 and 3.72 in Section 3.4.3). Square deviation σ in both cases does not exceed the mean values of this parameter averaged between the participating models (in "reference" set of results m = 281 kg/year, σ = 193 kg/year; in "own/alternative" set of results m = 449 kg/year, σ = 405 kg/year). Comparison of annual values of PCB-153 dry deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.135. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.135. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to water: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the data presented, the difference in absolute values obtained on the basis of both data sets ("reference" and "own/alternative") between models' results varies from 4 to 48% (Table 3.73 in Section 3.4.3). For the calculation results obtained by CliMoChem and MSCE-POP, the annual values of PCB-153 dry deposition mass flows from the atmosphere to water calculated with "own or alternative" data sets are less than those obtained with "reference" data set; and vice versa for G-CIEMS and SimpleBox model results. The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.0 calculations based on initial conditions.

According to the presented results on PCB-153 wet deposition mass flows from the atmosphere to water, the difference in results obtained on the basis of "own/alternative" data set is larger than that in results based on "reference" data set (Tables 3.74 and 3.75 in Section 3.4.3). Square deviation between participating models' results based on "reference" data set is less than the averaged value (in "reference" set of results m = 1105 kg/year, σ = 919 kg/year; in "own/alternative" set of results m = 1511 kg/year, σ = 1595 kg/year). Comparison of annual values of PCB-153 wet deposition mass flows from the atmosphere to water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.136. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

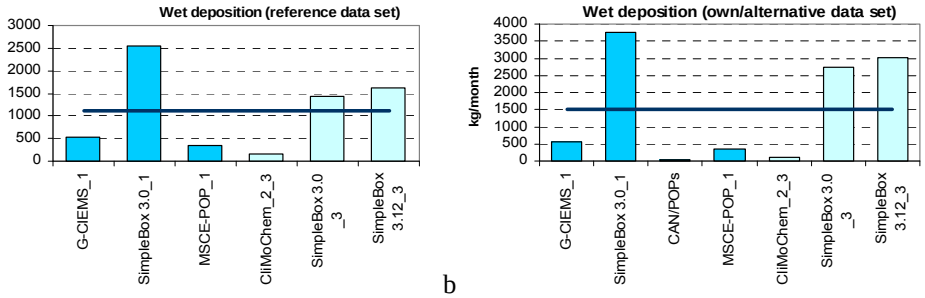


Fig.3.136. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to water: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The difference between the presented results obtained on the basis of both physical-chemical data sets varies from 4 to 90% (Table 3.76 in Section 3.4.3). The largest difference in the results obtained with two data sets is characteristic of SimpleBox 3.0 and 3.12 calculations performed on the basis of historical emissions. The lowest sensitivity to variations of pollutant-related parameters is observed in calculation results of MSCE-POP model obtained on the basis of initial conditions. Annual values of PCB-153 wet deposition mass flows from the atmosphere to water calculated by CliMoChem and MSCE-POP models with the use of "reference" data set exceed those based on "own or alternative" data sets; and vice versa for G-SIEMS and SimpleBox model results.

In comparison with the results on gaseous exchange flow obtained for the atmosphere-soil interface, the difference in values on gaseous exchange mass flows between the atmosphere and water calculated on the basis of "reference" data set is essentially lower since square deviation of these calculated values does not exceed the mean value averaged between all models (m = 444 kg/year, σ = 256 kg/year) (Tables 3.77 given in Section 3.4.3). The scattering of "own/alternative" set of results (m = 338 kg/year, σ = 409 kg/year) (Tables 3.78 given in Section 3.4.3) is noticeably higher than that for results based on "reference" data set. Comparison of annual values of PCB-153 gaseous exchange mass flows between the atmosphere and water calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.137. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

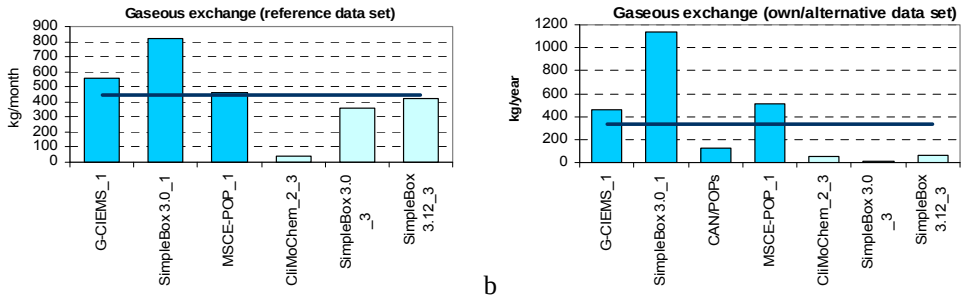


Fig.3.137. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to water: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the data presented, results of CliMoChem, SimpleBox 3.0 (initial conditions) and MSCE-POP models obtained on the basis of "own/alternative" data set are higher than those calculated with the use of

"reference" data set; and vice versa for the rest of other models' results (see also Table 3.79 in Section 3.4.3). The most considerable difference in absolute values calculated with the use of "reference" and "own/alternative" data sets is characteristic of SimpleBox 3.0 and 3.12 calculations carried out on the basis of initial conditions and historical emissions.

Thus, in the results obtained most participating models provided rather close values of net intermedia mass flows between the atmosphere and water. All models obtained net flows directed from the atmosphere to water. The scattering in results calculated by different models on the basis of "reference" data set is higher than that in the results obtained with "own or alternative" data set. The difference in absolute values of wet deposition and gaseous exchange flows is more noticeable in comparison with dry deposition flows. Maximum difference between results on all flows calculated with the use of "reference" and "own or alternative" data sets does not exceed 90%.

Model results on concentrations of PCB-153 in the atmosphere at its interface with ocean and in the surface water layer, which are conditioned by the considered above intermedia flows calculated with "reference" and "own/alternative" data sets are considered below.

Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with ocean calculated by the models on the basis of "reference" and "own/alternative" data sets (see Tables 3.94 and 3.95 in Section 3.5.2) is presented in Fig.3.138. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

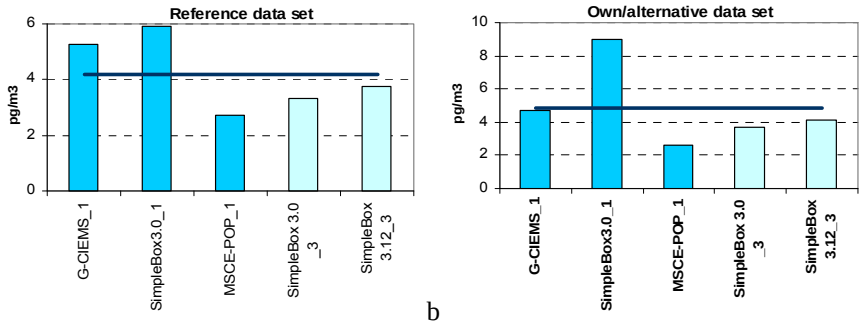
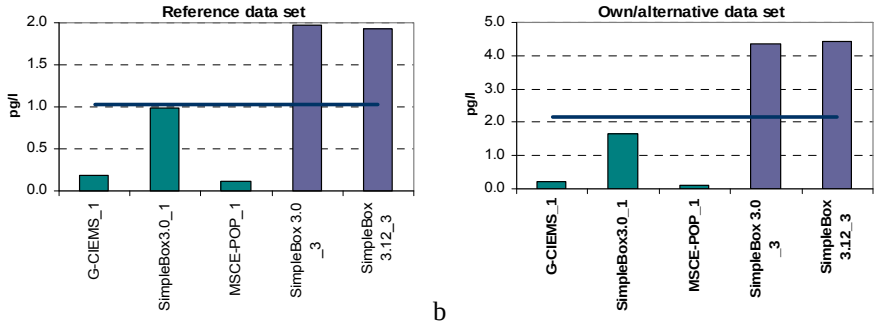


Fig.3.138. *Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with ocean (pg/m^3) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

Similar to the case with PCB-153 air concentrations formed at its interface with soil, in both sets of results obtained all models predicted rather close values of air concentrations formed at its interface with ocean. For both sets of results square deviation of annual values does not exceed the mean value averaged between different models (in "reference" set of results m = 4.20 pg/m^3, σ = 1.34 pg/m^3; in "own/alternative" set of results m = 4.83 pg/m^3, σ = 2.43 pg/m^3). Difference between two sets of results obtained on the basis of "reference" and "own/alternative" data sets is in the range from 3 to 52 % (results of MSCE-POP and SimpleBox 3.0 obtained on the basis of initial conditions, respectively) (see Table 3.96 in Section 3.5.2). For the calculation results of G-CIEMS and MSCE-POP models, the values of PCB-153 concentration in the atmosphere at its interface with ocean obtained with the use of "own or alternative" data sets are smaller than those obtained with "reference" data set, and vice versa for all SimpleBox results.

Comparison of annual values of PCB-153 concentration in surface ocean layer calculated by the models on the basis of "reference" and "own/alternative" data sets (see Tables 3.100 and 3.101 in Section 3.5.4) is presented in Fig.3.139. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



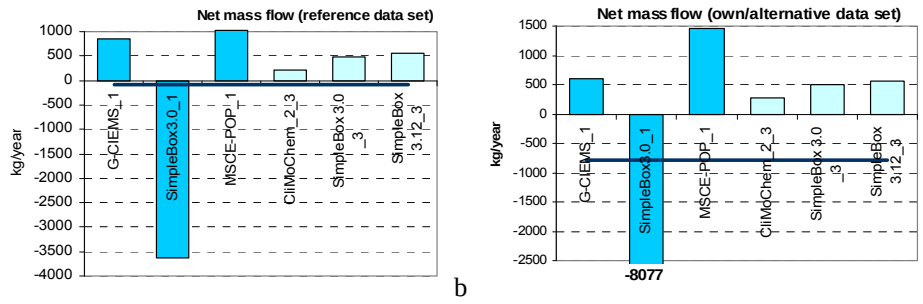
a b

Fig.3.139. *Comparison of annual values of PCB-153 concentration in surface ocean layer (pg/l) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The variability of water concentrations for most models is not very large but it is higher than that for air concentrations. The maximum values are obtained by SimpleBox 3.12 model on the basis of "own/alternative" data set. MSCE-POP model's results are characterized by the lowest values of water concentrations in both cases. At that, square deviation σ between different model results is slightly lower than the mean averaged value in the both cases (in "reference" set of results m = 1.04 pg/l, σ = 0.90 pg/l; in "own/alternative" set of results m = 2.16 pg/l, σ = 2.13 pg/l). Results of all models obtained on the basis of "reference" data set differ from those based on "own/alternative" data set in the range from 3 to 130% (see Table 3.102 given in Section 3.5.4). The maximum difference is characteristic of SimpleBox 3.12 results based on historical emissions); and the minimum difference – of MSCE-POP results. For the calculation results of all models, the values of PCB-153 concentration in surface ocean layer obtained with the use of "own or alternative" data sets exceed those obtained with "reference" data set.

The values of PCB-153 concentrations in the atmosphere at its interface with ocean are close for most participating models. The scattering in calculated values of water concentrations is more considerable. However, square deviation between different models' results is practically equal to the mean averaged value in the both cases. The difference between absolute values of air and water concentrations obtained with both physical-chemical data sets totals to 50 and 130 %, respectively.

Atmosphere – vegetation. Comparison of annual values of net exchange flow between the atmosphere and vegetation obtained on the basis of "reference" data set is presented in Table 3.90 (see Section 3.4.4). Annual values of net exchange flow between atmosphere and vegetation calculated on the basis of two data sets ("reference" and "own/alternative") are compared between different models in Fig. 3.140. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

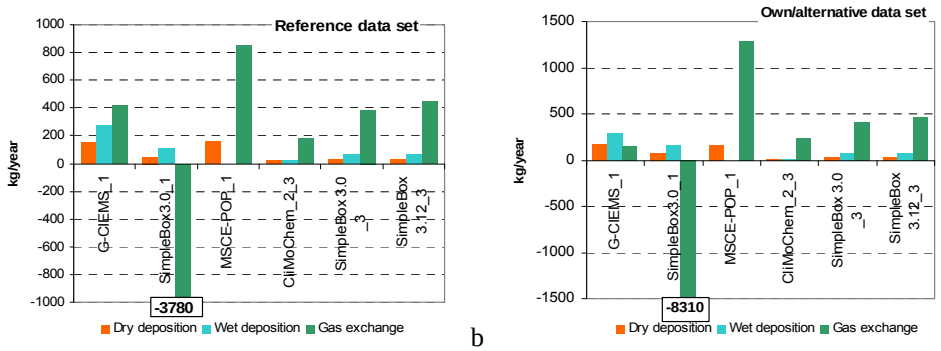


a b

Fig.3.140. *Comparison of PCB-153 annual values of net exchange flow between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the comparison of results on net exchange flow between the atmosphere and vegetation, the difference in annual values obtained by the participating models both on the basis of "reference" (m = -88 kg/year; σ = 1756 kg/year) and "own/alternative" (m = -779 kg/year; σ = 3598 kg/year) data sets is very large. Square deviation σ of absolute annual values obtained by the participating models is much higher than the mean value of this parameter averaged between the models. That testifies a considerable discrepancy in simulation of intermedia transport between these compartments by different models. A comparison of model results on net exchange flow of PCB-153 for the atmosphere and vegetation interface demonstrates that for most models this flow is transported from the atmosphere to vegetation. Calculations made by SimpleBox 3.0 model on the basis of initial conditions show high re-emission flux from vegetation. In spite of the fact that the scattering in absolute values is very large, the most models - CliMoChem, G-CIEMS, MSCE-POP and SimpleBox 3.0 and 3.12 (historical emissions) models demonstrate relatively close results. The difference in net exchange values obtained on the basis of two data sets is noticeable for G-CIEMS, MSCE-POP, and Simple Box 3.0 (initial conditions).

Comparison of annual values of dry and wet deposition and gaseous exchange flows between the atmosphere and vegetation calculated by models on the basis of two physical-chemical data sets is presented in Fig. 3.141.



a b

Fig.3.141. *Comparison of PCB-153 annual values of dry and wet deposition and gaseous exchange flows between atmosphere and vegetation calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

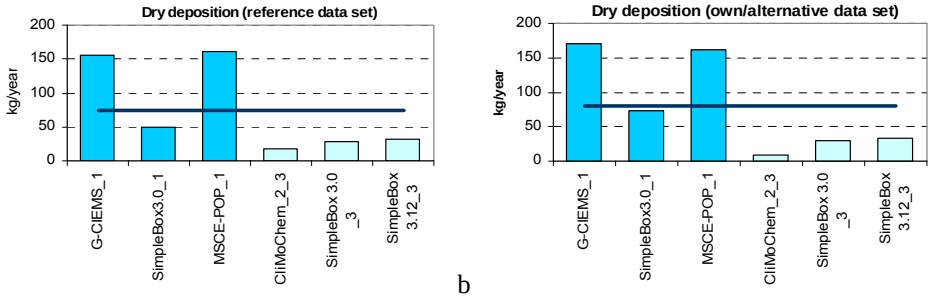
For model results calculated by the participating models on the basis of both physical-chemical data sets ("reference" and "own/alternative"), the absolute values of dry and wet deposition between the atmosphere and vegetation are closer to each other than those of gaseous exchange flows. The difference between results of both calculations on dry depositions is rather small for all models. Higher variability of absolute

values of wet deposition is observed. The maximum value of wet deposition flow is characteristic of G-CIEMS. It should be noted that wet deposition on vegetation is not taken into account in MSCE-POP model. For most models PCB-153 gaseous exchange flows are directed from the atmosphere to vegetation. MSCE-POP results presented the highest value of this gaseous flow among them. At that, calculations performed by SimpleBox 3.0 model on the basis of initial conditions show high re-emission flow from vegetation. For G-CIEMS, MSCE-POP and SimpleBox 3.0 (initial conditions) models noticeable difference in gaseous exchange flux between calculations on "reference" and "own/alternative" data sets can be seen.

To reveal differences in calculated values obtained on "reference" and "own/alternative" data sets, model results on dry and wet depositions and gaseous exchange between the atmosphere and soil are considered below in more detail.

According to the results on dry deposition of PCB-153 from the atmosphere to vegetation calculated on the basis of both data sets, most models predicted rather close absolute annual values (see Tables 3.81 and 3.82 in Section 3.4.4). Square deviation σ_φ does not exceed the mean values of this parameter averaged between the participating models in both cases (in "reference" set of results m = 74 kg/year, σ = 66 kg/year; in "own/alternative" set of results m = 79 kg/year, σ = 70 kg/year). Comparison of annual values of PCB-153 dry deposition mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.142. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

According to the data presented, the difference between two sets of model results varies from 0.3 to 50% depending on a model (see Table 3.83 in Section 3.4.4). The largest difference in the values obtained with two data sets is characteristic of CliMoChem results based on historical emissions. Negligible difference between values obtained on "reference" and "own/alternative" data sets is characteristic of MSCE-POP results based on initial conditions. For CliMoChem results, the annual values of PCB-153 dry deposition mass flows from the atmosphere to vegetation calculated with "own or alternative" data sets are smaller than those obtained with "reference" data set; and vice versa for G-CIEMS, MSCE-POP and all SimpleBox results.



a b

Fig.3.142. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to vegetation: dry deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The scattering between different models' results on PCB-153 wet deposition mass flows transported from the atmosphere to vegetation is higher than that on dry depositions (Tables 3.84 and 3.85 in Section 3.4.4). However, according to the results presented (in "reference" set of results m = 106 kg/year, σ = 97 kg/year; in "own/alternative" set of results m = 121 kg/year, σ = 111 kg/year), square deviation of this parameter values is less than the averaged value in both sets of obtained results. Comparison of annual values of PCB-153 wet

deposition mass flows transported from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.143. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

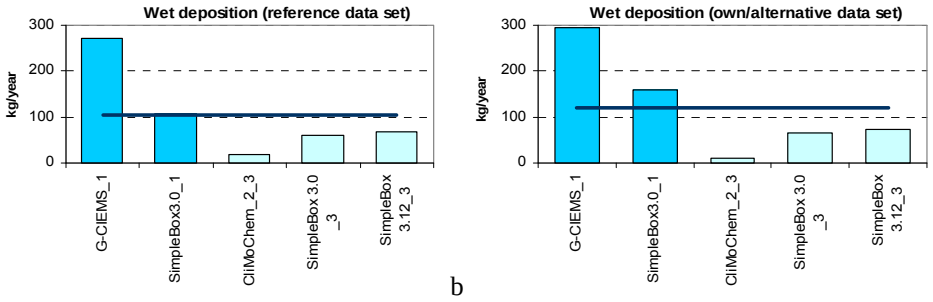


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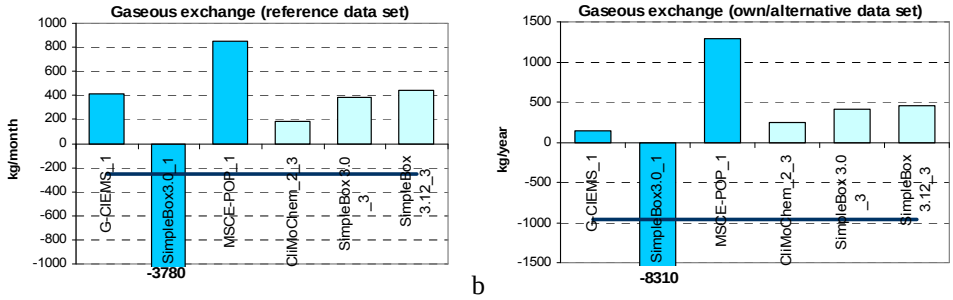
Fig.3.143. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to vegetation: wet deposition (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

For the calculation results of G-CIEMS and SimpleBox 3.0 and 3.12 models (initial conditions and historical emissions), the values of PCB-153 wet deposition mass flows transported from the atmosphere to vegetation obtained with the use of "own or alternative" data sets exceed those obtained with "reference" data set; and vice versa for CliMoChem model (see Table 3.86 in Section 3.4.4). The largest difference in the results obtained with two data sets making up approximately 50% is characteristic of SimpleBox 3.0 results based on initial conditions; the lowest difference equal to 9% is observed in results of MSCE-POP model.

According to the results on PCB-153 gaseous exchange flows for the atmosphere - vegetation interface calculated by the participating models on the basis of two physical-chemical data sets, the differences in both annual and monthly absolute values are very large (see Tables 3.87 and 3.88 given in Section 3.4.1). Square deviation of these values is higher than mean values averaged between all models results (in "reference" set of results m = -250 kg/year, σ = 1745 kg/year; in "own/alternative" set of results m = -960 kg/year, σ = 3624 kg/year). Comparison of annual values of PCB-153 gaseous exchange mass flows from the atmosphere to vegetation calculated by the models on the basis of "**reference**" and "**own or alternative**" data sets is presented in Fig.3.144. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.144. *Comparison of annual values of PCB-153 mass flows transported from the atmosphere to vegetation: gaseous exchange (kg/year) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

According to the results presented (see also Table 3.89 in Section 3.4.4), the most considerable difference in the values obtained on “reference” and “own/alternative” data sets is characteristic of SimpleBox 3.0 model results calculated on the basis of initial conditions. The less noticeable difference among different models is obtained in the rest of this model’s results. Results of MSCE-POP and CliMoChem models obtained with the use of “own/alternative” data set exceed those based on “reference” data set; and vice versa for G-CIEMS.

Thus, it can be noted that considerable scattering of net exchange flows for the atmosphere - vegetation interface obtained by different models is conditioned by the difference in gaseous exchange flows that is the most pronounced among other flows. The most participating models provided a reasonable agreement in description of dry and wet mass flows from the atmosphere to vegetation. One model predicted high re-emission flux from vegetation to the atmosphere in the case of values obtained on the basis of initial conditions. The difference between results of calculations carried out with the use of “reference” and “own/alternative” data sets is about 120%.

Model results on concentrations of PCB-153 in the atmosphere at its interface with vegetation and in vegetation, which are conditioned by the considered above intermedia flows calculated with “reference” and “own/alternative” data sets are considered below.

Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with vegetation calculated by the models on the basis of “reference” and ‘own/alternative” data sets (see Tables 3.97 and 3.98 in Section 3.5.3) is presented in Fig.3.145. The blue line in the plots shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).

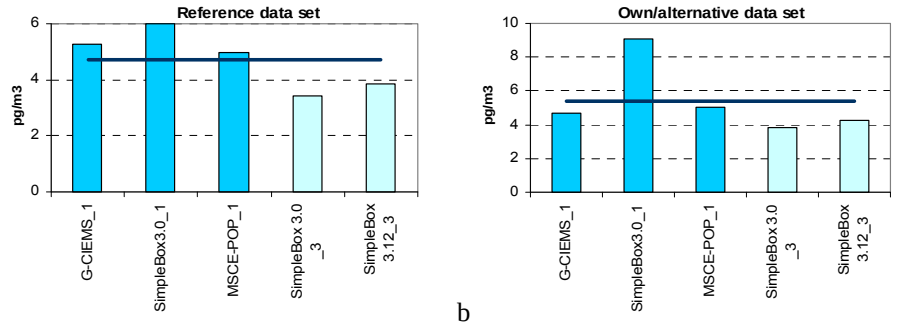
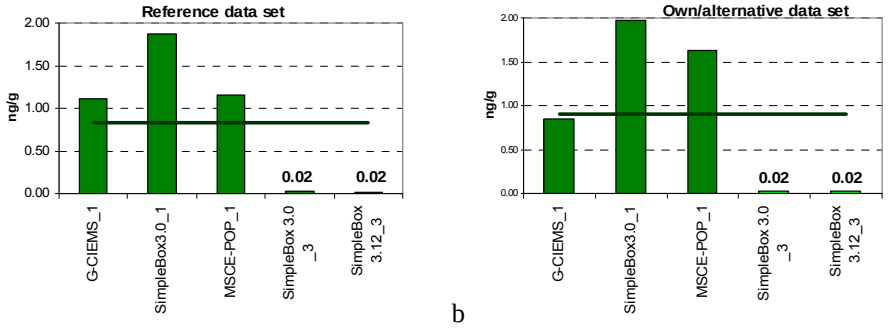


Fig.3.145. *Comparison of annual values of PCB-153 concentration in the atmosphere at its interface with vegetation (pg/m3) calculated by different models on the basis of “reference”(a) and “own or alternative” (b) data sets*

According to the results presented, PCB-153 concentrations in the atmosphere at its interface with vegetation are close to each other for all participating models. For two sets of results obtained the differences in annual values of PCB-153 concentration in the atmosphere at its interface with vegetation are not considerable (in “reference” set of results m = 4.70 pg/m^3, σ = 1.06 pg/m^3; in “own/alternative” set of results m = 5.37 pg/m^3, σ = 2.13 pg/m^3). Square deviation of these values in all cases is lower than the mean values averaged between all models results. For the calculation results of G-CIEMS, the values of PCB-153 concentration in the atmosphere at its interface with vegetation obtained with the use of “own or alternative” data sets are smaller than those obtained with “reference” data set; and vice versa for MSCE-POP and all SimpleBox results (see Table 3.99 in Section 3.5.3). The largest difference in the results obtained with two data sets (52%) is characteristic of SimpleBox 3.0 calculations performed on the basis of initial conditions. For MSCE-POP this difference is minimum among all others and totals to 1%.

Comparison of annual values of PCB-153 concentration in vegetation calculated by the models on the basis of "reference" and 'own/alternative" data sets (see Tables 3.103 and 3.104 in Section 3.5.5) is presented in Fig.3.146. The green line in the plot shows the value of the corresponding parameter averaged between models. Different color of columns corresponds to the different types of calculations (one-year calculations on the basis of initial data; and then long-tem calculations with historical emissions).



a b

Fig.3.146. *Comparison of annual values of PCB-153 concentration in vegetation (ng/g) calculated by different models on the basis of "reference"(a) and "own or alternative" (b) data sets*

The differences between annual values of PCB-153 concentration in vegetation calculated by the participating models are rather considerable for two sets of results obtained (in "reference" set of results m = 0.84 pg/m^3, σ = 0.80 pg/m^3; in "own/alternative" set of results m = 0.90 pg/m^3, σ = 0.90 pg/m^3). The highest and the lowest values of the considered parameter are obtained by different versions of SimpleBox model (3.0_1 and 3.12_3). Square deviation of these values is not higher than the mean values averaged between all models results. For the calculation results of all models except G-CIEMS and SimpleBox 3.0 (historical emissions), the values of PCB-153 concentration in vegetation obtained with the use of "own or alternative data sets" exceed those obtained with "reference" data set (see Table 3.105). The largest difference in the results obtained with two data sets equal to 42% is characteristic of MSCE-POP results. Results of SimpleBox 3.0 are the less sensitive to the changes in pollutant-related parameters.

Results on PCB-153 concentrations in the atmosphere at its interface with vegetation are in good agreement for most models. The variation in values of concentrations in vegetation is higher than that in the air concentrations. The difference between absolute values of air and vegetation concentrations obtained with "reference" and "own or alternative" physical-chemical data sets totals to 50 and 42 %, respectively.

According to the comparison presented above, it can be concluded that:

- All model provide reasonable agreement in description of intermedia mass flows and concentrations in the main environmental media.

- In particular, air concentrations as the most important output of the participating models are in good agreement for all models' results. Several models predict 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 predict 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. Very close absolute values of soil concentrations are characteristic of most models' results.

- Most participating models provide a reasonable agreement in description of net intermedia mass flows from the atmosphere to soil and to water. The scattering in results on net intermedia mass flows between the atmosphere and 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 calculate 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 calculate 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 "reference" and "own/alternative" 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 show 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).

3.6. Spatial distribution of depositions and concentrations in different compartments (optional)

Five models present results on spatial distribution of depositions and concentrations of PCB-153 in different environmental compartments: ADEPT, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox.

Calculated fields of PCB-153 concentrations in the atmosphere, soil, water and vegetation and net deposition fluxes in 2000 obtained by the participating models with the use of two different data sets ("reference" and "own or alternative") are compared below. The results on spatial distribution of PCB-153 deposition and concentrations in the main environmental media are obtained with the use of the two physical-chemical data sets by DEHM-POP, MSCE-POP and different versions of SimpleBox model.

The comparison of calculated deposition and concentration fields presented in Sections 3.6.1 and 3.6.2 below includes results of one-year calculations made on the basis of initial conditions (DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP, SimpleBox), zero initial concentrations (ADEPT, DEHM-POP, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox) together with results of long-term calculations performed with historical emissions (EVN-BETR and UK-MODEL, SimpleBox 3.0 and 3.12) (See Table 3.109). The model results obtained taking into account initial concentrations of pollutants in media and historical emissions, and on the basis of zero initial concentrations in the environmental media are compared in two different groups.

In Subsection 3.6.1 a preliminary analysis of the comparison of calculated deposition and concentration fields is made for the model results based on "reference" data set and obtained on the basis of non-zero initial conditions (initial concentrations and historical emissions).