Simultaneous Estimation of Glass-Water Distribution and PDMS-Water Partition Coefficients of Hydrophobic Organic Compounds Using Simple Batch Method

Supporting Information

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Number of pages = 24

Number of tables = 5

Number of figures = 2

S-1 First-Order Mass Transferring Kinetic Model

Based on the assumption that the rate-determining step is the diffusion in headspace boundary layer near PDMS, the overall mass transfer rate into PDMS in a glass-water-headspace-PDMS system can be expressed as

$$\frac{\mathrm{d}C_{\mathrm{P}}}{\mathrm{d}t} = \frac{A_{\mathrm{P}}}{V_{\mathrm{P}}} k_{\mathrm{A/P}} (C_{\mathrm{A}} - K_{\mathrm{AP}} C_{\mathrm{P}}) \tag{S5}$$

where C_{P} is the concentration in PDMS (mol/μm^3), V_{P} is the PDMS volume (μm^3), C_{A} is the concentration in headspace (mol/μm^3), and K_{AP} is the air-PDMS partition coefficient (μm^3/μm^3).

Since the rate-determining step is the diffusion in headspace boundary layer near PDMS, there is equilibration between glass, water, and headspace. That is,

$$C_{\mathrm{W}} = \frac{C_{\mathrm{G}}}{K_{\mathrm{GW}}} = \frac{C_{\mathrm{A}}}{K_{\mathrm{AW}}} \tag{S6}$$

where C_{W} is the concentration in water (mol/μm^3), C_{G} is the surface concentration on glass (mol/μm^2), K_{GW} is the glass-water distribution coefficient (μm^3/μm^2). The total amount of a chemical in the system can be expressed as

$$M = C_{\mathrm{G}} A_{\mathrm{G}} + C_{\mathrm{W}} V_{\mathrm{W}} + C_{\mathrm{A}} V_{\mathrm{A}} + C_{\mathrm{P}} V_{\mathrm{P}} \tag{S7}$$

where M is the total amount of a chemical (mol), V_{W} is the water volume (μm^3) and V_{A} is the headspace volume (μm^3). After rearrangement, Equation S7 becomes

$$C_{\mathrm{A}} = \frac{M - C_{\mathrm{P}} V_{\mathrm{P}}}{\frac{K_{\mathrm{GW}}}{K_{\mathrm{AW}}} A_{\mathrm{G}} + \frac{1}{K_{\mathrm{AW}}} V_{\mathrm{W}} + V_{\mathrm{A}}} \tag{S8}$$

When equilibration in the system is reached

$$M = C_{\mathrm{G,t}\to\infty} A_{\mathrm{G}} + C_{\mathrm{W,t}\to\infty} V_{\mathrm{W}} + C_{\mathrm{A,t}\to\infty} V_{\mathrm{A}} + C_{\mathrm{P,t}\to\infty} V_{\mathrm{P}} \tag{S9}$$

$$C_{\mathrm{P,t}\to\infty} = \frac{C_{\mathrm{G,t}\to\infty} K_{\mathrm{AW}}}{K_{\mathrm{GW}} K_{\mathrm{AP}}} = \frac{C_{\mathrm{W,t}\to\infty} K_{\mathrm{AW}}}{K_{\mathrm{AP}}} = \frac{C_{\mathrm{A,t}\to\infty}}{K_{\mathrm{AP}}} \tag{S10}$$

where $t \to \infty$ indicates the achievement of equilibration in the system. By expressing $C_{\mathrm{G,t}\to\infty}$, $C_{\mathrm{G,t}\to\infty}$, and $C_{\mathrm{G,t}\to\infty}$ using $C_{\mathrm{P,t}\to\infty}$ in Equation S9 through S10, and substituting M from Equation S9 into S8, and then substituting Equation S8 into S5, which then becomes

$$\frac{\mathrm{d}C_{\mathrm{P}}}{\mathrm{d}t} = \frac{A_{\mathrm{P}}}{V_{\mathrm{P}}} k_{\mathrm{A/P}} \left[\frac{C_{\mathrm{P,t}\to\infty}\left(\frac{K_{\mathrm{GW}} K_{\mathrm{AP}}}{K_{\mathrm{AW}}} A_{\mathrm{G}} + \frac{K_{\mathrm{AP}}}{K_{\mathrm{AW}}} V_{\mathrm{W}} + K_{\mathrm{AP}} V_{\mathrm{A}} + V_{\mathrm{P}} \right) - C_{\mathrm{P}} V_{\mathrm{P}}}{\frac{K_{\mathrm{GW}}}{K_{\mathrm{AW}}} A_{\mathrm{G}} + \frac{1}{K_{\mathrm{AW}}} V_{\mathrm{W}} + V_{\mathrm{A}}} - K_{\mathrm{AP}} C_{\mathrm{P}} \right] \tag{S11}$$

The solution of Equation S11 is

$$C_{\mathrm{P}} = C_{\mathrm{P,t}\to\infty}(1 - \mathrm{e}^{-\alpha t}) \tag{S12}$$

where α is the overall mass transfer rate (1/s). In Equation S12, $C_{\mathrm{P,t}\to\infty}$ and α are

$$C_{\mathrm{P},t\to\infty} = \frac{K_{\mathrm{PW}} M}{V_{\mathrm{W}} + K_{\mathrm{AW}} V_{\mathrm{A}} + K_{\mathrm{PW}} V_{\mathrm{P}} + K_{\mathrm{GW}} A_{\mathrm{G}}} \tag{S13}$$

$$\alpha = \frac{A_{\mathrm{P}} k_{\mathrm{A/P}} K_{\mathrm{AP}}}{V_{\mathrm{P}}} \times \frac{\frac{K_{\mathrm{GW}} K_{\mathrm{AP}}}{K_{\mathrm{AW}}} A_{\mathrm{G}} + \frac{K_{\mathrm{AP}}}{K_{\mathrm{AW}}} V_{\mathrm{W}} + K_{\mathrm{AP}} V_{\mathrm{A}} + V_{\mathrm{P}}}{\frac{K_{\mathrm{GW}} K_{\mathrm{AP}}}{K_{\mathrm{AW}}} A_{\mathrm{G}} + \frac{K_{\mathrm{AP}}}{K_{\mathrm{AW}}} V_{\mathrm{W}} + K_{\mathrm{AP}} V_{\mathrm{A}}} \tag{S14}$$

If the headspace capacity is negligible, and let K_{PW} is the product of K_{AW} and K_{PA}, Equations S13 and S14 become

$$C_{\mathrm{P},t\to\infty} = \frac{K_{\mathrm{PW}} M}{V_{\mathrm{W}} + K_{\mathrm{PW}} V_{\mathrm{P}} + K_{\mathrm{GW}} A_{\mathrm{G}}} \tag{S15}$$

$$\alpha = \frac{A_{\mathrm{P}} k_{\mathrm{A/P}} K_{\mathrm{AW}}}{V_{\mathrm{P}} K_{\mathrm{PW}}} \times \frac{\frac{K_{\mathrm{GW}}}{K_{\mathrm{PW}}} A_{\mathrm{G}} + \frac{1}{K_{\mathrm{PW}}} V_{\mathrm{W}} + V_{\mathrm{P}}}{\frac{K_{\mathrm{GW}}}{K_{\mathrm{PW}}} A_{\mathrm{G}} + \frac{1}{K_{\mathrm{PW}}} V_{\mathrm{W}}} \tag{S16}$$

Equations S15 and S16 are Equations 1 and 2 in the manuscript, respectively.

S-2 Derivation of Equations for Refilling and Non-refilling Experiments

In a glass-water-headspace-PDMS system, where headspace capacity of a HOC is negligible, at equilibrium:

$$C_{\mathrm{W}} = \frac{C_{\mathrm{P}}}{K_{\mathrm{PW}}} = \frac{C_{\mathrm{G}}}{K_{\mathrm{GW}}} = \frac{C_{\mathrm{A}}}{K_{\mathrm{AW}}} \tag{S17}$$

In the refilling experiment, when the first equilibrium is reached in the system, PDMS and water phases are replaced with clean ones for the second equilibration cycle. The procedure can be repeated for several times and in each cycle the system has total HOC mass equal to the mass retained on the glass surface from the previous cycle, since only the glass surface has not been replaced. Thus, the mass balance in each cycle can be written as

$$C_{\mathrm{G,n-1}} A_{\mathrm{G}} = C_{\mathrm{W,n}} V_{\mathrm{W}} + C_{\mathrm{G,n}} A_{\mathrm{G}} + C_{\mathrm{P,n}} V_{\mathrm{P}} \tag{S18}$$

In Equation S18, C_{G} and C_{W} can be expressed in terms of C_{P} according to Equation S17, that is, C_{W} is $C_{\mathrm{P}}/K_{\mathrm{PW}}$ and C_{G} is $C_{\mathrm{P}}K_{\mathrm{GW}}/K_{\mathrm{PW}}$. Equation S18 then becomes

$$\frac{C_{\mathrm{P,n-1}} K_{\mathrm{GW}} A_{\mathrm{G}}}{K_{\mathrm{PW}}} = \frac{C_{\mathrm{P,n}} V_{\mathrm{W}}}{K_{\mathrm{PW}}} + \frac{C_{\mathrm{P,n}} K_{\mathrm{GW}} A_{\mathrm{G}}}{K_{\mathrm{PW}}} + C_{\mathrm{P,n}} V_{\mathrm{P}} \tag{S19}$$

Equation S19 can be rewritten as

$$R \equiv \frac{C_{\mathrm{P,n}}}{C_{\mathrm{P,n-1}}} = \frac{K_{\mathrm{GW}} A_{\mathrm{G}}}{K_{\mathrm{GW}} A_{\mathrm{G}} + V_{\mathrm{W}} + K_{\mathrm{PW}} V_{\mathrm{P}}} \tag{S20}$$

The parallel non-refilling experiment is similar to the refilling experiment except that the aqueous phase is not replaced either in each cycle. Thus, in each cycle the total mass of HOC in the system is the mass on the glass surface and in the aqueous phase retained from the previous cycle. Thus, the mass balance equation in the non-refilling experiment is

$$C'_{\mathrm{W,n-1}} V_{\mathrm{W}} + C'_{\mathrm{G,n-1}} A_{\mathrm{G}} = C'_{\mathrm{W,n}} V_{\mathrm{W}} + C'_{\mathrm{G,n}} A_{\mathrm{G}} + C'_{\mathrm{P,n}} V'_{\mathrm{P}} \tag{S21}$$

where the prime superscript denotes non-refilling experiment and V'_{P} is PDMS volume used in non-refilling experiment. Again, C_G and C_W can be expressed in terms of C_P according to Equation S18. Equation S21 becomes,

$$\frac{C_{P,n-1}V_W}{K_{PW}} + \frac{C_{P,n-1}K_{GW}A_G}{K_{PW}} = \frac{C_{P,n}V_W}{K_{PW}} + \frac{C_{P,n}K_{GW}A_G}{K_{PW}} + C_{P,n}V'_P \tag{S22}$$

After rearrangement, Equation S22 becomes

$$r \equiv \frac{C'_{P,n}}{C'_{P,n-1}} = \frac{K_{GW}A_G + V_W}{K_{GW}A_G + V_W + K_{PW}V'_P} \tag{S23}$$

Equation S23 can be written as

$$K_{GW} = \frac{K_{PW}V'_P\, r - V_W(1-r)}{A_G(1-r)} \tag{S24}$$

Equation S24 can substitute K_{GW} in Equation S20,

$$R = \frac{\dfrac{K_{PW}V'_P\, r - V_W(1-r)}{(1-r)}}{\dfrac{K_{PW}V'_P\, r - V_W(1-r)}{(1-r)} + V_W + K_{PW}V_P} \tag{S25}$$

or

$$K_{PW} = \frac{V_W(1-r)}{V'_P\, r(1-R) - V_P R(1-r)} \tag{S26}$$

Equation S26 express K_{PW} in terms of R and r which can be obtained from refilling and non-refilling experiments, respectively. Equation S26 can substitute into Equation S24, which then becomes

$$K_{GW} = \frac{\dfrac{V_W(1-r)}{V'_P\, r(1-R) - V_P R(1-r)} V'_P\, r - V_W(1-r)}{A_G(1-r)}$$

$$K_{GW} = \frac{V_W R(V'_P\, r - V_P r + V_P)}{A_G[V'_P\, r(1-R) - V_P R(1-r)]} \tag{S27}$$

Equations S26 and S27 are Equations 11 and 12, respectively, in the main paper. If V'_P is equal to V_P, Equations S26 and S27 become

$$K_{PW} = \frac{V_W(1-r)}{V_P(r-R)} \tag{S28}$$

$$K_{GW} = \frac{V_W R}{A_G(r-R)} \tag{S29}$$

Equations S28 and S29 are Equations 9 and 10, respectively, in the main paper.

S-3 Verification of Negligible Headspace Capacity

The PCB capacity ratio of headspace to water can be expressed as

$$\frac{C_{\mathrm{A}}V_{\mathrm{A}}}{C_{\mathrm{W}}V_{\mathrm{W}}}=\frac{K_{\mathrm{AW}}V_{\mathrm{A}}}{V_{\mathrm{W}}} \tag{S30}$$

Fang et al. (2006) reported that the air-water Henry's law constants for PCB congeners were lower than 30 Pa/mole/m^3, which can be translated to K_{AW} of 0.012 since

$$30\frac{Pa}{mole/m^3}\cong 30\times10^{-5}\frac{atm}{mole/m^3}=30\times10^{-5}\times41\frac{mole/m^3}{mole/m^3}=0.012$$

Since the present study $V_{\mathrm{A}}/V_{\mathrm{W}}$ was 0.2, the capacity ratio of headspace to water was lower than 0.0025, indicating that the assumption of negligible headspace capacity was appropriate.

S-4 Experimental Data of Kinetic Study

TABLE S.1 Experimental data of kinetic study (reponse (peak area) of GC analysis)

IUPAC	1 hr	3 hr	6.33 hr	12 hr	24 hr	48 hr	91 hr	188 hr	Logα (α: s^{-1})	Rsq for α	Equilibration % after 4-day (95% confidence equilibration
PCB18	111840	143974	149169	80130	108699	84252	90192	114808			NA
PCB16,32	127509	154075	160882	126917	127499	106779	98498	120316			NA
PCB28,31	448743	748299	880929	850198	700396	608276	636118	687936	-3.56	0.52	100 (90)
PCB33,53	142976	282226	348125	329686	338059	250607	225670	292012	-3.55	0.5	100 (86)
PCB22		141020	222459	193292	150996	148357	128056	186512	-3.70	0.07	100 (81)
PCB52	297632	487361	780438	779066	693410	605328	545080	758560	-3.84	0.3	100 (90)
PCB47,48	240589	218851	351685	421917	495272	270087	240850	341728	-3.70	0.17	100 (81)
PCB44	230380	392247	739709	762437		593332	507228	746020	-3.94	0.4	100 (70)
PCB41,71	183494	344613	709906	769698	643516	566007	470794	728508			NA
PCB70		178089	484318	570827	484183	483904	410606	546616			NA
PCB66		457763	1122200	1350525	1223486	1279727	1047966	1398236			NA
PCB95	542644	1100253	2517821	3167318	2999683	2921089	2263892	3186236			NA
PCB56,60		398568	1107929	1412789	1326104	1455388	1184530	1591856	-4.28	0.81	100 (91)
PCB101	544432	1198469	2957384	3844259	4030232	4109771	3232372	4474628	-4.30	0.92	100 (92)
PCB99	178121	325037	923893	1173931	1211367	1200389	1039012	1375916	-4.31	0.92	100 (93)
PCB83	91451	245360	727755	958773	1000269	1145246	926892	1268696	-4.42	0.92	100 (92)
PCB97	169980	478213	1465893	1945626	2104727	2484188	1980092	2751996	-4.47	0.92	100 (92)
PCB87	24744	133166	460527	591643	581325	789638	590830	834100	-4.48	0.89	100 (90)
PCB85	104675	252681	715683	886429	988054	1174232	948128	1188268	-4.44	0.95	100 (94)
PCB110	311647	794688	2469666	3322150	3651952	4557468	3732786	5145632	-4.54	0.94	100 (92)
PCB151	228803	522549	1613161	2137998	2458029	3015298	2529688	3379756	-4.56	0.94	100 (93)
PCB135	102592	303032	926420	1244287	1556705	1917238	1568526	2064644	-4.60	0.95	100 (94)
PCB149		908730	2731184	3645823	4009848	5591250	4782266	6302996	-4.64	0.89	100 (92)
PCB118		449712	1525260	2166985	2313977	3191782	3367302	4132668	-4.81	0.91	100 (92)
PCB146	48558	132556	503240	704498	818815	1194940	1143528	1451836	-4.82	0.95	99 (93)
PCB153	308956	801455	2730490	3939522	4665111	6863886	6599412	8501180	-4.85	0.96	99 (93)
PCB105,132	167753	520884	1890254	2685542	3080546	4858172	4968104	5952000	-4.91	0.96	99 (93)
PCB141,179	163018	463429	1760983	2430384	2832049	4048258	4600094	5571812	-4.94	0.95	98 (92)
PCB138	262397	797678	3135022	4340155	5484807	8766834	9567418	11897604	-5.03	0.97	96 (91)
PCB163		109519	446231	615036	796681	1283432	1534034	1754192	-5.08	0.98	94 (91)
PCB158	52697	110617	491648	596164	763948	1269604	1487756	1625404	-5.03	0.98	96 (92)
PCB182,187	130449	385035	1452858	1906161	2477688	4277682	4650712	4963596	-5.01	0.98	97 (93)
PCB183	61581	170537	717733	999791	1263597	2248306	2459750	2660280	-5.02	0.98	96 (93)
PCB128	17850	91753	421731	601416	926428	1471682	1832212	2065488	-5.14	0.99	92 (90)
PCB185	17335	40678	211419	315641	523809	784872	985514	1002524	-5.07	1	95 (93)
PCB174	93512	250668	1036886	1470575	1948583	3426274	4211850	4520860	-5.13	0.99	92 (89)
PCB177	40003	125328	553406	830111	1104133	1978504	2278008	2554604	-5.10	0.98	94 (91)
PCB171,202	14645	85453	565023	823295	898293	2012704	2481840	2817092	-5.21	0.98	88 (84)
PCB180	110235	367986	1950957	2692469	3271043	5941560	7805650	9030620	-5.20	0.98	88 (85)
PCB170	33935	146080	814686	1040587	1392182	2488066	3588930	3867024	-5.25	0.98	86 (82)
PCB201	21426	71038	451917	558167	597608	1292994	1701338	1808004	-5.18	0.97	90 (85)
PCB203	25489	79294	533388	650465	708050	1539518	1878888	2096188	-5.17	0.97	90 (86)
PCB195	8161	21735	159151	178773	182072	425296	530482	601884	-5.20	0.96	88 (83)
PCB194	6774	25532	256967	236778	264128	579282	751000	913332	-5.26	0.96	85 (80

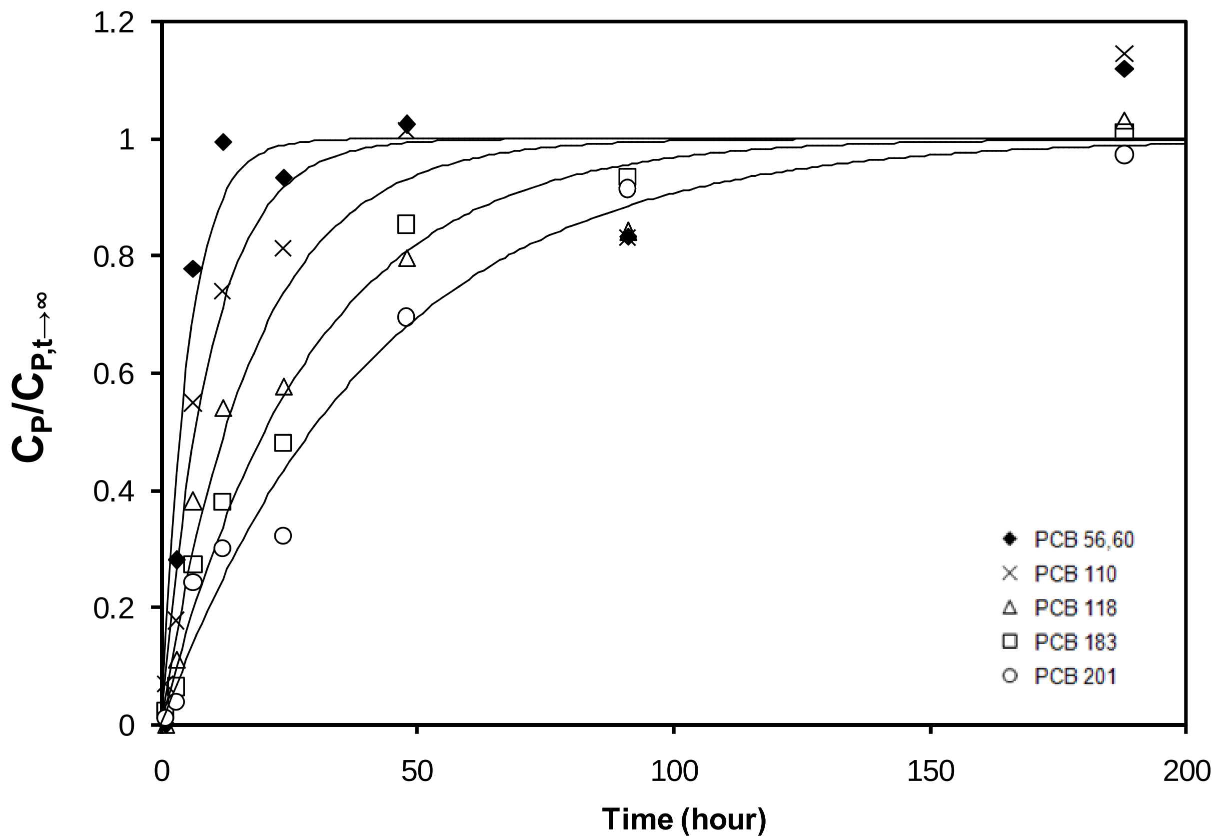

Figure S.1 Adsorption kinetic curves of some selected PCB congeners.

S-5 Values of *R* and *r* Obtained from Refilling and Non-refilling Experiments

Values of *R* and *r* obtained from refilling and non-refilling experiments are shown in Table S.2. The average and standard deviation values of *R* and *r* are also shown in Tabld S.2. Assuming that the experimental measurements of *R* and *r* values of each PCB congener are normally distributed, the averages and standard deviations of $\log K_{PW}$ and $\log K_{GW}$ can be obtained through Monte Carlo simulation (for each congener, 1000 pairs of *R* and *r* were produced having the average and standard deviation as the experimentally obtained values from this study; *R* and r values produced in simulation were considered only if they were in the range of 0 to 1). The results of averages and standard deviations $\log K_{PW}$ and $\log K_{GW}$ are also shown in Table S.2.

TABLE S.2 Values of *R* and *r* obtained from refilling and non-refilling experiments; logK_{PW} and logK_{GW} obtained from *R* and r

	R (unitless)					r (unitless)					logK_{PW} ($\mu m^3/\mu m^3$)		logK_{GW} ($\mu m^3/\mu m^2$)	
IUPAC	1st cycle	2nd cycle	3rd cycle	Avg	Stdev	1st cycle	2nd cycle	3rd cycle	Avg	Stdev	Avg	Stdev	Avg	Stdev
PCB18	ND	ND	ND	NA	NA	0.91	1.00	0.82	0.91	0.09	4.91	0.45	NA	NA
PCB16,32	ND	ND	ND	NA	NA	0.74	0.95	0.86	0.85	0.10	5.12	0.39	NA	NA
PCB28,31	ND	ND	ND	NA	NA	0.82	0.91	0.80	0.84	0.06	5.17	0.22	NA	NA
PCB33,53	ND	ND	ND	NA	NA	0.85	0.93	0.71	0.83	0.11	5.18	0.39	NA	NA
PCB22	ND	ND	ND	NA	NA	0.88	0.97	0.62	0.82	0.18	5.30	0.49	NA	NA
PCB52	0.03	ND	ND	0.03	NA	0.65	0.83	0.70	0.73	0.09	5.48	0.23	2.98	0.02
PCB47,48	0.03	ND	ND	0.03	NA	0.62	0.80	0.76	0.73	0.09	5.49	0.24	3.02	0.01
PCB44	0.09	ND	ND	0.09	NA	0.63	0.83	0.80	0.75	0.11	5.44	0.29	3.49	0.01
PCB41,71	0.06	ND	ND	0.06	NA	0.60	0.82	0.76	0.73	0.12	5.49	0.30	3.33	0.01
PCB70	0.06	ND	ND	0.06	NA	0.49	0.71	0.56	0.59	0.11	5.79	0.23	3.32	0.01
PCB66	0.06	ND	ND	0.06	NA	0.50	0.75	0.63	0.63	0.12	5.70	0.26	3.28	0.01
PCB95	0.08	0.11	ND	0.10	0.02	0.44	0.70	0.66	0.60	0.14	5.77	0.29	3.52	0.12
PCB56,60	0.08	0.15	ND	0.12	0.05	0.41	0.71	0.57	0.56	0.15	5.86	0.30	3.58	0.29
PCB101	0.11	0.10	ND	0.10	0.01	0.36	0.60	0.49	0.48	0.12	6.01	0.23	3.57	0.03
PCB99	0.09	0.12	ND	0.10	0.02	0.30	0.50	0.39	0.40	0.10	6.17	0.19	3.58	0.09
PCB83	0.09	0.02	ND	0.05	0.05	0.32	0.57	0.49	0.46	0.12	6.02	0.24	3.24	0.42
PCB97	0.08	0.03	ND	0.06	0.04	0.31	0.56	0.47	0.45	0.12	6.05	0.24	3.23	0.38
PCB87	0.08	0.05	ND	0.07	0.02	0.27	0.50	0.36	0.38	0.12	6.19	0.26	3.34	0.20
PCB85	0.15	0.07	ND	0.11	0.05	0.21	0.40	0.29	0.30	0.10	6.38	0.25	3.58	0.32
PCB110	0.09	0.09	ND	0.09	0.00	0.30	0.58	0.51	0.47	0.14	6.03	0.29	3.52	0.03
PCB151	0.14	0.14	ND	0.14	0.00	0.21	0.43	0.37	0.34	0.11	6.31	0.26	3.75	0.06
PCB135	0.13	0.05	ND	0.09	0.06	0.17	0.36	0.22	0.25	0.10	6.48	0.29	3.48	0.37
PCB149	0.19	0.14	ND	0.16	0.03	0.17	0.36	0.34	0.29	0.10	6.42	0.26	3.84	0.12
PCB118	0.12	0.12	ND	0.12	0.00	0.24	0.49	0.39	0.37	0.13	6.23	0.28	3.66	0.04
PCB146	0.15	0.19	0.42	0.25	0.15	0.15	0.28	0.24	0.22	0.07	6.66	0.24	4.07	0.46
PCB153	0.19	0.20	0.37	0.25	0.10	0.15	0.30	0.25	0.23	0.08	6.62	0.26	4.07	0.31
PCB105,132	0.16	0.16	0.31	0.21	0.08	0.21	0.41	0.34	0.32	0.10	6.40	0.26	3.93	0.28
PCB141,179	0.19	0.36	0.32	0.29	0.09	0.14	0.31	0.18	0.21	0.09	6.73	0.32	4.20	0.26
PCB138	0.18	0.21	0.41	0.27	0.12	0.16	0.29	0.27	0.24	0.07	6.61	0.24	4.09	0.37
PCB163	0.17	0.13	0.54	0.28	0.22	0.13	0.51	0.09	0.24	0.23	6.56	0.56	4.13	0.58
PCB158	0.22	0.25	0.52	0.33	0.16	0.11	0.25	0.21	0.19	0.07	6.83	0.34	4.28	0.46
PCB182,187	0.30	0.31	0.53	0.38	0.13	0.09	0.18	0.23	0.17	0.07	6.96	0.37	4.44	0.37
PCB183	0.28	0.32	0.77	0.45	0.27	0.10	0.32	0.86	0.43	0.39	6.26	0.73	4.41	0.58
PCB128	0.18	0.23	0.42	0.28	0.12	0.17	0.28	0.27	0.24	0.06	6.61	0.19	4.11	0.34
PCB185	0.22	0.22	0.70	0.38	0.28	0.08	0.28	NA	0.18	0.14	6.86	0.51	4.36	0.64
PCB174	0.33	0.35	0.56	0.41	0.13	0.12	0.17	0.15	0.15	0.03	7.04	0.23	4.52	0.33
PCB177	0.32	0.32	0.62	0.42	0.18	0.12	0.21	0.16	0.16	0.05	7.02	0.37	4.53	0.49
PCB171,202	0.23	0.38	0.55	0.39	0.16	0.11	0.26	0.31	0.23	0.11	6.78	0.42	4.40	0.43
PCB180	0.29	0.42	0.62	0.44	0.17	0.14	0.21	0.27	0.21	0.07	6.89	0.34	4.53	0.43
PCB170	0.33	0.41	0.66	0.47	0.17	0.17	0.31	0.24	0.24	0.07	6.82	0.34	4.55	0.43
PCB201	0.43	0.54	0.83	0.60	0.21	0.14	0.31	0.18	0.21	0.09	7.06	0.48	4.83	0.53
PCB203	0.41	0.56	0.85	0.61	0.22	0.14	0.22	0.24	0.20	0.05	7.09	0.43	4.83	0.55
PCB195	0.45	0.57	1.00	0.67	0.29	0.17	0.38	NA	0.28	0.15	6.89	0.54	4.81	0.62
PCB194	0.44	0.52	0.95	0.64	0.27	0.21	0.42	0.32	0.32	0.11	6.79	0.46	4.77	0.57

ND: non-detectable. NA: not available

S-6 Verification of C_G-C_W Linear Relationship

In the present study, it was assumed that the surface density (C_G) and the aqueous concentration (C_W) of a HOC have linear relationship at low aqueous concentration. The assumption sustains only when trace amount of adsorbate was adsorbed on glass, and it might be verified by the coverage ratio of surface area of PCBs on glass surface.

Coverage ratio, in this study, is defined as the summation of all individual congeners' projected area to the interior surface area of the glass bottle. The unit projected area of a PCB molecule is estimated from its total surface area (TSA) by assuming that each molecule is a sphere. Hawker and Connell (1988) reported that TSA of PCBs ranges approximately from 200×10^{-20} m^2 to 300×10^{-20} m^2. To be conservative and for simplicity, we assumed that each PCB's TSA is 300×10^{-20} m^2. Thus the projection area of each PCB molecule is 75×10^{-20} m^2.

The calculation procedure for the coverage ratio is shown as following. At equilibrium, C_G of a particular PCB congener can be determined using C_P of that congener through the equilibrium relationship

$$C_G = \frac{K_{GW} C_P}{K_{PW}} \tag{S31}$$

The projected area of that PCB congener is

$$A_{\text{Porjection}} = \frac{C_G A_G}{W_M} \times (6.02\times10^{23}\,\text{mole}^{-1}) \times (75\times10^{-20}\,\text{m}^2) \tag{S32}$$

where $A_{\text{Projection}}$ is the total projection area of the particular PCB congener (m^2), W_M is the molecular weight of the PCB congener (g/mole), 6.20×10^{-20} mole^{-1} is Avogadro's number, 75×10^{-20} m^2 is the projection area of each PCB molecule. The total projection area ($A_{\text{Projection,TOT}}$) of all PCBs is then

$$A_{\mathrm{Projection,TOT}} = \sum_{1}^{209} A_{\mathrm{Projection,PCBn}} \quad \text{(S33)}$$

The coverage ratio is then $A_{\mathrm{P,TOT}}/A_{\mathrm{G}}$.

The sorption kinetic test at 188 hr, which should be at equilibrium, was used as an example to verify that the PCB surface coverage ratio was low. In the system, A_{G} was 0.086 m^2 (860 cm^2). As shown in the following table, the total projection area of PCBs on glass surface was 2.16×10^{-5} m^2. Thus, the coverage ratio was 2.16×10^{-5} / 0.086 = 0.0025. That is the glass surface covered by PCBs was around 0.03%, which indicates that the sorption of chemicals on glass bottles was far from saturation. Thus, the assumption of the linear relationship between C_{G} and C_{W} should be appropriate.

TABLE S.3 Projection area of PCBs on glass surface in 2-L reactor

	C_P (g/m^3)	C_G (g/m^2)	W_M (g/mole)	$A_{Projection}$ (m^2)
PCB18	0.21		234	
PCB16,32	0.12		234	
PCB28,31	0.58		234	
PCB33,53	0.61		238	
PCB22	0.13		234	
PCB52	0.76	2.38E-09	268	3.45E-07
PCB47,48	0.21	7.12E-10	268	1.03E-07
PCB44	0.51	5.74E-09	268	8.32E-07
PCB41,71	0.18	1.22E-09	268	1.77E-07
PCB70	0.99	3.41E-09	268	4.95E-07
PCB66	0.58	2.20E-09	268	3.19E-07
PCB95	1.34	7.42E-09	303	9.53E-07
PCB56,60	0.62	3.25E-09	268	4.70E-07
PCB101	2.26	8.17E-09	303	1.05E-06
PCB99	0.79	2.03E-09	303	2.61E-07
PCB83	0.14	2.21E-10	303	2.84E-08
PCB97	0.73	1.11E-09	303	1.42E-07
PCB87	1.28	1.80E-09	303	2.31E-07
PCB85	0.44	6.82E-10	303	8.75E-08
PCB110	2.69	8.29E-09	303	1.06E-06
PCB151	1.13	3.09E-09	337	3.56E-07
PCB135	0.56	5.59E-10	337	6.44E-08
PCB149	4.12	1.07E-08	337	1.23E-06
PCB118	2.41	6.50E-09	303	8.35E-07
PCB146	0.70	1.78E-09	337	2.05E-07
PCB153	4.81	1.34E-08	337	1.55E-06
PCB105,132	2.83	9.74E-09	323	1.17E-06
PCB141,179	2.39	7.03E-09	350	7.80E-07
PCB138	4.79	1.44E-08	337	1.66E-06
PCB163	1.32	5.00E-09	337	5.76E-07
PCB158	0.58	1.61E-09	337	1.85E-07
PCB182,187	2.07	6.34E-09	372	6.62E-07
PCB183	1.00	1.43E-08	372	1.49E-06
PCB128	0.71	2.24E-09	337	2.59E-07
PCB185	0.21	6.63E-10	372	6.93E-08
PCB174	1.84	5.61E-09	372	5.86E-07
PCB177	0.98	3.13E-09	372	3.27E-07
PCB171,202	0.60	2.47E-09	379	2.53E-07
PCB180	3.60	1.59E-08	372	1.66E-06
PCB170	1.11	6.01E-09	372	6.28E-07
PCB201	0.05	3.02E-10	406	2.88E-08
PCB203	0.30	1.63E-09	406	1.56E-07
PCB195	0.14	1.16E-09	406	1.11E-07
PCB194	0.21	2.05E-09	406	1.96E-07
			$A_{Projection,TOT}$	2.16E-05

S-7 Values of K_{PW} and K_{OW} in Figure 6

Values of K_{PW} and K_{OW} in Figure 6 in the main paper are shown in Table S.4.

In a traditional approach using a glass-water-PDMS system to determine K_{PW} without considering glass adsorption effect (that is, the total mass of a HOC in water and on glass is mistaken as total mass in water), the K_{PW} of the HOC will be underestimated. At equilibrium, the mass in water should be $C_P V_W / K_{PW}$ and the mass on glass should be $C_P K_{GW} A_G / K_P W$. Because of the ignoring of the glass adsorption, the K_{PW} (noted as $K_{PW,\text{ignore glass}}$) was incorrectly estimated and it has the relationship with actual K_{PW} and K_{GW} (noted as $K_{PW,\text{actual}}$ and $K_{GW,\text{actual}}$)

$$K_{PW,\text{ignore glass}} = \frac{K_{PW,\text{actual}}}{1 + \dfrac{K_{GW,\text{actual}} A_G}{V_W}} \tag{S34}$$

With the scenario of using a 50 mL vial (inner glass surface area of 74 cm^2) in a traditional approach, values of $K_{PW,\text{ignore glass}}$ were obtained (using KPW and KPW from this study as $K_{PW,\text{actual}}$ and $K_{GW,\text{actual}}$ in Equation S31) and shown as open circles in Figure 6 in the main paper and in column (c) in Table S.4.

TABLE S.4 Values of logK_{PW} and logK_{OW} in Figure 6.

	logK_{OW}	logK_{PW}										
PCB IUPAC	(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)	(j)	(k)	(l)
1	4.46				4.03				4.44	4.09		
2	4.69										4.18	
4												4.59
10												4.55
14	5.38										4.94	5.14
15	5.30				4.65				5.11	4.83		
16	5.16	5.12	5.12									
18	5.24	4.91	4.91					5.11			5.13	5.23
21												5.43
22	5.58	5.30	5.30									
28	5.67	5.17	5.17		5.04	4.65	4.76	5.24	5.47	5.18	5.34	5.53
29												5.43
30												5.24

31	5.67	5.17	5.17									5.49
32	5.44	5.12	5.12									
33	5.60	5.18	5.18									
35	5.82										5.30	
41	5.69	5.49	5.37									
44	5.75	5.44	5.28					5.49				5.82
47	5.85	5.49	5.43						5.85	5.64		5.78
48	5.78	5.49	5.43									
49												5.88
50												5.70
52	5.84	5.48	5.43	5.38	5.55	4.98	5.14	5.49			5.65	5.81
53	5.62	5.18	5.18									
55												6.00
56	6.11	5.86	5.66									6.04
60	6.11	5.86	5.66									
65	5.86			5.35								
66	6.20	5.70	5.59					5.57				
70	6.20	5.79	5.67									
71	5.98	5.49	5.37									
72	6.26										5.86	
77	6.36							5.80			5.67	
78												6.05
83	6.26	6.02	5.93									
85	6.30	6.38	6.19									6.24
87	6.29	6.19	6.07									6.35
95	6.13	5.77	5.60									
97	6.29	6.05	5.95									6.21
99	6.39	6.17	5.97									6.37
101	6.38	6.01	5.82	5.71		5.48	5.48	5.61	6.21	6.08	6.14	6.28
104												6.17
105	6.65	6.40	6.04	5.89				5.73				6.42
110	6.48	6.03	5.86									6.30
112	6.45			5.71								
118	6.74	6.23	6.01	5.87	5.97			5.67			6.14	6.42
126	6.89							5.73			6.14	
128	6.74	6.61	6.15					5.52				6.76
132	6.58	6.40	6.04									
135	6.64	6.48	6.32									
137												6.82
138	6.83	6.61	6.16	6.20		5.98	5.65	5.49				6.76
141	6.82	6.73	6.21									6.70
145												6.65
146	6.89	6.66	6.22									
149	6.67	6.42	6.12									6.64
151	6.64	6.31	6.05									6.58
153	6.92	6.62	6.19	6.16	6.05	6.01	5.67	5.45	6.68	6.45	6.53	6.72
154	6.76			6.17								
155	6.41			6.03								6.79
156	7.18			6.28				5.44				6.72
158	7.02	6.83	6.25									
163	6.99	6.56	6.08									
170	7.27	6.82	6.02					5.02				7.10
171	7.11	6.78	6.11									
174	7.11	7.04	6.27									
177	7.08	7.02	6.25									
179	6.73	6.73	6.21									
180	7.36	6.89	6.11	6.40	6.24	6.37	5.55	5.07	6.76	6.54	6.78	6.99
183	7.20	6.26	5.58									
185	7.11	6.86	6.22									

187	7.17	6.96	6.25					5.14				6.87
194	7.80	6.79	5.80									
195	7.56	6.89	5.86									
201	7.62	7.06	6.02					4.77				
202	7.24	6.78	6.11						6.77	6.20		
203	7.65	7.09	6.05								7.05	
204												7.56
206	8.09							4.46	7.04	6.16		
209	8.18							4.27	6.84	5.59		

(a) Hawker and Connell, 1988
(b) Present study
(c) Present study ignore glass
(d) Mayer et al., 2000
(e) Poerschmann et al., 2000
(f) Paschke and Popp (1), 2003
(g) Paschke and Popp (2), 2003
(h) Zeng et al., 2005
(i) Yang et al. (1), 2006
(j) Yang et al. (2), 2006
(k) Ter Laak et al., 2008
(l) Smedes et al., 2009 (average of AlteSil polymers)

S-8 PCB Composition in Aroclors

TABLE S.5 PCB composition in Aroclors (weight %)

IUPAC	Sturcture	Aroclor[a] 1242	Aroclor[a] 1254	Aroclor[a] 1260	Aroclors mixture in this study
1	2	0.54		0.02	0.1867
2	3	0.03			0.0100
3	4	0.18			0.0600
4	22’	3.08	0.06	0.02	1.0533
5	23	0.14			0.0467
6	23’	1.43	0.02	0.01	0.4867
7	24	0.26			0.0867
8	24’	7.05	0.13	0.04	2.4067
9	25	0.5			0.1667
10	26	0.2			0.0667
11	33’				0.0000
12	34	0.06			0.0200
13	34’	0.22			0.0733
14	35				0.0000
15	44’	2.1	0.03	0.01	0.7133
16	22’3	3.14	0.09	0.01	1.0800
17	22’4	3.13	0.08	0.02	1.0767
18	22’5	8.53	0.25	0.05	2.9433
19	22’6	0.8			0.2667
20	233’	0.72			0.2400
21	234				0.0000
22	234’	2.84	0.04	0.01	0.9633
23	235	0.01			0.0033
24	236	0.13			0.0433
25	23’4	0.59			0.1967
26	23’5	1.28	0.03		0.4367
27	23’6	0.41			0.1367
28	244’	6.86	0.19	0.03	2.3600
29	245	0.08			0.0267
30	246				0.0000
31	24’5	7.34	0.28	0.04	2.5533
32	24’6	1.9	0.05	0.01	0.6533
33	2’34	5.01	0.16	0.03	1.7333
34	2’35	0.02			0.0067
35	33’4	0.08			0.0267
36	33’5				0.0000
37	344’	2.03	0.07	0.01	0.7033
38	345				0.0000
39	34’5				0.0000
40	22’33’	0.76	0.12		0.2933
41	22’34	0.68	0.01		0.2300
42	22’34’	1.19	0.15	0.01	0.4500
43	22’35	0.18			0.0600
44	22’35’	3.55	2.31	0.03	1.9633
45	22’36	0.89	0.05		0.3133
46	22’36’	0.36			0.1200
47	22’44’	0.93	0.14		0.3567
48	22’45	1.18	0.12		0.4333
49	22’45’	2.53	1.1	0.01	1.2133
50	22’46				0.0000
51	22’46’	0.23			0.0767

52	22’55’	3.53	5.38	0.24	3.0500
53	22’56’	0.71	0.12		0.2767
54	22’66’	0.01			0.0033
55	233’4	0.1			0.0333
56	233’4’	1.81	0.55	0.02	0.7933
57	233’5	0.02			0.0067
58	233’5’				0.0000
59	233’6	0.32	0.02		0.1133
60	2344’	1.18	0.18	0.04	0.4667
61	2345				0.0000
62	2346				0.0000
63	234’5	0.12	0.02		0.0467
64	234’6	1.7	0.59	0.01	0.7667
65	2356				0.0000
66	23’44’	3.39	1.01	0.02	1.4733
67	23’45	0.16			0.0533
68	23’45’				0.0000
69	23’46				0.0000
70	23’4’5	3.73	3.49	0.04	2.4200
71	23’4’6	1.03	0.15	0.01	0.3967
72	23’55’	0.01			0.0033
73	23’5’6				0.0000
74	244’5	1.81	0.84	0.05	0.9000
75	244’6	0.04			0.0133
76	2’345	0.08	0.02		0.0333
77	33’44’	0.31	0.03		0.1133
78	33’45				0.0000
79	33’45’				0.0000
80	33’55’				0.0000
81	344’5	0.01			0.0033
82	22’33’4	0.26	1.11		0.4567
83	22’33’5	0.11	0.48	0.01	0.2000
84	22’33’6	0.41	2.32	0.11	0.9467
85	22’344’	0.31	1.28	0.01	0.5333
86	22’345	0.03	0.06	0	0.0300
87	22’345’	0.46	3.99	0.41	1.6200
88	22’346				0.0000
89	22’346’	0.09	0.09		0.0600
90	22’34’5				0.0000
91	22’34’6	0.21	0.93	0.01	0.3833
92	22’355’	0.09	1.29	0.3	0.5600
93	22’356				0.0000
94	22’356’	0.01	0.02		0.0100
95	22’35’6	0.61	6.25	2.45	3.1033
96	22’366’	0.03	0.04		0.0233
97	22’3’45	0.38	2.62	0.096	1.0320
98	22’3’46				0.0000
99	22’44’5	0.46	3.02	0.04	1.1733
100	22’4’4’6				0.0000
101	22’455’	0.69	8.02	3.13	3.9467
102	22’456’	0.07	0.15		0.0733
103	22’45’6		0.03		0.0100
104	22’466’				0.0000
105	233’44’	0.47	2.99	0.22	1.2267
106	233’45				0.0000
107	233’4’5				0.0000
108	233’45’				0.0000
109	233’46	0.06	0.37	0.01	0.1467
110	233’4’6	0.83	9.29	1.33	3.8167

111	233’55’				0.0000
112	233’56				0.0000
113	233’5’6				0.0000
114	2344’5	0.04	0.18		0.0733
115	2344’6	0.04	0.2		0.0800
116	23456				0.0000
117	234’56	0.03	0.23		0.0867
118	23’44’5	0.66	7.35	0.48	2.8300
119	23’44’6		0.08		0.0267
120	23’455’				0.0000
121	23’45’6				0.0000
122	2’33’45	0.01	0.1		0.0367
123	2’344’5	0.03	0.15		0.0600
124	2’3455’	0.03	0.29	0.01	0.1100
125	2’3456’	0.02	0.02		0.0133
126	33’44’5				0.0000
127	33’455’				0.0000
128	22’33’44’	0.02	1.42	0.53	0.6567
129	22’33’45		0.38	0.14	0.1733
130	22’33’45’		0.6	0.22	0.2733
131	22’33’46		0.19	0.07	0.0867
132	22’33’46’	0.04	2.29	2.9	1.7433
133	22’33’55’		0.11	0.07	0.0600
134	22’33’56		0.37	0.34	0.2367
135	22’33’56’		0.61	1.08	0.5633
136	22’33’66’		0.7	1.46	0.7200
137	22’344’5		0.42	0.02	0.1467
138	22’344’5’	0.1	5.8	6.54	4.1467
139	22’344’6		0.15		0.0500
140	22’344’6’	0.01			0.0033
141	22’3455’		0.98	2.62	1.2000
142	22’3456				0.0000
143	22’3456’				0.0000
144	22’345’6		0.24	0.61	0.2833
145	22’34’66’				0.0000
146	22’34’55’		0.67	1.15	0.6067
147	22’34’56		0.1		0.0333
148	22’34’56’				0.0000
149	22’34’5’6	0.06	3.65	8.75	4.1533
150	22’34’56’				0.0000
151	22’355’6		0.69	3.04	1.2433
152	22’3566’				0.0000
153	22’44’55’	0.06	3.77	9.39	4.4067
154	22’44’56’		0.04		0.0133
155	22’44’66’				0.0000
156	233’44’5	0.01	0.82	0.52	0.4500
157	233’44’5’		0.19	0.02	0.0700
158	233’44’6	0.01	0.81	0.58	0.4667
159	233’455’				0.0000
160	233’456				0.0000
161	233’45’6				0.0000
162	233’4’55’				0.0000
163	233’4’5’6	0.01	1.03	2.42	1.1533
164	233’55’6		0.4	0.69	0.3633
165	2344’56				0.0000
166	23’44’55’		0.05		0.0167
167	23’44’55’		0.27	0.19	0.1533
168	23’44’5’6				0.0000
169	33’44’55’				0.0000

170	22’33’44’5		0.52	4.11	1.5433
171	22’33’44’6		0.14	1.11	0.4167
172	22’33’455’		0.07	0.7	0.2567
173	22’33’456			0.1	0.0333
174	22’33’456’		0.34	4.96	1.7667
175	22’33’45’6			0.17	0.0567
176	22’33’466’		0.04	0.59	0.2100
177	22’33’4’56		0.2	2.57	0.9233
178	22’33’55’6		0.03	0.83	0.2867
179	22’33’566’		0.1	2.03	0.7100
180	22’344’55’		0.67	11.38	4.0167
181	22’344’56			0.01	0.0033
182	22’344’56’				0.0000
183	22’344’5’6		0.18	2.41	0.8633
184	22’344’66’				0.0000
185	22’3455’6			0.55	0.1833
186	22’34566’				0.0000
187	22’34’55’6		0.25	5.4	1.8833
188	22’34’566’				0.0000
189	233’44’55’		0.01	0.1	0.0367
190	233’44’56		0.07	0.82	0.2967
191	233’44’5’6			0.17	0.0567
192	233’455’6				0.0000
193	233’4’55’6		0.03	0.53	0.1867
194	22’33’44’55’		0.01	2.07	0.6933
195	22’33’44’56			0.84	0.2800
196	22’33’44’56’			1.09	0.3633
197	22’33’44’66’			0.07	0.0233
198	22’33’455’6			0.1	0.0333
199	22’33’455’6’		0.01	0.78	0.2633
200	22’33’4566’			0.25	0.0833
201	22’33’45’66’			0.24	0.0800
202	22’33’55’66’			0.33	0.1100
203	22’344’55’6		0.02	1.4	0.4733
204	22’344’566’				0.0000
205	233’44’55’6			0.1	0.0333
206	22’33’44’55’6		0.03	0.53	0.1867
207	22’33’44’566’			0.05	0.0167
208	22’33’455’66’		0.01	0.13	0.0467
209	22’33’44’55’66’				0.0000
Total		100	100.31	99.276	99.8620

a: ATSDR (2000)

S-9 Schematic of A Batch Reactor Used in This Study

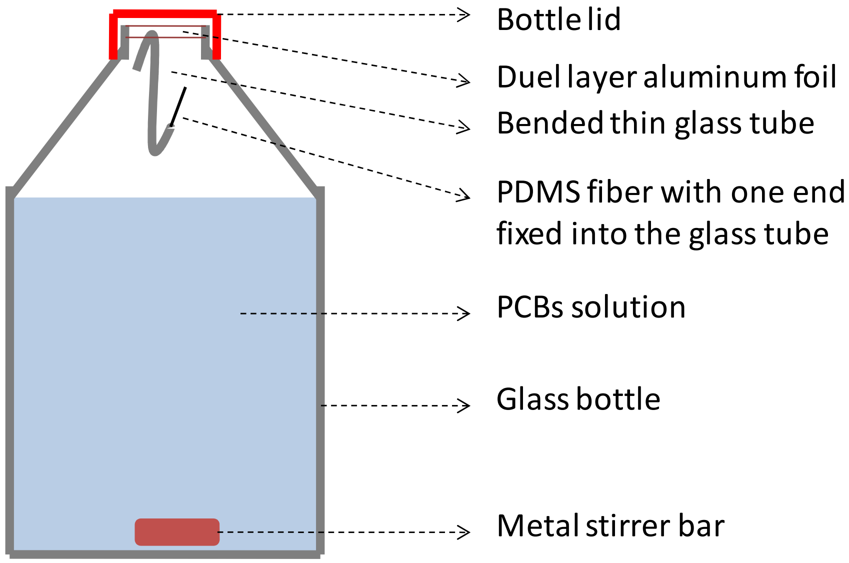

FIGURE S.2 Schematic of a batch reactor used in this study.

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