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

Graphical Tools for the Planning and Interpretation of Polyurethane Foam Based Passive Air Sampling Campaigns

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Content

The following poly-parameter linear free energy relationships (ppLFERs) were used to estimate the $K_{Q/G}$ at 15 °C:[29]

$$\log K_{\mathrm{Q/G\ 15\ ^\circ C}}\,(\mathrm{Berlin\ (winter)}) = 1.38S + 3.21A + 0.63L + 0.98V - 7.24 + \log \rho_{\mathrm{Q1}} \quad \text{(S1)}$$

$$\log K_{\mathrm{Q/G\ 15\ ^\circ C}}\,(\mathrm{Dübendorf\ (winter)}) = 1.63S + 3.20A + 0.51L + 1.51V - 7.33 + \log \rho_{\mathrm{Q2}} \quad \text{(S2)}$$

$$\log K_{\mathrm{Q/G\ 15\ ^\circ C}}\,(\mathrm{Aspvreten}) = 0.95S + 2.52A + 0.64L + 0.49V - 5.95 + \log \rho_{\mathrm{Q3}} \quad \text{(S3)}$$

$$\log K_{\mathrm{Q/G\ 15\ ^\circ C}}\,(\mathrm{Roost}) = 1.45S + 3.12A + 0.60L + 0.86V - 6.99 + \log \rho_{\mathrm{Q4}} \quad \text{(S4)}$$

The original ppLFERs yield $K_{Q/Gas}$ in units of $m^3\ g^{-1}$ and the last terms in Eqs. (S1-4) containing the density of the particles convert the K into units of $m^3\ m^{-3}$. We used densities ρ_{Q1} to ρ_{Q4} of 1784000, 1784000, 1728000 and 1588000 g m^{-3}, respectively. log $K_{Q/G}$ of a chemical at 15 °C was the mean of the values calculated using Eqs. (S1-4). The internal energy of phase transfer between particle and the gas phase ($\Delta U_{\mathrm{Q/G}}$) of a compound was assumed equal to the corresponding $\Delta U_{\mathrm{PUF/G}}$.[28]

Table S1 Abraham solute descriptors for selected native SVOCs.

Chemical	E	S	A	B	L	V
Naphthalene	1.34	0.9200	0	0.2000	5.1610	1.0854
Phenanthrene	2.06	1.2900	0	0.2600	7.6320	1.4544
Pyrene	2.81	1.7100	0	0.2800	8.8330	1.5846
Chrysene	3.03	1.7300	0	0.3300	10.3340	1.8234
Benzo(a)pyrene	3.625	1.9800	0	0.4400	11.7360	1.9536
PCB 1	1.48	1.07	0	0.2	6.338	1.4466
PCB 11	1.66	1.18	0	0.16	7.477	1.569
PCB 16	1.75	1.35	0	0.17	7.647	1.6914
PCB-28	1.76	1.3300	0	0.1500	7.9040	1.6910
PCB-52	1.9	1.4800	0	0.1500	8.1440	1.8140
PCB-101	2.04	1.6100	0	0.1300	8.8680	1.9360
PCB-118	2.06	1.5900	0	0.1100	9.3960	1.9360
PCB-138	2.18	1.7400	0	0.1100	9.7720	2.0590
PCB-153	2.18	1.7400	0	0.1100	9.5870	2.0590
PCB-180	2.29	1.8700	0	0.0900	10.4150	2.1810
PCB-194	2.48	2.0000	0	0.0600	11.1860	2.3030
BDE-47	2.45	1.4500	0	0.3400	10.6600	2.0830
BDE-99	2.74	1.5100	0	0.4400	11.7100	2.2580
BDE-100	2.76	1.4800	0	0.4100	11.4800	2.2580
BDE-153	2.88	1.5400	0	0.5200	12.6500	2.4330
HCB	1.49	0.7500	0	0.0900	6.9860	1.4508
alpha-HCH	1.45	0.7300	0	0.7100	7.3170	1.5800
beta-HCH	1.45	0.8800	0	0.6900	7.4930	1.5800
delta-HCH	1.45	0.9400	0	0.6300	7.6260	1.5800
gamma-HCH (Lindane)	1.45	0.9100	0	0.6800	7.4670	1.5800
4:2-FTOHs	-0.39	-0.140	0.4000	0.3000	2.3070	1.1711
6:2-FTOHs	-0.7	-0.390	0.4000	0.2800	2.5880	1.5233
8:2-FTOHs	-1.02	-0.640	0.4000	0.2500	2.8680	1.8755
10:2-FTOHs	-1.33	-0.890	0.4000	0.2300	3.1480	2.2277
hexamethylcyclotrisiloxane (D3)	-0.25	0.0100	0	0.5100	3.6230	1.7500
octamethylcyclotetrasiloxane (D4)	-0.47	-0.080	0	0.3200	4.4730	2.3450
decamethylcyclopentasiloxane (D5)	-0.7	-0.100	0	0.5000	5.2420	2.9310
dodecamethylcyclohexasiloxane (D6)	-0.88	-0.120	0	0.7400	6.0800	3.5170
Hexachlorobutadiene	1.02	0.42	0	0.16	5.347	1.3206
2,4,6-tribromoanisole	1.55	1.12	0	0.21	7.085	1.441
Pentachloroanisole	1.42	1.07	0	0.04	7.566	1.528
triethyl phosphate	0	1.12	0	1.05	5.04	1.3934

Table S2 Abraham solute descriptors for selected DCs

Chemical	**E**	**S**	**A**	**B**	**V**	**L**
PCB 30	1.74	1.35	0	0.17	1.6914	7.286
PCB 54	1.84	1.48	0	0.15	1.8138	7.753
PCB 107	2.07	1.59	0	0.11	1.9362	9.334
PCB 108	2.04	1.59	0	0.11	1.9362	9.349
PCB 198	2.46	2	0	0.06	2.3034	10.583
13C-PCB 3	1.5	1.05	0	0.18	1.4466	6.718
13C-PCB 9	1.63	1.2	0	0.18	1.569	7.001
13C-PCB 15	1.64	1.18	0	0.16	1.569	7.58
13C-PCB 28	1.76	1.33	0	0.15	1.6914	7.904
13C-PCB 31	1.77	1.33	0	0.15	1.6914	7.862
13C-PCB 32	1.74	1.35	0	0.17	1.6914	7.667
13C-PCB 101	2.04	1.61	0	0.13	1.9362	8.868
13C-PCB 111	2.08	1.59	0	0.11	1.9362	9.082
13C-PCB 118	2.06	1.59	0	0.11	1.9362	9.396
13C-HCB	1.49	0.75	0	0.09	1.4508	6.986
d6-gamma-HCH	1.45	0.91	0	0.68	1.5798	7.467

Table S3 Partition coefficients between PUF and the gas phase $K_{PUF/G}$ and their temperature dependence $\Delta U_{PUF/G}$ estimated for selected SVOCs using the ppLFERs.

Chemical	**log $K_{PUF/G}$**					**$\Delta U_{PUF/G}$**
	At -40 °C	At -15 °C	At 5 °C	At 25 °C	At 50 °C	(J·mol^{-1})
Naphthalene	5.76	4.73	4.05	3.45	2.81	-47182
Phenanthrene	9.15	7.65	6.65	5.78	4.84	-69042
Pyrene	11.33	9.52	8.31	7.26	6.13	-83265
Chrysene	12.91	10.89	9.54	8.36	7.10	-93128
Benzo(a)pyrene	14.87	12.59	11.05	9.73	8.30	-105223
PCB 1	7.46	6.17	5.30	4.55	3.75	-59506
PCB 11	8.84	7.37	6.38	5.52	4.60	-67907
PCB 16	9.50	7.91	6.84	5.92	4.93	-73196
PCB-28	9.68	8.08	7.00	6.07	5.07	-73944
PCB-52	10.35	8.63	7.48	6.48	5.41	-79191
PCB-101	11.41	9.54	8.29	7.20	6.03	-86154
PCB-118	11.83	9.92	8.64	7.53	6.34	-88072
PCB-138	12.63	10.59	9.22	8.04	6.77	-93903
PCB-153	12.46	10.44	9.09	7.91	6.65	-93108
PCB-180	13.61	11.43	9.97	8.70	7.34	-100518
PCB-194	14.71	12.37	10.81	9.45	7.99	-107683
BDE-47	12.75	10.73	9.38	8.21	6.95	-92925
BDE-99	13.97	11.79	10.32	9.05	7.69	-100736
BDE-100	13.70	11.54	10.10	8.85	7.51	-99219
BDE-153	15.03	12.70	11.13	9.78	8.32	-107546
HCB	7.28	6.05	5.22	4.51	3.74	-56714
alpha-HCH	7.63	6.34	5.48	4.73	3.93	-59439
beta-HCH	8.15	6.79	5.87	5.08	4.23	-62836
delta-HCH	8.41	7.01	6.07	5.26	4.39	-64464
gamma-HCH (Lindane)	8.20	6.83	5.90	5.11	4.25	-63252
4:2-FTOHs	2.90	2.12	1.60	1.14	0.66	-35991
6:2-FTOHs	2.85	2.04	1.49	1.02	0.52	-37307
8:2-FTOHs	2.79	1.95	1.39	0.90	0.38	-38619
10:2-FTOHs	2.73	1.86	1.28	0.78	0.24	-39931
hexamethylcyclotrisiloxane (D3)	2.76	2.04	1.56	1.14	0.69	-33059
octamethylcyclotetrasiloxane (D4)	3.79	2.86	2.24	1.70	1.12	-42746
decamethylcyclopentasiloxane (D5)	4.91	3.75	2.98	2.31	1.59	-53202
dodecamethylcyclohexasiloxane (D6)	6.09	4.70	3.77	2.96	2.10	-63954
Hexachlorobutadiene (HCBD)	4.92	4.01	3.39	2.86	2.29	-42192
2,4,6-tribromoanisole (TBA)	8.24	6.86	5.94	5.14	4.28	-63527
Pentachloroanisole (PCA)	8.62	7.20	6.24	5.41	4.52	-65829
triethyl phosphate (TP)	6.38	5.20	4.41	3.73	3.00	-54124

Table S4 Molecular weights, partition coefficients between PUF and the gas phase $K_{PUF/G}$ and their temperature dependence $\Delta U_{PUF/G}$ for selected depuration compounds

DCs	MW (g/mol)	log $K_{PUF/G}$					$\Delta U_{PUF/G}$ (J/mol)
		-40 °C	-15 °C	5 °C	25 °C	50 °C	
PCB 30	257.5	9.18	7.62	6.58	5.68	4.70	-71644
PCB 54	292	10.00	8.32	7.19	6.22	5.17	-77507
PCB 107	326.4	11.78	9.87	8.59	7.49	6.30	-87808
PCB 108	326.4	11.79	9.88	8.61	7.50	6.31	-87872
PCB 198	429.8	14.17	11.89	10.36	9.04	7.61	-105095
13C-PCB 3	200.65	7.75	6.43	5.55	4.78	3.96	-60788
13C-PCB 9	235.09	8.46	7.03	6.06	5.23	4.33	-66212
13C-PCB 15	235.09	8.93	7.45	6.46	5.59	4.67	-68350
13C-PCB 28	269.5	9.68	8.08	7.00	6.07	5.07	-73949
13C-PCB 31	269.5	9.64	8.04	6.97	6.04	5.04	-73769
13C-PCB 32	269.5	9.52	7.93	6.86	5.94	4.94	-73282
13C-PCB 101	338.4	11.41	9.54	8.29	7.20	6.03	-86156
13C-PCB 111	338.4	11.55	9.67	8.41	7.32	6.14	-86724
13C-PCB 118	338.4	11.83	9.92	8.64	7.53	6.34	-88074
13C-HCB	290.8	7.28	6.05	5.22	4.51	3.74	-56714
d6-gamma-HCH	296.8	8.20	6.82	5.90	5.11	4.25	-63250

Table S5 Partition coefficients between atmospheric particles and the gas phase $K_{Q/G}$ and their temperature dependence $\Delta U_{Q/G}$ estimated for selected SVOCs using the ppLFERs.

Chemical	**log $K_{Q/G}$**					**$\Delta U_{Q/G}$**
	At -40 °C	At -15 °C	At 5 °C	At 25 °C	At 50 °C	(J·mol^{-1})
Naphthalene	6.81	5.79	5.10	4.51	3.87	-47182
Phenanthrene	10.10	8.60	7.60	6.73	5.79	-69042
Pyrene	12.12	10.31	9.10	8.05	6.93	-83265
Chrysene	13.71	11.69	10.34	9.16	7.90	-93128
Benzo(a)pyrene	15.57	13.29	11.76	10.43	9.01	-105223
PCB 1	8.59	7.30	6.43	5.68	4.88	-59506
PCB 11	9.88	8.40	7.42	6.56	5.64	-67907
PCB 16	10.56	8.97	7.90	6.98	5.99	-73196
PCB-28	10.71	9.10	8.03	7.09	6.09	-73944
PCB-52	11.39	9.68	8.52	7.53	6.45	-79191
PCB-101	12.41	10.54	9.28	8.20	7.03	-86154
PCB-118	12.77	10.86	9.58	8.47	7.27	-88072
PCB-138	13.56	11.52	10.16	8.98	7.70	-93903
PCB-153	13.42	11.40	10.04	8.87	7.61	-93108
PCB-180	14.51	12.33	10.87	9.60	8.24	-100518
PCB-194	15.56	13.22	11.66	10.30	8.84	-107683
BDE-47	13.77	11.76	10.40	9.23	7.97	-92925
BDE-99	15.02	12.84	11.37	10.10	8.74	-100736
BDE-100	14.77	12.61	11.17	9.92	8.58	-99219
BDE-153	16.11	13.78	12.21	10.86	9.40	-107546
HCB	8.38	7.15	6.33	5.61	4.84	-56714
alpha-HCH	9.04	7.76	6.89	6.14	5.34	-59439
beta-HCH	9.49	8.13	7.21	6.42	5.57	-62836
delta-HCH	9.70	8.30	7.36	6.55	5.67	-64464
gamma-HCH (Lindane)	9.53	8.16	7.24	6.44	5.58	-63252
4:2-FTOHs	4.53	3.75	3.23	2.77	2.29	-35991
6:2-FTOHs	4.75	3.94	3.39	2.92	2.42	-37307
8:2-FTOHs	4.96	4.12	3.56	3.07	2.55	-38619
10:2-FTOHs	5.17	4.31	3.72	3.22	2.68	-39931
hexamethylcyclotrisiloxane (D3)	4.83	4.11	3.63	3.21	2.76	-33059
octamethylcyclotetrasiloxane (D4)	6.12	5.19	4.57	4.03	3.45	-42746
decamethylcyclopentasiloxane (D5)	7.63	6.48	5.70	5.03	4.31	-53202
dodecamethylcyclohexasiloxane (D6)	9.22	7.84	6.91	6.10	5.23	-63954
Hexachlorobutadiene (HCBD)	6.24	5.33	4.71	4.18	3.61	-42192
2,4,6-tribromoanisole (TBA)	9.27	7.89	6.97	6.17	5.31	-63527
Pentachloroanisole (PCA)	9.60	8.18	7.22	6.39	5.50	-65829
triethyl phosphate (TP)	7.95	6.77	5.99	5.31	4.57	-54124