Annex A

ALTERNATIVE DATA SET OF PHYSICAL-CHEMICAL PROPERTIES OF PCB-153, PCB-28 AND PCB-180

For models using “reference data sets” as own sets of physical-chemical properties, it is proposed to carry out sensitivity studies of Stage II with the use of alternative data sets. Data on physical-chemical properties (including degradation rate constants) are mostly taken from CliMoChem and DEHM-POP models.

Description		Numerical values			**Comments**	**Reference**
		PCB-153	PCB-28	PCB-180		
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; a_{KAW} is a parameter of temperature dependence.	K^0_{AW} (T_0), dimensionless	2.01E-03	4.63E-03	1.83E-03	$K_{AW}(T) = K_{AW}(T_{ref}) \exp(\mathrm{d}HK_{AW}/R(1/T_{ref} - 1/T))$ (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 153: $9.18 \cdot 10^{-3}$; PCB 28: $1.27 \cdot 10^{-2}$; PCB 180: $8.92 \cdot 10^{-3}$ $\mathrm{d}HK_{AW}$ = phase transfer enthalpy (J/mol) PCB 153: 71000; PCB 28: 47200; PCB 180: 74100 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{KAW}	8536	5680	8917		
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; a_p is a parameter of temperature dependence.	p^0_{OL} (T_0),	6.89E-05	6.26E-03	1.77E-05	Not used in DEHM-POP and CliMoChem models $p_{OL}(T) = p_{OL}(T_{ref}) \exp(\mathrm{d}Hp_{OL}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $p_{OL}(T_{ref})$ = Subcooled liquid vapour pressure at T_{ref} (Pa) PCB 153: $4.62 \cdot 10^{-4}$; PCB 28: $3.15 \cdot 10^{-2}$; PCB 180: $1.32 \cdot 10^{-4}$ $\mathrm{d}Hp_{OL}$ = phase transfer enthalpy (J/mol) PCB 153: 89030; PCB 28: 75620; PCB 180: 94140 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_p	10707.8	9095.0	11322.4		
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; a_{KOW} is a parameter of temperature dependence.	K^0_{OW} (T_0), dimensionless	8.17E+06	9.41E+05	1.84E+07	$K_{OW}(T) = K_{OW}(T_{ref}) \exp((\mathrm{d}HK_{OW}/R)(1/T_{ref}-1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{OW}(T_{ref})$ = octanol/water partitioning coefficient at T_{ref} PCB 153: $5.62 \cdot 10^6$; PCB 28: $5.13 \cdot 10^5$; PCB 180: $1.54 \cdot 10^7$ $\mathrm{d}HK_{OW}$ = phase transfer enthalpy (J/mol) PCB 153: -17500; PCB 28: -28400; PCB 180: -8270 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{KOW}	2102.4	3414.5	994.6		
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; a_{KOA} is a parameter of temperature dependence.	K^0_{OA} (T_0), dimensionless	2.74E+10	5.84E+08	9.78E+10	Not used in CliMoChem model $K_{OA}(T) = K_{OA}(T_{ref}) \exp((\mathrm{d}HK_{OA}/R)(1/T_{ref} - 1/T))$ dimensionless T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K) $K_{OA}(T_{ref})$ = octanol/water partitioning coefficient at T_{ref} PCB 153: $4.14 \cdot 10^9$; PCB 28: $1.16 \cdot 10^8$; PCB 180: $1.68 \cdot 10^{10}$ $\mathrm{d}HK_{OA}$ = phase transfer enthalpy (J/mol) PCB 153: -88440; PCB 28: -75620; PCB 180: -82410 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
	a_{KOA}	10636.8	9095.0	9911.6		

Description		Numerical values			Comments	Reference
		PCB-153	PCB-28	PCB-180		
Organic carbon/water partition coefficient, K_{OC} (dimensionless)						
Regression relation: $K_{OC} = regc\ K_{OW}^{b}$	*regc*	0.35	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
where *regc* and b are regression coefficients	*b*	1	1	1		
Water solubility, S_{WL} (mol/m^3)						
Temperature independent	S_{WL} (T), mol/m^3	1.38E-05	5.45E-04	3.88E-06	Not used in DEHM-POP and CliMoChem models. Values are calculated for T = 283.15 with the help of the following temperature dependence: $S_{WL}(T) = S_{WL}(T_{ref})\ \exp(d_{HS_{WL}}/R(1/T_{ref} - 1/T))$ (dimensionless) T = temperature (283.15 K); T_{ref} = reference temperature (298.15 K); $S_{WL}(T_{ref})$ = water solubility at T_{ref} (mol/m^3) PCB 153: $2.03 \cdot 10^{-5}$; PCB 28: $1.00 \cdot 10^{-3}$; PCB 180: $5.95 \cdot 10^{-6}$ $d_{HS_{WL}}$ = phase transfer enthalpy (J/mol) PCB 153: 18060; PCB 28: 28390; PCB 180: 20000 R = universal gas constant (8.3145 J/molK)	*Beyer at al.,* 2002
Degradation rate constants, k_d (1/s)						
Degradation in atmosphere: Temperature independent	k_{air} (T), 1/s	9.78E-08	6.53E-07	5.93E-08	The rate constants of the second order degradation process in air used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe. Then multiplying the second order rate constants by mean annual OH-radical concentration in the surface layer of 2 km depth at the latitude of 450N (0.8·106 molec/cm^3) [*Yu Lu and Khall,* 1991], the first order degradation rate constants were calculated.	*This study*
Degradation in soil: Temperature independent	k_{soil} (T), 1/s	7.29E-10	4.62E-09	3.64E-10	The rate constants of the first order degradation process in soil used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*
Degradation in water: Temperature independent	k_{water} (T), 1/s	8.27E-10	6.85E-08	4.13E-10	The rate constants of the first order degradation process in water used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*
Degradation in vegetation: Temperature independent	K_{veg}(T), 1/s	1.18E-07	7.92E-07	7.19E-08	The rate constants of the first order degradation process in vegetation used in CliMoChem model which keep this parameter temperature dependent were yearly averaged. This calculation was made with the use of monthly averaged temperatures calculated on the basis of meteorological data for 1997, 1998 and 1999 in Europe.	*This study*

* - 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".