Annex E

SENSITIVITY STUDY WITH RESPECT TO SUBSTANCE-SPECIFIC PROPERTIES USED IN THE DESCRIPTION OF BASIC PROCESSES FOR PCB-180

4.1. Gas/particle partitioning

Reference data set. Calculation results for PCB-180 together with m_φ and σ_φ are presented in Table E.1.

Table E.1. *Calculation results: fractions of particulate phase of PCB-180 calculated by models and statistical parameters used for evaluation ("reference" data set)*

Exp.No	T (°C)	DEHM-POP	CliMoChem	SimpleBox*	m_φ	σ_φ
1	-12	0.96	0.24	1.00	**0.73**	**0.43**
2	-5	0.88	0.20	0.99	**0.69**	**0.43**
3	0	0.79	0.20		**0.50**	**0.42**
4	3	0.69	0.17		**0.43**	**0.37**
5	5	0.49	0.10		**0.29**	**0.28**
6	8	0.46	0.12		**0.29**	**0.24**
7	10	0.44	0.14	0.92	**0.50**	**0.40**
8	12	0.37	0.13	0.90	**0.25**	**0.17**
9	15	0.35	0.16		**0.25**	**0.13**
10	17	0.25	0.13		**0.19**	**0.09**
11	20	0.19	0.12		**0.15**	**0.05**
12	25	0.10	0.09		**0.10**	**0.00**

* - only 4 experiments for Simple Box

The plot of dependence of φ on T calculated by participating models is presented in Fig. E.1.

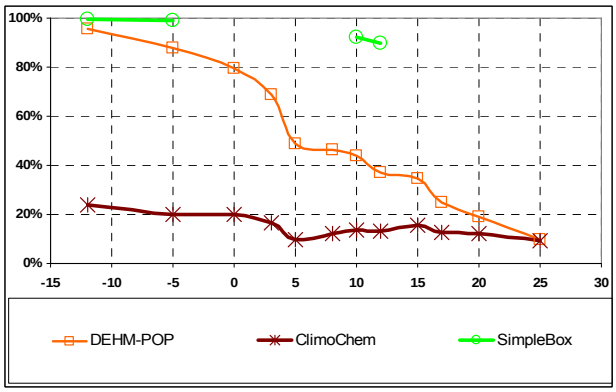


Fig. E.1. *Calculation results of the participating models (gas-particle partitioning) obtained with reference data set*

Calculated correlation coefficients between the results of participating models are given in Table E.2.

Table E.2. *Correlation coefficients* r_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.88	0.99
CliMoChem	-	0.96

* - by 4 experiments only

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.3.

Table E.3. *Coefficients of regression dependence between the models (α / β)*

	CliMoChem	SimpleBox*
DEHM-POP	0.14 / 0.08	0.16 / 0.84
CliMoChem	–	0.91 / 0.79

* - by 9 experiments only

Results of the calculation of pairwise residual square deviation σ are given in Table E.4.

Table E.4. *Residual square deviation,* σ^{res}_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.069	0.009
CliMoChem	-	0.024

* - by 9 experiments only

Own/altenative data set. Calculation results for PCB-180 together with m_φ and $\sigma_{.\varphi}$ are presented in Table E.5. The data set used in calculations by each model is indicated in the first row.

Table E.5. *Calculation results: fractions of particulate phase of PCB-180 calculated by models and statistical parameters used for evaluation (own/alternative data set)*

Exp.No	*T* (°C)	EVN-BETR and UK-MODEL	DEHM-POP	CAN/ POPs	MSCE-POP_1	MSCE-POP_2	CliMoChem	SimpleBox	m_φ	σ_φ
Data set		own	own	own	own	own	own	alt		
1	-12	0.98	0.93	0.99	0.98	0.97	0.22	0.99	**0.87**	**0.29**
2	-5	0.95	0.84	0.97	0.94	0.92	0.14	0.98	**0.82**	**0.30**
3	0	0.92	0.75	0.95	0.87	0.87	0.12	0.96	**0.75**	**0.32**
4	3	0.86	0.64	0.92	0.81	0.80	0.09	0.94	**0.69**	**0.31**
5	5	0.73	0.45	0.82	0.76	0.64	0.05	0.88	**0.62**	**0.29**
6	8	0.71	0.44	0.81	0.67	0.62	0.05	0.88	**0.60**	**0.28**
7	10	0.69	0.42	0.79	0.60	0.60	0.05	0.88	**0.58**	**0.27**
8	12	0.63	0.36	0.74	0.53	0.54	0.05	0.85	**0.47**	**0.24**
9	15	0.60	0.34	0.71	0.43	0.52	0.05	0.85	**0.44**	**0.23**
10	17	0.49	0.25	0.60	0.36	0.41	0.04	0.79	**0.36**	**0.20**
11	20	0.40	0.20	0.51	0.27	0.33	0.03	0.73	**0.29**	**0.17**
12	25	0.23	0.11	0.31	0.16	0.19	0.02	0.60	**0.17**	**0.10**

The plot of dependence of φ on *T* calculated by participating models with “own or alternative” data set is presented in Fig. E.2.

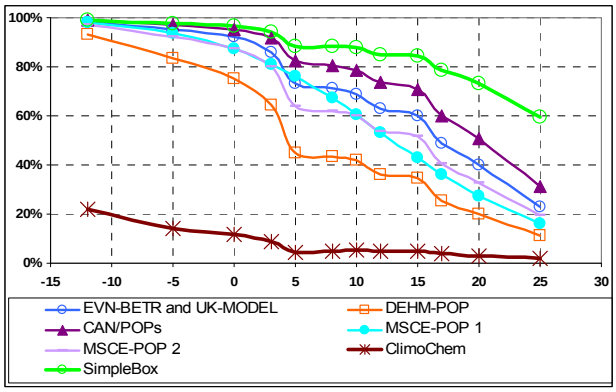


Fig. E.2. *Calculation results of the participating models (gas-particle partitioning) obtained with "own/alternative" data set*

Calculated correlation coefficients between the results of participating models are given in Table E.6.

Table E.6. *Correlation coefficients* r_{12}

	DEHM-POP	CAN/POPs	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.96	0.99	0.98	0.99	0.81	0.99
DEHM-POP	-	0.92	0.96	0.98	0.93	0.91
CAN/POPs	-	-	0.97	0.97	0.75	1.00
MSCE-POP 1	-	-	-	0.98	0.80	0.95
MSCE-POP 2	-	-	-	-	0.86	0.96
CliMoChem	-	-	-	-	-	0.74

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.7.

Table E.7. *Coefficients of regression dependence between the models* (α / β)

	DEHM-POP	CAN/POPs	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	1.08 / - 0.0001	0.88 /	1.15 / -0.17	1.04 / -0.09	0.20 / -0.06	0.48 / 0.53
DEHM-POP	–	0.72 /	0.99 / 0.14	0.92 / 0.18	0.21 / -0.02	0.39 / 0.67
CAN/POPs			1.28 / -0.35	1.15 / -0.26	0.21 / -0.09	0.55 / 0.44
MSCE-POP 1	–		–	0.88 / 0.07	0.17 / -0.03	0.40 / 0.62
MSCE-POP 2	–		–	–	0.21/ -0.05	0.45 / 0.58
CliMoChem	–		–	–	–	1.44 / 0.75

Results of calculations of pairwise residual square deviation σ are given in Table E.8.

Table E.8. *Residual square deviation,* σ^{res}_{12}

	DEHM-POP	CAN/POPs	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.25	0.08	0.16	0.09	0.11	0.06
DEHM-POP	-	0.27	0.26	0.15	0.07	0.16
CAN/POPs	-	-	0.22	0.18	0.13	0.03
MSCE-POP 1	-	-	-	0.15	0.11	0.12
MSCE-POP 2	-	-	-	-	0.10	0.10
CliMoChem	-	-	-	-	-	0.25

Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table E.9.

Table E.9. *Difference between calculations with two data sets*

Exp.No	*T* (°C)	DEHM-POP	CliMoChem	SimpleBox
1	-12	-2%	-8%	-1%
2	-5	-5%	-29%	-1%
3	0	-5%	-42%	
4	3	-6%	-49%	
5	5	-8%	-54%	
6	8	-6%	-59%	
7	10	-5%	-61%	-5%
8	12	-3%	-64%	-5%
9	15	0%	-67%	
10	17	2%	-70%	
11	20	6%	-74%	
12	25	13%	-78%	

This difference is visualized in Fig. E.3.

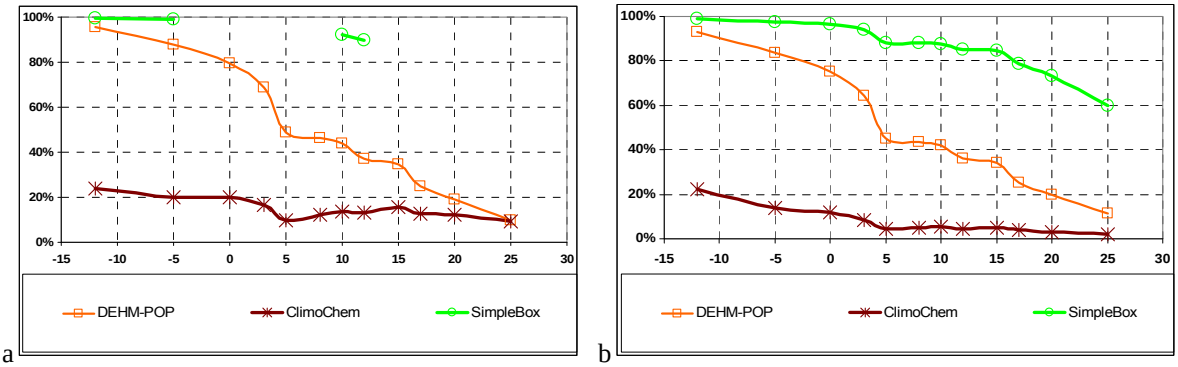


Fig. E.3. *Calculation results of the participating models obtained with "reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

4.2. Wet deposition

Reference data set. Calculation results for PCB-180 together with *m* and σ are presented in Tables 4. 4.10 and 4.11.

Table E.10. *Calculation results: concentrations in precipitation (pg/L) ("reference" data set)*

Exp. No	*T* (°C)	CliMoChem	SimpleBox	*m*	σ
1	-1	273	929	**601**	**464**
2	3	81	277	**179**	**139**
3	10	121	410	**265**	**204**
4	15	33	113	**73**	**56**
5	-1	27	929	**478**	**638**
6	3	8	277	**143**	**190**
7	10	12	410	**211**	**281**
8	15	3	113	**58**	**77**

Table E.11. *Calculation results: wet deposition flux, ng/m^2/hour ("reference" data set)*

Exp. No	*T* (°C)	CliMoChem	SimpleBox	*m*	σ
1	-1	0.273	0.929	**0.601**	**0.464**
2	3	0.081	0.277	**0.179**	**0.139**
3	10	0.121	0.410	**0.265**	**0.204**
4	15	0.033	0.113	**0.073**	**0.056**
5	-1	0.273	9.293	**4.783**	**6.379**
6	3	0.081	2.770	**1.426**	**1.901**
7	10	0.121	4.099	**2.110**	**2.813**
8	15	0.033	1.126	**0.579**	**0.773**

The comparison of calculated values of concentrations in precipitation is displayed in Fig. E.4.

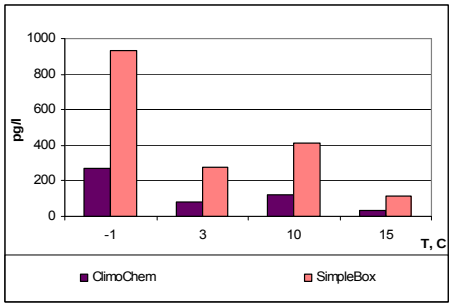


Fig. E.4. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (reference data set)*

Calculated correlation coefficients between the results of participating models are given in Table E.12.

Table E.12. *Correlation coefficients* r_{12}

	SimpleBox
CliMoChem	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.13.

Table E.13. *Coefficients of regression dependence between the models* (α / β)

	SimpleBox
CliMoChem	3.41 / -0.305

Pairwise residual square deviation σ are shown in Table E.14.

Table E.14. *Residual square deviation,* σ^{res}_{12}

	SimpleBox
CliMoChem	2.76

Own/alternative data set. Calculation results for PCB-180 together with *m* and σ are presented in Tables 4. 4.15 and 4.16.

Table E.15. *Calculation results: concentrations in precipitation (pg/L) (own/alternative data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1	138	5720	663	254	882	**1531**	**2361**
2	3	609	1403	199	76	266	**511**	**537**
3	10	3900	9110	250	91	341	**2738**	**3901**
4	15	570	1048	78	30	105	**366**	**439**
5	-1	–	–	663	25	882	**523**	**445**
6	3	–	–	199	8	266	**157**	**134**
7	10	–	–	250	9	341	**200**	**172**
8	15	–	–	78	3	105	**62**	**53**

Table E.16. *Calculation results: wet deposition flux, ng/m*^{2}*/hour (own/alternative data set)*

Exp. No	*T* (°C)	EVN-BETR and UK-MODEL	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox	*m*	σ
1	-1	0.138	5.720	0.663	0.254	0.882	**1.531**	**2.361**
2	3	0.609	1.403	0.199	0.076	0.266	**0.511**	**0.537**
3	10	3.900	9.110	0.250	0.091	0.341	**2.738**	**3.901**
4	15	0.570	1.048	0.078	0.030	0.105	**0.366**	**0.439**
5	-1	–	–	6.630	0.254	8.821	**5.235**	**4.451**
6	3	–	–	1.990	0.076	2.658	**1.575**	**1.340**

7	10	–	–	2.500	0.091	3.413	**2.001**	**1.716**
8	15	–	–	0.780	0.030	1.051	**0.620**	**0.529**

The comparison of calculated values of concentrations in precipitation is displayed in Fig. E.5.

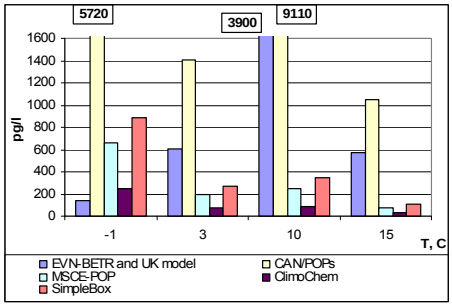


Fig. E.5. *Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (own/alternative data set)*

Calculated correlation coefficients between the results of participating models are given in Table E.17.

Table E.17. *Correlation coefficients* r_{12}

	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	0.76	-0.24	-0.26	-0.23
CAN/POPs	-	0.44	0.42	0.45
MSCE-POP	-	-	1.00	1.00
CliMoChem	-	-	-	1.00

The values of regression coefficients α and β calculated for all pairs of models are shown in Table E.18.

Table E.18. *Coefficients of regression dependence between the models* (α / β)

	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	1.67 / 2143	-0.04 / 343.3	-0.01 / 131.8	-0.04 / 456.5
CAN/POPs		0.03 / 171.2	0.01 / 66.41	0.04 / 227.1
MSCE-POP		–	0.38 / -1.43	1.33 / 3.96
CliMoChem		–	–	3.45 / 9.18

Finally, pairwise residual square deviation σ are shown in Table E.19.

Table E.19. *Residual square deviation,* σ^{res}_{12}

	CAN/POPs	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	4322	427	163	568
CAN/POPs	-	395	153	521
MSCE-POP	-	-	4	7
CliMoChem	-	-	-	19

Comparison between two data sets. The difference between calculation results obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table E.20.

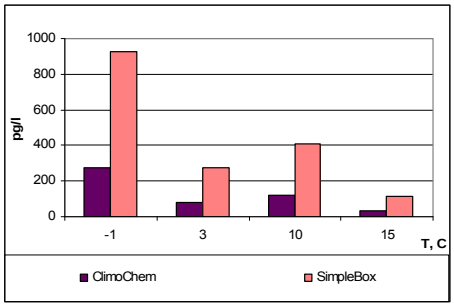
Table E.20. *Difference between calculations with two data sets*

Exp. No	*T* (°C)	CliMoChem	SimpleBox
1	-1	-7%	-5%
2	3	-6%	-4%
3	10	-25%	-17%
4	15	-10%	-7%

5	-1	-7%	-5%
6	3	-6%	-4%
7	10	-25%	-17%
8	15	-10%	-7%

These results are visualized in Fig. E.6.

a



b

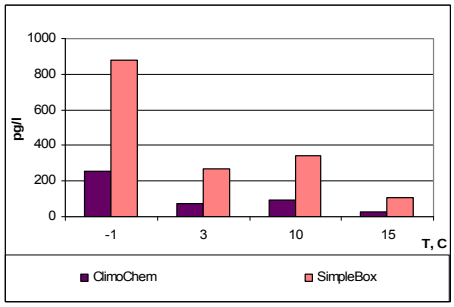


Fig. E.6. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

4.3. Gaseous exchange between atmosphere and soil

Here we present numerical results of calculations of soil concentrations and net gaseous flux to soil obtained by the participating models and their analysis for PCB-180 with "reference" and "own/alternative" data sets.

Fig. E.7 illustrates air concentration trend used in calculations for Experiment 1.

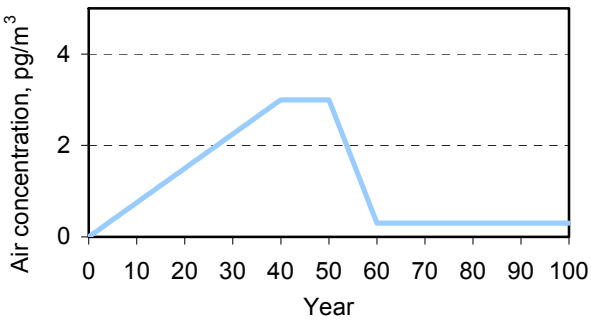


Fig. E.7. *Air concentration trend used for calculations for MSCE-POP model (MSCE-POP 2) for Experiment 1*

Reference data set. Calculation results for soil concentrations together with m and σ calculated with "reference" data set of PCB-180 properties are presented in Table E.21. Net gaseous fluxes to soil of PCB-180 calculated by the models and statistical parameters used for its evaluation are given in Table E.22.

Table E.21. *Calculation results: soil concentrations of PCB-180 (ng/g) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	DEHM-POP	CAN/POPs	CliMoChem	SimpleBox	m	σ
1	0.3	0.240	0.368	0.0001	0.0001	**0.15**	**0.18**
2	1.3	0.071	3.317	0.0007	0.0003	**0.85**	**1.65**

3	2.4	0.083	4.119	0.0016	0.0005	**1.05**	**2.05**
4	0.7	0.013	0.390	0.0003	0.0001	**0.10**	**0.19**

Table E.22. *Calculation results: net gaseous flux to soil, of PCB-180 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("reference" data set)*

No	Air conc, pg/m^3	CAN/POPs	CliMoChem	SimpleBox	*m*	σ
1	0.3	1.75E-13	5.40E-03	2.71E-02	**1.083E-02**	**1.434E-02**
2	1.3	2.33E-12	2.34E-02	1.18E-01	**4.698E-02**	**6.221E-02**
3	2.4	1.92E-12	4.32E-02	2.17E-01	**8.662E-02**	**1.147E-01**
4	0.7	1.97E-13	1.26E-02	6.31E-02	**2.522E-02**	**3.337E-02**

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Values of pairwise correlation coefficients are presented in Table E.23.

Table E.23. *Correlation coefficients for soil concentrations of PCB-180 ("reference" data set)*

	CAN/POPs	CliMoChem	SimpleBox
DEHM-POP	-0.28	-0.31	-0.29
CAN/POPs	-	0.91	0.97
CliMoChem	-	-	0.98

Correlation coefficients for net gaseous flux are presented in Table E.24.

Table E.24. *Correlation coefficients for net gaseous flux to soil of PCB-180 ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.77	0.77
CliMoChem	-	1.00

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Tables 4.25 and 4.26, respectively.

Table E.25. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-180 ("reference" data set)*

	CAN/POPs	CliMoChem	SimpleBox
DEHM-POP	-5.700 / 2.629	-0.002 /0.0009	-0.001 /0.0003
CAN/POPs		0.0003 / 0.0001	0.0001 / 0.00001
CliMoChem		–	0.338 / 0.00001

Table E.26. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-180 ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	1.12E+10 / 0.008	5.64E+10 / 0.041
CliMoChem	-	5.019 / -0.00001

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table E.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-180 ("reference" data set)*

	CAN/POPs	CliMoChem	SimpleBox
DEHM-POP	3.2485	0.0011	0.0004
CAN/POPs	-	0.0005	0.0001
CliMoChem	-	-	0.0001

Table E.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-180 ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.018	0.091
CliMoChem	-	0.0002

Own/alternative data set. Calculation results soil concentrations together with *m* and σ calculated with "own/alternative" data set of PCB-180 properties are presented in Table E.29. Net gaseous fluxes to soil of PCB-180 calculated by the models and statistical parameters used for its evaluation are given in Table E.30. Table E.29 contains also the information of the data set used for calculations for each model.

Table E.29. *Calculation results: soil concentrations of PCB-180 (ng/g) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	CAN/ POPs	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	*m*	σ
					1	2				
		own		own	own		own	alt		
1	0.3	0.004	0.355	0.638	0.013	0.075	0.002	0.602	**0.241**	**0.287**
2	1.3	0.019	3.742	6.604	0.064	0.363	0.008	3.667	**2.067**	**2.624**
3	2.4	0.034	4.808	7.203	0.139	0.792	0.016	5.680	**2.668**	**3.112**
4	0.7	0.006	0.768	0.710	0.027	0.154	0.003	0.747	**0.345**	**0.375**

Table E.30. *Calculation results: net gaseous flux to soil, of PCB-180 (ng/m^2/d) calculated by models and statistical parameters used for evaluation ("own/alternative" data set)*[*]

No	Air conc, pg/m^3	EVN-BETR and UK-MODEL	CAN/ POPs	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	*m*	σ
					1	2				
1	0.3	3.59E-04	3.51E-13	–	6.75E-03	3.62E-03	5.28E-03	-4.42E-02	**-4.69E-03**	**1.95E-02**
2	1.3	1.62E-03	3.27E-12	–	3.15E-02	2.50E-02	2.31E-02	-7.09E-02	**1.72E-03**	**3.78E-02**
3	2.4	2.89E-03	3.84E-12	–	5.40E-02	2.94E-02	4.24E-02	-2.69E-01	**-2.33E-02**	**1.22E-01**
4	0.7	8.47E-04	3.94E-13	–	1.26E-02	-4.37E-03	1.20E-02	-1.45E-01	**-2.06E-02**	**6.13E-02**

* - statistical parameters are calculated for models using steady-state and dynamic approaches.

Pairwise correlation coefficients are given in Table E.31.

Table E.31. *Correlation coefficients for soil concentrations of PCB-180 ("own/alternative" data set)*

		DEHM-POP	CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
				1	2		
EVN-BETR and UK MODEL		0.97	0.93	0.99	0.99	1.00	0.99
DEHM-POP		-	0.99	0.93	0.93	0.94	0.99
CAN/POPs		-	-	0.87	0.87	0.89	0.96
MSCE-POP	1	-	-	-	1.00	1.00	0.97
	2	-	–	–	1.00	1.00	0.97
CliMoChem		-	–	–	–	–	0.98

Correlation coefficients for net gaseous flux are presented in Table E.32.

Table E.32. *Correlation coefficients for net gaseous flux to soil of PCB-180 ("own/alternative" data set)*

		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.92	1.00	0.86	1.00	-0.82
CAN/POPs		–	0.94	0.98	0.91	-0.53
MSCE-POP	1	–	–	0.90	1.00	-0.78
	2	–	–	–	0.85	-0.43
CliMoChem		–	–	–	–	-0.83

Calculated regression coefficients α and β for soil concentrations and deposition fluxes are given in Table E.33 and 34, respectively.

Table E.33. *Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-180 ("own/alternative" data set)*

		DEHM-POP	CAN/POPS	MSCE-POP		CliMoChem	SimpleBox
				1	2		
EVN-BETR and UK MODEL		152.1 / -0.01	239 / 0.02	4.00 / -0.003	22.8 / -0.02	0.46 / -0.0003	175 / -0.11
DEHM-POP		–	1.62 / -0.14	0.02 / 0.003	0.14 / 0.02	0.003 / 0.0003	1.10 / 0.003
CAN/POPs				0.01 / 0.01	0.08 / 0.05	0.002 / 0.001	0.65 / 0.19
MSCE-POP	1		–	–	5.70 / -0.004	0.11 / 0.0001	42.18 / 0.11
	2		–	–	–	0.02 / 0.0001	7.39 / 0.11
CliMoChem		–		–	–	–	373 / 0.07

Table E.34. *Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-180 ("own/alternative" data set)*

		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		1.54E+09 / -2.40E-13	19.26 / -0.001	12.69 / -0.005	14.72 / -0.0004	-75.04 / -0.02
CAN/POPs		–	1.09E+10 / 0.005	8.62E+09 / -0.004	8.01E+09 / 0.005	-2.89E+10 / -0.08
MSCE-POP	1	–	–	0.69 / -0.005	0.76 / 0.0008	-3.67 / -0.04
	2	–	–	–	0.85 / 0.009	-2.63 / -0.10
CliMoChem		–	–	–	–	-5.13 / -0.03

Residual square deviation for soil concentrations and net gaseous flux are shown in Tables 4.27 and 4.28, respectively.

Table E.27. *Residual square deviation, σ^{res}_{12} for soil concentrations of PCB-180 ("own/alternative" data set)*

		DEHM-POP	CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
				1	2		
EVN-BETR and UK MODEL		0.96	2.36	0.01	0.08	0.001	0.48
DEHM-POP		-	0.93	0.04	0.21	0.004	0.64
CAN/POPs		-	-	0.05	0.28	0.005	1.15
MSCE-POP	1	-	-	-	0.001	0.001	1.04
	2	-	–	–		0.001	1.04
CliMoChem		-	–	–	–	–	0.85

Table E.28. *Residual square deviation, σ^{res}_{12} for net gaseous flux to soil of PCB-180 ("own/alternative" data set)*

		CAN/POPs	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		1.27E-12	0.003	0.015	0.001	0.099
CAN/POPs		-	0.012	0.006	0.011	0.147
MSCE-POP	1	–	–	0.012	0.003	0.109
	2	–	–	–	0.015	0.157
CliMoChem		–	–	–	–	0.097

Comparison between two data sets. The difference between calculated values of soil concentrations obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Table E.29. The corresponding differences between calculated values of net flux to soil were not calculated since near the equilibrium small changes in pollutant properties can lead to essential changes of fluxes (in relative values).

Table E.29. *Difference between calculations with two data sets*

No	Air conc, pg/m^3	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox
1	0.3	73%	48%	1014%	1192427%
2	1.3	99%	5158%	979%	1182447%
3	2.4	75%	5667%	884%	1072561%
4	0.7	82%	5938%	812%	988515%

Accumulation/clearance dynamics of PCBs in soil.

Fig. E.8 shows the results of the experiment obtained by CAN/POPs, CliMoChem and SimpleBox models with the use of “reference” data set.

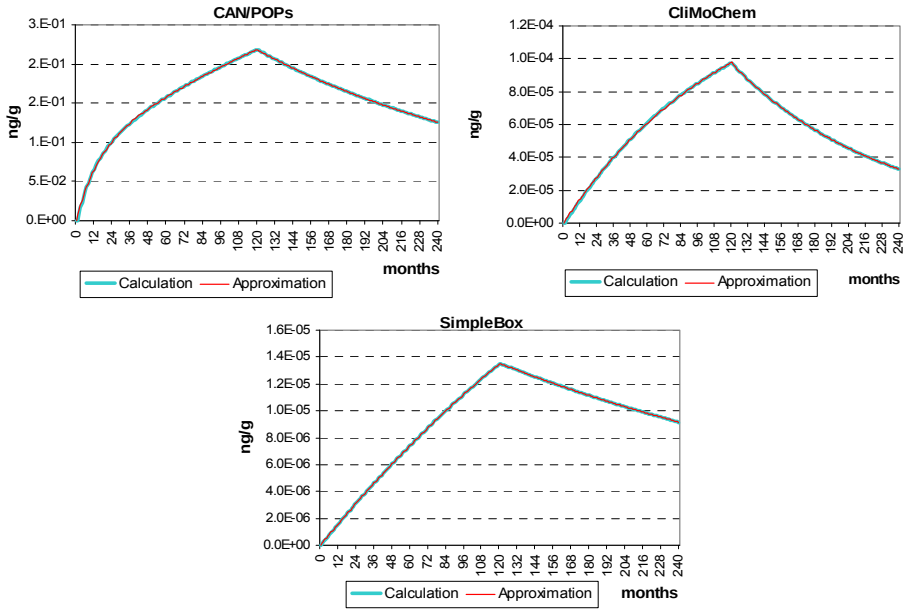


Fig. E.8. *Long-term trends of accumulation and clearance obtained by participating models (“reference” data set)*

The results obtained by CliMoChem, EVN-BETR and UK-MODEL, MSCE-POP and SimpleBox models with the use of “own/alternative” data sets are presented in Fig. E.9.

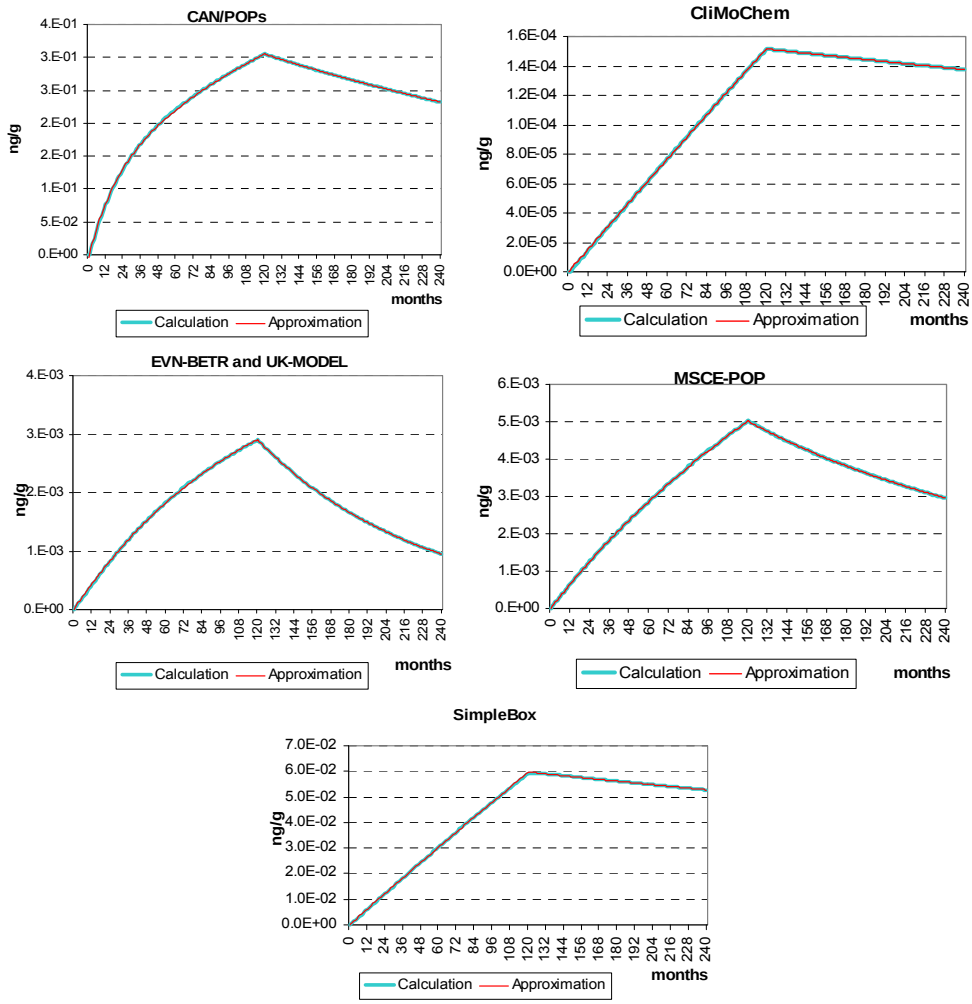


Fig. E.9. *Long-term trends of accumulation and clearance obtained by participating models ("own/alternative" data set)*

The values of characteristic times obtained by the approximation are shown in Table E.30.

Table E.30. *Parameters of multi-exponential approximation*

	CAN/POPs		CliMoChem		EVN-BETR and UK model		MSCE-POP		SimpleBox	
	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast
"Reference" data set										
Accumulation phase	15.0	0.8	6.9	6.9	–	–	–	–	17.9	17.9
Clearance phase	23.1	9.3	6.4	6.4	–	–	–	–	17.8	17.8
"Own/alternative" data set										
Accumulation phase	10.5	1.0	172.4	172.1	6.7	6.7	18.8	3.3	84.4	84.6
Clearance phase	30.5	11.6	70.8	71.0	6.3	6.2	17.7	5.8	55.8	55.8

The difference between results obtained with "reference" and "own/alternative" data sets (for those models which have performed both calculations) is illustrated by Fig. E.10.

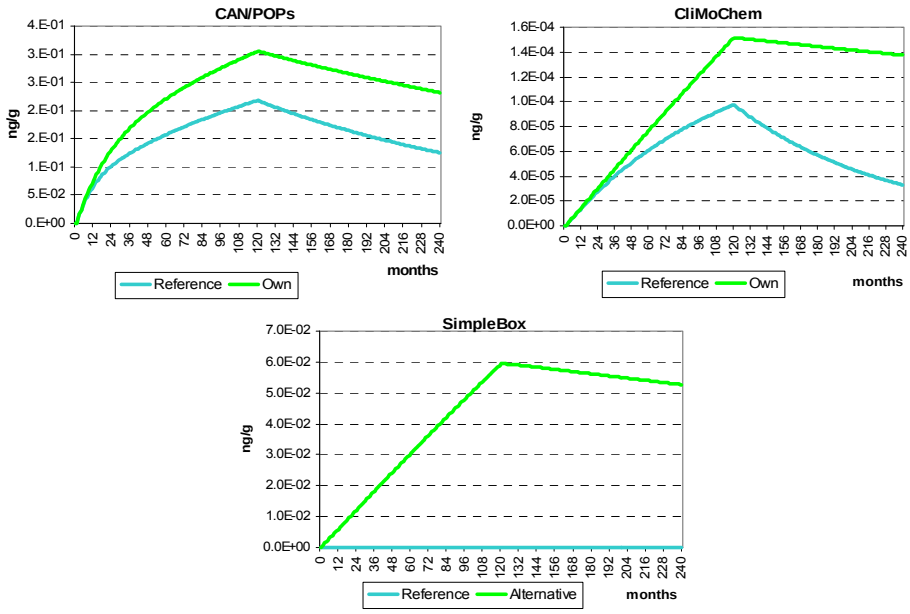


Fig. E.10. *Difference in long-term trends due to usage of different sets of PCB properties*

4.4. Gaseous exchange between atmosphere and water

Reference data set. Calculation results for water concentrations together with m and σ calculated with "reference" data set of PCB-180 properties are presented in Table E.31.

Table E.31. *Calculation results: water concentrations of PCB-180 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	m	σ
1	1.70	1.20	2.71	2.10	**1.92**	**0.64**
2	5.20	1.23	2.79	3.72	**3.23**	**1.66**
3	23.10	4.87	4.07	7.07	**9.78**	**8.97**
4	50.00	11.52	13.26	14.94	**22.43**	**18.43**

Fig. E.11 displays the result on water concentrations of PCB-180 calculated by the participating models with the use of "reference" data set.

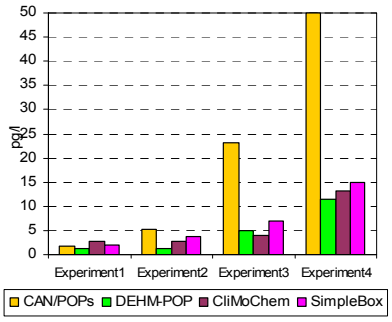


Fig. E.11. *Calculation results of the participating models (water concentrations) obtained with "reference" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-180 calculated by the participating models are given in Table E.32.

Table E.32*. Calculation results: fluxes of PCB-180 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CAN/POPs	CliMoChem	SimpleBox	*m*	σ
Gaseous flux to water					
1	-	0.22	0.63	**0.43**	**0.29**
2	-	0.23	1.15	**0.69**	**0.65**
3	-	0.29	1.57	**0.93**	**0.90**
4	-	0.98	3.57	**2.27**	**1.83**
Gaseous flux from water					
1	0.11	0.06	0.02	**0.06**	**0.05**
2	1.57	0.06	0.05	**0.56**	**0.87**
3	2.31	0.04	0.03	**0.79**	**1.31**
4	4.63	0.18	0.07	**1.62**	**2.60**
Net gaseous flux					
1	0.11	0.16	0.62	**0.30**	**0.28**
2	1.57	0.17	1.10	**0.95**	**0.71**
3	2.31	0.25	1.54	**1.36**	**1.04**
4	4.63	0.80	3.50	**2.98**	**1.97**

Below we present parwise comparison of modelling results for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table E.32.

Table E.32. *Correlation coefficients for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	SimpleBox
CAN/POPs	1.00	0.95	1.00
DEHM-POP	-	0.97	0.99
CliMoChem	-	-	0.97

Correlation coefficients for net gaseous flux are demonstrated in Table E.33.

Table E.33. *Correlation coefficients for net gaseous flux ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.92	0.98
CliMoChem	-	0.98

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4.34 and s.35, respectively.

Table E.34. *Coefficients of regression dependence between the models (α / β) for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	SimpleBox
CAN/POPs	0.22 /0.32	0.22 / 1.34	0.26 / 1.81
DEHM-POP	-	1.01 / 0.93	1.17 / 1.46
CliMoChem	-	–	1.09 / 0.74

Table E.35. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.15 / 0.02	0.66 / 0.28
CliMoChem	- CliMoChem	4.04 / 0.30

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.36 and 4.37.

Table E.36. *Residual square deviation, σ for water concentrations ("reference" data set)*

	DEHM-POP	CliMoChem	SimpleBox
CAN/POPs	0.79	2.73	0.94
DEHM-POP	-	2.08	1.12
CliMoChem	-	-	2.49

Table E.37. *Residual square deviation, σ for net gaseous flux ("reference" data set)*

	CliMoChem	SimpleBox
CAN/POPs	0.21	0.47
CliMoChem	-	0.44

Own/alternative data set. Calculation results for water concentrations together with *m* and σ calculated with "own/alternative" data set of PCB-180 properties are presented in Table E.38. Here data set of PCB-180 properties used for calculations by each model is indicated (second row).

Table E.38*. Calculation results: water concentrations of PCB-180 (pg/L) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own		own	own	alt	own		
1	0.96	1.70	2.24	0.80	19.17	0.89	**4.29**	**7.31**
2	0.96	5.20	4.99	0.82	20.03	0.91	**5.49**	**7.41**
3	5.16	23.10	0.45	3.79	93.35	3.87	**21.62**	**36.05**
4	12.50	50.00	0.47	8.63	208.43	8.98	**48.17**	**80.42**

Fig. E.12 displays the result on water concentrations of PCB-180 calculated by the participating models with the use of "own / alternative" data set.

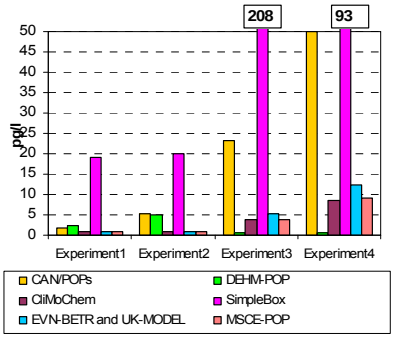


Fig. E.12. *Calculation results of the participating models (water concentrations) obtained with "own/alternative" data set*

Gaseous fluxes to water, from water and net gaseous flux of PCB-180 calculated by the models are given in Table E.39.

Table E.39*. Calculation results: fluxes of PCB-180 to/from water (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to water							
1	0.47	0.32	0.14	0.44	0.43	**0.36**	**0.14**
2	0.47	0.35	0.14	0.84	0.50	**0.46**	**0.26**
3	1.03	0.29	0.25	1.30	0.67	**0.71**	**0.46**

4	3.47	0.76	0.79	2.73	2.14	**1.98**	**1.19**
Gaseous flux from water							
1	0.02	-	0.13	0.35	0.42	**0.23**	**0.19**
2	0.02	-	0.13	0.68	0.49	**0.33**	**0.31**
3	0.04	-	0.22	1.55	0.64	**0.61**	**0.67**
4	0.14	-	0.71	2.86	2.08	**1.45**	**1.25**
Net gaseous flux							
1	0.45	0.32	0.01	0.09	0.01	**0.17**	**0.20**
2	0.45	0.35	0.01	0.16	0.01	**0.19**	**0.20**
3	0.99	0.29	0.03	-0.25	0.03	**0.22**	**0.47**
4	3.33	0.76	0.07	-0.14	0.07	**0.82**	**1.44**

The parwise comparison of modelling results is done for water concentrations and net gaseous flux to water. Correlation coefficients for water concentrations are shown in Table E.40.

Table E.40. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	1.00	-0.71	1.00	1.00	1.00
CAN/POPs	-	-0.70	1.00	1.00	1.00
DEHM-POP	-	-	-0.72	-0.72	-0.71
CliMoChem	-	-	-	1.00	1.00
SimpleBox	-	-	-	-	1.00

Correlation coefficients for net gaseous flux are demonstrated in Table E.41.

Table E.41. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.96	1.00	-0.53	0.98
CAN/POPs	-	0.93	-0.26	0.89
CliMoChem	-	-	-0.59	0.99
SimpleBox	-	-	-	-0.67

Values of regression coefficients α and β for water concentrations and net gaseous flux calculated for all pairs of models are given in Tables 4. 4.42 and 4.43, respectively.

Table E.42. *Coefficients of regression dependence between the models (α / β) for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	4.04 / 0.22	-0.28 / 3.40	0.68 / 0.19	16.38 / 5.07	0.70 / 0.23
CAN/POPs	-	-0.07 / 3.40	0.17 / 0.18	4.03 / 4.68	0.17 / 0.22
DEHM-POP	-	-	-1.24 / 6.03	-30.02 / 146.4	-1.26 / 6.23
CliMoChem	-	-	-	24.15 / 0.49	1.03 / 0.04
SimpleBox	-	-	-	-	0.04 / 0.02

Table E.43. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.16 / 0.23	0.02 / 0.002	-0.07 / 0.06	0.02 / 0.01
CAN/POPs	-	0.13 / -0.02	-0.22 / 0.06	0.11 / -0.02
CliMoChem	-	-	-3.72 / 0.08	0.94 / -0.001
SimpleBox	-	-	-	-0.10 / 0.02

Finally, values of residual square deviation for water concentrations and net gaseous flux are collected in Tables 4.44 and 4.45.

Table E.44. *Residual square deviation, σ for water concentrations ("own/alternative" data set)*

	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP

EVN-BETR and UK MODEL	3.409	2.612	0.113	4.393	0.029
CAN/POPs	-	2.641	0.486	10.70	0.559
DEHM-POP	-	-	4.463	107.1	4.652
CliMoChem	-	-	-	1.666	0.094
SimpleBox	-	-	-	-	0.165

Table E.45. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	CAN/POPs	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.113	0.004	0.282	0.009
CAN/POPs	-	0.019	0.320	0.023
CliMoChem	-	-	0.267	0.005
SimpleBox	-	-	-	0.037

Comparison between two data sets. The difference between calculated values of concentrations in water and gaseous fluxes to/from water obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.46 and 4.47, respectively.

Table E.46. *Difference between calculations with two data sets (water concentrations)*

N	CAN/POPs	DEHM-POP	CliMoChem	SimpleBox
1	0.0%	87%	-71%	815%
2	0.0%	305%	-71%	439%
3	0.0%	-91%	-7%	1220%
4	0.0%	-96%	-35%	1295%

This difference is visualized in Fig. E.13.

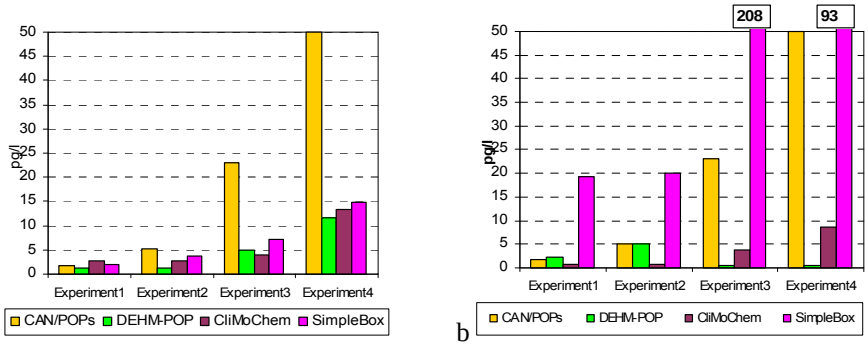


Fig. E.13. *Calculation results of the participating models obtained with " reference" (a) and "own/alternative" (b) data sets (for models presented both calculations)*

Table E.47. *Difference between calculations with two data sets (net gaseous flux)*

N	CAN/POPs	CliMoChem	SimpleBox
1	192%	-94%	-86%
2	-78%	-94%	-85%
3	-88%	-89%	-116%
4	-84%	-91%	-104%

4.5. Gaseous exchange between atmosphere and vegetation

Reference data set. Calculation results for concentrations in vegetation together with m and σ calculated with "reference" data set of PCB-180 properties are presented in Table E.48. Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-180 calculated by the models are given in Table E.49.

Table E.48*. Calculation results: concentrations of PCB-180 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CliMoChem	SimpleBox	m	σ
1	4.28	0.08	**2.18**	**2.97**
2	20.26	0.46	**10.36**	**14.00**
3	2.54	0.05	**1.30**	**1.76**
4	9.05	0.21	**4.63**	**6.25**

Table E.49*. Calculation results: fluxes of PCB-180 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("reference" data set)*

N	CliMoChem	SimpleBox	m	σ
Gaseous flux to vegetation				
1	0.06	3.03	**1.55**	**2.10**
2	0.65	33.36	**17.00**	**23.13**
3	0.05	2.34	**1.19**	**1.62**
4	0.24	12.13	**6.18**	**8.41**
Gaseous flux from vegetation				
1	0.06	0.18	**0.12**	**0.09**
2	0.65	6.11	**3.38**	**3.86**
3	0.05	0.21	**0.13**	**0.12**
4	0.24	1.81	**1.02**	**1.11**
Net gaseous flux				
1	0	2.85	-	-
2	0	27.25	-	-
3	0	2.12	-	-
4	0	10.32	-	-

Below we present pairwise comparison of modelling results for concentrations in vegetation and net gaseous flux. Correlation coefficients for concentrations in vegetation are shown in Table E.50.

Table E.50. *Correlation coefficients for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	1.00

Values of regression coefficients α and β for concentrations in vegetation calculated for all pairs of models are given in Table E.51.

Table E.51. *Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	43.26 / 0.39

Regression coefficients α and β between SimpleBox and MSCE-POP models equal 0.94 and –0.02, respectively. This testifies good agreement of net flux calculated by these two models.

Finally, values of residual square deviation for concentrations in vegetation are collected in Table E.52.

Table E.52. *Residual square deviation, σ for concentrations in vegetation ("reference" data set)*

	CliMoChem
SimpleBox	0.50

Own/alternative data set. Calculation results for concentrations in vegetation together with *m* and σ calculated with "own/alternative" data set of PCB-180 properties are presented in Table E.53. Here data set of PCB-180 properties used for calculations by each model is indicated (second row). Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-180 calculated by the models are given in Table E.54.

Table E.53*. Calculation results: concentrations of PCB-180 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Set	own	own	alt	own		
1	0.12	0.12	0.16	0.02	**0.10**	**0.06**
2	0.13	0.69	0.52	0.19	**0.38**	**0.27**
3	0.06	0.08	0.08	0.01	**0.06**	**0.03**
4	0.10	0.31	0.24	0.07	**0.18**	**0.11**

Table E.54*. Calculation results: fluxes of PCB-180 to/from vegetation (ng/m^2/day) calculated by all participating models and statistical parameters used for evaluation ("own/alternative" data set)*

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	*m*	σ
Gaseous flux to vegetation						
1	0.57	0.06	0.09	–	**0.24**	**0.29**
2	9.44	0.65	0.95	–	**3.68**	**4.99**
3	0.67	0.05	0.07	–	**0.26**	**0.35**
4	3.64	0.24	0.35	–	**1.41**	**1.93**
Gaseous flux from vegetation						
1	0.59	0.01	0.04	–	**0.21**	**0.33**
2	9.5	0.34	0.62	–	**3.48**	**5.21**
3	0.68	0.01	0.03	–	**0.24**	**0.38**
4	3.68	0.09	0.20	–	**1.32**	**2.04**
Net gaseous flux						
1	-0.02	0.05	0.04	0.06	**0.03**	**0.04**
2	-0.06	0.31	0.33	0.62	**0.30**	**0.28**
3	-0.01	0.04	0.03	0.04	**0.03**	**0.02**
4	-0.04	0.15	0.14	0.23	**0.12**	**0.11**

The parwise comparison of modelling results is done for concentrations in vegetation and net gaseous flux to vegetation. Correlation coefficients for concentrations in vegetation are shown in Table E.55.

Table E.55. *Correlation coefficients for water concentrations ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.73	0.63	0.65
SimpleBox	-	0.99	0.99
CliMoChem	-	-	1.00

Correlation coefficients for net gaseous flux are demonstrated in Table E.56.

Table E.56. *Correlation coefficients for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and	-0.97	-0.95	-0.98

UK MODEL			
SimpleBox	-	1.00	1.00
CliMoChem	-	-	1.00

Values of regression coefficients α and β for concentrations in vegetation and net gaseous flux calculated for all pairs of models are given in Tables 4.57 and 4.58, respectively.

Table E.57. *Coefficients of regression dependence between the models (α / β) for concentrations in vegetation ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	4.55 / -0.22	1.69 / -0.10	5.94/ –0.31
SimpleBox	-	0.43 / -0.03	1.45 / -0.06
CliMoChem	-	-	3.36 / 0.05

Table E.58. *Coefficients of regression dependence between the models (α / β) for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-6.04 / -0.06	-11.51 / -0.14	-5.61 / -0.04
SimpleBox		1.93 / -0.03	0.92 / 0.01
CliMoChem			0.47 / 0.03

Finally, values of residual square deviation for concentrations in vegetation and net gaseous flux are collected in Tables 4.59 and 4.60.

Table E.59. *Residual square deviation, σ for concentrations in vegetation ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.23	0.11	0.37
SimpleBox	-	0.02	0.05
CliMoChem	-	-	0.03

Table E.60. *Residual square deviation, σ for net gaseous flux ("own/alternative" data set)*

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.06	0.14	0.05
SimpleBox	-	0.02	0.01
CliMoChem	-	-	0.02

Comparison between two data sets. The difference between calculated values of water concentrations and net gaseous flux obtained with two data sets of pollutant properties (for those models who provided calculations for both these sets) is shown in Tables 4.61 – 4.64.

Table E.61. *Difference between calculations with two data sets (concentrations in vegetation)*

N	CliMoChem	SimpleBox
1	-97%	92%
2	-97%	13%
3	-97%	46%
4	-97%	18%

Table E.62. *Difference between calculations with two data sets (gaseous flux to vegetation)*

N	CliMoChem	SimpleBox
1	0%	-97%
2	0%	-97%

3	0%	-97%
4	0%	-97%

Table E.63. *Difference between calculations with two data sets (gaseous flux from vegetation)*

N	CliMoChem	SimpleBox
1	-90%	-77%
2	-48%	-90%
3	-82%	-84%
4	-64%	-89%

Table E.64. *Difference between calculations with two data sets (net gaseous flux)*[*]

N	SimpleBox
1	-98%
2	-99%
3	-98%
4	-99%

* The difference between values of net gaseous flux calculated by CliMoChem model is not calculated because for "reference" data set this flux is reported to be zero