

Annex A

PHYSICAL CHEMICAL PROPERTIES OF SELECTED POPs AND SUBSTANCE-SPECIFIC PARAMETERS

The values of physical-chemical properties, substance-specific parameters and degradation rates of POPs in the main environmental media (atmosphere, soil, seawater and vegetation) are presented below in Tables A.1-A.11.

A.1. Subcooled liquid-vapour pressure

The value of subcooled liquid-vapour pressure (p_{OL} , Pa) is used in the modelling of the process of POP partitioning between its particulate and gaseous phase in the atmosphere in accordance with the Junge-Pankow adsorption model [Junge, 1977; Pankow, 1987]. Thus, the value of p_{OL} determining the particle-bound fraction of a pollutant in air strongly influences such subsequent important processes as dry and wet deposition and degradation in air.

The value of subcooled liquid-vapour pressure (p_{OL} , Pa) depends on the air temperature and is included in the model in the following form:

$$p_{OL} = p_{OL}^0 \exp \left[-a_P \left(\frac{1}{T} - \frac{1}{T_0} \right) \right], \quad (\text{A.1})$$

where T is the ambient temperature, K;
 T_0 is the reference temperature, K;
 p_{OL}^0 is the value of p_{OL} at the reference temperature T_0 ;
 a_P is the coefficient of the vapour pressure temperature dependence, K.

Coefficients of p_{OL} temperature dependence and base values given at the temperature 283.15 K (T_0) for the selected POPs are presented in Table A.1. The way in which these coefficients of the temperature dependence were obtained or recalculated from original data presented in the literature used is specified in the field "Comments".

The temperature dependence of p_{OL} essentially affects the long-range transport of a pollutant. It increases with increasing temperature for all considered compounds. POPs with the lowest values of vapour pressure the same as PAHs, heavier congeners of PCDD/Fs and PCBs exist in the atmosphere preferably sorbed on atmospheric aerosol particles thereby increasing the probability of their subsequent deposition and washout with precipitation.

Table A.1. Coefficients of p_{OL} temperature dependence used in model parameterization

Compound		Values			Comments	Reference
		p_{OL}^0 , Pa	a_p , K	T_0 , K		
PAHs	B[a]P	$9.34 \cdot 10^{-7}$	11488	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{OL} \text{ (Pa)} = -A/T(K) + B$ with the help of the following formulas: $a_p = \ln(10) \cdot A$, $p_{OL}^0 = 10^{(-A/T_0 + B)}$ where for: B[a]P $A = 4989$, $B = 11.59$; B[b]F $A = 4578$, $B = 9.48$; B[k]F $A = 4427$, $B = 9.48$; I_P $A = 4839$, $B = 9.6$.	Hinckley et al., 1990
	B[b]F	$2.05 \cdot 10^{-7}$	10541	283.15		
	B[k]F	$7.00 \cdot 10^{-7}$	10194	283.15		
	I_P	$3.24 \cdot 10^{-8}$	11142	283.15		
PCDDs	2,3,7,8-TCDD	$8.11 \cdot 10^{-5}$	10113	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{OL} \text{ (Pa)} = -A/T(K) + B$ with the help of the following formulas: $a_p = \ln(10) \cdot A$, $p_{OL}^0 = 10^{(-A/T_0 + B)}$ where for: 2,3,7,8-TCDD $A = 4392$, $B = 11.42$ 1,2,3,7,8-PeCDD $A = 4778$, $B = 11.90$ 1,2,3,4,7,8-HxCDD $A = 4840$, $B = 11.75$ 1,2,3,6,7,8-HxCDD $A = 4803$, $B = 11.41$ 1,2,3,7,8,9-HxCDD $A = 4957$, $B = 12.01$ 1,2,3,4,6,7,8-HpCDD $A = 5017$, $B = 11.91$ OCDD $A = 4676$, $B = 11.20$	Bulgakov and Ioannisian, 1998
	1,2,3,7,8-PeCDD	$1.06 \cdot 10^{-5}$	11002	283.15		
	1,2,3,4,7,8-HxCDD	$4.54 \cdot 10^{-6}$	11145	283.15		
	1,2,3,6,7,8-HxCDD	$2.8 \cdot 10^{-6}$	11059	283.15		
	1,2,3,7,8,9-HxCDD	$3.19 \cdot 10^{-6}$	11414	283.15		
	1,2,3,4,6,7,8-HpCDD	$1.55 \cdot 10^{-6}$	11552	283.15		
	OCDD	$4.85 \cdot 10^{-6}$	10767	283.15		
PCDFs	2,3,7,8-TCDF	$1.31 \cdot 10^{-4}$	10002	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{OL} \text{ (Pa)} = -A/T(K) + B$ with the help of the following formulas: $a_p = \ln(10) \cdot A$, $p_{OL}^0 = 10^{(-A/T_0 + B)}$ where for: 2,3,7,8-TCDF $A = 4344$, $B = 11.46$ 1,2,3,7,8-PeCDF $A = 4504$, $B = 11.54$ 2,3,4,7,8-PeCDF $A = 4607$, $B = 11.70$ 1,2,3,4,7,8-HxCDF $A = 4655$, $B = 11.54$ 1,2,3,6,7,8-HxCDF $A = 4645$, $B = 11.49$ 1,2,3,7,8,9-HxCDF $A = 4643$, $B = 11.51$ 2,3,4,6,7,8-HxCDF $A = 4629$, $B = 11.49$ 1,2,3,4,6,7,8-HpCDF $A = 4735$, $B = 11.49$ 1,2,3,4,7,8,9-HpCDF $A = 4777$, $B = 11.43$ OCDF $A = 4805$, $B = 11.24$	Bulgakov and Ioannisian, 1998
	1,2,3,7,8-PeCDF	$4.30 \cdot 10^{-5}$	10371	283.15		
	2,3,4,7,8-PeCDF	$2.69 \cdot 10^{-5}$	10608	283.15		
	1,2,3,4,7,8-HxCDF	$1.26 \cdot 10^{-5}$	10719	283.15		
	1,2,3,6,7,8-HxCDF	$1.22 \cdot 10^{-5}$	10696	283.15		
	1,2,3,7,8,9-HxCDF	$1.30 \cdot 10^{-5}$	10691	283.15		
	2,3,4,6,7,8-HxCDF	$1.39 \cdot 10^{-5}$	10659	283.15		
	1,2,3,4,6,7,8-HpCDF	$5.85 \cdot 10^{-6}$	10903	283.15		
	1,2,3,4,7,8,9-HpCDF	$3.62 \cdot 10^{-6}$	10999	283.15		
	OCDF	$1.86 \cdot 10^{-6}$	11064	283.15		
PCBs	PCB-28	$6.43 \cdot 10^{-3}$	9383	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{OL} \text{ (Pa)} = -A/T(K) + B$ with the help of the following formulas: $a_p = \ln(10) \cdot A$, $p_{OL}^0 = 10^{(-A/T_0 + B)}$ where for: PCB-28 $A = 4075$, $B = 12.20$ PCB-105 $A = 4758$, $B = 12.9$ PCB-118 $A = 4664$, $B = 12.72$ PCB-153 $A = 4775$, $B = 12.85$ PCB-180 $A = 5042$, $B = 13.03$	Falconer and Bidleman, 1994
	PCB-105	$1.25 \cdot 10^{-4}$	10956	283.15		
	PCB-118	$1.77 \cdot 10^{-4}$	10739	283.15		
	PCB-153	$9.69 \cdot 10^{-5}$	10995	283.15		
	PCB-180	$1.67 \cdot 10^{-5}$	11610	283.15		
γ -HCH		$1.424 \cdot 10^{-2}$	8474	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{OL} \text{ (Pa)} = -3680/T(K) + 11.15$ with the help of the following formulas: $a_p = \ln(10) \cdot 3680$, $p_{OL}^0 = 10^{(-3680/T_0 + 11.15)}$	Hinckley et al., 1990
HCB		$2.88 \cdot 10^{-2}$	8248	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log p_{OL} \text{ (Pa)} = -3582/T(K) + 11.11$ with the help of the following formulas: $a_p = \ln(10) \cdot 3582$, $p_{OL}^0 = 10^{(-3582/T_0 + 11.11)}$	Hinckley et al., 1990

A.2. Henry's law constant and air/water partition coefficient

The value of the air-water Henry's law constant or the air/water partition coefficient are used in the description of the gaseous exchange process between the atmosphere and soil, between the atmosphere and seawater, as well as of wet deposition of the POP gaseous phase. Relation between the air-water Henry's law constant, (K_H , Pa·m³/mol) and the air/water partition coefficient (K_{aw} , dimensionless) is as follows:

$$K_{aw} = K'_H = \frac{K_H}{RT}, \quad (\text{A.2})$$

where T - temperature, K;

$R = 8.314 \text{ J/(mol·K)}$ - universal gas constant.

The temperature dependence of Henry's law constant in the dimensionless form (K'_H) used in the model parameterization is expressed by the following equation:

$$K'_H = \frac{K_{H0}}{RT} \exp \left[-a_H \left(\frac{1}{T} - \frac{1}{T_0} \right) \right], \quad (\text{A.3})$$

where T is the ambient air temperature, K;

T_0 is the reference temperature;

R is the universal gas constant, J/(mol·K),

a_H is the coefficient of Henry's law constant temperature dependence, K;

K_{H0} is the value of Henry's law constant at reference temperature, Pa·m³/mol.

Coefficients of the temperature dependence of the Henry's law constant for the selected POPs are presented in Table A.2. The way in which these coefficients of the temperature dependence were obtained or recalculated from original data presented in the literature used is specified in the field "Comments".

Table A.2. Coefficients of temperature dependence of Henry's law constant used in model parameterization

Compound		Values			Comments	Reference
		K_{H0} , Pa·m ³ /mol	a_H , K	T_0 , K		
PAHs	B[a]P	$5.44 \cdot 10^{-2}$	7866	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_H \text{ (Pa·m}^3\text{/mol)} = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $K_{H0} = 10^{(-A/T_0 + B)}$ where for: B[a]P $A = 3416$, $B = 10.8$ B[b]F $A = 3416$, $B = 10.4$ B[k]F $A = 3416$, $B = 10.7$ I_P $A = 3416$, $B = 10.0$	Ten Hulscher et al., 1992 cited by Galarnau et al., 2000
	B[b]F	$2.166 \cdot 10^{-2}$	7866	283.15		
	B[k]F	$4.322 \cdot 10^{-2}$	7866	283.15		
	I_P	$8.684 \cdot 10^{-3}$	7866	283.15		
PCDDs	2,3,7,8-TCDD	0.333	10104	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_H \text{ (Pa·m}^3\text{/mol)} = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $K_{H0} = 10^{(-A/T_0 + B)}$ where for: 2,3,7,8-TCDD $A = 4388$, $B = 15.02$ 1,2,3,7,8-PeCDD $A = 4522$, $B = 15.32$ 1,2,3,4,7,8-HxCDD $A = 4978$, $B = 16.08$ 1,2,3,6,7,8-HxCDD $A = 4936$, $B = 15.92$ 1,2,3,7,8,9-HxCDD $A = 5090$, $B = 16.60$ 1,2,3,4,6,7,8-HpCDD $A = 5621$, $B = 17.95$ OCDD $A = 4004$, $B = 13.27$	Bulgakov and Ioannian, 1998
	1,2,3,7,8-PeCDD	0.224	10412	283.15		
	1,2,3,4,7,8-HxCDD	$3.16 \cdot 10^{-2}$	11462	283.15		
	1,2,3,6,7,8-HxCDD	$3.07 \cdot 10^{-2}$	11366	283.15		
	1,2,3,7,8,9-HxCDD	$4.2 \cdot 10^{-2}$	11720	283.15		
	1,2,3,4,6,7,8-HpCDD	$1.25 \cdot 10^{-2}$	12943	283.15		
	OCDD	0.135	9219.6	283.15		

Table A.2. (continued)

PCDFs	2,3,7,8-TCDF	0.274	8998.5	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_H (\text{Pa} \cdot \text{m}^3/\text{mol}) = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $K_{H0} = 10^{(-A/T_0 + B)}$ where for: 2,3,7,8-TCDF $A = 3908$, $B = 13.24$ 1,2,3,7,8-PeCDF $A = 4392$, $B = 14.11$ 2,3,4,7,8-PeCDF $A = 4468$, $B = 14.69$ 1,2,3,4,7,8-HxCDF $A = 4832$, $B = 16.35$ 1,2,3,6,7,8-HxCDF $A = 4816$, $B = 15.91$ 1,2,3,7,8,9-HxCDF $A = 4816$, $B = 16.00$ 2,3,4,6,7,8-HxCDF $A = 4801$, $B = 15.93$ 1,2,3,4,6,7,8-HpCDF $A = 5211$, $B = 16.42$ 1,2,3,4,7,8,9-HpCDF $A = 5241$, $B = 16.62$ OCDF $A = 4537$, $B = 14.59$	
	1,2,3,7,8-PeCDF	$3.97 \cdot 10^{-2}$	10113	283.15		
	2,3,4,7,8-PeCDF	$8.14 \cdot 10^{-2}$	10288	283.15		
	1,2,3,4,7,8-HxCDF	0.193	11126	283.15		
	1,2,3,6,7,8-HxCDF	$7.97 \cdot 10^{-2}$	11089	283.15		
	1,2,3,7,8,9-HxCDF	$9.80 \cdot 10^{-2}$	11089	283.15		
	2,3,4,6,7,8-HxCDF	$9.43 \cdot 10^{-2}$	11055	283.15		
	1,2,3,4,6,7,8-HpCDF	$1.04 \cdot 10^{-2}$	11999	283.15		
	1,2,3,4,7,8,9-HpCDF	$1.29 \cdot 10^{-2}$	12068	283.15		
	OCDF	$3.69 \cdot 10^{-2}$	10447	283.15		
PCBs	PCB-28	7.642	7430	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_H (\text{Pa} \cdot \text{m}^3/\text{mol}) = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $K_{H0} = 10^{(-A/T_0 + B)}$, where $A = \Delta H_W / 2.303R$; $B = \log H_{298} + \Delta H_W / 2.303R(298)$. H_{298} is Henry's law constant ($\text{Pa} \cdot \text{m}^3/\text{mol}$) at 25°C taken from [Dunnivant et al., 1992]: PCB-28: 28.58 PCB-105: 10.03 PCB-118: 12.69 PCB-153: 16.48 PCB-180: 10.74 ΔH_W is the enthalpy of volatilization from water, kJ/mol taken from [Burkhard et al., 1985 cited in Wania, 1997]: PCB-28: 61.8 PCB-105: 67.2 PCB-118: 67.2 PCB-153: 69.4 PCB-180: 71.3	estimated
	PCB-105	2.365	8082	283.15		
	PCB-118	3.046	8082	283.15		
	PCB-153	3.781	8347	283.15		
	PCB-180	2.388	8575	283.15		
γ -HCH		0.1341	5485	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_H (\text{Pa} \cdot \text{m}^3/\text{mol}) = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $K_{H0} = 10^{(-A/T_0 + B)}$ where for: distilled water $A = 2382$, $B = 7.54$ sea water $A = 2703$, $B = 8.68$.	distilled water: Kucklick et al., 1991
		0.1361	6224	283.15		sea water: Kucklick et al., 1991
HCB		26.4	6190	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_H (\text{Pa} \cdot \text{m}^3/\text{mol}) = -A/T(K) + B$ with the help of the following formulas: $a_H = \ln(10) \cdot A$, $K_{H0} = 10^{(-A/T_0 + B)}$ where for HCB: $A = 2715$, $B = 11.009$ A and B were estimated with the use of temperature dependencies of p_{OL} and S_{WL} given in [Beyer and Matthies, 2001] $\log K_H = \log p_{OL} - \log S_{WL}$	estimated

A.3. Dry deposition velocities over land, sea, and forest

Velocities of dry deposition over land, sea, and forest are used for modelling of PAHs, PCDD/Fs, and PCBs which exist in the atmosphere mainly particle bounded. For γ -HCH and HCB, these parameters are not required because these pollutants are assumed to occur in the atmosphere only in the gas-phase.

Based on the measurement data on the distribution of low volatile POPs with particle sizes in the atmosphere, the velocity of dry deposition to different underlying surfaces for PAHs and PCDD/Fs is calculated for particles-carriers with effective aerodynamic diameter 0.84 μm and for PCBs – for particles with effective diameter 0.55 μm [Tsyro and Erdman, 2000; Pekar *et al.*, 1999; Shatalov *et al.*, 2000; Mantseva *et al.*, 2002].

Dry deposition velocities over sea from 10 m height and over land (except forests) from 1 m height are determined using Eq. 1.5 and 1.6 in Section 1.2.2 with the use of constants presented in Table A.3. The table also provides the constants defining velocities of dry deposition to a forest, which are calculated by Eq. 1.7 and 1.8 in Section 1.2.2.

Table A.3. Constants for the calculation of dry deposition velocities over land, sea, and forest used in the model parameterization

Compound		Aerodynamic diameter of particle-carriers, μm	Values						
			Dry deposition velocity over land			Dry deposition velocity over sea		Dry deposition velocity over forest	
			A_{soil}	B_{soil}	C_{soil}	A_{sea}	B_{sea}	α	β
PAHs	B[a]P	0.84	0.04	0.02	0.3	0.15	0.023	0.06	0.3
	B[b]F		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	B[k]F		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	I_P		0.04	0.02	0.3	0.15	0.023	0.06	0.3
PCDDs	2,3,7,8-TCDD	0.84	0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,7,8-PeCDD		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,4,7,8-HxCDD		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,6,7,8-HxCDD		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,7,8,9-HxCDD		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,4,6,7,8-HpCDD		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	OCDD		0.04	0.02	0.3	0.15	0.023	0.06	0.3
PCDFs	2,3,7,8-TCDF	0.84	0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,7,8-PeCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	2,3,4,7,8-PeCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,4,7,8-HxCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,6,7,8-HxCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,7,8,9-HxCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	2,3,4,6,7,8-HxCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,4,6,7,8-HpCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	1,2,3,4,7,8,9-HpCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
	OCDF		0.04	0.02	0.3	0.15	0.023	0.06	0.3
PCBs	PCB-28	0.55	0.02	0.01	0.33	0.15	0.013	0.048	0.3
	PCB-105		0.02	0.01	0.33	0.15	0.013	0.048	0.3
	PCB-118		0.02	0.01	0.33	0.15	0.013	0.048	0.3
	PCB-153		0.02	0.01	0.33	0.15	0.013	0.048	0.3
	PCB-180		0.02	0.01	0.33	0.15	0.013	0.048	0.3

A.4. Washout ratio

In the model parameterization for HCB total washout ratio determined on the basis of measurement data (W_T , dimensionless) is used. For other considered POPs, wet depositions of the gaseous and particulate phases are considered separately in the model (See Eqs. (1.11) and (1.13) in Section 1.2.3 “Wet deposition”). In the model description of gaseous phase scavenging with precipitation it is assumed that equilibrium between the vapour phase and the dissolved phase in a raindrop is attained rapidly and washout ratios for the gaseous phase (W_g , dimensionless) of PAHs, PCDD/Fs and PCBs is determined as inverse values to dimensionless Henry’s law constant:

$$W_g = 1/K'_H \quad (\text{A.5})$$

where K'_H is the dimensionless Henry’s law constant.

W_g may be also defined experimentally by the relationship of a substance concentration in the dissolved phase in wet depositions and in the gaseous phase in air. In particular, γ -HCH washout ratio for the gaseous phase is empirically obtained on the basis of simultaneous measurements in air and precipitation [Wania *et al.*, 1999].

For the description of particle bound phase scavenging of PAHs, PCDD/Fs, and PCBs with precipitation (W_p , dimensionless), values of the washout ratio determined experimentally or derived theoretically are used. Wet deposition of POP particle bound phase is the dominant removal mechanism by precipitation for pollutants, which are present in the atmosphere in the most part associated with particles.

Table A.4 gives washout ratio values of the considered pollutants used in the model parameterization. The way in which these values were selected is specified in the field "Comments".

Table A.4. Washout ratio, (dimensionless) used in the model parameterization

Compound		Values rain	Comments	Reference
PAHs	B[a]P	$5.0 \cdot 10^4$	W_p selected on the basis of geometric mean values of 4 indicator PAHs estimated from measurement data: B[a]P $7.37 \cdot 10^4$ B[k]F $5.90 \cdot 10^4$ B[b]F $2.62 \cdot 10^4$ I _P $9.03 \cdot 10^4$	Ligocki <i>et al.</i> , 1985, Poster and Baker, 1996, Hoff <i>et al.</i> , 1996, Franz and Eisenreich, 1998
	B[b]F			
	B[k]F			
	I _P			
PCDDs	2,3,7,8-TCDD	$5.50 \cdot 10^4$	Values of W_p (homologue-specific) determined experimentally were selected in [Harrad and Smith, 1997; Meneses <i>et al.</i> , 2002] for modelling; For 2,3,7,8-TCDD the value is assumed to equal that of TCDFs.	Koester and Hites, 1992; Standley and Hites, 1991 cited by Harrad and Smith, 1997; Meneses <i>et al.</i> , 2002
	1,2,3,7,8-PeCDD	$1.80 \cdot 10^4$		
	1,2,3,4,7,8-HxCDD	$1.20 \cdot 10^4$		
	1,2,3,6,7,8-HxCDD	$1.20 \cdot 10^4$		
	1,2,3,7,8,9-HxCDD	$1.20 \cdot 10^4$		
	1,2,3,4,6,7,8-HpCDD	$5.90 \cdot 10^4$		
PCDFs	OCDD	$7.20 \cdot 10^4$	Values of W_p (homologue-specific) determined experimentally were selected in [Harrad and Smith, 1997; Meneses <i>et al.</i> , 2002] for modelling	Koester and Hites, 1992; Standley and Hites, 1991 cited by Harrad and Smith, 1997; Meneses <i>et al.</i> , 2002
	2,3,7,8-TCDF	$5.50 \cdot 10^4$		
	1,2,3,7,8-PeCDF	$1.80 \cdot 10^4$		
	2,3,4,7,8-PeCDF	$1.80 \cdot 10^4$		
	1,2,3,4,7,8-HxCDF	$1.0 \cdot 10^4$		
	1,2,3,6,7,8-HxCDF	$1.0 \cdot 10^4$		
	1,2,3,7,8,9-HxCDF	$1.0 \cdot 10^4$		
	2,3,4,6,7,8-HxCDF	$1.0 \cdot 10^4$		
	1,2,3,4,6,7,8-HpCDF	$3.0 \cdot 10^4$		
PCBs	PCB-28	$1.5 \cdot 10^5$	W_p for PCB-28, PCB-105, PCB-118, PCB-180 is assumed to be equal W_p of PCB-153, which experimentally determined value is selected in [Sweetman and Jones 2000] for modelling	Swackhamer, <i>et al.</i> , 1988 cited by Sweetman and Jones, 2000
	PCB-105			
	PCB-118			
	PCB-153			
	PCB-180			
γ -HCH		$3.7 \cdot 10^4$	Experimentally determined value of W_g [Ma <i>et al.</i> , 2003]	Atlas and Giam, 1988 cited by Ma <i>et al.</i> , 2003
HCB		$1.0 \cdot 10^4$	W_i selected on the basis of measurement data	Berg and Hjelbrekke, 1998, 1999; Berg <i>et al.</i> , 1996, 1997, 2000, 2001, 2002; Hoff <i>et al.</i> , 1996; Eisenreich <i>et al.</i> , 1981

A.5. Degradation rate constants in environmental media

Degradation process of POPs in the atmosphere is considered as the gas-phase reaction of pollutants with hydroxyl radicals and all other reactions are neglected. In MSCE-POP model, the degradation process in the atmosphere is expressed by the equation of the second order (see Eq. (1.14) in Section 1.2.4 “Degradation in air”). Temperature dependence of degradation rate constant of the gas-phase reaction with OH-radical is taken in the form of Arrhenius equation:

$$k_{air} = A \cdot \exp(-E_a / RT), \quad (\text{A.6})$$

where A is the pre-exponential multiplier; $\text{cm}^3/(\text{molec} \cdot \text{s})$;

E_a is the activation energy of interaction with OH-radical in air, J/mol;

R is the universal gas constant, J/(mol · K);

T is the ambient temperature, K.

This equation is applied for the gaseous phase of a pollutant only. Values of the pre-exponential multiplier and the activation energy for the temperature dependence of degradation rate constant in the atmosphere for the considered pollutants are displayed in Table A.5. Temperature dependent degradation rate constant are implied for PCBs, γ -HCH and HCB. Of note that for PAHs and PCDD/Fs no such temperature dependence exists in the literature and the values of second order rate constant for the gas-phase reaction with OH-radical at 25°C are used in the calculations.

Table A.5. Coefficients of temperature dependence of degradation rate constants in air k_{air} , used in model parameterization

Compound		Values		Reference
		$A, \text{cm}^3/(\text{molec} \cdot \text{s})$	$E_a, \text{J/mol}$	
PAHs	B[a]P	$5 \cdot 10^{-11}$	-	Meylan and Howard, 1993 cited in SRC PhysProp Database
	B[b]F	$1.86 \cdot 10^{-11}$	-	
	B[k]F	$5.36 \cdot 10^{-11}$	-	
	I ₁ P	$6.447 \cdot 10^{-11}$	-	
PCDDs	2,3,7,8-TCDD	$1.05 \cdot 10^{-12}$	-	Brubaker and Hites, 1997
	1,2,3,7,8-PeCDD	$5.6 \cdot 10^{-13}$	-	
	1,2,3,4,7,8-HxCDD	$2.7 \cdot 10^{-13}$	-	
	1,2,3,6,7,8-HxCDD	$2.7 \cdot 10^{-13}$	-	
	1,2,3,7,8,9-HxCDD	$2.7 \cdot 10^{-13}$	-	
	1,2,3,4,6,7,8-HpCDD	$1.3 \cdot 10^{-13}$	-	
	OCDD	$5.0 \cdot 10^{-14}$	-	
PCDFs	2,3,7,8-TCDF	$6.1 \cdot 10^{-13}$	-	Brubaker and Hites, 1997
	1,2,3,7,8-PeCDF	$3.0 \cdot 10^{-13}$	-	
	2,3,4,7,8-PeCDF	$3.0 \cdot 10^{-13}$	-	
	1,2,3,4,7,8-HxCDF	$1.4 \cdot 10^{-13}$	-	
	1,2,3,6,7,8-HxCDF	$1.4 \cdot 10^{-13}$	-	
	1,2,3,7,8,9-HxCDF	$1.4 \cdot 10^{-13}$	-	
	2,3,4,6,7,8-HxCDF	$1.4 \cdot 10^{-13}$	-	
	1,2,3,4,6,7,8-HpCDF	$6.0 \cdot 10^{-14}$	-	
	1,2,3,4,7,8,9-HpCDF	$6.0 \cdot 10^{-14}$	-	
	OCDF	$3.0 \cdot 10^{-14}$	-	
PCBs	PCB-28	$2.7 \cdot 10^{-10}$	13720	Anderson and Hites, 1996; Beyer and Matthies, 2001
	PCB-105	$6.15 \cdot 10^{-11}$	12920	
	PCB-118	$6.15 \cdot 10^{-11}$	12920	
	PCB-153	$8.12 \cdot 10^{-11}$	15380	
	PCB-180	$1.4 \cdot 10^{-10}$	17840	
γ -HCH		$6 \cdot 10^{-11}$	14200	Brubaker and Hites, 1998
HCB		$4.9 \cdot 10^{-10}$	24300	Brubaker and Hites, 1998

In the MSCE-POP model the degradation process of POPs in soil and seawater is described as a first-order process by Eq. (1.28) (Section 1.3.3 “Degradation in soil”) and Eq. (1.36) (Section 1.5.2 “Degradation in seawater”). The degradation rate constants in these media for the considered POPs are presented in Table A.6. Of note that degradation rate constant for γ -HCH hydrolysis in seawater at pH = 8 used in model parameterization is taken to be temperature dependent.

Table A.6. Degradation rate constants in environmental media k_{soil} and k_{sea} used in model parameterization

Compound		Values		Comments	Reference
PAHs	B[a]P	$k_{\text{soil}}, \text{s}^{-1}$	$1.13 \cdot 10^{-8}$	Temperature independent; recalculated from recommended half-lives	Mackay et al., 1992b
		$k_{\text{sea}}, \text{s}^{-1}$	$1.13 \cdot 10^{-7}$		
	B[b]F	$k_{\text{soil}}, \text{s}^{-1}$	$1.13 \cdot 10^{-8}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.13 \cdot 10^{-7}$		
	B[k]F	$k_{\text{soil}}, \text{s}^{-1}$	$1.13 \cdot 10^{-8}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.13 \cdot 10^{-7}$		
PCDDs	2,3,7,8-TCDD	$k_{\text{soil}}, \text{s}^{-1}$	$2.14 \cdot 10^{-10}$	Temperature independent; recalculated from recommended half-lives	Sinkkonen and Paasivirta, 2000
		$k_{\text{sea}}, \text{s}^{-1}$	$4.81 \cdot 10^{-8}$		
	1,2,3,7,8-PeCDD	$k_{\text{soil}}, \text{s}^{-1}$	$1.93 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$2.67 \cdot 10^{-8}$		
	1,2,3,4,7,8-HxCDD	$k_{\text{soil}}, \text{s}^{-1}$	$8.02 \cdot 10^{-11}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.30 \cdot 10^{-8}$		
	1,2,3,6,7,8-HxCDD	$k_{\text{soil}}, \text{s}^{-1}$	$3.50 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.30 \cdot 10^{-8}$		
	1,2,3,7,8,9-HxCDD	$k_{\text{soil}}, \text{s}^{-1}$	$2.75 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.30 \cdot 10^{-8}$		
PCDFs	2,3,7,8-TCDF	$k_{\text{soil}}, \text{s}^{-1}$	$3.50 \cdot 10^{-10}$	Temperature independent; recalculated from recommended half-lives	Sinkkonen and Paasivirta, 2000
		$k_{\text{sea}}, \text{s}^{-1}$	$3.01 \cdot 10^{-8}$		
	1,2,3,7,8-PeCDF	$k_{\text{soil}}, \text{s}^{-1}$	$4.28 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.46 \cdot 10^{-8}$		
	2,3,4,7,8-PeCDF	$k_{\text{soil}}, \text{s}^{-1}$	$3.50 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.46 \cdot 10^{-8}$		
	1,2,3,4,7,8-HxCDF	$k_{\text{soil}}, \text{s}^{-1}$	$3.21 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$6.88 \cdot 10^{-9}$		
	1,2,3,6,7,8-HxCDF	$k_{\text{soil}}, \text{s}^{-1}$	$2.75 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$6.88 \cdot 10^{-9}$		
	1,2,3,7,8,9-HxCDF	$k_{\text{soil}}, \text{s}^{-1}$	$3.85 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$6.88 \cdot 10^{-9}$		
	2,3,4,6,7,8-HxCDF	$k_{\text{soil}}, \text{s}^{-1}$	$4.28 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$6.88 \cdot 10^{-9}$		
PCBs	PCB-28	$k_{\text{soil}}, \text{s}^{-1}$	$7.4 \cdot 10^{-9}$	Temperature independent (on the average for +7 °C); recalculated from recommended half-lives	Sinkkonen and Paasivirta, 2000
		$k_{\text{sea}}, \text{s}^{-1}$	$1.33 \cdot 10^{-7}$		
	PCB-105	$k_{\text{soil}}, \text{s}^{-1}$	$2.20 \cdot 10^{-9}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$3.21 \cdot 10^{-9}$		
	PCB-118	$k_{\text{soil}}, \text{s}^{-1}$	$3.21 \cdot 10^{-9}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$3.21 \cdot 10^{-9}$		
	PCB-153	$k_{\text{soil}}, \text{s}^{-1}$	$1.17 \cdot 10^{-9}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$1.6 \cdot 10^{-9}$		
	PCB-180	$k_{\text{soil}}, \text{s}^{-1}$	$5.83 \cdot 10^{-10}$		
		$k_{\text{sea}}, \text{s}^{-1}$	$8.02 \cdot 10^{-10}$		
γ -HCH	$k_{\text{soil}}, \text{s}^{-1}$	for soil depth <5cm	$5.73 \cdot 10^{-7}$	Temperature independent; recalculated from half-lives	Dowd et al., 1993 cited by Mackay et al., 1997
		for soil depth 5-20cm	$8.91 \cdot 10^{-8}$		Rao and Davidson 1980 cited by Mackay et al., 1997
		Bio-degradation	$4.46 \cdot 10^{-8}$		
	$k_{\text{sea}}^0, \text{s}^{-1}$		$1.905 \cdot 10^{-9}$	The following temperature dependence is used: $k_{\text{sea}} = k_{\text{sea}}^0 \cdot \exp(-B(1/T - 1/T_0) - C \cdot (T - T_0))$ where $T_0 = 283.15$ $B = Ea/R + 4471 \cdot \ln(10)$; $C = 0.03928$ $Ea = 84.6 \text{ kJ/mol}$; $R = 8.314 \text{ J/(mol}\cdot\text{K)}$	Ngabe et al., 1993; Harner et al., 1999
HCB		$k_{\text{soil}}, \text{s}^{-1}$	$5.24 \cdot 10^{-9}$	Temperature independent; recalculated from half-lives	Sheringer, 1997
		$k_{\text{sea}}, \text{s}^{-1}$	$5.24 \cdot 10^{-9}$		

A.6. Octanol-water partition coefficient

The octanol-water partition coefficient (K_{OW} , dimensionless) is a measure of substance hydrophobicity and characterizes its partitioning between water and lipid media substituted for octanol. K_{OW} is used for the estimation of the partition coefficient in the organic carbon-water system (K_{OC}), the partition coefficient in the octanol-air system (K_{OA}), and the bioconcentration factor (BCF). For the considered POPs partition coefficients in the “octanol-water” system selected for modelling are given in Table A.7.

Table A.7. Octanol-water partition coefficient (K_{OW}), dimensionless used in the model parameterization

Compound		Value K_{OW}	Comments	References
PAHs	B[a]P	$1.1 \cdot 10^6$	Temperature independent B[a]P $\log K_{OW} = 6.04$ B[b]F $\log K_{OW} = 5.80$ B[k]F $\log K_{OW} = 6.00$ I_P $\log K_{OW} = 6.584$	Mackay et al., 1992b
	B[b]F	$6.31 \cdot 10^5$		
	B[k]F	$1.00 \cdot 10^6$		SRC Calculated Values, 1988 cited in database SRC Chemfate, 2001
	I_P	$3.84 \cdot 10^6$		
PCDDs	2,3,7,8-TCDD	$9.12 \cdot 10^6$	Temperature independent;	Govers and Krop, 1998
	1,2,3,7,8-PeCDD	$1.86 \cdot 10^7$	2,3,7,8-TCDD $\log K_{OW} = 6.96$	Paasivirta et al., 1999
	1,2,3,4,7,8-HxCDD	$6.31 \cdot 10^7$	1,2,3,7,8-PeCDD $\log K_{OW} = 7.27$	Beyer and Matthies, 2002
	1,2,3,6,7,8-HxCDD	$9.12 \cdot 10^7$	1,2,3,4,7,8-HxCDD $\log K_{OW} = 7.80$	Paasivirta et al., 1999
	1,2,3,7,8,9-HxCDD	$5.75 \cdot 10^7$	1,2,3,6,7,8-HxCDD $\log K_{OW} = 7.96$	
	1,2,3,4,6,7,8-HpCDD	$1.00 \cdot 10^8$	1,2,3,7,8,9-HxCDD $\log K_{OW} = 7.76$	Beyer and Matthies, 2002
	OCDD	$1.58 \cdot 10^8$	1,2,3,4,6,7,8-HpCDD $\log K_{OW} = 8.0$ OCDD $\log K_{OW} = 8.20$	
PCDFs	2,3,7,8-TCDF	$3.80 \cdot 10^6$	Temperature independent;	Paasivirta et al., 1999
	1,2,3,7,8-PeCDF	$6.17 \cdot 10^6$	2,3,7,8-TCDF $\log K_{OW} = 6.58$	Sijm et al., 1989
	2,3,4,7,8-PeCDF	$7.94 \cdot 10^6$	1,2,3,7,8-PeCDF $\log K_{OW} = 6.79$	Paasivirta et al., 1999
	1,2,3,4,7,8-HxCDF	$3.47 \cdot 10^7$	2,3,4,7,8-PeCDF $\log K_{OW} = 6.90$	
	1,2,3,6,7,8-HxCDF	$3.72 \cdot 10^7$	1,2,3,4,7,8-HxCDF $\log K_{OW} = 7.54$	Govers and Krop, 1998
	1,2,3,7,8,9-HxCDF	$5.75 \cdot 10^7$	1,2,3,6,7,8-HxCDF $\log K_{OW} = 7.57$	
	2,3,4,6,7,8-HxCDF	$4.17 \cdot 10^7$	1,2,3,7,8,9-HxCDF $\log K_{OW} = 7.76$	Paasivirta et al., 1999
	1,2,3,4,6,7,8-HpCDF	$8.32 \cdot 10^7$	2,3,4,6,7,8-HxCDF $\log K_{OW} = 7.62$	
	1,2,3,4,7,8,9-HpCDF	$9.77 \cdot 10^7$	1,2,3,4,6,7,8-HpCDF $\log K_{OW} = 7.92$	Sijm et al., 1989
	OCDF	$1.00 \cdot 10^8$	1,2,3,4,7,8,9-HpCDF $\log K_{OW} = 7.99$ OCDF $\log K_{OW} = 8.0$	Paasivirta et al., 1999 Beyer and Matthies, 2002
PCBs	PCB-28	$6.31 \cdot 10^5$	Temperature independent;	Mackay et al., 1992a
	PCB-105	$4.47 \cdot 10^6$	PCB-28 $\log K_{OW} = 5.8$	Hawker and Connell, 1988
	PCB-118	$5.5 \cdot 10^6$	PCB-105 $\log K_{OW} = 6.65$	
	PCB-153	$7.94 \cdot 10^6$	PCB 118 $\log K_{OW} = 6.74$	Mackay et al., 1992a
	PCB-180	$2.29 \cdot 10^7$	PCB-153 $\log K_{OW} = 6.9$ PCB-180 $\log K_{OW} = 7.36$	Hawker and Connell, 1988
γ -HCH		$7.943 \cdot 10^3$	Temperature independent $\log K_{OW} = 3.9$	Chu and Chan, 2000
HCB		$2.426 \cdot 10^5$	Temperature independent; estimated with the use of K_{OA} from [Harner and Mackay, 1995] and used value of K_H obtained on the basis of data from [Beyer and Matthies, 2001]	estimated

A.7. Organic carbon-water partition coefficient

The organic carbon-water partition coefficient (K_{OC} , m^3/kg) is used for the description of POP sorption by soil and bottom sediments. K_{OC} values used in the model parameterization for the most part of the considered POPs were obtained from K_{OW} values using the following relation:

$$K_{OC} = 0.41K_{OW} \text{ [Karickhoff, 1981]} \quad (A.7)$$

Partition coefficients in the “organic carbon-water” system selected for modelling are presented in Table A.8.

Table A.8. Organic carbon-water partition coefficient (K_{OC}), m^3/kg used in the model parameterization

Compound		Values	Comments	Reference
		K_{oc} , m ³ /kg		
PAHs	B[a]P	$4.496 \cdot 10^2$	calculated from K_{ow} by Eq. (A.7) from <i>Karickhoff</i> , 1981	estimated
	B[b]F	$2.59 \cdot 10^2$		
	B[k]F	$4.10 \cdot 10^2$		
	I_P	$1.57 \cdot 10^3$		
PCDDs	2,3,7,8-TCDD	$3.74 \cdot 10^3$	calculated from K_{ow} by Eq. (A.7) from <i>Karickhoff</i> , 1981	
	1,2,3,7,8-PeCDD	$7.63 \cdot 10^3$		
	1,2,3,4,7,8-HxCDD	$2.59 \cdot 10^4$		
	1,2,3,6,7,8-HxCDD	$3.74 \cdot 10^4$		
	1,2,3,7,8,9-HxCDD	$2.36 \cdot 10^4$		
	1,2,3,4,6,7,8-HpCDD	$4.10 \cdot 10^4$		
	OCDD	$6.50 \cdot 10^4$		
PCDFs	2,3,7,8-TCDF	$1.56 \cdot 10^3$		
	1,2,3,7,8-PeCDF	$2.53 \cdot 10^3$		
	2,3,4,7,8-PeCDF	$3.26 \cdot 10^3$		
	1,2,3,4,7,8-HxCDF	$1.42 \cdot 10^4$		
	1,2,3,6,7,8-HxCDF	$1.52 \cdot 10^4$		
	1,2,3,7,8,9-HxCDF	$2.36 \cdot 10^4$		
	2,3,4,6,7,8-HxCDF	$1.71 \cdot 10^4$		
	1,2,3,4,6,7,8-HpCDF	$3.41 \cdot 10^4$		
	1,2,3,4,7,8,9-HpCDF	$4.01 \cdot 10^4$		
PCBs	OCDF	$4.10 \cdot 10^4$		
	PCB-28	$2.59 \cdot 10^2$	calculated from K_{ow} by Eq. (A.7) from <i>Karickhoff</i> , 1981	
	PCB-105	$1.83 \cdot 10^3$		
	PCB-118	$2.255 \cdot 10^3$		
	PCB-153	$3.26 \cdot 10^3$		
PCB-180	$9.39 \cdot 10^3$			
γ -HCH		1.08	predicted	<i>Chu and Chan</i> , 2000
HCB		$9.946 \cdot 10^1$	calculated from K_{ow} by Eq. (A.7) from <i>Karickhoff</i> , 1981	estimated

A.8. Octanol-air partition coefficient

The octanol-air partition coefficient (K_{OA} , dimensionless) is used for the description of a substance partitioning between air and the cuticle of plants, between the gaseous phase and the organic film of atmospheric aerosol particles, etc. In experiments this coefficient is determined by the ratio of equilibrium concentrations of a substance in octanol and air. Additionally, this coefficient can be defined with the use of coefficients “octanol-water” and “air-water”.

$$K_{OA} = C_O / C_A = K_{OW} / K_{AW} = K_{OW} \cdot RT / K_H, \quad (\text{A.8})$$

where C_O is the equilibrium concentration of a substance in octanol;

C_A is the equilibrium concentration of a substance in air;

K_{OW} is octanol-water partition coefficient;

R is universal gas constant equal to 8.314 J/(mol·K);

T is temperature, K;

K_H is Henry's law constant, Pa·m³/mol.

Parameter K_{OA} of the considered POPs depends on temperature. The temperature dependence of partition coefficient in the “octanol-air” system is expressed in the following form:

$$K_{OA} = K_{OA}^0 \exp \left[a_K \left(\frac{1}{T} - \frac{1}{T_0} \right) \right], \quad (\text{A.9})$$

where $T_0 = 283.15$ K is the reference temperature;

K_{OA}^0 is the K_{OA} value at the reference temperature;

a_K is the coefficient of K_{OA} temperature dependence, K.

Coefficients for K_{OA} temperature dependence of the considered POPs used for modelling are presented in Table A.9. The way in which these coefficients of the temperature dependence were obtained or recalculated from original data presented in the literature used is specified in the field “Comments”.

Table A.9. Octanol-air partition coefficient (K_{OA}), dimensionless used in the model parameterization

Compound		Values			Comments	Reference
		K_{OA}^0 dimensionless	a_K K	T_0 K		
PAHs	B[a]P	$4.99 \cdot 10^{10}$	7866	283.15	<p>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: $a_K = \ln(10) \cdot A$, $K_{OA}^0 = 10^{(A/T_0 - B)}$ where for: B[a]P $A = 3416$, $B = 1.37$ B[b]F $A = 3416$, $B = 1.21$ B[k]F $A = 3416$, $B = 1.31$ estimated with the use of basic value of K_{OA} at 25°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Mackay <i>et al.</i>, 1992b; K_H from Ten Hulscher <i>et al.</i>, 1992) together with temperature dependence coefficient for Henry's law constant</p>	estimated
	B[b]F	$7.16 \cdot 10^{10}$	7866	283.15		
	B[k]F	$5.69 \cdot 10^{10}$	7866	283.15		
	I_P	$1.11 \cdot 10^{12}$	7866	283.15		
PCDDs	2,3,7,8-TCDD	$6.44 \cdot 10^{10}$	10104	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Govers and Krop, 1998; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,7,8-PeCDD	$1.96 \cdot 10^{11}$	10412	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,4,7,8-HxCDD	$4.71 \cdot 10^{12}$	11462	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Beyer and Matthies, 2002; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,6,7,8-HxCDD	$6.99 \cdot 10^{12}$	11366	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,7,8,9-HxCDD	$3.22 \cdot 10^{12}$	11720	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,4,6,7,8-HpCDD	$1.88 \cdot 10^{13}$	12943	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Beyer and Matthies, 2002; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	OCDD	$2.77 \cdot 10^{12}$	9219.6	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
PCDFs	2,3,7,8-TCDF	$3.26 \cdot 10^{10}$	8998.5	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,7,8-PeCDF	$3.66 \cdot 10^{11}$	10113	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Sijm <i>et al.</i> , 1989; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	2,3,4,7,8-PeCDF	$2.30 \cdot 10^{11}$	10288	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,4,7,8-HxCDF	$4.24 \cdot 10^{11}$	11126	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T/K_H$ (K_{OW} from Paasivirta <i>et al.</i> , 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated

Table A.9. (continued)

Compound		Values			Comments	Reference
		K_{OA}^0 dimensionless	a_K K	T_0 K		
PCDFs	1,2,3,6,7,8-HxCDF	$1.10 \cdot 10^{12}$	11089	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T / K_H$ (K_{OW} from Govers and Krop, 1998; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,7,8,9-HxCDF	$1.38 \cdot 10^{12}$	11089	283.15		estimated
	2,3,4,6,7,8-HxCDF	$1.04 \cdot 10^{12}$	11055	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T / K_H$ (K_{OW} from Paasivirta et al., 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,4,6,7,8-HpCDF	$1.89 \cdot 10^{13}$	11999	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T / K_H$ (K_{OW} from Sijm et al., 1989; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	1,2,3,4,7,8,9-HpCDF	$1.78 \cdot 10^{13}$	12068	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T / K_H$ (K_{OW} from Paasivirta et al., 1999; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
	OCDF	$6.38 \cdot 10^{12}$	10447	283.15	Coefficients of the exponential equation are estimated with the use of basic value of K_{OA} at 10°C calculated by equation: $K_{OA} = K_{OW} \cdot R \cdot T / K_H$ (K_{OW} from Beyer and Matthies, 2002; K_H from Bulgakov and Ioannisian, 1998) together with temperature dependence coefficient for Henry's law constant	estimated
PCBs	PCB-28	$5.78 \cdot 10^8$	8731	283.15	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: $a_k = \ln(10) \cdot A$, $K_{OA}^0 = 10^{(A/T_0 - B)}$ where for: PCB-28 $A = 3792$, $B = 4.63$ A was taken to be equal to the corresponding coefficient for PCB-29 taken from [Harner and Bidleman, 1996], B was estimated from the formula $B = A/293 - \log K_{OA}^{293}$, where $\log K_{OA}^{293} = (-1.268) \log p_L^0 + 6.135$ [Harner and Bidleman, 1996]	estimated
	PCB-105	$6.94 \cdot 10^{10}$	10772	283.15	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: $a_k = \ln(10) \cdot A$, $K_{OA}^0 = 10^{(A/T_0 - B)}$	Harner and Bidleman, 1996
	PCB-118	$4.51 \cdot 10^{10}$	10806	283.15	where for: PCB-105 $A = 4678$, $B = 5.68$ PCB-118 $A = 4693$, $B = 5.92$	
	PCB-153	$3.64 \cdot 10^{10}$	10811	283.15	PCB-153 $A = 4695$, $B = 6.02$	
	PCB-180	$2.07 \cdot 10^{11}$	10442	283.15	PCB-180 $A = 4535$, $B = 4.70$	
γ -HCH		$1.45 \cdot 10^8$	5485	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_{OA} = 2382/T(K) - 0.25$ estimated with the use of basic value of K_{OA} at 25°C calculated by equation: $\log K_{OA} = \log K_{OW} - \log K_H / RT$ (K_{OW} from Chu and Chan, 2000; K_H from Kucklick et al., 1991) together with temperature dependence coefficient for Henry's law constant for fresh water	estimated
HCB		$3.74 \cdot 10^7$	9045	283.15	Coefficients of the exponential equation are recalculated from the standard form of temperature dependence: $\log K_{OA} = 3928/T(K) - 6.3$ with the help of the following formulas: $a_k = \ln(10) \cdot 3928$, $K_{OA}^0 = 10^{(3928/T_0 - 6.3)}$	Harner and Mackay, 1995

A.9. Molecular diffusion coefficients in air and water

Molecular diffusion coefficients (D_A , D_W , cm²/s) are used in the description of the POP air-soil exchange process. The molecular diffusion coefficient of an organic compound in air (D_A , cm²/s) can be estimated by the formula [Schwarzenbach *et al.*, 1993]:

$$D_A = 10^{-3} \cdot \frac{T^{1.75} [(1/M_{air}) + (1/M)]^{1/2}}{p [\bar{V}_{air}^{1/3} + \bar{V}_m^{1/3}]^2} \quad (A.10)$$

where T is the absolute temperature, 298 K;
 M_{air} is the mean molecular air weight, ~29 g/mol;
 M is the molecular weight of an organic substance, g/mol;
 p is the pressure, 1 atm;
 \bar{V}_{air} is the mean molar gas volume in the air, ~20.1 cm³/mol;
 \bar{V}_m is the molar volume of an organic substance, cm³/mol.

For the determination of molecular diffusion coefficients for organic substances in water (D_W , cm²/s), the following ratio [Schwarzenbach *et al.*, 1993] can be used:

$$D_W = \frac{13.26 \times 10^{-5}}{\mu^{1.14} \cdot (\bar{V}_m)^{0.589}} \quad (A.11)$$

where μ is the solution viscosity in centipoise at a certain temperature, taken to be equal to water viscosity, 0.894 cps at 298K;
 \bar{V}_m is the mean molar volume of a substance, cm³/mol.

In order to calculate molecular diffusion coefficients for the selected POPs, molecular weights (M) and molar volumes (V_m) of these compounds found in the literature (Table A.10) were used.

Table A.11 demonstrates values of molecular diffusion coefficients for air and water calculated with the use of data from Table A.10.

Table A.11. Molecular diffusion coefficients in air and water, m^2/s used in the model parameterization

Compound		Values		Comments	Reference
		D_A	D_W		
PAHs	B[a]P	$5.44 \cdot 10^{-6}$	$6.24 \cdot 10^{-10}$	calculated by Eqs. (A.10) and (A.11) taken from [Schwarzenbach <i>et al.</i> , 1993]	estimated
	B[b]F	$5.44 \cdot 10^{-6}$	$6.24 \cdot 10^{-10}$		
	B[k]F	$5.44 \cdot 10^{-6}$	$6.24 \cdot 10^{-10}$		
	I_P	$5.3 \cdot 10^{-6}$	$6.06 \cdot 10^{-10}$		
PCDDs	2,3,7,8-TCDD	$5.575 \cdot 10^{-6}$	$6.534 \cdot 10^{-10}$		
	1,2,3,7,8-PeCDD	$5.40 \cdot 10^{-6}$	$6.30 \cdot 10^{-10}$		
	1,2,3,4,7,8-HxCDD	$5.24 \cdot 10^{-6}$	$6.09 \cdot 10^{-10}$		
	1,2,3,6,7,8-HxCDD	$5.24 \cdot 10^{-6}$	$6.09 \cdot 10^{-10}$		
	1,2,3,7,8,9-HxCDD	$5.24 \cdot 10^{-6}$	$6.09 \cdot 10^{-10}$		
	1,2,3,4,6,7,8-HpCDD	$5.10 \cdot 10^{-6}$	$5.90 \cdot 10^{-10}$		
	OCDD	$4.97 \cdot 10^{-6}$	$5.73 \cdot 10^{-10}$		
PCDFs	2,3,7,8-TCDF	$5.67 \cdot 10^{-6}$	$6.66 \cdot 10^{-10}$		
	1,2,3,7,8-PeCDF	$5.49 \cdot 10^{-6}$	$6.42 \cdot 10^{-10}$		
	2,3,4,7,8-PeCDF	$5.49 \cdot 10^{-6}$	$6.42 \cdot 10^{-10}$		
	1,2,3,4,7,8-HxCDF	$5.32 \cdot 10^{-6}$	$6.20 \cdot 10^{-10}$		
	1,2,3,6,7,8-HxCDF	$5.32 \cdot 10^{-6}$	$6.20 \cdot 10^{-10}$		
	1,2,3,7,8,9-HxCDF	$5.32 \cdot 10^{-6}$	$6.20 \cdot 10^{-10}$		
	2,3,4,6,7,8-HxCDF	$5.32 \cdot 10^{-6}$	$6.20 \cdot 10^{-10}$		
	1,2,3,4,6,7,8-HpCDF	$5.17 \cdot 10^{-6}$	$6.00 \cdot 10^{-10}$		
	1,2,3,4,7,8,9-HpCDF	$5.17 \cdot 10^{-6}$	$6.00 \cdot 10^{-10}$		
	OCDF	$5.03 \cdot 10^{-6}$	$5.82 \cdot 10^{-10}$		
PCBs	PCB-28	$5.43 \cdot 10^{-6}$	$6.08 \cdot 10^{-10}$	recalculated from molecular diffusion coefficients in air and water for PCB-153	estimated
	PCB-105	$4.82 \cdot 10^{-6}$	$5.40 \cdot 10^{-10}$		
	PCB-118	$4.82 \cdot 10^{-6}$	$5.40 \cdot 10^{-10}$	calculated by Eqs. (A.10) and (A.11) taken from [Schwarzenbach <i>et al.</i> , 1993]	
	PCB-153	$4.59 \cdot 10^{-6}$	$5.14 \cdot 10^{-10}$		
	PCB-180	$4.38 \cdot 10^{-6}$	$4.91 \cdot 10^{-10}$		
γ -HCH		$6 \cdot 10^{-6}$	$7 \cdot 10^{-10}$	calculated by Eqs. (A.10) and (A.11) taken from [Schwarzenbach <i>et al.</i> , 1993]	estimated
HCB		$6.166 \cdot 10^{-6}$	$7.399 \cdot 10^{-10}$		

Table A.10. Molar volume and molar masses

Compound		Values		Reference
		M , g/mol	V_m , cm ³ /mol	
PAHs	B[a]P	252.29	222.8	Paasivirta <i>et al.</i> , 1999; Ruelle and Kesselring, 1997
	B[b]F	252.29	222.8	
	B[k]F	252.29	222.8	
	I_P	276.31	233.8	
PCDDs	2,3,7,8-TCDD	321.98	206	Mackay <i>et al.</i> , 1992b; Ruelle and Kesselring, 1997
	1,2,3,7,8-PeCDD	356.40	218.9*	
	1,2,3,4,7,8-HxCDD	390.87	231.8	
	1,2,3,6,7,8-HxCDD	390.87	231.8	
	1,2,3,7,8,9-HxCDD	390.87	231.8	
	1,2,3,4,6,7,8-HpCDD	425.2	244.7	
PCDFs	OCDD	460.0	257.6	
	2,3,7,8-TCDF	306.00	199.4	
	1,2,3,7,8-PeCDF	340.42	212.3	
	2,3,4,7,8-PeCDF	340.42	212.3	
	1,2,3,4,7,8-HxCDF	374.87	225.2	
	1,2,3,6,7,8-HxCDF	374.87	225.2	
	1,2,3,7,8,9-HxCDF	374.87	225.2	
	2,3,4,6,7,8-HxCDF	374.87	225.2	
	1,2,3,4,6,7,8-HpCDF	409.31	238.1	
PCBs	1,2,3,4,7,8,9-HpCDF	409.31	238.1	
	OCDF	443.8	251	
	PCB-28	257.5	247.3	Mackay <i>et al.</i> , 1992a
	PCB-105	326.4**	289.1**	
	PCB-118	326.4	289.1	
	PCB-153	360.9	310	
	PCB-180	395.3	330.9	
γ -HCH		290.85	179.5	Mackay <i>et al.</i> , 1997; Ruelle and Kesselring, 1997
HCB		284.8	166.8	Mackay <i>et al.</i> , 1992a; Ruelle and Kesselring, 1997

* molar volume is given for congener – 1,2,3,4,7- PeCDD

** - this congener description is not presented in detail in [Mackay *et al.*, 1992a]. However, parameter values are taken to be equal to these values of other pentachlorobiphenyls given in [Mackay *et al.*, 1992a].