Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts

Field Calibration of Low Density Polyethylene Passive Samplers for Gaseous POPs

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Text SI 1: More details on the passive sampling theory

Passive sampling relies on diffusion to accumulate analytes of interests, thus accumulating only the gaseous molecules in the atmosphere. The exchange of chemicals between the passive sampler and the atmosphere can be presented in three stages. Initially uptake can be assumed to be linear and then enters a curvilinear stage before approaching equilibrium. To estimate the atmospheric concentrations (C_g; ng/m^3) from the accumulated amounts in the passive samplers, it is important first to know the stage reached by each analyte. It has been shown that the loss of performance reference compounds (PRCs) loaded into passive samplers prior to deployment allows in-situ calibration of exchange kinetics. This will therefore reflects exposure conditions at different sites (Huckins et al., 2001). This approach is based on theoretical and experimental evidence which shows that both the loss of the PRCs and the uptake of the target compounds are related (Huckins et al., 2001). Furthermore, site-specific loss rate constants (k_e) can potentially be used with sampler-air partitioning coefficients (K_{PE-A}) to measure the air concentration at deployment sites. k_e is calculated as (equation SI 1):

$$k_e = \ln\left(\frac{C^0_{PRC}}{C^t_{PRC}}\right).t^{-1} \qquad \text{(SI 1)}$$

where C^0_{PRC} is the initial concentration of PRC in the sampler before deployment, C^t_{PRC} is the concentration of PRC after deployment time t (days). PRCs also allow for identifying the compounds that attain sorption equilibrium during the exposure. A PRC that completely dissipates indicates that all compounds with similar or lower K_{PE-A} values have attained equilibrium. C_g (ng/L) can then be calculated as (equation SI 2):

$$C_g = \frac{C_{LDPE}}{K_{PE-A}} \qquad \text{(SI 2)}$$

where C_{LDPE} is the compound's concentration (ng/kg PE) in the LDPE. When a PRC is partially dissipated, then C_g can be calculated as (equation SI 3):

$$C_g = \frac{C_{LDPE}}{(1 - e^{-k_e t}) \,.\, K_{PE-A}} \qquad \text{(SI 3)}$$

where k_e is the loss rate constant (day^{-1}) and t is the deployment period (days).

Figure SI 1: Sampling location at East Providence, USA.

Table SI 1: Meteorological information and sampled air volumes (m^3) of the active sampling in East Providence, USA.

Sampling periods	Sampling dates	Volume of sampled air (m^3)	Temperature ^0C	Wind speed (m/s)
P1	20.11.-23.11.12	1884	8.20	2.22
P2	23.11.-27.11.12	2456	6.92	3.52
P3	27.11.-30.11.12	1700	8.92	4.23
P4	30.11.-4.12.12	2425	8.14	3.98
P5	4.12.-7.12.12	1570	9.31	3.88
P6	7.12.-11.12.12	2384	8.10	4.29

Text SI 2: More details on the instrumental analysis

Samples were injected in the splitless mode onto the GC/MSMS. High purity helium gas was used as the carrier gas with a flow rate of 1 mL/min for OCPs and PCBs, and 2 mL/min for PBDEs. For OCPs and PCBs, injection port, GC-MS-MS interface, and ion trap temperatures were set to 250˚C, 250˚C, 180˚C, respectively. OCPs were measured using the following temperature program: initial temperature 100˚C, hold 1 min, 5˚C/min to 220 ˚C (10 min), 4 ˚C/min to 280 ˚C, and hold for 5 min. p,p'-DDD and o,p'-DDT isomers were not chromatographically separated, and thus detected concentrations represents the sum of both isomers (p,p'-DDD/o,p'-DDT). PCBs were analyzed using the following temperature program: 100˚C, hold 1 min, 11˚C/min to 180 ˚C, 3 ˚C/min to 260 ˚C, 20 ˚C/min to 300, and hold for 6 min.

For PBDEs, injection port, GC-MS-MS interface, and ion trap temperatures were set to 260˚C, 280˚C, 220˚C, respectively. PBDEs were measured using the following temperature program: initial temperature 140˚C, hold 2 min, 10˚C/min to 180 ˚C, 3 ˚C/min to 220 ˚C, 10 ˚C/min to 310, and hold for 5 min.

In all the above mentioned methods, the ion trap was operated in electron ionization-MS-MS mode. The filament emission current was 150 μA.

Text SI 3: Quality Assurance/Quality control

All samples were processed in a clean trace laboratory, which received HEPA-filtered air under positive pressure. Calibration standard were run at the beginning of each working day to develop the calibration curves for the measured POPs. All samples were spiked with surrogate standards composed of labeled compounds. Ranges of the surrogate recoveries in the PUFs and LDPEs respectively were as follows: $^{13}C_6$ HCBz: 81 %-98 %, 84 %-102 %; $^{13}C_{12}$ p,p'-DDT: 83 %-86 %, 87 %-95 %; $^{13}C_{12}$ PCB 8: 85 %-91 %, 82 %-86 %; $^{13}C_{12}$ PCB 28: 81 %-84 %, 86 %-93 %; $^{13}C_{12}$ PCB 52: 91 %-97 %; 94 %-101 %; $^{13}C_{12}$ PCB 118: 78 %-84 %, 84 %-91 %; $^{13}C_{12}$ PCB 138: 90 %-94 %; 85 %-96 %; $^{13}C_{12}$ PCB 180: 81 %-89 %, 84 %-97 %; $^{13}C_{12}$ PCB 209: 73 %-81 %; 77 %-94 %; $^{13}C_{12}$ BDE 28: 82 %-95 %, 89 %-97 %; $^{13}C_{12}$ BDE 47: 80 %-89 %, 87 %-98 %; $^{13}C_{12}$ BDE 99: 78 %-91 %; 82 %-93 %; $^{13}C_{12}$ BDE 153: 74 %-79 %; 75 %-86 %; $^{13}C_{12}$ BDE 183: 71 %-80 %; 74 %-86 %.

Six LDPE and seven PUF procedural and field blanks were included in the analysis. OCPs were not detected in the procedural and the field blanks. Trace amounts of PCB 11, PCB 18, PCB 28, PCB 52, PCB 101, PCB 118, PCB 153, BDE 47, BDE 100 and BDE 99 were detected in the procedural and field blanks with no major differences between both blanks. Detected analytes in the blanks were < 5 % of the amounts detected in any of the samples, so results were not blank corrected. LODs were determined as the concentration of analytes in a sample giving a peak with a signal-to-noise (S/N) of 3. LODs ranges in the LDPE and PUFs were as follows: OCPs: 0.020 - 0.096 ng/PE, 0.012 - 0.191 pg/m^3 in the PUFs; PCBs: 0.015 - 0.09 ng/PE, 0.018-0.109 pg/m^3; PBDEs: 0.009-0.046 ng/PE, 0.008-0.086 pg/m^3. PUFs LOD are based on an average sampled air volume of 2070 m^3.

Matrix spikes were included during the analysis of the samples. Recoveries of POPs in the matrix spikes generally ranged from 91.0 % to 107 % with a relative standard deviation percentage (RSD %) < 20 %.

To study the reproducibility, all PE samples were analyzed in duplicates. Reproducibility ranged from 0.203-14.4 %

Instrumental calibrations were checked by injection of the continuing calibration solution. Instruments calibrations were verified before, during, and after each analytical sequence. Three calibration standards were continuously injected every 15 samples and the calibration check was maintained within ±15% for all analytes.

Table SI 2: Calculated % equilibrium of PRCs in the deployed LDPE samplers.

Deployment Period	PBB 9	PBB 52	PBB 103	OCN
3 days	5	1	0	0
7 days	8	2	0	0
10 days	14	3	0	0
14 days	24	4	0	0
17 days	43	5	1	1
21 days	60	7	1	1

Text SI 4: Physico-Chemical Properties of POPs

Internally consistent (adjusted for thermodynamic consistency) physicochemical properties were chosen as far as possible for the investigated POPs. OCP parameters were obtained from Khairy and Lohmann (2013). For PCBs, octanol-water partitioning coefficients (K_{OW}), air-water partitioning coefficients (K_{AW}), solubility in water (S_W in mol/m^3), octanol-air partitioning coefficients (K_{OA}) and the sub-cooled liquid vapor pressure (P_L/Pa) were all obtained from Schenker et al. (2005). To obtain K_{OW} values for all PCB congeners investigated here, available values from Schenker et al. (2005) were regressed against K_{OW} values from Hawker and Connell (1988). Similarly, available S_w and K_{OA} values were regressed separately against K_{OW}s to obtain S_w and K_{OA} values for all PCBs. P_L values were regressed against values from Falconer and Bidleman (1994). Available K_{AW} values were regressed against calculated K_{AW}s using equation SI 4 (Reinhard and Drefahl, 1999) to obtain values for the other congeners:

$$K_{AW} = \frac{H_c}{RT} \qquad \text{(SI 4)}$$

where H_c is Henry's law constant ($atm.L.mol^{-1}$), R is the gas constant (0.08206 in L.atm/mol.K) and T is the absolute temperature in Kelvin. H_c values were obtained from Mackay et al. (2006). Enthalpies of vaporization (ΔH_{vap} in KJ/mol) were obtained from Kömp and McLachlan (1997). Available ΔH_{vap} values were regressed against P_L to obtain values for all the PCB congeners.

For PBDEs, final adjusted values (FAV) of K_{OW}, K_{OA}, K_{AW}, S_W and P_L obtained from Wania and Dugani (2003) were used. Except for P_L, missing values for the other 4 parameters were obtained from a regression relationship against molecular weight. Available P_L values were regressed against ΔH_{vap} to extrapolate for the investigated PBDE congeners. ΔH_{vap} values were obtained from Tittlemier et al. (2002). H_c values were obtained from Cetin and Odabasi (2005). Available H_c values were regressed against values obtained from SPARC online calculator to extrapolate for all the congeners.

FAV of K_{AW}, S_W and P_L for dioxins and furans were obtained from Aberg et al. (2008). Missing values were obtained from a correlation with molecular weight. P_L values for PAHs were taken from Khairy and Lohmann (2012). $K_{PE\text{-}W}$ values for PCBs, PBDEs and dioxins/furans were calculated as shown in Lohmann (2012). Physico-chemical parameters of OCPs, PCBs and PBDEs are given in Tables (SI 2-5) respectively.

Table SI 3: Selected and derived physico-chemical constants (at 25 ^{0}C) for OCPs (Khairy and Lohmann, 2013).

	log K_{OA}	log K_{AW}	log P_L (Pa)	ΔH_{VAP} (KJ/mol)	log K_{PE-W} (L/kg)
Hexachlorobenzene	7.1	-1.5	-1.03	68.6	5.2
α-hexachlorocyclohexane	7.5	-3.6	-0.59	68.5	2.8
β-hexachlorocyclohexane	8.7	-4.8	-1.28	66.5	2.2
γ-hexachlorocyclohexane	7.7	-4.1	-1.12	70.5	3.0
δ-hexachlorocyclohexane	8.9	-4.8	-1.52	76.4	2.8
Heptachlor	7.7	-1.8	-0.89	76.5	4.8
Aldrin	8.3	-2.0	-1.19	75.1	4.9
Heptachlor-epoxide	8.6	-3.2	-1.66	77.9	4.7
Oxychlordane	8.5	-3.4	-1.92	78.4	5.6
Trans- chlordane	8.8	-2.5	-2.00	80.7	5.2
Cis- chlordane	8.8	-2.7	-2.14	80.4	5.2
Endosulfan I	8.5	-3.6	-2.36	82.0	4.5
Trans- nonachlor	9.6	-3.0	-2.43	82.5	5.7
p,p'-DDE	9.7	-2.8	-2.47	85.6	5.5
Dieldrin	8.8	-3.4	-1.85	87.2	4.2
o,p'-DDD	9.4	-3.7	-3.77	97.6	5.1
Endrin	8.3	-3.3	-2.51	86.1	4.9
Endosulfan II	9.5	-4.8	-2.40	85.0	3.4
p,p'-DDD	10.1	-3.7	-2.92	88.5	5.0
o,p'-DDT	9.4	-3.0	-2.84	88.6	5.7
Endrin Aldehyde	8.60[a]	-7.4	-1.68	77.0	4.2
Endosulfan sulfate	9.97[a]	-6.9	-2.89	88.9	2.6
p,p'-DDT	9.70	-3.3	-3.32	93.2	5.8
Endrin ketone	10.2[a]	-3.3	-1.80	78.1	5.4
Methoxychlor	10.1	-4.1	-3.79	97.8	5.3

a: From Odabasi and Cetin, 2012

Table SI 4: Selected and derived physico-chemical constants (at 25 ^{0}C) for PCBs.

	log K_{OW}[a]	log K_{OA}[a]	log K_{AW}[a]	log S_W (mol/m^3)[a]	log P_L (Pa)[a]	H_c (Pa m^3/mol)[b]	ΔH_{VAP} (KJ/mol)[c]	log K_{PE-W} (L/kg)[d]
PCB 8	5.29	7.35	-2.06	-2.20	-0.86	25.7	72.0	4.50
PCB 11	**5.57**	**7.56**	**-2.16**	**-2.64**	**-1.21**	20.3	**75.0**	**4.93**
PCB 18	**5.53**	**7.51**	**-2.07**	**-2.59**	**-1.22**	25.3	75.0	4.90
PCB 28	5.92	7.86	-1.93	-3.10	-1.59	36.5	78.0	5.40
PCB 44	**6.09**	**8.22**	**-2.04**	**-3.16**	**-1.99**	27.0	81.0	5.50
PCB 52	6.26	8.16	-1.96	-3.40	-1.94	31.3	81.0	5.70
PCB 66	**6.59**	**8.72**	**-1.92**	**-3.67**	**-2.53**	35.4	**85.3**	6.00
PCB 101	6.76	8.83	-2.08	-4.00	-2.67	24.0	85.0	6.30
PCB 81	**6.77**	**8.93**	**-2.06**	**-3.85**	**-2.62**	25.8	**86.0**	**6.17**
PCB 77	**6.77**	**8.93**	**-2.25**	**-3.85**	**-2.73**	16.7	**86.9**	**6.17**
PCB 123	**7.19**	**9.40**	**-1.90**	**-4.28**	**-2.95**	36.7	**88.6**	**6.61**
PCB 118	7.08	9.44	-2.36	-4.10	-3.05	14.5	**89.4**	6.40
PCB 114	**7.09**	**9.29**	**-1.90**	**-4.18**	**-2.97**	36.7	**88.8**	**6.51**
PCB 153	7.31	9.45	-2.13	-4.50	-3.26	20.0	91.0	6.80
PCB 105	7.22	9.62	-2.39	-4.10	-3.05	13.8	**89.4**	6.40
PCB 138	7.70	9.67	-1.97	-4.70	-3.27	30.2	92.0	7.00
PCB 126	**7.36**	**9.59**	**-2.14**	**-4.45**	**-3.37**	21.3	**91.9**	**6.78**
PCB 187	**7.67**	**9.95**	**-1.64**	**-4.76**	**-3.78**	65.9	**94.0**	7.10
PCB 128	**7.19**	**9.40**	**-1.95**	**-4.28**	**-3.51**	32.7	**93.0**	6.60
PCB 167	**7.78**	**10.1**	**-1.87**	**-4.87**	**-3.60**	39.2	**93.7**	**7.22**
PCB 156	**7.68**	**9.96**	**-1.90**	**-4.77**	**-3.71**	37.0	**94.6**	7.20
PCB 157	**7.68**	**9.96**	**-1.97**	**-4.77**	**-3.75**	31.6	**94.9**	**7.11**
PCB 180	7.66	10.2	-2.51	-4.80	-3.88	8.51	97.0	7.10
PCB 169	**7.95**	**10.3**	**-2.10**	**-5.04**	**-4.21**	23.4	**98.6**	**7.39**
PCB 170	**7.78**	**10.1**	**-2.18**	**-4.87**	**-4.20**	19.4	**98.5**	7.30
PCB 189	**8.27**	**10.6**	**-2.01**	**-5.37**	**-4.35**	28.8	**99.6**	**7.72**
PCB 195	**8.11**	**10.4**	**-1.89**	**-5.20**	**-4.38**	38.1	**99.9**	**7.55**
PCB 206	**8.69**	**11.1**	**-2.30**	**-5.80**	**-4.95**	15.1	**103**	**8.16**
PCB 209	**8.79**	**11.2**	**-2.15**	**-5.90**	**-4.83**	20.8	**107**	**8.26**

a: Final adjusted values from Schenker et al., (2005). Highlighted bold K_{OW} values were calculated as: log K_{OW} = 1.11 x log K_{OW} (Hawker and Connell, 1988) - 0.293 (n = 9; R^2 = 0.99). Highlighted bold K_{OA} values were calculated as: log K_{OA} = 1.14 x log K_{OW} + 1.24 (n = 9; R^2 = 0.99). Highlighted bold K_{AW} values were calculated as: log K_{AW} = 1.02 x log K_{AW} (calculated from H_c using equation SI 4) - 0.034 (n = 9; R^2 = 0.99). Highlighted bold S_W values were calculated as: log S_w = -1.01 x log K_{OW} + 3.0 (n = 9; R^2 = 0.99). Highlighted bold P_L values were calculated as: log P_L = 0.96 x log P_L (Falconer and Bidleman, 1994) - 0.19 (n = 9; R^2 = 0.99).

b: Henry's law constant values obtained from Mackay et al., (2006).

c: Enthalpies of vaporization obtained from Kömp and McLachlan (1997). Highlighted bold values were calculated as: ΔH_{VAP} = -7.90 x log P_L + 65.28 (n = 9; R^2 = 0.99).

d: Sampler-water partitioning coefficients obtained from Lohmann (2012). Highlighted bold values were calculated as: log K_{PE-W} = 1.02 x log S_W + 2.24 (n = 16; R^2 = 0.99).

Table SI 5: Selected and derived physico-chemical constants (at 25 ^{0}C) for PCBs.

	log K_{OW}[a]	log K_{OA}[a]	log K_{AW}[a]	log S_W (mol/m^3)[a]	log P_L (Pa)[a]	H_c (Pa m^3/mol)[b]	ΔH_{VAP} (KJ/mol)[c]	log K_{PE-W} (L/kg)[d]
BDE-2	**5.07**	**7.83**	-2.52	**-2.13**	**-1.53**	**36.0**	**61.0**	**4.54**
BDE-8	**5.47**	**8.66**	-2.80	**-2.62**	**-2.16**	**11.3**	**70.3**	**5.11**
BDE-15	5.48	8.63	-2.78	-2.62	-2.00	**11.8**	**67.6**	5.10
BDE-30	**5.88**	**9.49**	**-3.09**	**-3.10**	**-2.57**	**4.70**	**76.3**	**5.69**
BDE-28	5.80	9.41	-3.11	-3.09	-2.80	4.83	79.7	5.70
BDE-49	**6.28**	**10.3**	**-3.37**	**-3.59**	**-3.55**	**1.56**	**90.9**	**6.26**
BDE-47	6.39	10.4	-3.35	-3.71	-3.67	0.850	94.6	6.30
BDE-100	6.53	11.0	-3.81	-4.02	-4.43	0.240	102	6.90
BDE-99	6.76	11.3	-3.67	-4.16	-4.44	0.600	108	6.90
BDE-154	**7.08**	**12.0**	**-3.94**	**-4.57**	**-5.04**	0.080	113	7.40
BDE-153	7.08	11.9	-3.86	-4.59	-5.05	0.260	110	7.40
BDE-183	**7.49**	**12.8**	**-4.22**	**-5.06**	**-5.38**	0.053	118	7.98

a: Final adjusted values of Wania and Dugani (2003). Highlighted bold K_{OW}, K_{OA}, K_{AW} and S_w values were calculated as:
log K_{OW} = 0.005 x molecular weight + 3.80 (n = 6; R^2 = 0.99)
log K_{OA} = 0.005 x molecular weight + 5.22 (n = 6; R^2 = 0.99)
log K_{AW} = -0.004 x molecular weight - 1.62 (n = 6; R^2 = 0.99)
log S_W = -0.006 x molecular weight - 0.58 (n = 6; R^2 = 0.99)
log P_L = -0.068 x ΔH_{VAP} + 2.59 (n = 6; R^2 = 0.99)

b: Henry's law constant values obtained from Cetin and Odabasi (2005). Highlighted bold values were calculated as: H_c = 1.65 x H_c (SPARC calculator) + 0.27 (n = 7; R^2 = 0.92).

c: obtained from Tittlemier et al. (2002). Highlighted bold values were calculated as: ΔH_{VAP} = 2.92 x ΔH_{VAP} (EPI suite) - 90.75 (n = 7; R^2 = 0.92).

d: K_{PE-W} values obtained from Lohmann (2012). Highlighted bold values were calculated as: log K_{PE-W} = -1.17 x log S_W + 2.05 (n = 7; R^2 = 0.99)

Table SI 6: Selected and derived physico-chemical constants (at 25 ^{0}C) for dioxins and furans.

	log K_{AW}[a]	log S_W (mol/m^3)[a]	log P_L (Pa)[a]	log K_{PE-W} (L/kg)[b]
2-CDF	-2.36	-1.13	-0.10	3.51
2,8-CDF	-2.71	-2.06	-1.37	4.43
2,4,8-CDF	-2.91	-2.76	-2.23	5.13
2,3,7,8-CDF	-3.16	-3.71	-3.48	6.07
1,2,3,7,8-CDF	-3.35	-4.13	-4.04	6.48
2,3,4,7,8-CDF	-3.35	-4.30	-4.25	6.65
1,2,3,4,7,8-CDF	-3.14	-5.21	-4.96	7.55
1,2,3,4,6,7,8-CDF	-3.11	-5.86	-5.57	8.19
1,2,3,4,6,7,8,9-CDF	-3.24	-6.83	-6.68	9.15
2-CDD	-2.38	-2.09	-1.08	4.46
2,7-CDD	-2.54	-3.47	-2.61	5.83
2,8-CDD	-2.53	-2.89	-2.03	5.25
2,3,7-CDD	**-2.61**	**-3.30**	**-2.57**	5.66
2,3,7,8-CDD	-2.46	-3.98	-3.05	6.33
1,2,3,7,8-CDD	-2.89	-3.99	-3.69	6.34
1,2,3,4,7,8-CDD	-3.02	-4.58	-4.21	6.92
1,2,3,6,7,8-CDD	**-3.02**	**-4.61**	**-4.24**	6.95
1,2,3,7,8,9-CDD	**-3.02**	**-4.61**	**-4.24**	6.95
1,2,3,4,6,7,8-CDD	-3.24	-4.80	-4.65	7.14
1,2,3,4,6,7,8,9-CDD	-3.28	-5.56	-5.44	7.89

a: values obtained from Aberg et al., (2008). Highlighted values were obtained from a correlation with molecular weight.
b: K_{PE-W} values obtained from Lohmann (2012).

Table SI 7: Calculated relative uncertainties (RU) for K_{PE-A}s of OCPs.

Compound	K_{PE-A} RU [a]	K_{PE-A} RU [b]	PRC equilibrium correction RU	RU from LDPE/PUF analysis	Overall RU %[a]	Overall RU %[b]	log K_{PE-A} ± RU in log units[a]	log K_{PE-A} ± RU in log units[b]
HCBz	0.33	0.32	5.9E-06	0.300/0.300	42.4	42.4	6.87±0.2	6.87±0.2
a-HCH	0.01	0.28	3.9E-03	0.300/0.300	42.4	42.4	6.87±0.2	6.87±0.2
b-HCH	0.14	0.25			14.0	25.0	7.27±0.1	8.03±0.1
g-HCH	0.06	0.21	2.3E-02	0.300/0.300	42.5	42.4	7.16±0.2	7.16±0.2
d-HCH	0.69[x]	0.57[x]			69.0	57.0	7.47±0.3	8.21±0.3
Heptachlor	0.00	0.31	2.3E-02	0.300/0.300	42.5	42.4	7.12±0.2	7.12±0.2
Aldrin	0.04	0.57			100	100	7.19±0.5	7.68±0.5
Heptachlor epoxide	0.69	0.07	5.2E-01	0.300/0.300	67.0	67.0	7.78±0.3	7.78±0.3
Oxychlordane	0.69[x]	0.57[x]	4.5E-01	0.300/0.300	61.9	61.9	8.21±0.3	8.21±0.3
Trans- chlordane	0.19	0.08	6.4E-01	0.300/0.300	76.8	76.8	7.99±0.4	7.99±0.4
Cis- chlordane	0.09	0.15	6.4E-01	0.300/0.300	76.8	76.8	8.09±0.4	8.09±0.4
Endosulfan I	0.26	0.29	4.5E-01	0.300/0.300	61.9	61.9	8.33±0.3	8.33±0.3
Trans- nonachlor	0.69[x]	0.57[x]	9.1E-01	0.300/0.300	100	100	8.35±0.5	8.35±0.5
p,p'-DDE	0.03	0.03	9.3E-01	0.300/0.300	102	102	8.37±0.5	8.37±0.5
Dieldrin	0.12	0.11			12.0	11.0	7.74±0.1	8.12±0.1
o,p'-DDD	0.69[x]	0.57[x]			69.0	57.0	9.33±0.3	8.66±0.3
Endrin	0.40	0.54			40.0	54.0	8.29±0.2	7.68±0.2
Endosulfan II	0.09	0.57	8.9E-01	0.300/0.300	98.8	98.8	8.35±0.5	8.35±0.5
p,p'-DDD	0.20	0.15	5.0E-01	0.300/0.300	46.9	45.0	8.63±0.2	9.28±0.2
o,p'-DDT	0.69[x]	0.57[x]		0.300/0.300	81.0	86.8	8.56±0.4	8.66±0.4
Endrin Aldehyde	0.69[x]	0.57[x]			69.0	57.0	7.60±0.3	10.2±0.3
Endosulfan sulfate	0.69[x]	0.57[x]		0.300/0.300	105	105	8.84±0.5	8.84±0.5
p,p'-DDT	0.14	0.16	9.6E-01	0.300/0.300	102	102	9.02±0.5	9.02±0.5
Endrin ketone	0.69[x]	0.57[x]	9.3E-01		69.0	57.0	7.70±0.3	10.1±0.3
Methoxychlor	0.69[x]	0.57[x]			69.0	57.0	9.35±0.3	9.28±0.3

a: Uncertainty estimates given by Shen and Wania, 2005 for P_L were used.
b: Uncertainty estimates given by Schenker et al., 2005 for K_{OA} were used.
x: Pesticides were assigned the highest uncertainty estimate as in Shen and Wania, 2005 and Schenker et al., 2005 (not internally consistent values).
Only highlighted K_{PE-A} RU values were used in the calculation of the overall uncertainty.

Table SI 8: Calculated relative uncertainties (RU) for K_{PE-A}s of PCBs.

Compound	K_{PE-A} RU [a]	K_{PE-A} RU [b]	PRC equilibrium correction RU	RU from LDPE/PUF analysis	Overall RU %[a]	Overall RU %[b]	log K_{PE-A} ± RU in log units[a]	log K_{PE-A} ± RU in log units[b]
PCB 8	0.21	0.55		0.300/0.300	42.4	42.4	6.66±0.2	6.66±0.2
PCB 11	0.38[x]	1.1[x]		0.300/0.300	42.4	42.4	7.15±0.2	7.15±0.2
PCB 18	0.38[x]	1.1[x]		0.300/0.300	42.4	42.4	6.91±0.2	6.91±0.2
PCB 28	0.15	0.65	0.05	0.300/0.300	42.7	42.7	7.26±0.2	7.26±0.2
PCB 52	0.13	0.55	0.21	0.300/0.300	47.4	47.4	7.55±0.2	7.55±0.2
PCB 44	0.38[x]	1.1[x]	0.23	0.300/0.300	48.4	48.4	7.62±0.2	7.62±0.2
PCB 66	0.15	1.1[x]	0.45	0.300/0.300	61.5	61.5	8.26±0.3	8.26±0.3
PCB 101	0.24	0.43	0.46	0.300/0.300	62.7	62.7	8.24±0.3	8.24±0.3
PCB 81	0.38[x]	1.1[x]	0.46	0.300/0.300	62.2	62.2	8.51±0.3	8.51±0.3
PCB 77	0.38[x]	1.1[x]	0.51	0.300/0.300	66.6	66.6	8.54±0.3	8.54±0.3
PCB 123	0.38[x]	1.1[x]	0.58	0.300/0.300	72.0	72.0	8.70±0.3	8.70±0.3
PCB 118	0.11	1.1	0.58	0.300/0.300	71.9	71.9	8.72±0.3	8.72±0.3
PCB 114	0.38[x]	1.1[x]	0.57	0.300/0.300	70.8	70.8	8.61±0.3	8.61±0.3
PCB 153	0.15	0.8	0.67	0.300/0.300	79.0	79.0	8.85±0.4	8.85±0.4
PCB 105	0.17	1.1	0.61	0.300/0.300	74.3	74.3	8.75±0.3	8.75±0.3
PCB 138	0.04	0.8	0.67	0.300/0.300	79.3	79.3	8.91±0.4	8.91±0.4
PCB 126	0.38[x]	1.1[x]	0.69	0.300/0.300	81.3	81.3	9.10±0.4	9.10±0.4
PCB 187	0.38[x]	1.1[x]	0.76	0.300/0.300	87.0	87.0	9.25±0.4	9.25±0.4
PCB 128	0.38[x]	1.1[x]	0.74	0.300/0.300	85.0	85.0	8.86±0.4	8.86±0.4
PCB 167	0.38[x]	1.1[x]	0.75	0.300/0.300	85.7	85.7	9.20±0.4	9.20±0.4
PCB 156	0.38[x]	1.1[x]	0.77	0.300/0.300	87.6	87.6	9.12±0.4	9.12±0.4
PCB 157	0.38[x]	1.1[x]	0.77	0.300/0.300	87.9	87.9	9.23±0.4	9.23±0.4
PCB 180	0.18	0.44	0.80	0.300/0.300	90.6	90.6	9.44±0.4	9.44±0.4
PCB 169	0.38[x]	1.1[x]	0.85	0.300/0.300	95.0	95.0	9.62±0.4	9.62±0.4
PCB 170	0.38[x]	1.1[x]	0.85	0.300/0.300	94.6	94.6	9.36±0.4	9.36±0.4
PCB 189	0.38[x]	1.1[x]	0.86	0.300/0.300	96.1	96.1	9.92±0.5	9.92±0.5
PCB 195	0.38[x]	1.1[x]	0.87	0.300/0.300	96.3	96.3	10.1±0.5	10.1±0.5
PCB 206	0.38[x]	1.1[x]	0.90		38.0	171	10.3±0.2	10.2±1.1
PCB 209	0.38[x]	1.1[x]	0.90		38.0	171	10.2±0.2	10.3±1.1

a: Uncertainty estimates given by Li et al., 2003 for P_L were used.
b: Uncertainty estimates given by Schenker et al., 2005 for K_{OA} were used.
x: PCBs were assigned the highest uncertainty estimate as in Shen and Wania, 2005 (not internally consistent values).
Only highlighted K_{PE-A} RU values were used in the calculation of the overall uncertainty.

Table SI 9: Calculated relative uncertainties (RU) for K_{PE-A}s of PBDEs.

Compound	K_{PE-A} RU [a]	K_{PE-A} RU [b]	PRC equilibrium correction RU	RU from LDPE/PUF analysis	Overall RU %[a]	Overall RU %[b]	log K_{PE-A} ± RU in log units[a]	log K_{PE-A} ± RU in log units[b]
BDE 2	0.30[x]	0.30[x]	0.03	0.300/0.300	42.5	42.5	6.60±0.2	6.60±0.2
BDE 8	0.30[x]	0.30[x]	0.31	0.300/0.300	52.3	52.3	7.59±0.2	7.59±0.2
BDE 15	0.30	0.30	0.24	0.300/0.300	48.6	48.6	7.53±0.2	7.53±0.2
BDE 30	0.30[x]	0.30[x]	0.46	0.300/0.300	62.4	62.4	8.64±0.3	8.64±0.3
BDE 28	0.20	0.20	0.54	0.300/0.300	68.4	68.4	8.49±0.3	8.49±0.3
BDE 49	0.30[x]	0.30[x]	0.74	0.300/0.300	84.9	84.9	9.46±0.4	9.46±0.4
BDE 47	0.19	0.19	0.76	0.300/0.300	87.0	87.0	9.49±0.4	9.49±0.4
BDE 100	0.08	0.08			8.00	8.00	9.88±0.04	10.1±0.04
BDE 99	0.21	0.11			21.0	21.0	9.89±0.1	10.4±0.1
BDE 154	0.30[x]	0.30[x]			30.0	30.0	10.4±0.1	11.0±0.1
BDE 153	0.17	0.17			17.0	17.0	10.4±0.1	10.9±0.1
BDE 183	0.30[x]	0.30[x]			30.0	30.0	10.7±0.1	11.8±0.1

a: Uncertainty estimates given by Wania and Dugani, 2003 for P_L were used.
b: Uncertainty estimates given by Wania and Dugani, 2003 for K_{OA} were used.
x: PBDEs were assigned the highest uncertainty estimate as in Wania and Dugani, 2003 (not internally consistent values).
Only highlighted K_{PE-A} RU values were used in the calculation of the overall uncertainty.

Table SI 10: Accumulated amounts of OCPs (ng/g PE) in the LDPE.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
HCBz	0.09	0.26	0.48	0.65	0.73	0.73
a-HCH	0.04	0.06	0.12	0.19	0.22	0.23
b-HCH	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
g-HCH	0.03	0.04	0.07	0.15	0.19	0.21
d-HCH	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Heptachlor	0.06	0.17	0.35	0.63	0.75	0.81
Aldrin	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Heptachlor epoxide	0.03	0.10	0.18	0.29	0.46	0.73
Oxychlordane	0.06	0.14	0.35	0.67	1.11	1.44
Trans- chlordane	0.06	0.16	0.31	0.90	1.71	2.42
Cis- chlordane	0.04	0.14	0.30	0.74	1.72	2.53
Endosulfan I	0.10	0.25	0.43	0.85	1.89	2.69
Trans- nonachlor	0.03	0.07	0.15	0.33	0.72	0.97
p,p'-DDE	0.04	0.06	0.12	0.24	0.49	0.66
Dieldrin	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
o,p'-DDD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Endrin	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Endosulfan II	0.07	0.12	0.21	0.33	0.69	1.00
p,p'-DDD/o,p'-DDT	0.03	0.08	0.18	0.35	0.60	0.90
Endrin Aldehyde	0.06	0.09	0.14	0.25	0.46	0.74
Endosulfan sulfate	0.11	0.17	0.30	0.38	0.72	1.53
p,p'-DDT	0.20	0.26	0.48	0.65	0.73	0.73
Endrin ketone	0.04	0.06	0.12	0.19	0.22	0.23
Methoxychlor	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD

<LOD: below the limit of detection

Table SI 11: Accumulated amounts of PCBs (ng/g PE) in the LDPE.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
PCB 8	0.07	0.09	0.27	0.40	0.43	0.43
PCB 11	0.05	0.09	0.15	0.29	0.58	0.75
PCB 18	0.06	0.09	0.26	0.49	0.63	0.67
PCB 28	0.08	0.15	0.33	0.62	0.99	1.07
PCB 52	0.08	0.20	0.40	0.63	0.86	0.99
PCB 44	0.08	0.20	0.42	0.63	0.96	1.10
PCB 66	0.08	0.20	0.43	0.73	1.05	1.56
PCB 101	0.10	0.19	0.32	0.57	0.84	1.48
PCB 81	0.04	0.06	0.14	0.20	0.27	0.96
PCB 77	0.05	0.09	0.16	0.26	0.40	0.82
PCB 123	0.03	0.07	0.13	0.22	0.36	0.51
PCB 118	0.05	0.13	0.24	0.37	0.51	0.67
PCB 114	0.03	0.08	0.13	0.19	0.25	0.37
PCB 153	0.06	0.11	0.17	0.25	0.35	0.55
PCB 105	0.04	0.08	0.11	0.13	0.16	0.33
PCB 138	0.03	0.08	0.11	0.13	0.19	0.39
PCB 126	<LOD	0.05	0.09	0.12	0.15	0.29
PCB 187	<LOD	0.07	0.12	0.19	0.24	0.42
PCB 128	<LOD	0.04	0.09	0.12	0.16	0.22
PCB 167	<LOD	0.04	0.08	0.11	0.13	0.20
PCB 156	<LOD	0.05	0.11	0.18	0.25	0.36
PCB 157	<LOD	0.04	0.10	0.15	0.19	0.35
PCB 180	<LOD	0.06	0.13	0.20	0.27	0.46
PCB 169	<LOD	0.05	0.10	0.14	0.17	0.35
PCB 170	<LOD	0.05	0.09	0.11	0.15	0.30
PCB 189	<LOD	0.07	0.11	0.15	0.19	0.44
PCB 195	<LOD	0.07	0.12	0.17	0.26	0.60
PCB 206	<LOD	<LOD	0.15	0.35	1.50	2.89
PCB 209	<LOD	<LOD	0.23	0.50	1.95	3.26

<LOD: below the limit of detection

Table SI 12: Accumulated amounts of PBDEs (ng/g PE) in the LDPE.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
BDE 2	0.005	0.02	0.03	0.04	0.06	0.07
BDE 8	0.01	0.02	0.02	0.04	0.09	0.18
BDE 15	0.01	0.02	0.03	0.05	0.10	0.22
BDE 30	<LOD	0.01	0.02	0.04	0.08	0.13
BDE 28	<LOD	0.01	0.02	0.03	0.05	0.12
BDE 49	<LOD	0.05	0.08	0.12	0.17	0.24
BDE 47	<LOD	0.03	0.05	0.08	0.16	0.23
BDE 100	<LOD	0.02	0.03	0.04	0.06	0.07
BDE 99	<LOD	0.02	0.02	0.04	0.09	0.18
BDE 154	<LOD	0.02	0.03	0.05	0.10	0.22
BDE 153	<LOD	0.01	0.02	0.04	0.08	0.13
BDE 183	<LOD	0.01	0.02	0.03	0.05	0.12

<LOD: below the limit of detection

Table SI 13: Gaseous concentrations of OCPs (pg/m^3) measured by the high volume sampler.

Compound	0-3 days	3-7 days	7-10 days	10-14 days	14-17 days	17-21 days
HCBz	25.3	25.7	36.3	21.0	25.0	31.0
a-HCH	7.31	2.80	2.52	10.2	8.68	10.1
g-HCH	3.03	1.25	1.54	5.20	2.90	3.86
Heptachlor	4.79	11.4	12.1	9.61	18.7	20.9
Heptachlor epoxide	3.32	3.25	7.90	3.39	8.94	5.93
Oxychlordane	3.05	3.15	9.08	9.33	17.2	10.0
Trans- chlordane	3.16	7.47	13.0	13.7	33.7	24.9
Cis- chlordane	1.51	4.59	9.04	14.5	18.1	10.1
Endosulfan I	3.74	3.11	10.7	5.74	15.8	13.2
Trans- nonachlor	1.91	2.80	7.87	7.29	11.9	9.50
p,p'-DDE	2.54	1.57	5.89	4.96	8.72	7.38
Endosulfan II	4.47	1.63	4.04	5.83	9.11	8.14
p,p'-DDD/o,p'-DDT	0.59	1.70	7.38	4.09	4.88	4.03
Endosulfan sulfate	3.20	2.03	3.08	4.26	8.27	8.22
p,p'-DDT	1.33	1.81	3.52	2.43	6.30	6.57

Table SI 14: Gaseous concentrations of PCBs (pg/m^3) measured by the high volume sampler.

Compound	0-3 days	3-7 days	7-10 days	10-14 days	14-17 days	17-21 days
PCB 8	10.9	13.0	21.0	7.99	14.4	24.6
PCB 11	4.78	4.78	10.8	18.2	8.92	1.70
PCB 18	6.58	6.59	18.6	17.4	13.3	19.1
PCB 28	5.92	6.46	11.4	12.6	13.3	14.4
PCB 52	6.28	7.94	13.1	7.18	7.01	9.92
PCB 44	3.25	5.26	9.65	12.4	9.86	4.60
PCB 66	2.15	3.75	5.65	8.22	5.84	4.82
PCB 101	2.38	2.38	4.48	3.78	4.18	6.13
PCB 81	0.67	1.23	0.84	7.43	3.81	1.52
PCB 77	0.87	1.07	0.58	4.14	2.52	3.60
PCB 123	0.44	0.70	1.23	1.04	1.70	1.04
PCB 118	0.82	1.22	3.42	1.48	1.52	1.09
PCB 114	0.53	0.80	1.24	0.23	0.15	1.16
PCB 153	0.95	0.74	0.60	0.54	1.06	0.82
PCB 105	0.83	1.07	0.83	0.24	1.30	0.80
PCB 138	0.53	0.87	0.39	0.30	1.01	0.53
PCB 126	0.40	0.40	0.68	0.62	0.18	0.34
PCB 187	0.32	0.39	0.87	0.41	0.93	0.42
PCB 128	0.22	0.28	0.88	0.39	0.40	0.24
PCB 167	0.21	0.28	0.49	0.44	0.22	0.29
PCB 156	0.24	0.42	1.02	0.39	0.54	0.44
PCB 157	0.25	0.27	0.75	0.39	0.67	0.35
PCB 180	0.22	0.47	0.56	0.85	0.66	0.59
PCB 169	0.24	0.35	0.53	0.63	0.68	0.31
PCB 170	0.24	0.25	0.68	0.14	0.66	0.25
PCB 189	0.32	0.61	1.52	0.57	0.32	0.12
PCB 195	0.33	0.35	1.16	0.50	0.93	0.48

Table SI 15: Gaseous concentrations of PBDEs (pg/m^3) measured by the high volume sampler.

Compound	0-3 days	3-7 days	7-10 days	10-14 days	14-17 days	17-21 days
BDE 2	3.25	5.25	4.22	2.73	5.74	5.74
BDE 8	1.25	1.28	0.81	0.62	1.93	2.56
BDE 15	1.58	2.18	1.22	2.82	1.30	1.40
BDE 30	0.26	0.23	0.27	0.21	0.96	0.91
BDE 28	0.23	0.37	0.38	0.22	0.52	0.52
BDE 49	0.33	0.32	0.54	0.37	0.24	0.29
BDE 47	0.24	0.19	0.24	0.28	0.71	0.71

Table SI 16: Derived % equilibrium for OCPs in LDPEs.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
HCBz	33	49	74	95	100	100
a-HCH	20	31	51	79	96	100
g-HCH	15	24	41	67	89	98
Heptachlor	15	24	41	67	89	98
Heptachlor epoxide	4	7	12	21	34	48
Oxychlordane	5	8	14	24	39	55
Trans- chlordane	3	5	9	15	25	36
Cis- chlordane	3	5	9	15	25	36
Endosulfan I	5	8	14	24	39	55
Trans- nonachlor	1	2	3	4	6	9
p,p'-DDE	1	1	2	4	5	7
Endosulfan II	1	2	3	5	7	11
p,p'-DDD/o,p'-DDT	1	1	2	3	5	7
Endosulfan sulfate	1	1	1	2	3	5
p,p'-DDT	1	1	2	4	5	7

Table SI 17: Derived % equilibrium for PCBs in LDPEs.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
PCB 8	24	37	60	86	98	100
PCB 11	11	17	30	51	75	90
PCB 18	19	30	49	77	95	100
PCB 28	12	20	34	57	81	94
PCB 52	6	9	16	29	49	63
PCB 44	7	12	21	36	60	75
PCB 66	2	4	7	12	18	27
PCB 101	3	5	8	15	24	34
PCB 81	1	2	4	6	9	13
PCB 77	2	3	4	7	12	17
PCB 123	1	2	4	6	10	14
PCB 118	1	2	3	5	8	12
PCB 114	2	3	5	8	13	19
PCB 153	1	2	3	5	8	12
PCB 105	1	2	2	4	6	9
PCB 138		1	2	4	6	8
PCB 126		1	2	2	4	5
PCB 187		1	2	3	4	5
PCB 128		2	3	6	9	13
PCB 167		1	2	2	3	5
PCB 156		1	2	3	5	7
PCB 157		1	2	2	4	5
PCB 180		1	1	2	2	3
PCB 169		0	1	1	1	2
PCB 170		1	1	2	3	4
PCB 189		1	1	1	2	2
PCB 195		0	1	1	1	2

Table SI 18: Derived % equilibrium for PBDEs in LDPEs.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
BDE 2	13	20	35	59	82	95
BDE 8	4	6	11	19	31	44
BDE 15	4	7	11	20	32	46
BDE 30		2	3	5	8	11
BDE 28		2	3	6	9	13
BDE 49		1	1	1	2	2
BDE 47		1	1	1	2	2

Table SI 19: Sampling rates (R_s m^3/d) of OCPs in LDPEs.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
HCBz	2.25	2.91	2.75	3.43	2.97	2.25
a-HCH	3.12	3.94	4.96	4.76	3.72	2.75
g-HCH	5.53	6.24	7.35	7.57	7.53	5.95
Heptachlor	6.06	6.31	8.57	9.42	7.23	5.25
Heptachlor epoxide	6.27	6.98	8.60	9.34	9.38	11.3
Oxychlordane	3.42	11.6	13.2	14.0	15.5	14.5
Trans- chlordane	3.04	6.65	8.47	13.1	14.6	13.8
Cis- chlordane	4.50	9.95	13.2	14.2	19.6	23.3
Endosulfan I	4.65	12.2	20.7	21.2	26.4	28.0
Trans- nonachlor	2.59	5.81	8.46	9.38	12.3	11.9
p,p'-DDE	2.45	5.80	8.53	9.28	11.1	10.7
Endosulfan II	2.46	10.8	10.2	11.6	14.9	15.2
p,p'-DDD/o,p'-DDT	8.44	9.59	14.5	17.5	19.6	20.0
Endosulfan sulfate	3.28	9.89	8.67	11.5	11.9	13.3
p,p'-DDT	13.7	22.3	24.0	25.4	30.0	35.1

Table SI 20: Sampling rates (R_s m^3/d) of PCBs in LDPEs.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
PCB 8	2.02	2.98	3.49	4.32	3.42	2.37
PCB 11	3.59	4.24	4.90	6.52	7.75	6.63
PCB 18	3.57	4.05	5.34	5.66	5.41	4.15
PCB 28	6.11	6.89	8.05	9.79	10.7	8.45
PCB 52	7.19	7.30	7.83	10.3	11.2	9.69
PCB 44	4.93	10.1	11.8	11.7	12.8	12.3
PCB 66	17.2	18.6	21.0	21.3	22.2	25.9
PCB 101	20.6	17.5	24.2	24.9	26.3	32.0
PCB 81	10.9	10.3	17.3	24.7	31.0	35.3
PCB 77	21.9	23.9	21.9	31.1	31.7	32.6
PCB 123	21.2	26.6	30.1	36.9	37.9	42.1
PCB 118	22.4	31.6	31.6	32.4	35.2	37.7
PCB 114	26.4	29.2	36.7	38.1	45.0	45.6
PCB 153	33.6	34.1	37.8	51.3	48.9	59.3
PCB 105	19.3	25.7	25.3	25.7	29.5	32.4
PCB 138	35.5	29.0	29.5	34.9	32.2	53.9
PCB 126		34.2	29.0	31.3	34.7	56.8
PCB 187		50.0	39.0	53.4	45.0	63.1
PCB 128		25.6	31.5	37.2	40.9	45.3
PCB 167		24.1	38.8	42.9	44.0	51.4
PCB 156		31.3	39.4	50.5	52.4	59.7
PCB 157		37.6	42.4	43.1	49.9	67.0
PCB 180		45.8	50.2	53.9	53.4	68.9
PCB 169		38.4	43.4	44.2	47.1	65.6
PCB 170		38.3	39.8	48.9	54.8	67.9
PCB 189		23.1	27.5	30.2	39.8	64.2
PCB 195		31.8	41.3	43.2	49.0	80.1

Table SI 21: Sampling rates (R_s m^3/d) of PBDEs in LDPEs.

Compound	0-3 days	0-7 days	0-10 days	0-14 days	0-17 days	0-21 days
BDE 2	0.92	1.02	1.02	1.57	1.78	1.37
BDE 8	3.52	3.28	5.76	6.38	8.99	10.6
BDE 15	3.04	3.26	3.97	4.64	6.22	10.8
BDE 30		14.3	14.0	21.3	23.0	24.9
BDE 28		11.6	13.5	15.6	17.9	27.5
BDE 49		33.6	42.2	42.2	55.4	58.9
BDE 47		36.7	35.1	49.8	48.0	54.9

Table SI 22: Calculated K_{PE-A} values (L/kg) for OCPs from the field study.

	Present study[a]	Khairy and Lohmann[6b]	% difference (a and b)	Predicted values[d]
HCBz	6.87±0.2	6.83±0.20	9	7.07±0.2
α-HCH	6.87±0.2	6.63±0.23	56	6.71±0.2
β-HCH				7.28±0.1
γ-HCH	7.16±0.2	7.22±0.30	14	7.15±0.2
δ-HCH				7.48±0.3
Heptachlor	7.12±0.2	7.41±0.21	64	6.96±0.2
Aldrin				7.20±0.5
Heptachlor- epoxide	7.78±0.3	7.58±0.21	45	7.59±0.5
Oxychlordane	8.21±0.3	8.26±0.23	12	7.80±0.4
Trans- chlordane	7.99±0.4	7.72±0.21	60	7.87±0.4
Cis- chlordane	8.09±0.4	7.97±0.22	28	7.98±0.4
Endosulfan I	8.33±0.3	8.13±0.41	45	8.17±0.3
Trans- nonachlor	8.35±0.5	8.12±0.22	52	8.22±0.6
p,p'-DDE	8.37±0.5	8.13±0.21	54	8.26±0.5
Dieldrin				7.75±0.1
o,p'-DDD				9.32±0.3
Endrin				8.29±0.2
Endosulfan II	8.35±0.5	8.24±0.42	25	8.20±0.5
p,p'-DDD				8.63±0.2
o,p'-DDT				8.56±0.4
Endrin Aldehyde				7.61±0.3
Endosulfan sulfate	8.84±0.5	8.57±0.44	60	8.60±0.6
p,p'-DDT	9.02±0.5	8.94±0.43	18	8.95±0.5
Endrin ketone				7.71±0.3
Methoxychlor				9.34±0.3

a: values obtained from the current field study

d: values predicted from equation 7 in the main text

Table SI 23: Calculated K_{PE-A} values (L/kg) for PBDEs from the field study.

	Present study[a]	K_{PE-W}/K_{AW}[b]	% difference (a and b)	Predicted values[c]
BDE-2	6.60±0.2	7.06	96	7.48±0.2
BDE-8	7.59±0.2	7.91	70	8.00±0.3
BDE-15	7.53±0.2	7.88	77	7.87±0.3
BDE-30	8.64±0.3	8.78	32	8.34±0.3
BDE-28	8.49±0.3	8.81	71	8.53±0.3
BDE-49	9.46±0.4	9.63	38	9.14±0.4
BDE-47	9.49±0.4	9.65	37	9.24±0.4
BDE-100				9.87±0.04
BDE-99				9.87±0.1
BDE-154				10.4±0.1
BDE-153				10.4±0.1
BDE-183				10.6±0.1

a: values obtained from the current field study
b: $K_{PE-A} = K_{PE-W}/K_{AW}$
d: values predicted from equation 7 in the main text

Table SI 24: Predicted K_{PE-A} values (L/kg) for PAHs

	Present study[a]	Khairy and Lohmann[5b]	% difference (a and b)
PAHs			
Nap	4.93	4.90	7
C_1-Nap	5.54	5.56	4
C_2-Nap	6.17	6.12	11
C_3-Nap	6.78	6.89	24
C_4-Nap	7.41	7.56	33
Biphenyl	6.08	6.15	17
Acenaphthylene	5.89	6.15	58
Acenapthene	6.03	6.05	5
Flr	6.45	6.42	7
C_1-Flr	7.23	7.37	31
C_2-Flr	7.85	8.03	40
C_3-Flr	8.48	8.69	49
DBT	7.41	7.56	33
C_1-DBT	8.03	8.22	42
C_2-DBT	8.65	8.89	55
C_3-DBT	9.27	9.56	63
Phn	7.04	7.26	50
Ant	7.24	7.30	15
C_1-Phn/Ant	7.76	7.94	39
C_2-Phn/Ant	8.39	8.60	48
C_3-Phn/Ant	9.01	9.27	59
C_4-Phn/Ant	9.62	9.92	66
Fluoranthene	8.01	8.38	81
Pyrene	8.18	8.33	35
Retene	9.46	9.74	63
1-Methyl pyrene	8.96	9.22	57
BaA	9.04	9.73	130
Chrysene	9.41	9.75	75
Benzo(b)fluoranthene	10.3	10.7	82
7,12-DMBaA	10.6	11.0	82
Benzo(k)fluoranthene	10.4	10.8	72
Benzo(a)pyrene	10.4	10.9	96
Perylene	10.4	10.8	80
Indeno[1,2,3 (cd)]pyrene	11.3	11.8	98
Dibenzo[a,h]anthracene	11.6	12.0	94
Bengo(ghi)perylene	11.4	11.9	95
2-MNap	5.54	5.61	15
1-MNap	5.54	5.56	4
1,5-DMNap	6.17	6.24	16
2,3/2-6-DMNap	6.17	6.30	30
2,3,5-TMNap	6.78	6.87	20
9-Ethyl fluorene	7.85	8.03	40
1,4,6,7-TeMNap	7.41	7.56	33
2/1-MFlr	7.23	7.37	31

Table SI 24: continued.

	Present study[a]	Khairy and Lohmann[5b]	% difference (a and b)
1,2,5,6- TeMNap	7.41	7.56	33
2-MDBT	8.03	8.22	42
4,5-MePhn	7.66	7.83	38
2-MPhn/Ant	7.76	7.94	39
1-MPhn	7.76	7.94	39
9-MAnt	7.76	7.94	39
3,6-DMPhn	8.39	8.60	48
1,2-DMDBT	8.65	8.89	55
2,4,7-TMDBT	9.27	9.56	63
1,2,5/1,2,7 TMPhn	9.01	9.27	59

a: Predicted $K_{PE\text{-}A}$ values from equation 11; b: converted from L/L to L/kg using ρ_{LDPE} = 0.91 kg/L; Nap = naphthalene; C1,2,3,4: alkylated PAHs and the number indicates alkylation level; Flr: fluorene; DBT: dibenzothiophene; Phn: phenanthrene; Ant: anthracene; BaA: benz(a)anthracene; DMBaA: dimethyl benz(a)anthracene; MNap: methyl naphthalene; DMNap: dimethyl naphthalene; TMNap: trimethyl naphthalene; TeMNap: tetramethyl naphthalene; MFlr: methyl fluorene; MDBT: methyl dibenzothiophene; MePhn: methylene phenanthrene; MPhn: methyl phenanthrene; MAnt: methyl anthracene; DMPhn: dimethyl phenanthrene; DMDBT: dimethyl dibenzothiophene; TMDBT: trimethyl dibenzothiophene; TMPhn: trimethyl phenanthrene.

Table SI 25: Predicted K_{PE-A} values (L/kg) for polychlorinated dibenzo-p-dioxins and dibenzofurans

	Present study[a]	K_{PE-W}/K_{AW}[b]	% difference (a and b)
2-CDF	6.31	5.87	93
2,8-CDF	7.35	7.14	48
2,4,8-CDF	8.06	8.04	5
2,3,7,8-CDF	9.09	9.23	32
1,2,3,7,8-CDF	9.54	9.83	64
2,3,4,7,8-CDF	9.72	10.0	62
1,2,3,4,7,8-CDF	10.3	10.7	83
1,2,3,4,6,7,8-CDF	10.8	11.3	103
1,2,3,4,6,7,8,9-CDF	11.7	12.4	130
2-CDD	7.11	6.84	61
2,7-CDD	8.37	8.36	3
2,8-CDD	7.89	7.78	26
2,3,7-CDD	8.33	8.27	15
2,3,7,8-CDD	8.74	8.79	13
1,2,3,7,8-CDD	9.26	9.22	8
1,2,3,4,7,8-CDD	9.68	9.94	58
1,2,3,6,7,8-CDD	9.71	9.97	58
1,2,3,7,8,9-CDD	9.71	9.97	58
1,2,3,4,6,7,8-CDD	10.0	10.4	74
1,2,3,4,6,7,8,9-CDD	10.7	11.2	99

a: predicted from equation 7 in the main text
b: $K_{PE-A} = K_{PE-W}/K_{AW}$
CDD: chlorinated dibenzo-p-dioxin
CDF: chlorinated dibenzofuran

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