

SENSITIVITY STUDY WITH RESPECT TO SUBSTANCE-SPECIFIC PROPERTIES USED IN THE DESCRIPTION OF BASIC PROCESSES FOR PCB-28

D.1. Gas/particle partitioning

Reference data set. Calculation results for PCB-28 together with m_φ and σ_φ are presented in Table D.1.

Table D.1. Calculation results: fractions of particulate phase of PCB-28 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	0.044	0.011	0.256	0.104	0.133
2	-5	0.018	0.009	0.123	0.050	0.064
3	0	0.009	0.008	0.071	0.029	0.036
4	6	0.004	0.007	0.036	0.016	0.018
5	10	0.003	0.006	0.023	0.011	0.011
6	15	0.002	0.006	0.014	0.007	0.006
7	20	0.001	0.005	0.008	0.005	0.004
8	25	0.001	0.008		0.004	0.005
9	25	0.001	0.005		0.003	0.003
10	26	0.001	0.008	0.004	0.004	0.003
11	32	0.001	0.009	0.002	0.004	0.005

* - only 9 experiments for Simple Box

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

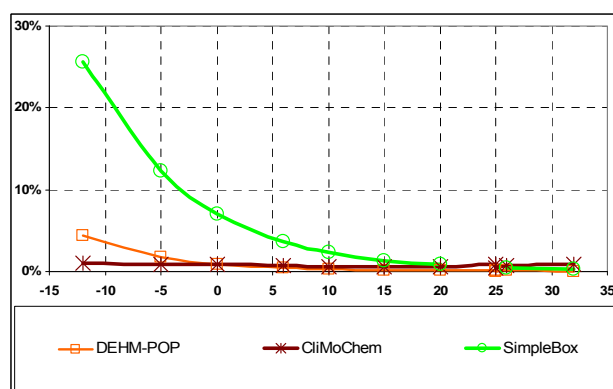


Fig. D.1. Calculation results of the participating models (gas-particle partitioning) obtained with reference data set

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

Table D.2. Correlation coefficients r_{12}

	CliMoChem	SimpleBox*
DEHM-POP	0.70	1.00
CliMoChem	—	0.75

* - by 9 experiments only

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

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

	CliMoChem	SimpleBox*
DEHM-POP	0.10 / 0.01	5.80 / 0.01
CliMoChem	—	35.44 / - 0.21

* - by 9 experiments only

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

Table D.4. Residual square deviation, σ_{12}^{res}

	CliMoChem	SimpleBox*
DEHM-POP	0.004	0.022
CliMoChem	—	0.156

* - by 9 experiments only

Own/alternative data set. Calculation results for PCB-28 together with m_φ and σ_φ are presented in Table D.5. The data set used in calculations by each model is indicated in the first row.

Table D.5. Calculation results: fractions of particulate phase of PCB-28 calculated by models and statistical parameters used for evaluation (own/alternative data set)

Exp.No	T (°C)	EVN-BETR and UK-MODEL	DEHM-POP	MSCE-POP_1	MSCE-POP_2	CliMoChem	SimpleBox	m_φ	σ_φ
Data set		own	own	own	own	own	alt		
1	-12	0.190	0.061	0.061	0.054	0.028	0.058	0.075	0.058
2	-5	0.083	0.025	0.025	0.023	0.017	0.034	0.034	0.024
3	0	0.045	0.014	0.013	0.013	0.012	0.023	0.020	0.013
4	6	0.022	0.007	0.006	0.007	0.008	0.015	0.011	0.006
5	10	0.014	0.004	0.004	0.004	0.007	0.011	0.007	0.004
6	15	0.008	0.002	0.002	0.002	0.005	0.008	0.005	0.003
7	20	0.004	0.001	0.001	0.001	0.004	0.006	0.003	0.002
8	25	0.004	0.001	0.001	0.001	0.005	0.006	0.002	0.002
9	25	0.003	0.001	0.001	0.001	0.003	0.004	0.002	0.001
10	26	0.004	0.001	0.001	0.001	0.004	0.006	0.003	0.002
11	32	0.003	0.001	0.0004	0.001	0.004	0.006	0.003	0.002

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

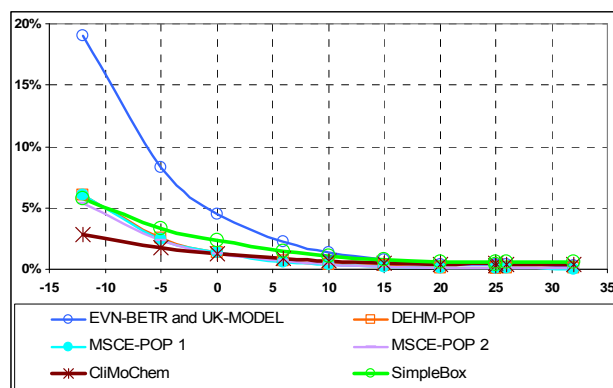


Fig. D.2. Calculation results of the participating models (gas-particle partitioning) obtained with “own/alternative” data set

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

Table D.6. Correlation coefficients r_{12}

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	1.00	1.00	1.00	0.98	0.99
DEHM-POP	–	1.00	1.00	0.98	0.99
MSCE-POP 1	–	–	1.00	0.98	0.98
MSCE-POP 2	–	–	–	0.98	0.99
CliMoChem	–	–	–	–	1.00

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

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

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.317 / - 0.0001	0.318 / -0.0004	0.283 / 0.00003	0.135 / 0.004	0.287 / 0.006
DEHM-POP	–	1.0021 / -0.0003	0.893 / 0.0002	0.423 / 0.004	0.901 / 0.006
MSCE-POP 1	–	–	0.890 / 0.0004	0.420 / 0.004	0.896 / 0.007
MSCE-POP 2	–	–	–	0.475 / 0.004	1.011 / 0.006
CliMoChem	–	–	–	–	2.118 / -0.003

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

Table D.8. Residual square deviation, σ_{12}^{res}

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK MODEL	0.001	0.002	0.001	0.004	0.008
DEHM-POP	–	0.001	0.001	0.005	0.009
MSCE-POP 1	–	–	0.002	0.005	0.009
MSCE-POP 2	–	–	–	0.004	0.008
CliMoChem	–	–	–	–	0.002

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 D.9.

Table D.9. Difference between calculations with two data sets

Exp.No	T (°C)	DEHM-POP	CliMoChem	SimpleBox
1	-12	37%	162%	-77%
2	-5	43%	91%	-73%
3	0	47%	53%	-68%
4	6	52%	19%	-59%
5	10	54%	1%	-52%
6	15	58%	-18%	-42%
7	20	61%	-32%	-30%
8	25	64%	-44%	
9	25	64%	-44%	
10	26	65%	-46%	42%
11	32	69%	-56%	136%

This difference is visualized in Fig. D.3.

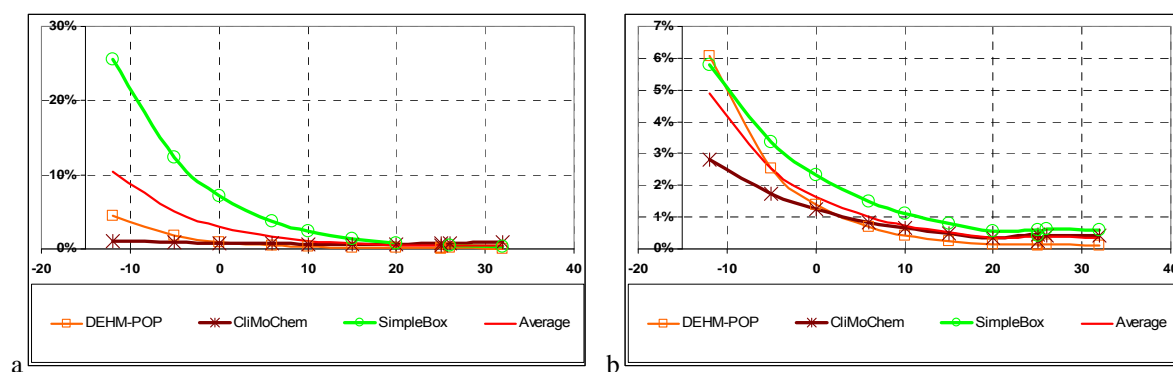


Fig. D.3. Calculation results of the participating models obtained with “reference” (a) and “own/alternative” (b) data sets (for models presented both calculations)

4.2. Wet deposition

Reference data set. Calculation results for PCB-28 together with m and σ are presented in Tables 4.10 and 4.11.

Table D.10. Calculation results: concentrations in precipitation (pg/L) (“reference” data set)

Exp. No	T (°C)	CliMoChem	SimpleBox	m	σ
1	-1	176	612	394	308
2	3	311	1077	694	542
3	10	28	202	115	123
4	-1	18	612	315	420
5	3	31	1077	554	740
6	10	3	202	103	141

Table D.11. Calculation results: wet deposition flux, ng/m²/hour (“reference” data set)

Exp. No	T (°C)	CliMoChem	SimpleBox	m	σ
1	-1	0.176	0.612	0.394	0.308
2	3	0.311	1.077	0.694	0.542
3	10	0.028	0.202	0.115	0.123
4	-1	0.176	6.119	3.147	4.202
5	3	0.311	10.773	5.542	7.398
6	10	0.028	2.022	1.025	1.410

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

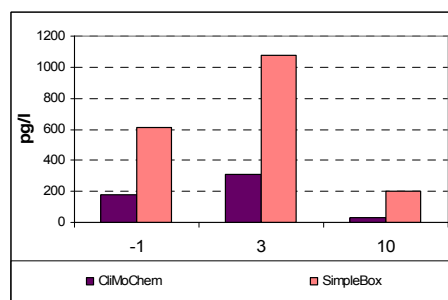


Fig. D.4. Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (reference data set)

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

Table D.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 D.13.

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

	SimpleBox
CliMoChem	3.09 / 100.33

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

Table D.14. Residual square deviation, σ_{12}^{res}

	SimpleBox
CliMoChem	39.84

Own/alternative data set. Calculation results for PCB-28 together with m and σ are presented in Tables 4. 4.15 and 4.16.

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

Exp. No	T (°C)	EVN-BETR and UK-MODEL	MSCE-POP	CliMoChem	SimpleBox	m	σ
1	-1	24	456	176	603	315	263
2	3	30	803	310	1065	552	468
3	10	166	99	26	109	100	58
4	-1	—	456	18	603	359	305
5	3	—	803	31	1065	633	538
6	10	—	99	3	109	70	59

Table D.16. Calculation results: wet deposition flux, ng/m²/hour (own/alternative data set)

Exp. No	T (°C)	EVN-BETR and UK-MODEL	MSCE-POP	CliMoChem	SimpleBox	m	σ
1	-1	0.024	0.456	0.176	0.603	0.315	0.263
2	3	0.030	0.803	0.310	1.065	0.552	0.468
3	10	0.166	0.099	0.026	0.109	0.100	0.058
4	-1	—	4.560	0.176	6.029	3.588	3.045
5	3	—	8.030	0.310	10.651	6.330	5.376
6	10	—	0.990	0.026	1.090	0.702	0.588

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

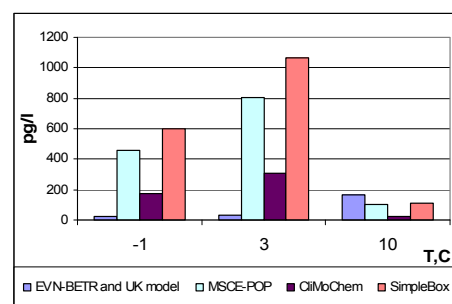


Fig. D.5. Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/L (own/alternative data set)

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

Table D.17. Correlation coefficients r_{12}

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	-0.85	-0.86	-0.86
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 D.18.

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

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	-3.73 / 726.24	-1.53 / 282.69	-5.10 / 966.39
MSCE-POP	–	0.40 / -12.32	1.36 / -22.48
CliMoChem	–	–	3.36 / 19.10

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

Table D.19. Residual square deviation, σ_{12}^{res}

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	261.38	101.63	348.77
MSCE-POP	–	4.68	7.33
CliMoChem	–	–	8.38

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 D.20.

Table D.20. Difference between calculations with two data sets

Exp. No	T (°C)	CliMoChem	SimpleBox
1	-1	-0.1%	-1.5%
2	3	-0.1%	-1.1%
3	10	-7.7%	-46.1%

These results are visualized in Fig. D.6.

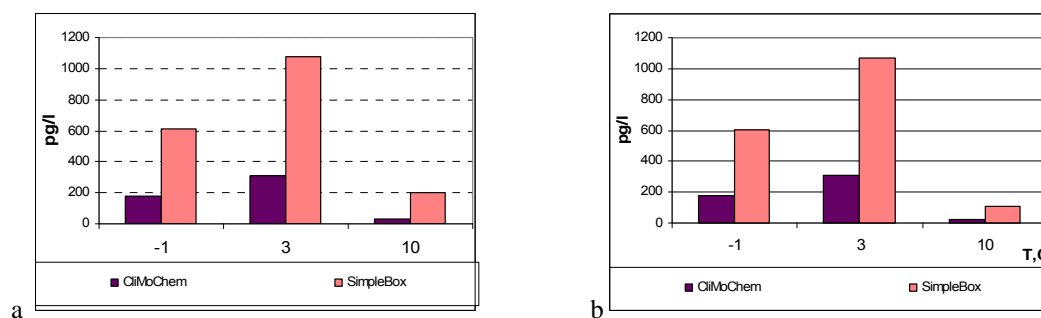


Fig. D.6. Calculation results of the participating models obtained with “reference” (a) and “own/alternative” (b) data sets (for models presented both calculations)

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-28 with “reference” and “own/alternative” data sets.

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

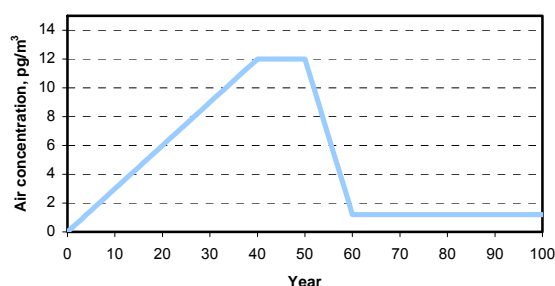


Fig. D.7. Air concentration trend used for calculations for MSCE-POP model (MSCE-POP 2) for Experiment 1

Reference data set. Calculation results for soil concentrations together with m and σ calculated with “reference” data set of PCB-28 properties are presented in Table D.21. Net gaseous fluxes to soil of PCB-28 calculated by the models and statistical parameters used for its evaluation are given in Table D.22.

Table D.21. Calculation results: soil concentrations of PCB-28 (ng/g) calculated by models and statistical parameters used for evaluation (“reference” data set)

No	Air conc. pg/m ³	DEHM-POP	CliMoChem	SimpleBox	m	σ
1	1.2	0.137	0.001	0.0001	0.046	0.079
2	5.6	0.043	0.003	0.001	0.016	0.024
3	4.2	0.020	0.003	0.001	0.008	0.011
4	1.8	0.004	0.001	0.0001	0.002	0.002

Table D.22. Calculation results: net gaseous flux to soil, of PCB-28 (ng/m²/d) calculated by models and statistical parameters used for evaluation (“reference” data set)

No	Air conc. pg/m ³	CliMoChem	SimpleBox	m	σ
1	1.2	0.02	0.07	0.05	0.04
2	5.6	0.09	0.40	0.25	0.22
3	4.2	0.07	0.25	0.16	0.13
4	1.8	0.03	0.08	0.05	0.04

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

Pairwise regression analysis is performed only for values of soil concentrations and deposition fluxes calculated by models using steady state and dynamic approaches. In spite of the fact that numerical values of soil concentrations are highly different, the variations of the corresponding numerical values

caused by change of environmental conditions between different experiments are similarly described by most of models. This can be seen from values of pairwise correlation coefficients (Table D.23).

Table D.23. Correlation coefficients for soil concentrations of PCB-28 (“reference” data set)

	CliMoChem	SimpleBox
DEHM-POP	-0.39	-0.26
CliMoChem	–	0.95

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

Table D.24. Correlation coefficients for net gaseous flux to soil of PCB-28 (“reference” data set)

	SimpleBox
CliMoChem	0.03

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

Table D.25. Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-28 (“reference” data set)

	CliMoChem	SimpleBox
DEHM-POP	-0.008 / 0.0021	-0.002 / 0.0006
CliMoChem	–	0.342 / -0.0001

Table D.26. Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-28 (“reference” data set)

	SimpleBox
CliMoChem	4.287 / -0.022

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

Table D.27. Residual square deviation, σ_{12}^{res} for soil concentrations of PCB-28 (“reference” data set)

	CliMoChem	SimpleBox
DEHM-POP	0.002	0.001
CliMoChem	–	0.0002

Table D.28. Residual square deviation, σ_{12}^{res} for net gaseous flux to soil of PCB-28 (“reference” data set)

	SimpleBox
CliMoChem	0.16

Own/alternative data set. Calculation results soil concentrations together with m and σ calculated with “own/alternative” data set of PCB-28 properties are presented in Table D.29. Net gaseous fluxes to soil of PCB-28 calculated by the models and statistical parameters used for its evaluation are given

in Table D.30. Table D.29 contains also the information of the data set used for calculations for each model.

Table D.29. Calculation results: soil concentrations of PCB-28 (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	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	<i>m</i>	<i>σ</i>
				1	2				
		own	own	own		own	alt		
1	1.2	0.0001	0.018	0.010	0.051	0.0005	0.003	0.014	0.020
2	5.6	0.0005	0.196	0.076	0.421	0.002	0.026	0.120	0.165
3	4.2	0.0004	0.089	0.045	0.241	0.002	0.016	0.066	0.092
4	1.8	0.0001	0.019	0.007	0.036	0.0004	0.003	0.011	0.014

Table D.30. Calculation results: net gaseous flux to soil, of PCB-28 (ng/m²/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	DEHM-POP	MSCE-POP		CliMoChem	SimpleBox	<i>m</i>	<i>σ</i>
				1	2				
1	1.2	0.001	–	-0.029	-0.152	0.019	0.044	-0.023	0.077
2	5.6	0.005	–	-0.031	-0.617	0.094	0.282	-0.053	0.338
3	4.2	0.004	–	-0.096	-0.509	0.068	0.158	-0.075	0.260
4	1.8	0.002	–	-0.071	-0.205	0.024	0.046	-0.041	0.102

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

Pairwise correlation coefficients are given in Table D.31.

Table D.31. Correlation coefficients for soil concentrations of PCB-28 (“own/alternative” data set)

		DEHM-POP	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.93	0.97	0.97	1.00	0.98
DEHM-POP		–	0.99	0.99	0.94	0.98
MSCE-POP	1	–	–	1.00	0.98	1.00
	2	–	–	–	0.97	1.00
CliMoChem		–	–	–	–	0.99

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

Table D.32. Correlation coefficients for net gaseous flux to soil of PCB-28 (“own/alternative” data set)

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
EVN-BETR and UK MODEL		-0.08	-1.00	1.00	0.97
MSCE-POP	1	–	-0.13	-0.02	0.14
	2	–	–	-0.99	-0.96
CliMoChem		–	–	–	0.99

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

Table D.33. Coefficients of regression dependence between the models (α / β) for soil concentrations of PCB-28 (“own/alternative” data set)

		DEHM-POP	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		398 / -0.026	164 / -0.010	903 / -0.056	5.4 / -0.0001	57.2 / -0.003
DEHM-POP		–	0.39 / 0.003	2.15 / 0.014	0.01 / 0.0004	0.13 / 0.001
MSCE-POP	1	–	–	5.55 / -0.004	0.03 / 0.0003	0.35 / 0.00004
	2	–	–	–	0.01 / 0.0003	0.06 / 0.0003
CliMoChem		–	–	–	–	10.62 / -0.002

Table D.34. Coefficients of regression dependence between the models (α / β) for net gaseous flux to soil of PCB-28 (“own/alternative” data set)

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
EVN-BETR and UK MODEL		-1.38 / -0.05	-120.5 / -0.01	19.21 / -0.01	58.68 / -0.04
MSCE-POP	1	–	0.90 / -0.32	-0.02 / 0.05	0.50 / 0.16
	2	–	–	-0.16 / -0.01	-0.48 / -0.04
CliMoChem		–	–	–	3.08 / -0.03

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

Table D.27. Residual square deviation, σ_{12}^{res} for soil concentrations of PCB-28 (“own/alternative” data set)

		DEHM-POP	MSCE-POP		CliMoChem	SimpleBox
			1	2		
EVN-BETR and UK MODEL		0.055	0.013	0.081	0.0001	0.004
DEHM-POP		–	0.009	0.043	0.0006	0.004
MSCE-POP	1	–	–	0.0074	0.0004	0.0008
	2	–	–	–	0.0004	0.0012
CliMoChem		–	–	–	–	0.003

Table D.28. Residual square deviation, σ_{12}^{res} for net gaseous flux to soil of PCB-28 (“own/alternative” data set)

		MSCE-POP		CliMoChem	SimpleBox
		1	2		
EVN-BETR and UK MODEL		0.056	0.031	0.004	0.044
MSCE-POP	1	–	0.390	0.063	0.194
	2	–	–	0.007	0.055
CliMoChem		–	–	–	0.034

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 D.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 D.29. Difference between calculations with two data sets

No	Air conc, pg/m ³	DEHM-POP	CliMoChem	SimpleBox
1	1.2	-87%	-11%	2089%
2	5.6	352%	-14%	2365%
3	4.2	342%	-23%	2547%
4	1.8	338%	-30%	2599%

Accumulation/clearance dynamics of PCBs in soil.

Fig. D.8 shows the results of the experiment obtained by CliMoChem and SimpleBox models with the use of “reference” data set.

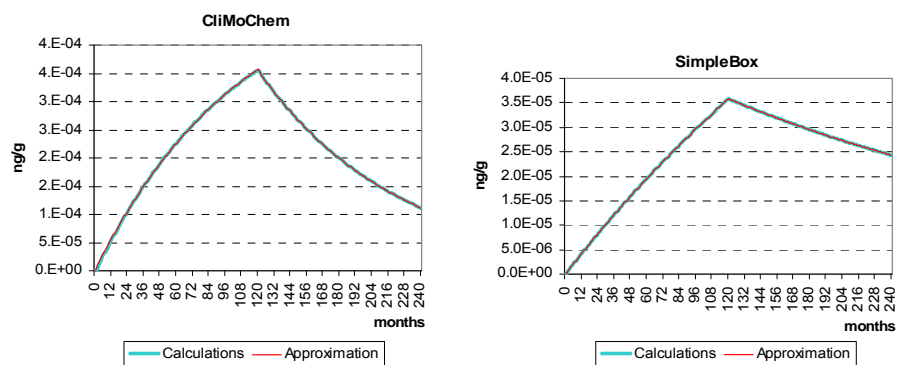


Fig. D.8. Long-term trends of accumulation and clearance obtained by participating models (“reference” data set)

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. D.9.

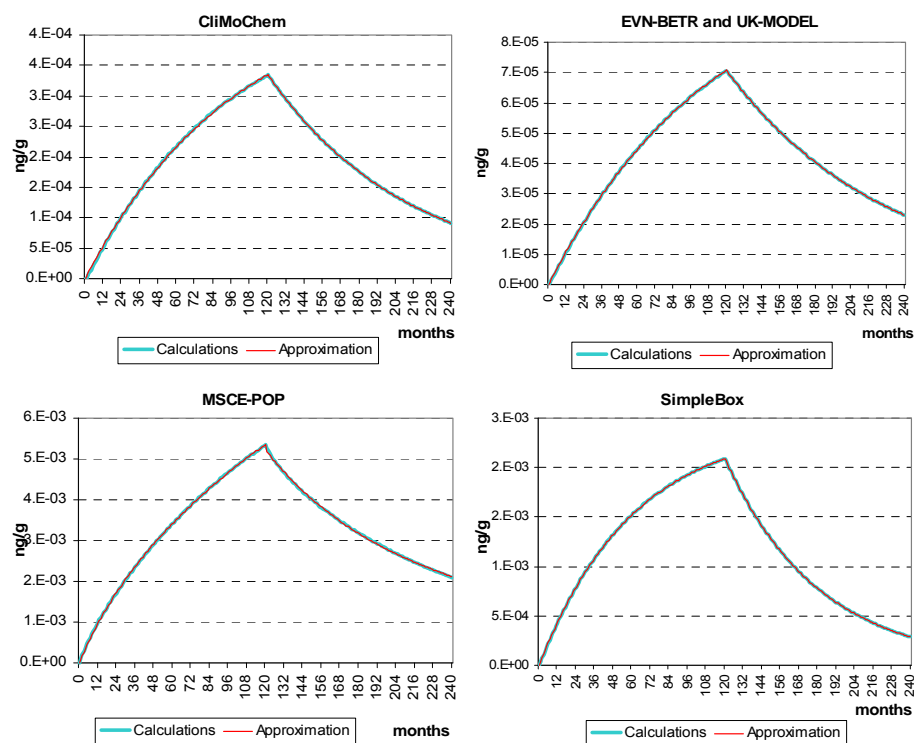


Fig. D.9. Long-term trends of accumulation and clearance obtained by participating models (“own/alternative” data set)

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

Table D.30. Parameters of multi-exponential approximation

	CliMoChem		EVN-BETR and UK model		MSCE-POP		SimpleBox	
	Slow	Fast	Slow	Fast	Slow	Fast	Slow	Fast
“Reference” data set								
Accumulation phase	6.4	6.4	–	–	–	–	18.7	18.7
Clearance phase	6.0	6.0	–	–	–	–	17.8	17.8
“Own/alternative” data set								
Accumulation phase	5.7	5.7	6.5	6.5	10.3	1.2	3.5	3.5
Clearance phase	5.3	5.4	6.2	6.0	10.7	2.9	3.5	3.5

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

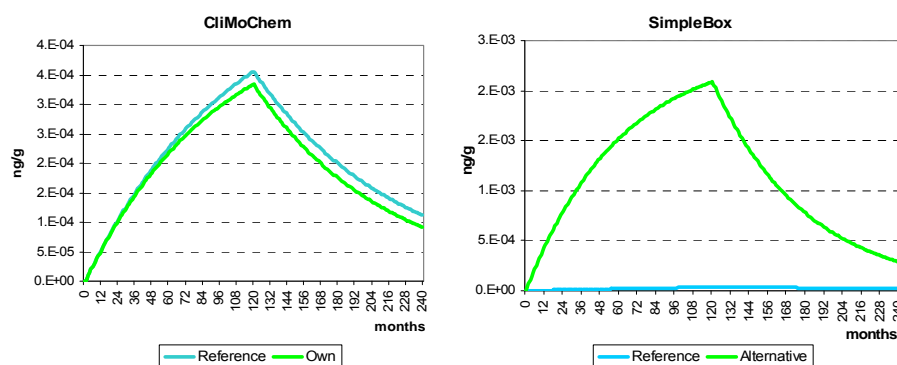


Fig. D.10. Difference in long-term trends due to usage of different sets of PCB properties

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-28 properties are presented in Table D.31.

Table D.31. Calculation results: water concentrations of PCB-28 (pg/L) calculated by all participating models and statistical parameters used for evaluation (“reference” data set)

N	DEHM-POP	CliMoChem	SimpleBox	m	σ
1	7.03	4.86	19.61	10.50	7.96
2	15.74	10.90	54.87	27.17	24.11
3	33.45	17.55	103.76	51.59	45.88
4	9.38	5.46	26.06	13.63	10.94

Fig. D.11 displays the result on water concentrations of PCB-28 calculated by the participating models with the use of “reference” data set.

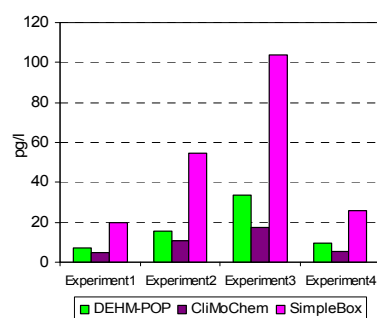


Fig. D.11. Calculation results of the participating models (water concentrations) obtained with “reference” data set

Gaseous fluxes to water, from water and net gaseous flux of PCB-28 calculated by the participating models are given in Table D.32.

Table D.32. Calculation results: fluxes of PCB-28 to/from water (ng/m²/day) calculated by all participating models and statistical parameters used for evaluation (“reference” data set)

N	CliMoChem	SimpleBox	m	σ
Gaseous flux to water				
1	2.61	5.92	4.27	2.34
2	5.85	26.28	16.07	14.44
3	6.90	31.32	19.11	17.27
4	2.38	6.64	4.51	3.01
Gaseous flux from water				
1	1.66	3.54	2.60	1.33
2	3.73	19.61	11.67	11.23
3	3.48	21.81	12.64	12.96
4	1.31	4.08	2.70	1.96
Net gaseous flux				
1	0.95	2.38	1.67	1.01
2	2.13	6.67	4.40	3.21
3	3.43	9.51	6.47	4.30
4	1.07	2.56	1.81	1.06

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

Table D.32. Correlation coefficients for water concentrations (“reference” data set)

	CliMoChem	SimpleBox
DEHM-POP	0.98	0.99
CliMoChem	-	1.00

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

Table D.33. Correlation coefficients for net gaseous flux (“reference” data set)

	SimpleBox
CliMoChem	0.99

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 D.34. Coefficients of regression dependence between the models (α / β) for water concentrations (“reference” data set)

	CliMoChem	SimpleBox
DEHM-POP	0.49 / 1.72	3.19 / -1.26
CliMoChem	-	6.48 / -11.70

Table D.35. Coefficients of regression dependence between the models (α / β) for net gaseous flux (“reference” data set)

	SimpleBox
CliMoChem	2.96 / -0.33

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

Table D.36. Residual square deviation, σ for water concentrations (“reference” data set)

	CliMoChem	SimpleBox
DEHM-POP	1.80	6.84
CliMoChem	-	5.01

Table D.37. Residual square deviation, σ for net gaseous flux (“reference” data set)

	SimpleBox
CliMoChem	0.82

Own/alternative data set. Calculation results for water concentrations together with m and σ calculated with “own/alternative” data set of PCB-28 properties are presented in Table D.38. Here data set of PCB-28 properties used for calculations by each model is indicated (second row).

Table D.38. Calculation results: water concentrations of PCB-28 (pg/L) calculated by all participating models and statistical parameters used for evaluation (“own/alternative” data set)

N	EVN-BETR and UK-MODEL	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP	m	σ
Set	own	own	own	alt	own		
1	4.74	290.37	1.02	13.29	7.46	63.38	126.97
2	10.43	83.90	2.30	39.02	16.77	30.48	32.83
3	17.00	67.16	4.62	39.70	39.43	33.58	24.05
4	5.32	150.45	1.34	11.44	10.72	35.85	64.19

Fig. D.12 displays the result on water concentrations of PCB-28 calculated by the participating models with the use of “own / alternative” data set.

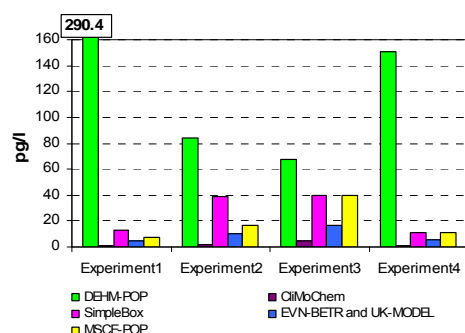


Fig. D.12. Calculation results of the participating models (water concentrations) obtained with “own/alternative” data set

Gaseous fluxes to water, from water and net gaseous flux of PCB-28 calculated by the models are given in Table D.39.

Table D.39. Calculation results: fluxes of PCB-28 to/from water (ng/m²/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 water						
1	4.29	2.55	4.97	7.81	4.90	2.19
2	9.44	5.71	22.37	21.08	14.65	8.33
3	15.82	6.61	19.20	20.17	15.45	6.18
4	4.89	2.28	4.27	6.75	4.55	1.84
Gaseous flux from water						
1	1.91	0.38	2.53	7.63	3.11	3.14
2	4.19	0.85	14.92	20.67	10.16	9.23
3	4.48	1.01	11.99	19.21	9.17	8.11
4	1.64	0.35	2.23	6.49	2.68	2.66
Net gaseous flux						
1	2.38	2.17	2.44	0.18	1.79	1.08
2	5.25	4.87	7.44	0.41	4.49	2.95
3	11.34	5.60	7.21	0.96	6.28	4.29
4	3.25	1.93	2.04	0.26	1.87	1.23

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

Table D.40. Correlation coefficients for water concentrations (“own/alternative” data set)

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	-0.78	0.99	0.89	0.98
DEHM-POP	-	-0.75	-0.80	-0.72
CliMoChem	-	-	0.81	1.00
SimpleBox	-	-	-	0.77

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

Table D.41. Correlation coefficients for net gaseous flux (“own/alternative” data set)

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.87	0.76	1.00
CliMoChem	-	0.98	0.85
SimpleBox	-	-	0.73

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 D.42. Coefficients of regression dependence between the models (α / β) for water concentrations (“own/alternative” data set)

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	-13.93 / 278.54	0.28 / -0.33	2.43 / 3.09	2.47 / -4.60
DEHM-POP	–	-0.01 / 4.10	-0.12 / 43.98	-0.10 / 33.77
CliMoChem	–	–	7.80 / 7.76	8.83 / -1.91
SimpleBox	–	–	–	0.71 / 0.26

Table D.43. Coefficients of regression dependence between the models (α / β) for net gaseous flux (“own/alternative” data set)

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	0.40 / 1.42	0.55 / 1.72	0.09 / -0.03
CliMoChem	–	1.55 / -0.86	0.16 / -0.13
SimpleBox	–	–	0.09 / 0.03

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

Table D.44. Residual square deviation, σ for water concentrations (“own/alternative” data set)

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	109.82	0.39	12.52	5.32
DEHM-POP	-	1.87	16.33	17.26
CliMoChem	-	-	15.73	1.87
SimpleBox	-	-	-	16.01

Table D.45. Residual square deviation, σ for net gaseous flux (“own/alternative” data set)

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK MODEL	1.61	3.33	0.02
CliMoChem	-	0.99	0.32
SimpleBox	-	-	0.41

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 D.46. Difference between calculations with two data sets (water concentrations)

N	DEHM-POP	CliMoChem	SimpleBox
1	4031%	-79%	-32%
2	433%	-79%	-29%
3	101%	-74%	-62%
4	1504%	-75%	-56%

This difference is visualized in Fig. D.13.

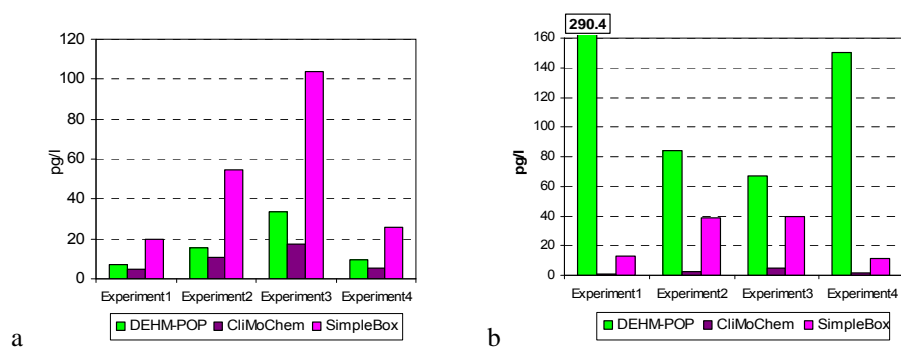


Fig. D.13. Calculation results of the participating models obtained with “reference” (a) and “own/alternative” (b) data sets (for models presented both calculations)

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

N	CliMoChem	SimpleBox
1	52%	115%
2	300%	5%
3	245%	-12%
4	70%	59%

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-28 properties are presented in Table D.48. Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-28 calculated by the models are given in Table D.49.

Table D.48. Calculation results: concentrations of PCB-28 in vegetation (ng/g) calculated by all participating models and statistical parameters used for evaluation (“reference” data set)

N	CliMoChem	SimpleBox	m	σ
1	0.180	0.067	0.12	0.08
2	0.299	0.057	0.18	0.17
3	0.242	0.073	0.16	0.12
4	0.142	0.034	0.09	0.08

Table D.49. Calculation results: fluxes of PCB-28 to/from vegetation (ng/m²/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	0.59	30.33	15.46	21.03
2	2.07	106.14	54.11	73.59
3	1.01	51.55	26.28	35.74
4	0.77	39.42	20.10	27.33
Gaseous flux from vegetation				
1	0.59	28.00	14.29	19.38
2	2.07	102.72	52.40	71.17
3	1.01	48.68	24.84	33.71
4	0.77	37.81	19.29	26.19
Net gaseous flux				
1	0	2.33	-	-
2	0	3.42	-	-
3	0	2.88	-	-
4	0	1.61	-	-

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 D.50.

Table D.50. Correlation coefficients for concentrations in vegetation (“reference” data set)

	CliMoChem
SimpleBox	0.51

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

Table D.51. Coefficients of regression dependence between the models (α / β) for concentrations in vegetation (“reference” data set)

	CliMoChem
SimpleBox	2.06 / 0.10

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 D.52.

Table D.52. Residual square deviation, σ for concentrations in vegetation (“reference” data set)

	CliMoChem
SimpleBox	0.10

Own/alternative data set. Calculation results for concentrations in vegetation together with m and σ calculated with “own/alternative” data set of PCB-28 properties are presented in Table D.53. Here data set of PCB-28 properties used for calculations by each model is indicated (second row).

Gaseous fluxes to vegetation, from vegetation and net gaseous flux of PCB-28 calculated by the models are given in Table D.54.

Table D.53. Calculation results: concentrations of PCB-28 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	<i>m</i>	σ
Set	own	own	alt	own		
1	0.010	0.083	0.026	0.126	0.06	0.05
2	0.004	0.084	0.057	0.150	0.07	0.06
3	0.008	0.104	0.038	0.171	0.08	0.07
4	0.003	0.052	0.025	0.089	0.04	0.04

Table D.54. Calculation results: fluxes of PCB-28 to/from vegetation (ng/m²/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	<i>m</i>	σ
Gaseous flux to vegetation						
1	8.69	0.59	0.86	—	3.38	4.60
2	30.58	2.07	3.02	—	11.89	16.19
3	14.52	1.01	1.47	—	5.66	7.67
4	11.31	0.77	1.12	—	4.40	5.99
Gaseous flux from vegetation						
1	8.60	0.18	0.81	—	3.20	4.69
2	30.55	1.65	2.91	—	11.70	16.33
3	14.45	0.46	1.39	—	5.44	7.82
4	11.28	0.49	1.07	—	4.28	6.07
Net gaseous flux						
1	0.09	0.41	0.05	0.41	0.24	0.19
2	0.03	0.42	0.11	0.48	0.26	0.22
3	0.07	0.54	0.07	0.55	0.31	0.27
4	0.03	0.28	0.05	0.29	0.16	0.14

The pairwise 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 D.55.

Table D.55. Correlation coefficients for water concentrations (“own/alternative” data set)

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-0.33	0.42	0.63
SimpleBox	-	0.62	0.43
CliMoChem	-	-	0.97

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

Table D.56. Correlation coefficients for net gaseous flux (“own/alternative” data set)

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	-0.43	0.32	0.51
SimpleBox	-	0.62	0.40
CliMoChem	-	-	0.97

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 D.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	-1.45 / 0.05	4.25 / 0.11	3.95 / 0.06

UK MODEL			
SimpleBox	–	1.43 / 0.08	0.61 / 0.06
CliMoChem	–	–	0.60 / 0.0001

Table D.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	-0.44 / 0.10	1.20 / 0.36	1.84 / 0.31
SimpleBox	–	2.29 / 0.27	1.45 / 0.31
CliMoChem	–	–	0.95 / 0.004

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

Table D.59. Residual square deviation, σ for concentrations in vegetation (“own/alternative” data set)

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.02	0.05	0.03
SimpleBox	-	0.05	0.03
CliMoChem	-	-	0.01

Table D.60. Residual square deviation, σ for net gaseous flux (“own/alternative” data set)

	SimpleBox	MSCE-POP	CliMoChem
EVN-BETR and UK MODEL	0.05	0.18	0.16
SimpleBox	-	0.15	0.17
CliMoChem	-	-	0.05

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 D.61. Difference between calculations with two data sets (concentrations in vegetation)

N	CliMoChem	SimpleBox
1	-54%	-61%
2	-72%	-0.2%
3	-57%	-48%
4	-64%	-28%

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

N	CliMoChem	SimpleBox
1	-69%	-97%
2	-20%	-97%
3	-54%	-97%
4	-36%	-97%

Table D.64. *Difference between calculations with two data sets (net gaseous flux)*^{*}

N	SimpleBox
1	-98%
2	-97%
3	-97%
4	-97%

* 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