

## COMPARISON OF RESULTS OF COMPUTATIONAL EXPERIMENTS FOR PCB-28

### D.1. Gas/particle partitioning:

#### D.1.1. Input data

Eleven sets of input data (different ambient temperatures in the range from – 12° C to 32° C) are proposed for modelling experiments with PCB-28.

**Table D.1.** Input data for computation experiments with PCB-28 describing gas/particle partitioning

	Exp. 1	Exp.2	Exp.3	Exp. 4	Exp. 5	Exp. 6	Exp. 7	Exp. 8	Exp. 9	Exp. 10	Exp. 11
Averaged ambient temperature, C	-12	-5	0	6	10	15	20	25	25	26	32
Total Suspended Matter, TSP, $\mu\text{g}/\text{m}^3$	30	30	30	30	30	30	30	51	29	49	66
Organic content in the aerosol, %	20	20	20	20	20	20	20	17	21	20	20

Output: PCB particulate fractions calculated for a range of temperatures (for PCB-28: from – 12°C to 32°C).

#### D.1.2. Comparison of the results

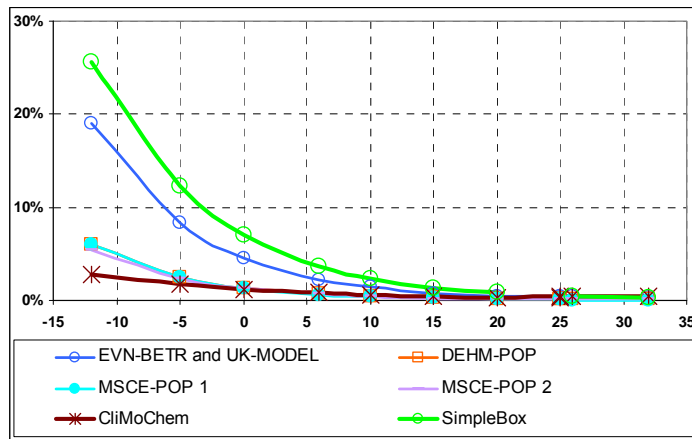
**Table D.2.** Calculation results: fractions of particulate phase of PCB-28 calculated by models and statistical parameters used for evaluation

N	Temperature (C)	EVN-BETR and UK-MODEL	DEHM-POP	MSCE-POP*		CliMoChem	SimpleBox**	$m_\phi$	$\sigma_\phi$
				1	2				
1	-12	0.190	0.061	0.061	0.054	0.028	0.256	0.108	0.092
2	-5	0.083	0.025	0.025	0.023	0.017	0.123	0.049	0.044
3	0	0.045	0.014	0.013	0.013	0.012	0.071	0.028	0.025
4	6	0.022	0.007	0.006	0.007	0.008	0.036	0.014	0.012
5	10	0.014	0.004	0.004	0.004	0.007	0.023	0.009	0.008
6	15	0.008	0.002	0.002	0.002	0.005	0.014	0.006	0.005
7	20	0.004	0.001	0.001	0.001	0.004	0.008	0.003	0.003
8	25	0.004	0.001	0.001	0.001	0.005	-	0.002	0.002
9	25	0.003	0.001	0.001	0.001	0.003	-	0.002	0.001
10	26	0.004	0.001	0.001	0.001	0.004	0.004	0.003	0.002
11	32	0.003	0.001	0.0004	0.001	0.004	0.002	0.002	0.001

\* - See process description of MSCE-POP model (MSCE-POP 1: current version; MSCE-POP 2: experimental version);

\*\* - Only 9 experiments for Simple Box.

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



**Fig. D.1.** Fractions of PCB-28 particulate phase for different ambient temperatures (Calculation results of the participating models)

**Table D.3.** Coefficients of regression dependence between the models ( $\alpha / \beta$ )

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox *
EVN-BETR and UK-MODEL	0.32/-0.0001	0.32/ -0.0004	0.28/ 0.00003	0.13 / 0.004	1.35 / 0.004
DEHM-POP	-	1.00/-0.0003	0.89 / 0.0002	0.42 / 0.004	4.25 / 0.005
MSCE-POP 1	-	-	0.89 / 0.0004	0.42 / 0.004	4.22 / 0.007
MSCE-POP 2			-	0.47 / 0.004	4.76 / 0.004
CliMoChem			-	-	10.05 / -0.040

\* - by 9 experiments only

**Table D.4.** Correlation coefficients

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

\* - by 9 experiments only

**Table D.5.** Residual square deviation ( $\sigma$ )

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox *
EVN-BETR and UK-MODEL	0.001	0.002	0.001	0.004	0.013
DEHM-POP	-	0.001	0.001	0.005	0.018
MSCE-POP 1	-	-	0.002	0.005	0.019
MSCE-POP 2	-	-	-	0.004	0.014
CliMoChem	-	-	-	-	0.026

\* - by 9 experiments only

## D.2. Dry deposition of particulate phase

### D.2.1. Input data

The following four sets of input data are proposed for modelling experiments with PCB-28.

**Table D.6.** Input data for computation experiments with PCB-28 describing dry deposition of particulate phase

N	Experiment 1	Experiment 2	Experiment 3	Experiment 4
Type of underlying surfaces	Grass	Forest	Bare soil	Seawater
Mean wind velocity, m/sec	4	4	4	4
Air concentration of particulate phase, ng/m <sup>3</sup>	1	1	1	1

### D.2.2. Comparison of the results

See chapter 4.2.3. According to EVN-BETR and UK-MODEL, DEHM-POP, G-CIEMS, CAM/POPs, CliMoChem, SimpleBox and MSCE-POP parameterizations, these calculations were made for all considered PCB congeners together.

## D.3. Wet deposition

### D.3.1. Input data

Six sets of input data are proposed for modeling experiments with PCB-28.

**Table D.7.** Input data for computation experiments with PCB-28 describing wet deposition

N	Experiment 1	Experiment 2	Experiment 3	Experiment 4	Experiment 5	Experiment 6
Precipitation intensity, mm/hour	1	1	1	10	10	10
Precipitation height, m	1000	1000	1000	1000	1000	1000
Average ambient temperature, °C	-1	3	10	-1	3	10
Air concentration, gaseous phase, pg/m <sup>3</sup>	7	14	225	7	14	225
Air concentration, particulate phase, pg/m <sup>3</sup>	3	5.3	0.2	3	5.3	0.2

**Output:** calculated wet deposition fluxes, ng/m<sup>2</sup>/hour and total (dissolved+particulate) concentrations of PCB in precipitation, pg/l.

### D.3.2. Comparison of the results

Since additional experiments on wet deposition (last three experiments) were made only by two participating models, statistical processing is performed for the calculation results of the first three experiments. It should be mentioned that results of Experiments 4, 5 and 6 calculated by MSCE-POP and SimpleBox show the same concentration in precipitation as in Experiments 1, 2, and 3, respectively. Fluxes between Experiments 1, 2, 3 and Experiments 4, 5, 6 differ ten times in accordance with the different values of precipitation intensity given (See Table D.7).

**Table D.8.** Calculation results: total (dissolved + particulate) concentrations of PCB-28 in precipitation, pg/l and statistical parameters used for evaluation

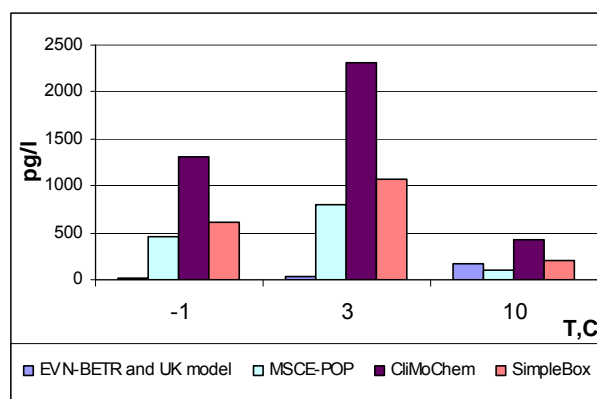
N	Temperature (C)	EVN-BETR and UK model	MSCE-POP	CliMoChem	SimpleBox	$m_p$	$\sigma_p$
1	-1	24	456	1307	612	600	533
2	3	30	803	2306	1077	1054	945
3	10	166	99	423	202	222	140

**Table D.9** Calculation results: wet deposition flux of PCB-28, ng/m<sup>2</sup>/hour and statistical parameters used for evaluation

N	Temperature (C)	EVN-BETR and UK model	MSCE-POP	CliMoChem	SimpleBox	$m_p$	$\sigma_p$
1	-1	0.024	0.456	0.176	0.612	0.317	0.266
2	3	0.030	0.803	0.311	1.077	0.555	0.472
3	10	0.166	0.099	0.031	0.202	0.124	0.076

**Table D.10.** Correlation coefficients for concentration in precipitation

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	-0.85	-0.83	-0.83
MSCE-POP	-	1.00	1.00
CliMoChem	-	-	1.00



**Fig. D.2.** Concentration in precipitation calculated by different models for different values of ambient temperatures, pg/l

**Table D.11.** Coefficients of regression dependence between the models,  $\alpha / \beta$  for concentration in precipitation

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	-3.73 / 726.24	-9.71 / 2057.25	-4.51 / 960.96
MSCE-POP	-	2.67 / 134.48	1.24 / 68.02
CliMoChem	-	-	0.46 / 5.50
Mean concentration in precipitation	452.67	1345.15	630.47

**Table D.12.** Residual square deviation ( $\sigma$ ) for concentration in precipitation

	MSCE-POP	CliMoChem	SimpleBox
EVN-BETR and UK model	261.38	748.22	348.44
MSCE-POP		57.76	27.82
CliMoChem			0.98

## D.4. Gaseous exchange between the atmosphere and soil

### D.4.1. Input data

Four sets of input data are proposed for modelling experiments with PCB-28.

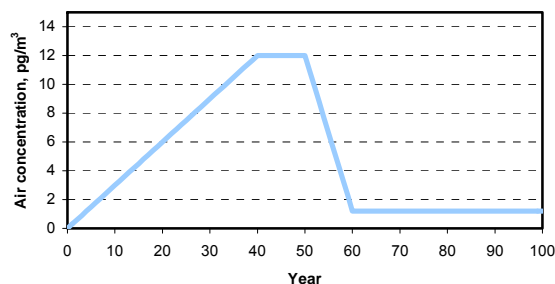
**Table D.13.** Input data for computation experiments with PCB-28 describing air/soil exchange

N	Experiment 1	Experiment 2	Experiment 3	Experiment 4
Average ambient temperature, °C	10	10.9	12.9	13.9
Air concentration, gaseous phase, pg/m <sup>3</sup>	1.2	5.6	4.2	1.8
Bulk soil density, kg/m <sup>3</sup>	1210	1080	890	1360
Volumetric water content in soil, %	20.6	41.4	26.4	16.8
Volumetric air content in soil, %	20	20	20	20
Fraction of organic carbon in soil, %	7.1	17.7	12.3	4

**Output:** calculation of PCB-28 soil concentrations, ng/g and gaseous fluxes from and to soil and/or net gaseous flux to soil, ng/m<sup>2</sup>/d.

## D.4.2. Comparison of the results

1) Fig. D.3. illustrates air concentration trend used in calculations for Experiment 1.



**Fig. D.3.** Air concentration trend used for calculations for MSCE-POP model (second version) for Experiment 1

**Table D.14.** Calculation results: soil concentrations of PCB-28 calculated by models and statistical parameters used for evaluation, ng/g

N	Air conc, pg/m <sup>3</sup>	EVN-BETR and UK-MODEL	DEHM-POP	MSCE-POP*		CliMoChem	SimpleBox	m	σ
				1	2				
1	1.2	0.0001	0.0184	0.0096	0.0513	0.0072	0.0001	0.0144	0.0193
2	5.6	0.0005	0.1961	0.0761	0.4213	0.0549	0.0011	0.1250	0.1619
3	4.2	0.0004	0.0890	0.0453	0.2411	0.0387	0.0006	0.0692	0.0904
4	1.8	0.0001	0.0195	0.0071	0.0360	0.0037	0.0001	0.0111	0.0142

\* - MSCE-POP 1: steady-state calculations; MSCE-POP 2: calculations from dynamic model

**Table D.15.** Calculation results: net gaseous flux to soil, of PCB-28 calculated by models and statistical parameters used for evaluation, ng/m<sup>2</sup>/d

N	Air conc, pg/m <sup>3</sup>	EVN-BETR and UK-MODEL	MSCE-POP		CliMo Chem	SimpleBox	m *	σ *
			1	2				
1	1.2	1.18E-03	-2.90E-02	-1.52E-01	0	7.15E-02	-2.70E-02	9.33E-02
2	5.6	5.18E-03	-3.12E-02	-6.17E-01	0	4.02E-01	-6.01E-02	4.20E-01
3	4.2	3.96E-03	-9.64E-02	-5.09E-01	0	2.52E-01	-8.76E-02	3.17E-01
4	1.8	1.73E-03	-7.12E-02	-2.05E-01	0	8.43E-02	-4.75E-02	1.23E-01

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

**Table D.16.** Correlation coefficients for soil concentrations of PCB-28

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK-MODEL	0.93	0.97	0.97	0.99	0.97
DEHM-POP	-	0.99	0.99	0.96	0.99
MSCE-POP 1	-	-	1.00	0.99	1.00
MSCE-POP 2	-	-	-	0.99	1.00
CliMoChem	-	-	-	-	0.99

**Table D.17.** Correlation coefficients for net gaseous flux to soil of PCB-28\*

	MSCE-POP 1	MSCE-POP 2	SimpleBox
EVN-BETR and UK-MODEL	-0.08	-1.00	0.99
MSCE-POP 1	-	0.13	0.08
MSCE-POP 2	-	-	-0.98

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

**Table D.18.** Coefficients of regression dependence between the models ( $\alpha / \beta$ ) for soil concentrations

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK-MODEL	398.33 / -0.03	163.59 / -0.01	902.92 / -0.06	126.57 / -0.01	2.26 / -0.0001
DEHM-POP	-	0.39 / 0.003	2.15 / 0.01	0.28 / 0.003	0.01 / 0.00004
MSCE-POP 1	-	-	5.55 / -0.004	0.75 / 0.0001	0.01 / -0.000002
MSCE-POP 2	-	-	-	0.14 / 0.001	0.003 / 0.00001
CliMoChem	-	-	-	-	0.02 / 0.000004
Mean soil concentration	0.0808	0.0345	0.1874	0.0261	0.0005

**Table D.19.** Coefficients of regression dependence between the models ( $\alpha / \beta$ ) for net gaseous flux to soil of PCB-28\*

	MSCE-POP 1	MSCE-POP 2	SimpleBox
EVN-BETR and UK-MODEL	-1.38 / -0.05	-120.50 / -0.01	82.07 / -0.05
MSCE-POP 1	-	0.90 / -0.32	0.38 / 0.22
MSCE-POP 2	-	-	-0.67 / -0.05
Mean flux	-0.06	-0.37	0.20

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

**Table D.20.** Residual square deviation ( $\sigma$ ) for soil concentrations

	DEHM-POP	MSCE-POP 1	MSCE-POP 2	CliMoChem	SimpleBox
EVN-BETR and UK-MODEL	0.055	0.013	0.081	0.005	0.0002
DEHM-POP	-	0.009	0.043	0.012	0.0001
MSCE-POP 1	-	-	0.007	0.005	0.0000
MSCE-POP 2	-	-	-	0.006	0.00001
CliMoChem	-	-	-	-	0.0001

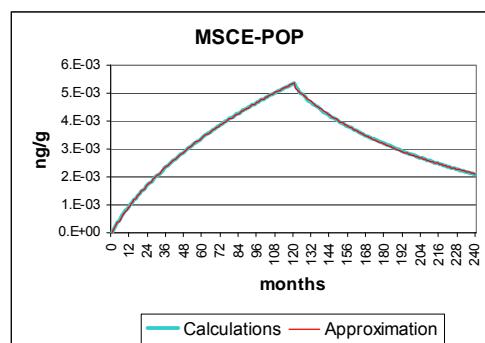
**Table D.21.** Residual square deviation ( $\sigma$ ) for net gaseous flux to soil of PCB-28\*

	MSCE-POP 1	MSCE-POP 2	SimpleBox
EVN-BETR and UK-MODEL	0.06	0.03	0.04
MSCE-POP 1	-	0.39	0.27
MSCE-POP 2	-	-	0.06

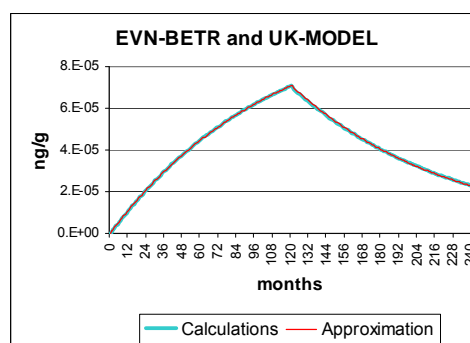
\* - statistical parameters are calculated for models using steady-state and dynamic approaches.

## 2) Accumulation/clearance dynamics of POPs in soil (optional):

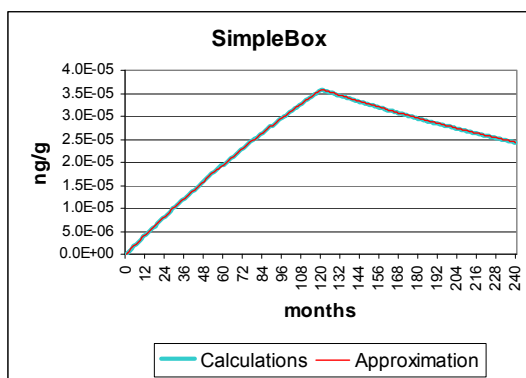
Figs. D.4, D.5, and D.6 below show the results of the experiment obtained by MSCE-POP, EVN-BETR and UK model, and SimpleBox models, respectively.



**Fig. D.4.** Long-term trends of accumulation and clearance obtained by MSCE-POP model



**Fig. D.5.** Long-term trends of accumulation and clearance obtained by EVN-BETR and UK-MODEL model



**Fig. D.6.** Long-term trends of accumulation and clearance obtained by SimpleBox model

**Table D.22.** Parameters of multi-exponential approximation

		EVN-BETR and UK model		SimpleBox		MSCE-POP	
		Slow	Fast	Slow	Fast	Slow	Fast
Accumulation phase	Lambda	8.94E-03	8.94E-03	3.09E-03	3.09E-03	5.61E-03	5.00E-02
	$t_{1/2}$ , years	6.46	6.46	18.68	18.68	10.30	1.16
Clearance phase	Lambda	9.38E-03	9.66E-03	3.24E-03	3.24E-03	5.38E-03	2.00E-02
	$t_{1/2}$ , years	6.16	5.98	17.84	17.83	10.73	2.89

## D.5. Gaseous exchange between the atmosphere and water

### D.5.1. Input data

Four sets of input data are proposed for modelling experiments with PCB-28.

**Table D.23.** Input data for calculation experiments with PCB-28 describing air/water exchange.

	Experiment 1	Experiment 2	Experiment 3	Experiment 4
Average ambient temperature, °C	23	23	10	13.9
Air concentration, gaseous phase, pg/m <sup>3</sup>	75	168	134.4	51
Mean wind velocity, m/sec	3	5.6	5	3.25

**Output:** calculation of PCB-28 water concentrations, pg/l and gaseous fluxes from and to water and/or net gaseous flux to water, ng/m<sup>2</sup>/d

### D.5.2. Comparison of the results

**Table D.24.** Calculation results: water concentrations of PCB-28 (pg/l) calculated by all participating models and statistical parameters used for evaluation

N	EVN-BETR and UK-MODEL	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP	$m$	$\sigma$
1	4.74	290.37	1024.85	19.61	7.46	269	439
2	10.43	83.90	2295.67	54.87	16.77	492	1009
3	17.00	67.16	4624.42	103.76	39.43	970	2043
4	5.32	150.45	1340.76	26.06	10.72	307	581

**Table D.25.** Calculation results: statistical evaluation of PCB-28 water concentrations (pg/l) calculated by models having results of the same order

N	EVN-BETR and UK-MODEL	DEHM-POP	SimpleBox	MSCE-POP	<i>m</i>	$\sigma$
1	4.74	290.37	19.61	7.46	80.5	140.0
2	10.43	83.90	54.87	16.77	41.5	34.4
3	17.00	67.16	103.76	39.43	56.8	37.4
4	5.32	150.45	26.06	10.72	48.1	68.8

**Table D.26.** Calculation results: Gaseous flux to water of PCB-28 (ng/m<sup>2</sup>/d) calculated by all participating models and statistical parameters used for evaluation

N	EVN-BETR and UK-MODEL	CliMoChem	SimpleBox	MSCE-POP	<i>m</i>	$\sigma$
1	4.29	2.55	5.92	7.81	5.14	2.25
2	9.44	5.71	26.28	21.08	15.63	9.66
3	15.82	6.61	31.32	20.17	18.48	10.26
4	4.89	2.28	6.64	6.75	5.14	2.09

**Table D.27.** Correlation coefficients for water concentrations

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

**Table D.28.** Correlation coefficients for gaseous flux to water

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	0.94	0.94	0.84
CliMoChem	-	1.00	0.98
SimpleBox	-	-	0.98

**Table D.29.** Coefficients of regression dependence between the models ( $\alpha$  /  $\beta$ ) for water concentrations

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	-13.93 / 278.54	283.18 / -332.68	6.72 / -11.90	2.47 / -4.60
DEHM-POP	-	-12.02 / 4099.41	-0.29 / 94.35	-0.10 / 33.77
CliMoChem	-	-	0.02 / -3.42	0.01 / -1.91
SimpleBox	-	-	-	0.37 / -0.39
Mean concentration in water	147.97	2321.43	51.08	18.60

**Table D.30.** Coefficients of regression dependence between the models ( $\alpha$  /  $\beta$ ) for gaseous flux to water

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	0.39 / 0.96	2.32 / -2.41	1.22 / 3.43
CliMoChem	-	5.98 / -8.11	3.44 / -0.79
SimpleBox	-	-	0.57 / 3.91
Mean gaseous flux to water	4.29	17.54	13.95

**Table D.31.** Residual square deviation,  $\sigma$  for water concentrations

	DEHM-POP	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	109.81	392.84	4.25	5.32
DEHM-POP	-	1866.32	41.96	17.26
CliMoChem	-	-	5.13	1.87
SimpleBox	-	-	-	3.79



**Table D.32.** Residual square deviation,  $\sigma$  for gaseous flux to water

	CliMoChem	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	1.33	7.93	7.21
CliMoChem	-	1.66	2.87
SimpleBox	-	-	2.91

## D.6. Gaseous exchange between the atmosphere and vegetation

### D.6.1. Input data

Four sets of input data are proposed for modelling experiments with PCB-28.

**Table D.33.** Input data for calculation experiments with PCB-28 describing air/vegetation exchange

N	Experiment 1	Experiment 2	Experiment 3	Experiment 4
Type of vegetation compartment:	Grass	Grass	Grass	Grass
Average ambient temperature, °C	5	25	11	18
Air concentration, gaseous phase, $\mu\text{g}/\text{m}^3$	10	35	17	13
Mean wind velocity, m/sec	4	4	4	4

**Output:** calculation of PCB-28 concentration in vegetation,  $\text{ng}/\text{g}$  dry weight and gaseous fluxes from and to vegetation and/or net gaseous flux to vegetation,  $\text{ng}/\text{m}^2/\text{d}$ ;

### D.6.2. Comparison of the results

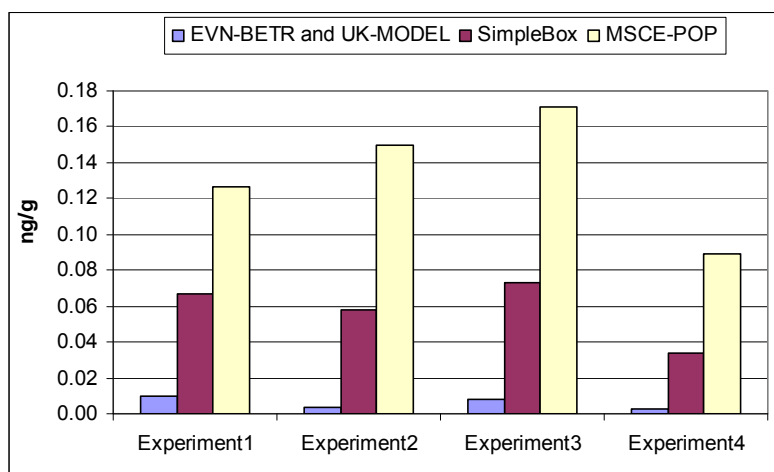
**Table D.34.** Calculation results: concentrations of PCB-28 in vegetation calculated by models,  $\text{ng}/\text{g}$  d.w

N	Air concentration, $\mu\text{g}/\text{m}^3$	EVN-BETR and UK-MODEL	SimpleBox*	MSCE-POP
1	10	0.010	0.067	0.126
2	35	0.004	0.057	0.150
3	17	0.008	0.073	0.171
4	13	0.003	0.034	0.089

\* -  $\text{ng}/\text{g}$  wet weight

**Table D.35.** Calculation results: net gaseous flux of PCB-28 to vegetation,  $\text{ng}/\text{m}^2/\text{d}$  calculated by models

N	Air concentration, $\mu\text{g}/\text{m}^3$	EVN-BETR and UK-MODEL	SimpleBox	MSCE-POP
1	10	0.09	2.33	0.41
2	35	0.03	3.42	0.48
3	17	0.07	2.88	0.55
4	13	0.03	1.61	0.29



**Fig. D.7.** Comparison of concentration in vegetation calculated by different models, ng/g

**Table D.36.** Correlation coefficients for concentrations in vegetation

	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	0.81	0.42
SimpleBox	–	0.87

**Table D.37.** Correlation coefficients for net gaseous flux

	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	-0.02	0.32
SimpleBox	–	0.86

**Table D.38.** Coefficients of regression dependence between the models ( $\alpha / \beta$ ) for concentrations in vegetation

	SimpleBox	MSCE-POP
EVN-BETR and UK-MODEL	3.98 / 0.033	4.25 / 0.11
SimpleBox	-	1.78 / 0.03

**Table D.39.** Coefficients of regression dependence between the models ( $\alpha / \beta$ ) for net gaseous flux

	SimpleBox
MSCE-POP	0.12/ 0.11