Annex B

COMPARISON OF PHYSICAL-CHEMICAL PROPERTIES AND DEGRADATION RATES OF PCB-28 AND PCB-180 BETWEEN INDIVIDUAL MODELS

Table B.1. *"Reference data sets" of physical-chemical properties and degradation rates of PCB-28 and PCB-180**

Description		Numerical values		**Comments**	**Reference**
		PCB-28	PCB-180		
Air/water Henry's law constant, K_H (Pa·m^3/mol)					
Temperature dependent: $H = H_0 \exp(-a_H (1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a_H is a parameter of temperature dependence.	H_0 (T_0), Pa·m^3/mol	9.46E+00	1.98E+00	Coefficients are recalculated from the following temperature dependence: $\log H = \log H(25^0C) - (\Delta U_{aw} + R \cdot 298.15)/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{aw} - internal energy of phase transfer, kJ/mol (PCB-28: 52.3; PCB-180: 63.6). $H(25^0C)$ - Henry 's law constant at 25^{0}C, Pa·m^3/mol (PCB-28: 30.5; PCB-180: 8.13).	*Li et al.*, 2003
	a_H	6588.7	7947.9		
Air/water partition coefficient, K_{aw} (dimensionless)					
Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{aw} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K^0_{AW} (T_0), dimensionless	4.02E-03	8.42E-04	Coefficients are recalculated from the following temperature dependence: $\log K_{aw} = \log K_{aw}(25\ ^0C) - \Delta U_{aw}/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{aw} - internal energy of phase transfer, kJ/mol (PCB-28: 52.3; PCB-180: 63.6). $K_{aw}(25^0C)$ - dimensionless air/water partition coefficient at 25^{0}C, estimated from: $K_{aw}(25^0C) = H(25\ ^0C)/(R \cdot 298.15)$	*Li et al.*, 2003
	a_{Kaw}	6290.6	7649.7		
Subcooled liquid vapour pressure, p_{ol} (Pa)					
Temperature dependent: $p_{ol} = p^0_{ol} \exp(-a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{ol} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{ol} (T_0),	5.24E-03	1.51E-05	Coefficients are recalculated from the following temperature dependence: $\log p_{ol} = \log p_{ol}(25\ ^0C) - (\Delta U_a + R \cdot 298.15)/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_a - internal energy of phase transfer, kJ/mol (PCB-28: 74.2; PCB-180:89.6). $p_{ol}(25^0C)$ - vapour pressure at 25^{0}C, *Pa* (PCB-28: 2.70E-2; PCB-180:1.08E-4).	*Li et al.*, 2003
	a_p	9222.9	11075.2		
Octanol/water partition coefficient, K_{ow} (dimensionless)					
Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	K^0_{ow} (T_0), dimensionless	8.09E+05	2.70E+07	Coefficients are recalculated from the following temperature dependence: $\log K_{ow} = \log K_{ow}(25\ ^0C) - \Delta U_{OW}/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{ow} - internal energy of phase transfer, kJ/mol (PCB-28: -26.3 ; PCB-180: -29.1). $K_{ow}(25^0C)$ - octanol/water partition coefficient at 25 ^{0}C, dimensionless (PCB-28: 4.61E+5; PCB-180:1.45E+7)	*Li et al.*, 2003
	a_{Kow}	3163.3	3500.1		

Description		Numerical values		Comments	Reference
		PCB-28	PCB-180		
Octanol/air partition coefficient, K_{oa} (dimensionless)					
Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	3.77E+08	1.06E+11	Coefficients are recalculated from the following temperature dependence: $\log K_{oa} = \log K_{oa}(25\ ^0C) - \Delta U_{oa}/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: T - temperature; R - Universal Gas Constant; ΔU_{oa} - internal energy of phase transfer, kJ/mol (PCB-28: -78.5; PCB-180: -92.8). K_{oa}(25 ^{0}C) - octanol/air partition coefficient at 25^{0}C, dimensionless (PCB-28: 7.05E+7; PCB-180:1.46E+10);	*Li et al.*, 2003
	a_{Koa}	9441.9	11161.9		
Organic carbon/water partition coefficient, K_{oc} (dimensionless)					
Regression relation: $K_{oc} = regc\ K_{ow}^b$ where *regc* and b are regression coefficients	*regc*	0.41	0.41	*Koc* is calculated from *Kow* , where *Kow* is the temperature dependent octanol-water partition coefficient	*Karikhoff*, 1981
	b	1	1		
Water solubility, S_{WL} (mol/m^3)					
Temperature independent	S_{WL} (T), mol/m^3	5.53E-04	7.57E-06	Values are calculated for T = 283.15 with the help of the following temperature dependence: $\log S_{WL} = \log S_{WL}(25^0C) - \Delta U_W/(\ln(10) \cdot R) \cdot (1/T - 1/298.15)$ where: R - Universal Gas Constant; ΔU_W - internal energy of phase transfer, kJ/mol (PCB-28: 22.0; PCB-180: 26.0). S_{WL}(25^{0}C) - water solubility, mol/m^3 at 25^{0}C (PCB-28: 8.85E-4; PCB-180:1.32E-5).	*Li et al.*, 2003
Degradation rate constants, k_d (1/s)					
Degradation in atmosphere: Temperature independent	k_{air} (T), 1/s	3.50E-07	3.50E-08	Degradation rate constant in the air is conversed from half-life values, *h* (PCB-28: 550; PCB-180: 5500): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	*Mackay et al*, 1992
Degradation in soil: Temperature independent	k_{soil} (T), 1/s	3.50E-09	3.50E-09	Degradation rate constant in soil is conversed from half-life values (PCB-28:55000; PCB-180: 55000): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	*Mackay et al*, 1992
Degradation in water: Temperature independent	k_{water} (T), 1/s	1.13E-08	3.50E-09	Degradation rate constant in water is conversed from half-life values (PCB-28: 17000; PCB-180: 55000): k_d = 0.693/ t1/2 where k_d is the first-order rate constant (s^{-1}) and t1/2 is the half-life (s).	*Mackay et al*, 1992
Degradation in sediment: Temperature independent	k_{sed} (T), 1/s	3.50E-09	3.50E-09	Degradation rate constant in sediment is conversed from half-life values (PCB-28: 55000; PCB-180: 55000): $k_d = 0.693/ t_{1/2}$ where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).	*Mackay et al*, 1992

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here for the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

Table B.2. *The Henry's law constant and the air/water partition coefficient of PCBs (data sets of the participating POP models)**

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
CAM/POPs	Temperature dependent: $H = H_0 \exp(-a_H(1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a is a parameter of temperature dependence. Temperature dependent: $K_{aw} = H/(R{\cdot}T)$	H_0, Pa·m^3/mol	-	2.53E-01	Coefficient a_H of the exponential equation are recalculated from the coefficient of the following temperature dependence: $H = H_0{\cdot}10^{(-3416\,(1/T - 1/To))}$ with the help of the following formula: $a_H = \ln(10){\cdot}\,3416$, It was obtained from the following temperature dependence: $\log(H/H(25^0C))$= slop $(1/T - 1/298)$ $H(25^0C)$ - Henry 's law constant at 25^{0}C, Pa·m^3/mol (PCB-180: 1.01)	*Achman, Hornbucle, Eisenreich* [1993]
		a_H	-	7865.6		
		T_0, K	-	283.15		
SimpleBox	Temperature dependent: $H = H_0 \exp(-a_H(1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a_H is a parameter of temperature dependence.	H_0, Pa·m^3/ mol	9.46E+00	1.98E+00	Same to the "reference data set"	*Li et al.*, 2003
		a_H	6588.7	7947.9		
		T_0, K	283.15	283.15		
EVN-BETR and UK-MODEL	H is temperature independent.	H, Pa·m^3/mol	30.5	8.18	Calculated as H = Vapour Pressure (Pa) / Water Solubility (mol/m^3) at 25^{o}C	*Li et al.*, 2003
	Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{aw} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K_{aw}, dimensionless	4.02E-03	8.48E-04	At 10^{o}C, calculated as: $K_{aw}(T_0) = 10^{\log Kaw} \cdot a$, $a = \exp[(\Delta H_{vap}/R) \cdot (1/T_0 - 1/T)]$. ΔH_{vap} = 62.8 KJ/mol: Enthalpy of vaporisation (from water to air) Here $a_{Kaw} = \Delta H_{vap}/R$	
		a_{Kaw}	7553.5	7553.5		
		T_0, ^{0}K	283.15			
CliMoChem	Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{aw} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K^0_{aw}, dimensionless	4.63E-03	1.83E-03	$K_{aw}(T) = K_{aw}(T_{ref}) \exp(dH_{Kaw}/R\,(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{aw}(T_{ref})$ = Henry 's law constant at T_{ref} (dimensionless): PCB 28: 1.27E -2 ; PCB 180: 8.92E-3 dH_{kaw} = phase transfer enthalpy (J/mol): PCB 28: 47200; PCB 180:74100 R = universal gas constant (8.3145 J/mol·K)	*Beyer et al.*, 2002
		a_{Kaw}	5680	8910		
		T_0, K	283.15			
DEHM-POP	Temperature dependent: $K_{aw} = K^0_{aw} \exp(-a_{Kaw}(1/T - 1/T_0))$ where T - temperature (K), K^0_{aw} is the value at the reference temperature T_0, and a_{Kaw} is a parameter of temperature dependence.	K^0_{aw}, dimensionless	4.63E-03	1.83E-03	$K_{aw}(283.15) = K^0_{aw}(298.15) \exp(-a_{Kaw}(1/T - 1/T_0))$, where $K^0_{AW}(298.15)$ = 1.27E-2, 8.92E-3 for PCB 28 and 180 respectively	*Beyer at al.*, 2002
		a_{Kaw}	5680	8917		
		T_0, K	283.15			
MSCE-POP	Temperature dependent: $H = H_0 \exp(-a_H(1/T - 1/T_0))$ where T - temperature (K), H_0 is the value at the reference temperature T_0, and a_H is a parameter of temperature dependence. Temperature dependent: $K_{aw} = H/(R \cdot T)$	H_0, Pa·m^3/mol	7.642	2.388	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log H = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10){\cdot}$ A; $H_0 = 10^{(-A/To + B)}$; where $A = \Delta H_W/2.303R$; $B = \log H_{298} + \Delta H_W/2.303R(298)$. where H_{298} is Henry's law constant (Pa·m^3/mol) at 25^{0}C (PCB-28: 28.58; PCB-180: 10.74); ΔH_W is the enthalpy of volatilization from water, kJ/mol (PCB-28: 61.8: PCB-180: 71.3)	*Burkhard et al.*, 1985 *Dunnivant et al.*, 1992
		a_H	7430	8575		
		T_0, K	283.15	283.15		

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here at the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

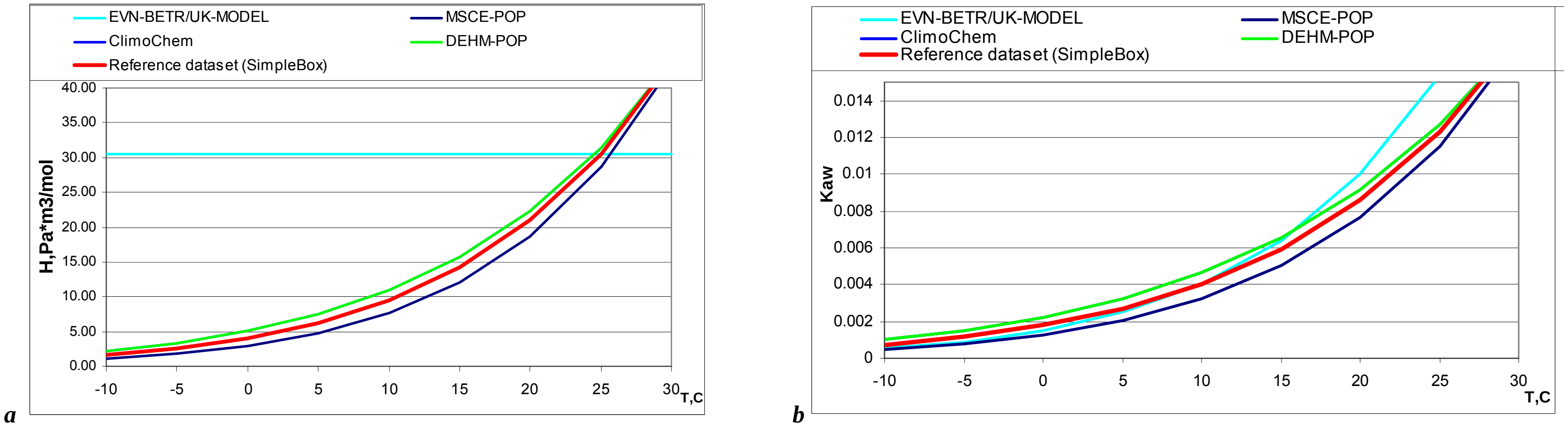

Fig. B.1. Comparison of temperature dependencies of Henry's law constant (H, Pa·m³/mol) and air/water partition coefficient (K_{aw}, dimensionless) of PCB-28.

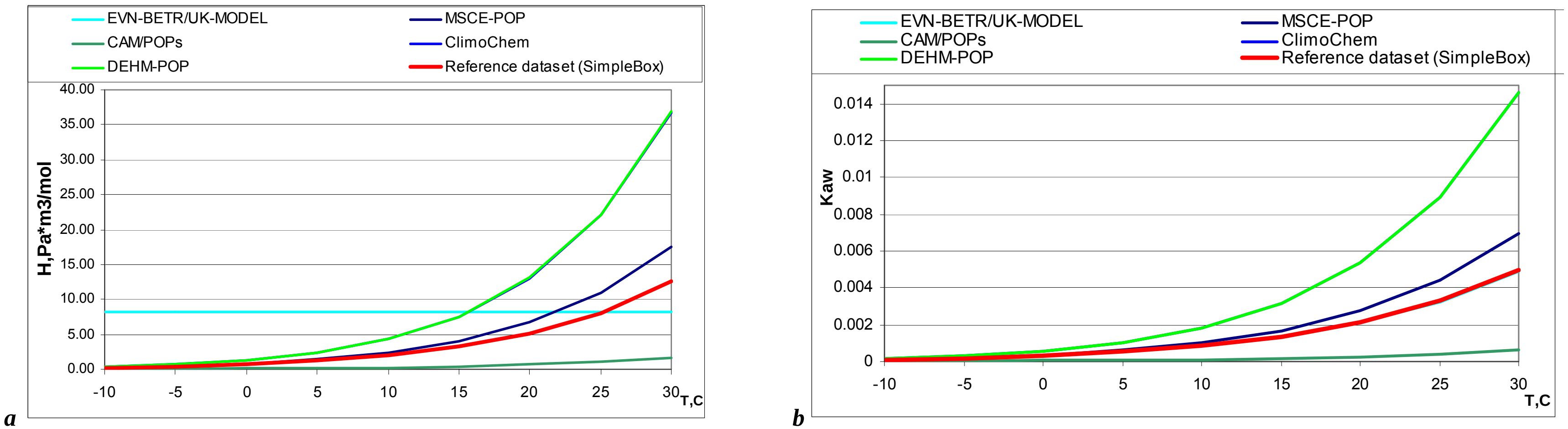

Fig. B. 2. Comparison of temperature dependencies of Henry's law constant (H, Pa·m3/mol) and air/water partition coefficient (Kaw, dimensionless) of PCB-180.

Table B.3. Absolute values and statistical parameters of Henry's law constant (H, Pa·m3/mol) and air/water partition coefficient (Kaw, dimensionless) of PCB-28 for three arbitrary temperatures (-10°C, 10°C and 25°C) and coefficients of temperature dependencies

	H, Pa·m3/mol				Kaw, dimensionless			
	-10°C	10°C	25°C	aH	-10°C	10°C	25°C	aKaw
SimpleBox	1.61E+00	9.46E+00	3.05E+01	6588.7	7.43E-04	4.02E-03	1.23E-02	6290.6
EVN-BETR and UK-MODEL	3.05E+01	3.05E+01	3.05E+01	-	5.29E-04	4.02E-03	1.54E-02	7553.5
CliMoChem	2.21E+00	1.09E+01	3.15E+01	-	1.01E-03	4.63E-03	1.27E-02	5680
DEHM-POP	2.21E+00	1.09E+01	3.15E+01	-	1.01E-03	4.63E-03	1.27E-02	5680
MSCE-POP	1.04E+00	7.64E+00	2.86E+01	7430	4.75E-04	3.25E-03	1.15E-02	-
"Reference data set"	1.61E+00	9.46E+00	3.05E+01	6588.7	7.43E-04	4.02E-03	1.23E-02	6290.6
min	1.04E+00	7.64E+00	2.86E+01	6588.7	4.75E-04	3.25E-03	1.15E-02	5680.0
max	3.05E+01	3.05E+01	3.15E+01	7430.0	1.01E-03	4.63E-03	1.54E-02	7553.5
arith. mean	6.53E+00	1.31E+01	3.05E+01	6869.1	7.51E-04	4.09E-03	1.28E-02	6298.9
median	1.91E+00	1.02E+01	3.05E+01	6588.7	7.43E-04	4.02E-03	1.25E-02	6290.6
geom. mean	2.72E+00	1.16E+01	3.05E+01	6858.0	7.22E-04	4.07E-03	1.28E-02	6263.9
max/min	2/29*	1/4*	1	1.1	2	1	1	1.3

* - the first value is calculated without the temperature independent value of H (EVN-BETR and UK-MODEL), the second value is calculated taking it into account.

Table B.4. *Absolute values and statistical parameters of Henry's law constant (H, Pa·m^3/mol) and air/water partition coefficient (K_{aw}, dimensionless) of PCB-180 for three arbitrary temperatures (-10°C, 10°C and 25°C) and coefficients of temperature dependencies*

	H, Pa·m^3/mol				K_{aw}, dimensionless			
	-10°C	10°C	25°C	a_H	-10°C	10°C	25°C	a_{Kaw}
CAM/POPs	3.06E-02	2.53E-01	1.02E+00	7865.6	1.40E-05	1.07E-04	4.13E-04	-
SimpleBox	2.35E-01	1.98E+00	8.13E+00	7947.9	1.08E-04	8.42E-04	3.28E-03	7649.7
EVN-BETR and UK-MODEL	8.18E+00	8.18E+00	8.18E+00	-	1.12E-04	8.48E-04	3.25E-03	7553.5
CliMoChem	3.66E-01	4.31E+00	2.21E+01	-	1.67E-04	1.83E-03	8.91E-03*	8910*
DEHM-POP	3.66E-01	4.31E+00	2.21E+01	-	1.67E-04	1.83E-03	8.92E-03*	8917*
MSCE-POP	2.39E-01	2.39E+00	1.10E+01	8575	1.09E-04	1.01E-03	4.42E-03	-
"Reference data set"	2.35E-01	1.98E+00	8.13E+00	7947.9	1.08E-04	8.42E-04	3.28E-03	7649.7
min	3.06E-02	2.53E-01	1.02E+00	7865.6	1.40E-05	1.07E-04	4.13E-04	7553.5
max	8.18E+00	8.18E+00	2.21E+01	8575.0	1.67E-04	1.83E-03	8.92E-03	8917.0
arith. mean	1.38E+00	3.34E+00	1.15E+01	8084.1	1.12E-04	1.04E-03	4.64E-03	8136.0
median	2.39E-01	2.39E+00	8.18E+00	7947.9	1.09E-04	8.48E-04	3.28E-03	7649.7
geom. mean	3.32E-01	2.32E+00	8.40E+00	8079.2	9.20E-05	8.05E-04	3.38E-03	8111.6
max/min	12/267***	17/32***	22/22***	1.1	12	17	22	1.2

*- difference in absolute values obtained from identical temperature dependencies can be explained by accuracy of coefficient recalculation.

*** - the first value is calculated without the temperature independent value of H (EVN-BETR and UK-MODEL), the second value is calculated taking it into account.

Table B.5. *The subcooled liquid vapour pressure of PCBs (data sets of the participating POP models)**

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
CAM/POPs	Temperature dependent: $p_{ol} = p^0_{ol}\exp(-a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{ol} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{ol}, Pa	-	1.67E-05	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $p_{ol} = 10^{(m/T + b)}$ where T - temperature (^{0}K); m = -5042 - parameter of temperature dependence, and b = 13.03 - parameter depended on molecular weight. It was obtained from the following original equation: $\log(p_{ol}) = -Q/(2.303\,RT) + b$ where: T - temperature; R - Universal Gas Constant; Q - the heat of vaporisation (kJ/mol)	*Harner et al*., 1996; *Falconer et al.,* 1995
		a_p	-	11610		
		$T_{0,}$ K	-	283.15		
SimpleBox	Temperature dependent: $p_{OL} = p^0_{OL}\exp(-a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{OL} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{OL},Pa	5.24E-03	1.51E-05	Same to the "reference data set"	*Li et al.,* 2003
		a_p	9222.9	11075.2		
		$T_{0,}$ K	283.15	283.15		
EVN-BETR and UK-MODEL	Temperature independent:	p_{OL}, Pa	2.70E-02	1.08E-04	T = 25°C	*Li et al.,* 2003
MSCE-POP	Temperature dependent: $p_{ol} = p^0_{ol}\exp(-a_p(1/T - 1/T_0))$ where T - temperature (K), p^0_{ol} is the value at the reference temperature T_0, and a_p is a parameter of temperature dependence.	p^0_{OL}, Pa	6.43E-03	1.67E-05	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{ol}$ (Pa) = $-A/T(K) + B$ with the help of the following formulas: $a_p = \ln(10)\cdot A$, $p^0_{ol} = 10^{(-A/To + B)}$ where; A = 4075 and 5072 for PCB-28 and PCB-180 respectively; B = 12.20 and 13.03 for PCB-28 and PCB-180 respectively	*Falconer and Bidleman,* 1994
		a_p	9383	11610		
		$T_{0,}$ K	283.15	283.15		

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here at the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

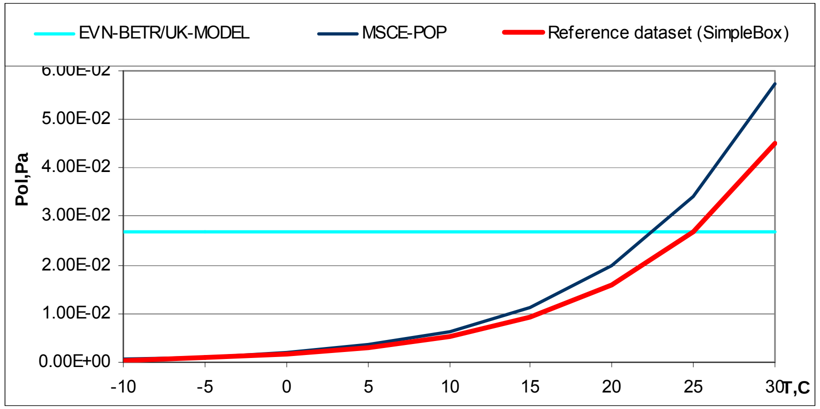

Fig. B.3. *Comparison of temperature dependencies of subcooled liquid vapour pressure of PCB-28 used in data sets of the participating POP models and in "reference data set"*

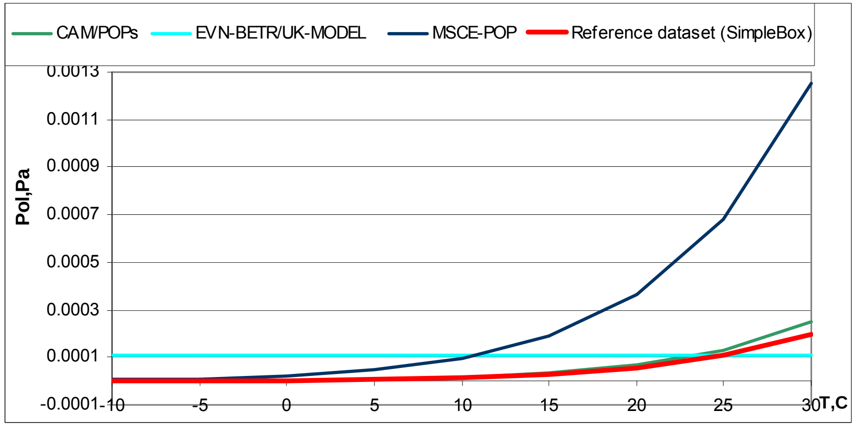

Fig. B.4. *Comparison of temperature dependencies of subcooled liquid vapour pressure of PCB-180 used in data sets of the participating POP models and in "reference data set"*

Table B.6. *Absolute values, coefficients of temperature dependence and statistical parameters of subcooled liquid vapour pressure of PCB-28 for three arbitrary temperatures (-10°C, 10°C and 25°C)*

	p_{0L}, Pa			a_p
	-10°C	10°C	25°C	
SimpleBox	4.41E-04	5.24E-03	2.70E-02	9222.9
EVN-BETR/UK-MODEL	2.70E-02	2.70E-02	2.70E-02	-
MSCE-POP	5.18E-04	6.43E-03	3.41E-02	9383
Reference data set	4.41E-04	5.24E-03	2.70E-02	9222.9
min	4.41E-04	5.24E-03	2.70E-02	9222.9
max	2.70E-02	2.70E-02	3.41E-02	9383.0
arith. mean	7.10E-03	1.10E-02	2.88E-02	9276.3
median	4.79E-04	5.84E-03	2.70E-02	9222.9
geom. mean	1.28E-03	8.31E-03	2.86E-02	9276.0
max/min	1.2/61.3*	1.2/5.2*	1.3	1.02

* - the first value is calculated without the temperature independent value of p_{0L} (EVN-BETR and UK-MODEL), the second value is calculated taking it into account

Table B.7. *Absolute values, coefficients of temperature dependence and statistical parameters of subcooled liquid vapour pressure of PCB-180 for three arbitrary temperatures (-10°C, 10°C and 25°C)*

	p_{0L}, Pa			a_p
	-10°C	10°C	25°C	
CAM/POPs	7.40E-07	1.67E-05	1.31E-04	11610
SimpleBox	7.73E-07	1.51E-05	1.08E-04	11075.2
EVN-BETR/UK-MODEL	1.08E-04	1.08E-04	1.08E-04	-
MSCE-POP	5.07E-06	9.69E-05	6.84E-04	11610
Reference data set	7.73E-07	1.51E-05	1.08E-04	11075.2
min	7.40E-07	1.51E-05	1.08E-04	11075.2
max	1.08E-04	1.08E-04	6.84E-04	11610.0
arith. mean	2.31E-05	5.04E-05	2.28E-04	11342.6
median	7.73E-07	1.67E-05	1.08E-04	11342.6
geom. mean	3.00E-06	3.31E-05	1.62E-04	11339.4
max/min	6.8/145.9*	6.4/7.2*	6.3	1.05

* - the first value is calculated without the temperature independent value of p_{0L} (EVN-BETR and UK-MODEL), the second value is calculated taking it into account

Table B.8. *The octanol/water partition coefficient of PCBs (data sets of the participating POP models)**

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
CAM/POPs	Temperature dependent: $K_{ow} = K_{oa} \cdot H/RT$ where T - temperature (K); R - Universal Gas Constant; H - Henry's law constant; K_{oa} - Octanol/air partition coefficient (dimensionless)		-	-	These values are calculated with the help of temperature dependencies of H and K_{oa}.	This study
SimpleBox	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	$K^0_{ow}(T_0)$, dimen-sionless	8.09E+05	2.70E+07	Same to the "reference data set"	*Li et al.*, 2003
		a_{Kow}	3163.3	3500.1		
		T_0, K	283.15	283.15		
EVN-BETR and UK-MODEL	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence.	K^0_{ow}, dimen-sionless	8.02E+05	2.69E+07	For 10°C, calculated as $K_{ow}(T_0) = 10^{\log Kow} \cdot a$, $a = \exp[(\Delta H_{sol} / R) \cdot (1/T_0 - 1/T)]$. ΔH_{sol} = -31.1 KJ/mol: Enthalpy of solution (from octanol to water) Here: $a_{Kow} = \Delta H_{sol} / R$	*Li et al.*, 2003
		a_{Kow}	3740.5	3740.5		
		T_0, K	283.15	283.15		
CliMoChem	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence (-dH/R)	K^0_{ow}, dimen-sionless	9.41E+05	1.84E+07	$K_{ow}(T) = K_{ow}(T_{ref}) \exp((dHK_{ow}/R)(1/T_{ref} - 1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{ow}(T_{ref})$ = Octanol/water partition coefficient at T_{ref} PCB 28: 5.13E+5; PCB 180: 1.54E+7 dHK_{ow} = phase transfer enthalpy (J/mol) PCB 28: -28400; PCB 180: -8270 R = universal gas constant (8.3145 J/mol·K)	*Beyer et al.*, 2002
		a_{Kow}	3415.7	994.6		
		T_0, K	283.15	283.15		
DEHM-POP	Temperature dependent: $K_{ow} = K^0_{ow} \exp(a_{Kow}(1/T - 1/T_0))$ where T - temperature (K), K^0_{ow} is the value at the reference temperature T_0, and a_{Kow} is a parameter of temperature dependence (-dH/R)	K^0_{ow}, dimen-sionless	9.41E+05	1.84E+07	K_{ow} (283.15) = K^0_{ow} (298.15) exp(aK_{ow} (1/T - 1/T_0), where K^0_{ow} (298.15) = 5.13E+5; 1.54E+7 for PCB-28 and 180 respectively; aK_{ow} = dHK_{ow}/R dHK_{ow} = phase transfer enthalpy (J/mol) PCB 28: -28400; PCB 180: -8270 R = universal gas constant (8.3145 J/mol·K)	*Beyer et al.*, 2002
		a_{Kow}	3414.5	994.6		
		T_0, K	283.15	283.15		
MSCE-POP	Temperature independent	K_{ow}, dimen-sionless	6.31E+5	2.29E+7	PCB-28: log K_{ow} = 5.8 PCB-180: log K_{ow} = 7.36	*Mackay et al.*, 1992; *Hawker and Connell*, 1988

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here for the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

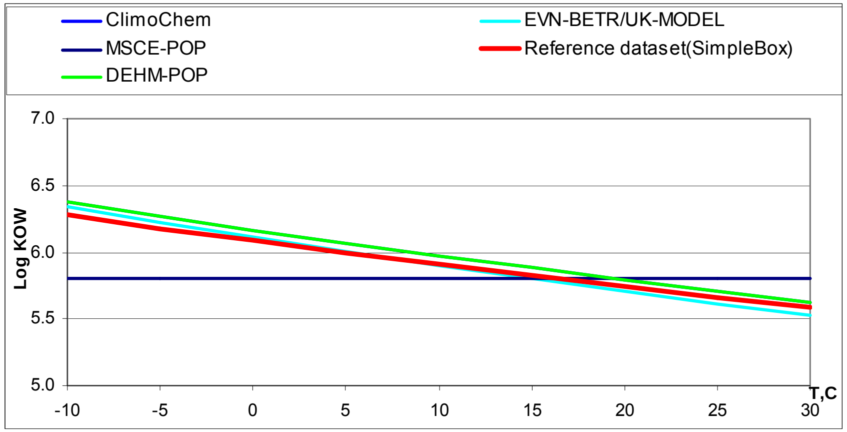

Fig. B.5. *Comparison of temperature dependencies of* $logK_{ow}$ *of PCB-28 used in the models and in "reference data set"*

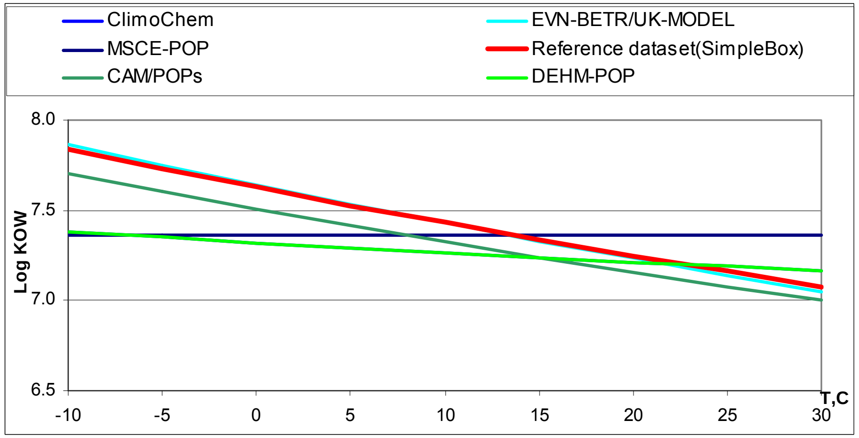

Fig. B.6. *Comparison of temperature dependencies of* $logK_{ow}$ *of PCB-180 used in the models and in "reference data set"*

Table B.9. *Absolute values, coefficients of temperature dependence and statistical parameters of octanol/water partition coefficient of PCB-28 for ttree arbitrary temperatures (-10°C, 10°C and 25°C)*

	K_{ow}			a_{Kow}
	-10°C	10°C	25°C	
SimpleBox	1.89E+06	8.09E+05	4.61E+05	3163.3
EVN-BETR/UK-MODEL	2.19E+06	8.02E+05	4.13E+05	3740.5
CliMoChem	2.35E+06	9.41E+05	5.13E+05	3415.7*
DEHM-POP	2.35E+06	9.41E+05	5.13E+05	3414.5*
MSCE-POP	6.31E+05	6.31E+05	6.31E+05	-
Reference data set	1.89E+06	8.09E+05	4.61E+05	3163.3
min	6.31E+05	6.31E+05	4.13E+05	3163.3
max	2.35E+06	9.41E+05	6.31E+05	3740.5
arith. mean	1.88E+06	8.25E+05	5.06E+05	3433.5
median	2.19E+06	8.09E+05	5.13E+05	3415.1
geom. mean	1.71E+06	8.16E+05	5.01E+05	3427.4
max/min	1.2/3.7**	1.2/1.5**	1.2/1.5**	1.2

** - difference in absolute values obtained for identical temperature dependencies can be explained by accuracy of coefficient recalculation;*

*** - the first value is calculated without the temperature independent value of Kow (MSCE-POP), the second value is calculated taking it into account*

Table B.10. *Absolute values, coefficients of temperature dependence and statistical parameters of octanol/water partition coefficient of PCB-180 for three arbitrary temperatures (-10°C,10°C and 25°C)*

	K_{ow}			a_{Kow}
	-10°C	10°C	25°C	
CAM/POPs	5.11E+07	2.12E+07	1.20E+07	-
SimpleBox	6.91E+07	2.70E+07	1.45E+07	3500.1*
EVN-BETR/UK-MODEL	7.34E+07	2.69E+07	1.38E+07	3740.5*
CliMoChem	2.40E+07	1.84E+07	1.54E+07	994.6
DEHM-POP	2.40E+07	1.84E+07	1.54E+07	994.6
MSCE-POP	2.29E+07	2.29E+07	2.29E+07	-
Reference data set	6.91E+07	2.70E+07	1.45E+07	3500.1*
min	2.29E+07	1.84E+07	1.20E+07	994.6
max	7.34E+07	2.70E+07	2.29E+07	3740.5
arith. mean	4.27E+07	2.27E+07	1.64E+07	2307.5
median	2.40E+07	2.29E+07	1.54E+07	2247.4
geom. mean	3.68E+07	2.24E+07	1.61E+07	1897.0
max/min	3.1/3.2**	1.5/1.5**	1.3/1.9**	3.8

** - difference in absolute values obtained from identical temperature dependencies can be explained by accuracy of coefficient recalculation*

*** - the first value is calculated without the temperature independent value of Kow (MSCE-POP), the second value is calculated taking it into account*

Table B.11. *The octanol/air partition coefficient of PCBs (data sets of the participating POP models)**

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
CAM/POPs	Temperature dependent: $K_{oa} = 10^{(a/T + b)}$ where T - temperature; P - liquid vapour pressure p_{ol} (Pa)	a	-	-529-19.25 logP	These values are calculated with the help of temperature dependencies of p_{ol}	*Harner et al,* 1996; 1998
		b	-	8.2995-0.95 logP		
SimpleBox	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	3.77E+08	1.06E+11	Same to the "reference data set"	*Li et al.,* 2003
		a_{Koa}	9441.9	11161.9		
		T_0, K	283.15	283.15		
EVN-BETR and UK-MODEL	Temperature dependent:	K^0_{oa} (T_0), dimensionless	1.99E+08	3.18E+10	At 10°C, calculated as $K_{oa} = K_{ow} / K_{aw}$	
		T_0, K	283.15	283.15		
DEHM-POP	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	5.84E+08	9.78E+10	K_{oa} (283.15) = K^0_{oa} (298.15) $\exp(a_{Koa}(1/T - 1/T_0))$, where K^0_{oa}(298.15) = 1.16E+8, 1.68E+10 for PCB-28 and 180 respectively $a_{Koa} = dHK_{oa}/R$ dHK_{oa} = phase transfer enthalpy (J/mol) PCB 28: -75620; PCB-180: -82410 R = universal gas constant (8.3145 J/mol·K)	*Beyer et al., 2002*
		a_{Koa}	9095.0	9911.6		
		T_0, K	283.15	283.15		
MSCE-POP	Temperature dependent: $K_{oa} = K^0_{oa} \exp(a_{Koa}(1/T - 1/T_0))$ where T - temperature (K), K^0_{oa} is the value at the reference temperature T_0, and a_{Koa} is a parameter of temperature dependence.	K^0_{oa} (T_0), dimensionless	5.78E+8	2.07E+11	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_{oa} = A/T(K) - B$ with the help of the following formulas: $a_p = \ln(10) \cdot A$, $K^0_{oa}(T_0) = 10^{(A/To - B)}$ where: $A = 3792^a$ and 4535^b for PCB-28 and PCB-180 respectively; $B = 4.63^a$ and 4.70^b for PCB-28 and PCB-180 respectively	[a]-estimated with the use of data [*Harner and Bidleman* 1996] for PCB-29 [b]-*Harner and Bidleman* [1996]
		a_{Koa}	8731	10442		
		T_0, K	283.15	283.15		

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here for the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

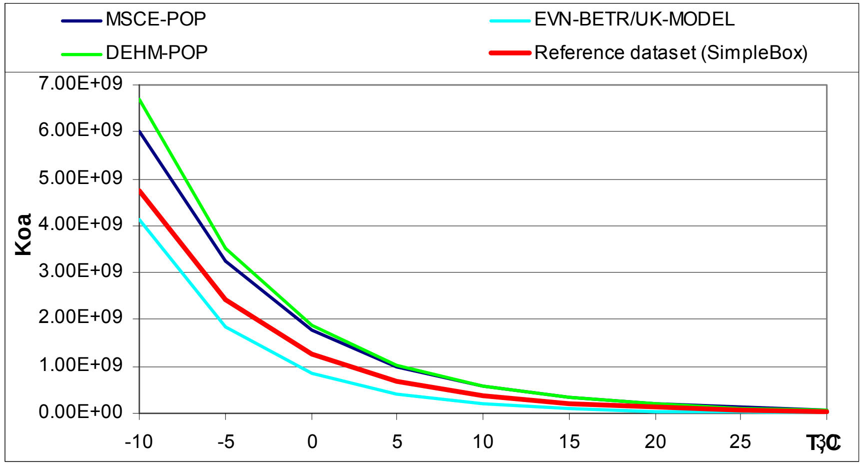

Fig. B.7. *Comparison of temperature dependencies of octanol/air partition coefficient of PCB-28 used in the participating POP models and in "reference data set"*

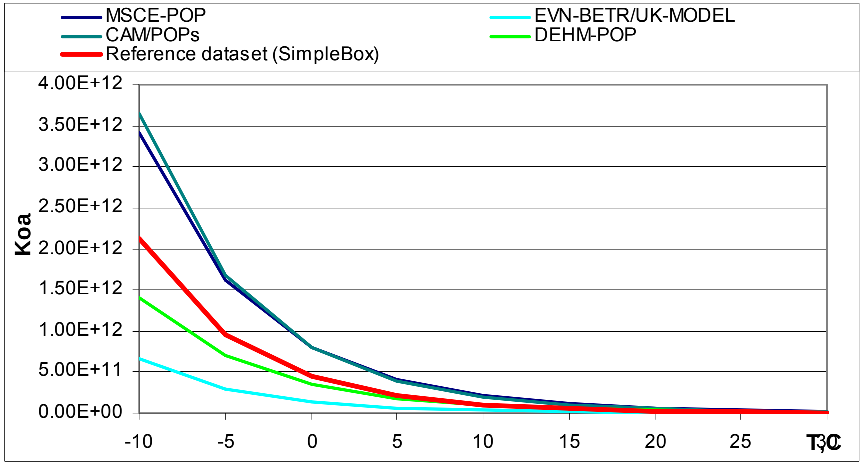

Fig. B.8. *Comparison of temperature dependencies of octanol/air partition coefficient of PCB-180 used in the participating POP models and in "reference data set"*

Table B.12. Absolute values, coefficients of temperature dependencies and statistical parameters of octanol/air partition coefficient of PCB-28 for three arbitrary temperatures (-10℃, 10℃ and 25℃)

	K_{oa}			a_{Koa}
	-10°C	10°C	25°C	
SimpleBox	4.75E+09	3.77E+08	7.04E+07	9441.9
EVN-BETR/UK-MODEL	4.14E+09	2.00E+08	2.68E+07	-
DEHM-POP	6.71E+09	5.84E+08	1.16E+08	9095.0
MSCE-POP	6.02E+09	5.78E+08	1.23E+08	8731
Reference data set	4.75E+09	3.77E+08	7.04E+07	9441.9
min	4.14E+09	2.00E+08	2.68E+07	8731.0
max	6.71E+09	5.84E+08	1.23E+08	9441.9
arith. mean	5.27E+09	4.23E+08	8.12E+07	9177.5
mediana	4.75E+09	3.77E+08	7.04E+07	9268.5
geom. mean	5.19E+09	3.95E+08	7.17E+07	9172.7
max/min	2	3	5	1.1

Table B.13. Absolute values, coefficients of temperature dependencies and statistical parameters of octanol/air partition coefficient of PCB-180 for three arbitrary temperatures (-10℃, 10℃ and 25℃)

	K_{oa}			a_{Koa}
	-10°C	10°C	25°C	
CAM/POPs	3.65E+12	1.97E+11	2.91E+10	-
SimpleBox	2.12E+12	1.06E+11	1.46E+10	11161.9
EVN-BETR/UK-MODEL	6.58E+11	3.17E+10	4.26E+09	-
DEHM-POP	1.40E+12	9.78E+10	1.68E+10	9911.6
MSCE-POP	3.41E+12	2.07E+11	3.24E+10	10442
Reference data set	2.12E+12	1.06E+11	1.46E+10	11161.9
min	6.58E+11	3.17E+10	4.26E+09	9911.6
max	3.65E+12	2.07E+11	3.24E+10	11161.9
arith. mean	2.23E+12	1.10E+11	1.65E+10	10669.4
mediana	2.12E+12	1.06E+11	1.46E+10	10802.0
geom. mean	1.93E+12	9.37E+10	1.38E+10	10656.2
max/min	6	7	8	1.1

Table B.14. *The organic carbon/water partition coefficient of PCBs (data sets of the participating POP models)*

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
CAM/POPs	Regression relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	-	0.41	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partition coefficient	*Karickhoff*, 1981; *Mackay*, 1991; *Schnoor*, 1996
		b	-	1		
SimpleBox	Regression relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	0.41	Same to the "reference data set" K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partition coefficient	*Karikhoff*, 1981
		b	1	1		
EVN-BETR and UK-MODEL	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	0.41		*Karikhoff*, 1981
		b	1	1		
CliMoChem	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.35	0.35	K_{oc} is calculated from K_{ow}, where K_{ow} is the temperature dependent octanol-water partition coefficient	*Seth et al.*, 1999
		b	1	1		
DEHM-POP	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	0.41		*Mackay*, 1999
		b	1	1		
MSCE-POP	Regresion relation: $K_{oc} = regc\ K_{ow}^{b}$ where *regc* and *b* are regression coefficients	*regc*	0.41	0.41		*Karikhoff*, 1981
		b	1	1		

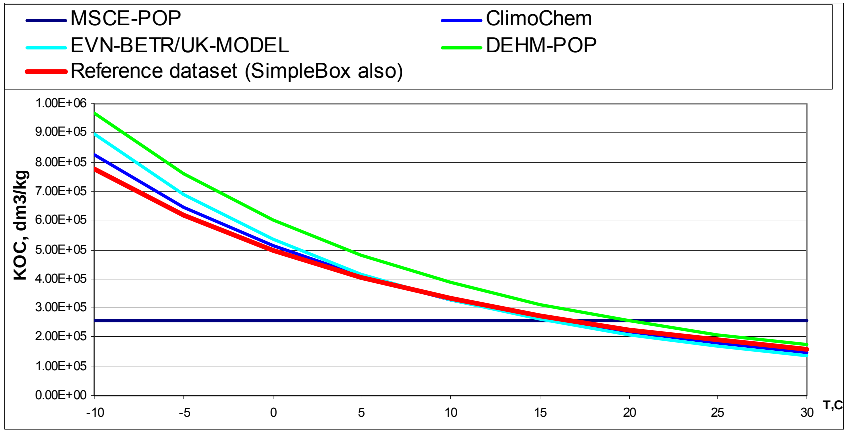

Fig. B.9. *Comparison of temperature dependencies of organic carbon/water partition coefficient of PCB-28 used in the participating POP models and in "reference data set"*

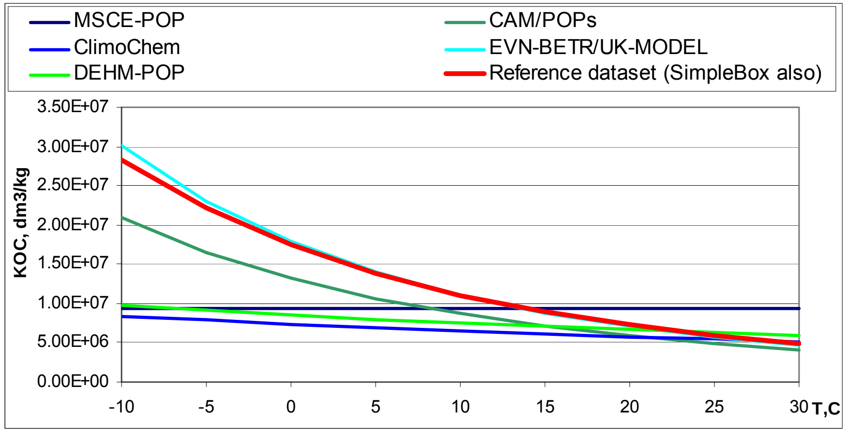

Fig. B.10. *Comparison of temperature dependencies of organic carbon/water partition coefficient of PCB-180 used in the participating POP models and in "reference data set"*

Table B.15. *Absolute values and statistical parameters of organic carbon/water partition coefficient of PCB-28 for three arbitrary temperatures (-10°C, 10°C and 25°C).*

	K_{oc}, dm^3/kg		
	-10°C	10°C	25°C
SimpleBox	7.75E+05	3.32E+05	1.89E+05
EVN-BETR/UK-MODEL	8.97E+05	3.29E+05	1.69E+05
CliMoChem	8.24E+05	3.29E+05	1.80E+05
DEHM-POP	9.65E+05	3.86E+05	2.10E+05
MSCE-POP	2.59E+05	2.59E+05	2.59E+05
Reference data set	7.75E+05	3.32E+05	1.89E+05
min	2.59E+05	2.59E+05	1.69E+05
max	9.65E+05	3.86E+05	2.59E+05
arith. mean	7.49E+05	3.28E+05	1.99E+05
mediana	8.00E+05	3.31E+05	1.89E+05
geom. mean	6.93E+05	3.25E+05	1.97E+05
max/min	3.7	1.5	1.5

Table B.16. *Absolute values and statistical parameters of organic carbon/water partition coefficient of PCB-180 for three arbitrary temperatures (-10°C, 10°C and 25°C).*

	K_{oc}, dm^3/kg		
	-10°C	10°C	25°C
CAM/POPs	2.09E+07	8.68E+06	4.92E+06
SimpleBox	2.83E+07	1.11E+07	5.94E+06
EVN-BETR/UK-MODEL	3.01E+07	1.10E+07	5.67E+06
CliMoChem	8.41E+06	6.44E+06	5.40E+06
DEHM-POP	9.85E+06	7.54E+06	6.32E+06
MSCE-POP	9.39E+06	9.39E+06	9.39E+06
Reference data set	2.83E+07	1.11E+07	5.94E+06
min	8.41E+06	6.44E+06	4.92E+06
max	3.01E+07	1.11E+07	9.39E+06
arith. mean	1.93E+07	9.32E+06	6.23E+06
mediana	2.09E+07	9.39E+06	5.94E+06
geom. mean	1.69E+07	9.15E+06	6.10E+06
max/min	3.6	1.7	1.9

Table B.17. *Water solubility of PCBs (data sets of the participating POP models)*

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
SimpleBox	Temperature independent	S_{WL} (T), mol/m^3	5.53E-04	7.57E-06	Same to the “reference data set” T = 10°C	*Li et al.*, 2003
EVN-BETR and UK-MODEL	Temperature independent.	S_{WL} (T), mol/m^3	8.85E-04	1.32E-05	T = 25°C	*Li et al.*, 2003

Table B.18. *Degradation rate constants of PCBs in the environmental media (data sets of the participating POP models)**

Model	Description	Numerical values			Comments	Reference
			PCB-28	PCB-180		
CAM/POPs	Degradation in atmosphere: Temperature dependent: $k_{air} = k^0_{air} \exp(-a_{kair}(1/T - 1/T_0))$ where T - temperature (K), k^0_{air} is the value at the reference temperature T_0, and a_{kair} is *a* parameter of temperature dependence	k^0_{air} T_0, cm^3/molec·s	-	1.25E-13	Coefficients of the exponential equation are recalculated from the following temperature dependence: $K_{OH} = K_{OH}^0 \exp(a(1/T_0 - 1/T)$ where K_{OH}^0 = 1.6E-13 is the value at the reference temperature T_0 (298 K), a = 1400 is parameter of temperature dependence.	This study
		a_{kair}	-	1400		
		T_0, *K*	-	283.15		
CliMoChem	Degradation in atmosphere: Temperature dependent: $k_{air} = k^0_{air} \exp(-a_{kair}(1/T - 1/T_0))$ where T - temperature (K), k^0_{air} is the value at the reference temperature T_0, and a_{kair} is *a* parameter of temperature dependence	k^0_{air} (T_0), cm^3/molec·s	7.95E-13	7.15E-14	$k_{air}(T) = k_{air}(T_{ref}) \exp((Ea_{air}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{air}(T_0)$ = degradation rate constant at T_0 (cm^3/d), PCB 28: 9.21E-8 ; PCB 180: 9.04E-9 Ea_{air} = activation energy (J/mol) PCB 28: 13700; PCB 180: 17800 R = universal gas constant (8.3145 J/mol·K) k^0_{air} = degradation rate constant at 283.15 (cm^3/d), PCB 28: 6.87E-08; PCB-180: 6.18E-09 $a_{kair} = Ea/R$	*Beyer et al.*, 2002
		a_{kair}	1647.7	2140.8		
		T_0, *K*	283.15	283.15		
	Degradation in soil: Temperature dependent: $k_{soil} = k^0_{soil} \exp(-a_{ksoil}(1/T - 1/T_0))$ where T - temperature (K), k^0_{soil} is the value at the reference temperature T_0, and a_{ksoil} is *a* parameter of temperature dependence	k^0_{soil} (T_0), 1/d	3.90E-09	3.07E-10	$k_{soil}(T) = k_{soil}(T_{ref}) \exp((Ea_{soil}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{soil}(T_0)$ = degradation rate constant at T_0 (1/*d*), PCB 28: 6.40E-4 ; PCB 180: 5.04E-5 Ea_{soil} = activation energy (J/mol) PCB 28: 30000; PCB 180: 30000 R = universal gas constant (8.3145 J/mol·K) k^0_{soil} = degradation rate constant at 283.15 (1/d) PCB 28: 3.37E-04; PCB-180: 2.65E-05 $a_{ksoil} = Ea_{soil} / R$	
		a_{ksoil}	3608.2	3608.2		
		T_0, *K*	283.15	283.15		
	Degradation in water: Temperature dependent: $k_{water} = k^0_{water} \exp(-a_{kwater}(1/T - 1/T_0))$ where T - temperature (K), k^0_{water} is the value at the reference temperature T_0, and a_{kwater} is *a* parameter of temperature dependence	k^0_{water} (T_0), 1/d	7.01E-08	4.22E-10	$k_{water}(T) = k_{water}(T_{ref}) \exp((Ea_{water}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{water}(T_0)$ = degradation rate constant at T_0 (1/d), PCB 28: 1.15E-2 ; PCB 180: 6.93E-5 Ea_{water} = activation energy (J/mol) PCB 153: 30000; PCB 28: 30000 ; PCB 180: 30000 R = universal gas constant (8.3145 J/mol·K) k^0_{water} = degradation rate constant at 283.15 (1/d), PCB 28: 6.06E-03; PCB-180: 3.65E-05 $a_{kwater} = Ea_{water}/R$	
		a_{kwater}	3608.2	3608.2		
		T_0, *K*	283.15	283.15		
	Degradation in vegetation*: Temperature dependent: $k_{veg} = k^0_{veg} \exp(-a_{kveg}(1/T - 1/T_0))$ where T - temperature (K), k^0_{veg} is the value at the reference temperature T_0, and a_{ksed} is *a* parameter of temperature dependence	k^0_{veg} (T_0), 1/d	7.71E-07	6.94E-08	$k_{veg}(T) = k_{veg}(T_{ref}) \exp((Ea_{veg}/R)(1/T - 1/T_0))$ T = temperature (283.15 K), T_0 = reference temperature (298.15 K) $k_{veg}(T_0)$ = degradation rate constant at T_0(1/d)*, PCB 28: 8.93E-2 ; PCB 180: 8.77E-3 Ea_{veg} = activation energy (J/mol) PCB 28: 13700 ; PCB 180: 17800 R = universal gas constant (8.3145 J/mol·K) $k_{veg}(T_0)$ = degradation rate constant at T_0 (1/d), PCB 28: 6.66E-02; PCB-180: 6.00E-03 $a_{kveg} = Ea_{veg} / R$	
		a_{kveg}	1647.7	2140.8		
		T_0, *K*	283.15	283.15		

<table>
<tr><th rowspan="2">Model</th><th rowspan="2">Description</th><th colspan="3">Numerical values</th><th rowspan="2">Comments</th><th rowspan="2">Reference</th></tr>
<tr><th></th><th>PCB-28</th><th>PCB-180</th></tr>
<tr><td rowspan="5">MSCE-POP</td><td rowspan="3">Degradation in atmosphere:
Temperature dependent:
$k_{air} = k^0_{air} \exp(-a_{kair}(1/T - 1/T_0))$
where T - temperature (K), k^0_{air} is the value at the reference temperature T_0, and a_{kair} is a parameter of temperature dependence</td><td>$k^0_{air}(T_0)$, $cm^3/(molec \cdot s)$</td><td>7.95E-13</td><td>7.16E-14</td><td rowspan="3">Coefficients of the exponential equation are recalculated from the following temperature dependence:
$k_{air} = A \cdot exp(-Ea/RT)$
with the help of the following formulas:
$a_{kair} = Ea/R$,
$k^0_{air} = A \cdot exp(-Ea/RT_0)$
where A = 2.70 E-10 and 1.40 E-10 are the pre-exponential multiplier values for PCB-28 and PCB-180 respectively, $m^3/(molec \cdot s)$;
E_A = 13720 and 17840 are the activation energies of interaction with OH-radical in air for PCB-28 and PCB-180 respectively, J/mol</td><td rowspan="3">Anderson and Hites, 1996; Beyer and Matthies, 2001</td></tr>
<tr><td>a_{kair}</td><td>1650.1</td><td>2145.6</td></tr>
<tr><td>T_0, K</td><td>283.15</td><td>283.15</td></tr>
<tr><td>Degradation in soil:
Temperature independent</td><td>k_{soil}, 1/s</td><td>7.4E-09</td><td>5.83E-10</td><td>Degradation rate constant in soil is conversed from half-life values (PCB-28: 26000 hours; PCB-180: 330000 hours):
$k_d = 0.693/ t_{1/2}$
where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).</td><td rowspan="2">Sinkkonen and Paasivirta, 2000</td></tr>
<tr><td>Degradation in water:
Temperature independent</td><td>k_{water}, 1/s</td><td>1.33E-07</td><td>8.02E-10</td><td>Degradation rate constant in water is conversed from half-life values (PCB-28: 1450 hours; PCB-180: 240000 hours):
$k_d = 0.693/ t_{1/2}$
where k_d is the first-order rate constant (s^{-1}) and $t_{1/2}$ is the half-life (s).</td></tr>
<tr><td rowspan="3">SimpleBox</td><td>Degradation in atmosphere:
Temperature independent</td><td>k_{air}, 1/s</td><td>3.50E-07</td><td>3.50E-08</td><td>Same half-lives as in "reference data set": PCB-28: 550; PCB-180: 5500 hours</td><td rowspan="3">Mackay et al. 1992</td></tr>
<tr><td>Degradation in soil:
Temperature independent</td><td>k_{soil}, 1/s</td><td>3.50E-09</td><td>3.50E-09</td><td>Same half-lives as in "reference data set": PCB-28: 55000; PCB-180: 55000 hours</td></tr>
<tr><td>Degradation in water:
Temperature independent</td><td>k_{water}, 1/s</td><td>1.13E-08</td><td>3.50E-09</td><td>Same half-lives as in "reference data set": PCB-28: 17000; PCB-180: 55000 hours</td></tr>
<tr><td rowspan="5">EVN-BETR and UK-MODEL</td><td>Degradation in atmosphere:
Temperature independent</td><td>k_{air}, 1/s</td><td>3.50E-07</td><td>3.50E-08</td><td>Same half-lives as in "reference data set": PCB-28: 550; PCB-180: 5500 hours</td><td rowspan="5">Mackay et al. 1992</td></tr>
<tr><td>Degradation in soil:
Temperature independent</td><td>k_{soil},1/s</td><td>3.50E-09</td><td>3.50E-09</td><td>Same half-lives as in "reference data set": PCB-28: 55000; PCB-180: 55000 hours</td></tr>
<tr><td>Degradation in water:
Temperature independent</td><td>K_{water},1/s</td><td>1.13E-08</td><td>3.50E-09</td><td>Same half-lives as in "reference data set": PCB-28: 17000; PCB-180: 55000 hours</td></tr>
<tr><td>Degradation in sediment:
Temperature independent</td><td>k_{sed},1/s</td><td>3.50E-09</td><td>3.50E-09</td><td>Same half-lives as in "reference data set": PCB-28: 55000; PCB-180: 55000 hours</td></tr>
<tr><td>Degradation in vegetation:
Temperature independent</td><td>K_{veg},1/s</td><td>1.13E-07</td><td>1.13E-08</td><td>Half-lives: PCB-28: 1700; PCB-180: 17000 hours</td></tr>
</table>

* - for the sake of comparability, the base values and coefficients of temperature dependences of the considered parameters are given here at the temperature 283.15 K (T_0) and the way they were recalculated from original dependencies is specified in the field "Comments".

** - because of insufficient data about vegetation degradation rate constants, the values are taken from atmospheric degradation [*Möller*, 2002] and multiplied with an average OH-radical concentration of 970000 $1/cm^3$ [*Beyer et al.*, 2002].

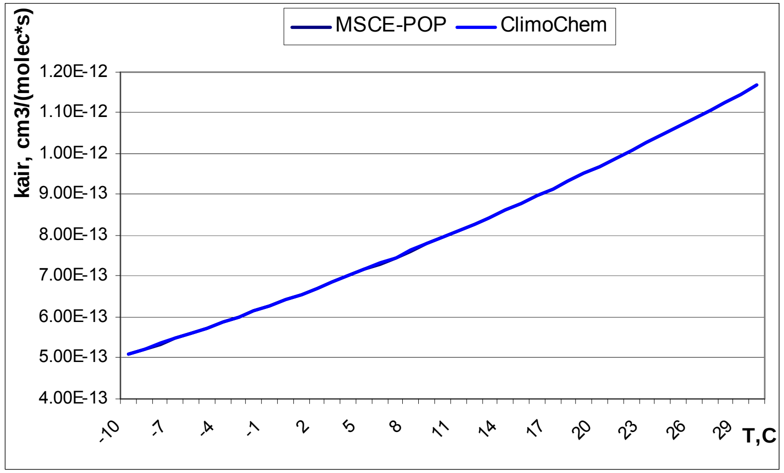

Fig. B.11. *Comparison of temperature dependencies of degradation rate constant of PCB-28 in the atmosphere*

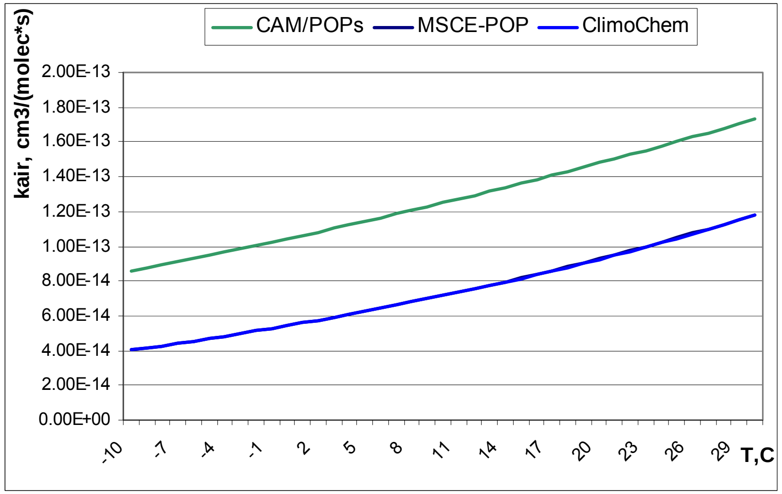

Fig. B.12. *Comparison of temperature dependencies of degradation rate constant of PCB-180 in the atmosphere*

Table B.19. *Monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe and the yearly average degradation rate constants of PCB-28 for the models which use temperature dependence of this parameter*

Month	Temperatures, °C			MSCE-POP	CliMoChem			
	Over land	Over sea	Average	air, $cm^3 \cdot molec^{-1} \cdot s^{-1}$	air, $cm^3 \cdot molec^{-1} \cdot s^{-1}$	soil, s^{-1} (for Over land temp)	sea, s^{-1} (for Over sea temp)	veg., s^{-1} (for aver. temp)
Jan	4	4	4	7.01E-13	7.01E-13	2.96E-09	5.32E-08	6.80E-07
Feb	4	3	4	7.01E-13	7.01E-13	2.96E-09	5.08E-08	6.80E-07
Mar	7	5	6	7.31E-13	7.31E-13	3.4E-09	5.57E-08	7.09E-07
Apr	11	6	9	7.79E-13	7.79E-13	4.08E-09	5.84E-08	7.55E-07
May	17	10	13	8.45E-13	8.45E-13	5.3E-09	7.01E-08	8.20E-07
Jun	21	14	17	9.15E-13	9.15E-13	6.28E-09	8.37E-08	8.87E-07
Jul	22	16	19	9.51E-13	9.51E-13	6.55E-09	9.13E-08	9.22E-07
Aug	22	16	19	9.51E-13	9.51E-13	6.55E-09	9.13E-08	9.22E-07
Sep	18	13	15	8.8E-13	8.79E-13	5.54E-09	8.01E-08	8.53E-07
Oct	14	10	12	8.28E-13	8.28E-13	4.66E-09	7.01E-08	8.03E-07
Nov	10	7	9	7.79E-13	7.79E-13	3.9E-09	6.12E-08	7.55E-07
Dec	6	5	6	7.31E-13	7.31E-13	3.25E-09	5.57E-08	7.09E-07
Averaged second-order rate constants, $cm^3 \cdot molec^{-1} \cdot s^{-1}$				8.16E-13	8.16E-13	-	-	-
Averaged first-order rate constants, s^{-1}				6.53E-07	6.53E-07	4.62E-09	6.85E-08	7.92E-07

Table B.20. *Absolute values and statistical parameters of degradation rate constants of first order (PCB-28)*

	k_{air} s^{-1}	k_{soil}, s^{-1}	k_{water}, s^{-1}	$k_{sediment}$, s^{-1}	k_{veg}, s^{-1}
CliMoChem	6.53E-07	4.62E-09	6.85E-08	-	7.92E-07
MSCE-POP	6.53E-07	7.4E-09	1.33E-07	-	-
SimpleBox	3.50E-07	3.50E-09	1.13E-08	-	-
EVN-BETR/UK-MODEL	3.50E-07	3.50E-09	1.13E-08	3.50E-09	1.13E-07
Reference data set	3.50E-07	3.50E-09	1.13E-08	3.50E-09	-
min	3.50E-07	3.50E-09	1.13E-08	-	-
max	6.53E-07	7.40E-09	1.33E-07	-	-
arith. mean	4.71E-07	4.50E-09	4.71E-08	-	-
median	3.50E-07	3.50E-09	1.13E-08	-	-
geom.mean	4.49E-07	4.30E-09	2.65E-08	-	-
max/min	1.9	2.1	11.8	1.0	7.0

Table B.21. *Monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe and the yearly average degradation rate constants of PCB-180 for the models which use temperature dependence of this parameter*

Month	Temperatures, °C			CAM/POPs	MSCE-POP	CliMoChem			
	Over land	Over sea	Average	air, $cm^3 \cdot molec^{-1} \cdot s^{-1}$	air, $cm^3 \cdot molec^{-1} \cdot s^{-1}$	air, $cm^3 \cdot molec^{-1} \cdot s^{-1}$	soil, s^{-1} (for Over land temp)	sea, s^{-1} (for Over sea temp)	veg., s^{-1} (for aver. temp)
Jan	4	4	4	1.12E-13	6.08E-14	6.07E-14	2.33E-10	3.2E-10	5.89E-08
Feb	4	3	4	1.12E-13	6.08E-14	6.07E-14	2.33E-10	3.06E-10	5.89E-08
Mar	7	5	6	1.16E-13	6.42E-14	6.42E-14	2.68E-10	3.36E-10	6.23E-08
Apr	11	6	9	1.23E-13	6.97E-14	6.96E-14	3.21E-10	3.52E-10	6.76E-08
May	17	10	13	1.32E-13	7.75E-14	7.74E-14	4.17E-10	4.22E-10	7.51E-08
Jun	21	14	17	1.41E-13	8.6E-14	8.58E-14	4.94E-10	5.04E-10	8.33E-08
Jul	22	16	19	1.46E-13	9.04E-14	9.03E-14	5.15E-10	5.5E-10	8.76E-08
Aug	22	16	19	1.46E-13	9.04E-14	9.03E-14	5.15E-10	5.5E-10	8.76E-08
Sep	18	13	15	1.36E-13	8.17E-14	8.15E-14	4.36E-10	4.82E-10	7.91E-08
Oct	14	10	12	1.29E-13	7.55E-14	7.54E-14	3.67E-10	4.22E-10	7.32E-08
Nov	10	7	9	1.23E-13	6.97E-14	6.96E-14	3.07E-10	3.68E-10	6.76E-08
Dec	6	5	6	1.16E-13	6.42E-14	6.42E-14	2.56E-10	3.36E-10	6.23E-08
Averaged second-order rate constants, $cm^3 \cdot molec^{-1} \cdot s^{-1}$				1.28E-13	7.42E-14	7.41E-14	-	-	-
Averaged first-order rate constants, s^{-1}				1.02E-07	5.94E-08	5.93E-08	3.64E-10	4.13E-10	7.19E-08

Table B.22. *Absolute values and statistical parameters of degradation rate constants of first order (PCB-180)*

	k_{air} s^{-1}	$k_{soil,}$ s^{-1}	$k_{water,}$ s^{-1}	$k_{sediment,}$ s^{-1}	$k_{veg,}$ s^{-1}
CAM/POPs	1.02E-07	-	-	-	
CliMoChem	5.93E-08	3.64E-10	4.13E-10	-	7.19E-08
MSCE-POP	5.94E-08	5.83E-10	8.02E-10	-	-
SimpleBox	3.50E-08	3.50E-09	3.50E-09	-	-
EVN-BETR/UK-MODEL	3.50E-08	3.50E-09	3.50E-09	3.50E-09	1.13E-08
Reference data set	3.50E-08	3.50E-09	3.50E-09	3.50E-09	-
min	3.50E-08	3.64E-10	4.13E-10	-	-
max	1.02E-07	3.50E-09	3.50E-09	-	-
arith. mean	5.43E-08	2.29E-09	2.34E-09	-	-
median	4.72E-08	3.50E-09	3.50E-09	-	-
geom.mean	4.99E-08	1.56E-09	1.70E-09	-	-
max/min	2.9	9.6	8.5	1.0	6.4