Volatilization of PCBs from Contaminated Sediments & Water

Contract NYS C001263
4/1/85 to 9/30/86

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I. Introduction

The goal of this work was to provide physio-chemical parameters for modeling the volatilization of PCB components that could be expected to occur as a result of the Hudson River PCB Reclamation Demonstration Project. These parameters include (a) particle/water distribution coefficients as a function of suspended matter concentration and temperature and (b) Henry's law constants (air/water distribution coefficients) as a function of temperature. Throughout this report, distribution coefficients are given in units of grams of PCB component per gram of suspended matter divided by grams of PCB component per gram of water. Henry's law constants are given in units of grams of PCB component per cubic centimeter of air divided by grams of PCB component per cubic centimeter of water.

Distribution coefficient experiments were performed using approximately 3 liters of water spiked with sediment either from (a) core 91.8 (near Kingston) 2-4 cm or (b) core 190.9 (from about five miles downstream of Fort Edward), 16-20 plus 24-29 cm. A few experiments were run using SLOSH III as a source of PCBs because the supply of 91.8 4-8 was depleted. This is a grab sample of Hudson River sediment from near Indian Point available in kilogram quantities. Samples were extracted and analyzed according to the procedures detailed in Bopp (1979).

Henry's law constant experiments were run with the sediments from core 190.9 in 19 l glass bottles with about 3 l of water. PCB components were extracted from the air using a florisil column (Giam et al., 1975). The florisil was pre-combusted at 500°C overnight and deactivated with 3% water (w/w). For PCB component analyses, the florisil was soxhlet extracted and the water and particles were treated exactly as in the distribution coefficient experiments.

During all experiments constant temperatures (±0.5°C) were maintained by immersing the bottles in a water or water/ethylene glycol bath regulated with a Neslab constant temperature circulator. Agitation of the samples was provided by a magnetic stirrer and teflon coated stir bars.

II. Peak Identification

Figures 1-4 show packed column chromatograms and peak numbering schemes for standards of Aroclors 1221, 1242, 1254 and 1260, respectively. Figures 5-8 show the capillary column chromatograms. Ballschmiter and Zell (1980) congener numbers are shown in table I and tables II-V indicate the congeners present in individual capillary peaks. Our peak assignments are based on about a dozen individual congener standards and the work of Mullin et al. (1984). They are consistent with the assignments of Brown et al. (1985) and with NYSDEC assignments (Mark Brown, personal communication).

III. Particle-Water Distribution Coefficients

a) Equilibration Time and Replication. All distribution coefficient (K_p) experiments were equilibrated for forty-eight hours. This time was chosen on the basis of lab experiments employing SLOSH III, a Lamont grab sample of Hudson River sediment. No consistent trend of K_p with time was observed for 1 day, one week and two week equilibrations. Data for packed column peaks 2-12 is shown in tables VI-VIII. Excellent agreement between the one day and two week values indicates essentially complete equilibration in 24 hours. 48 hours was chosen for subsequent experiments to provide assurance of equilibration.

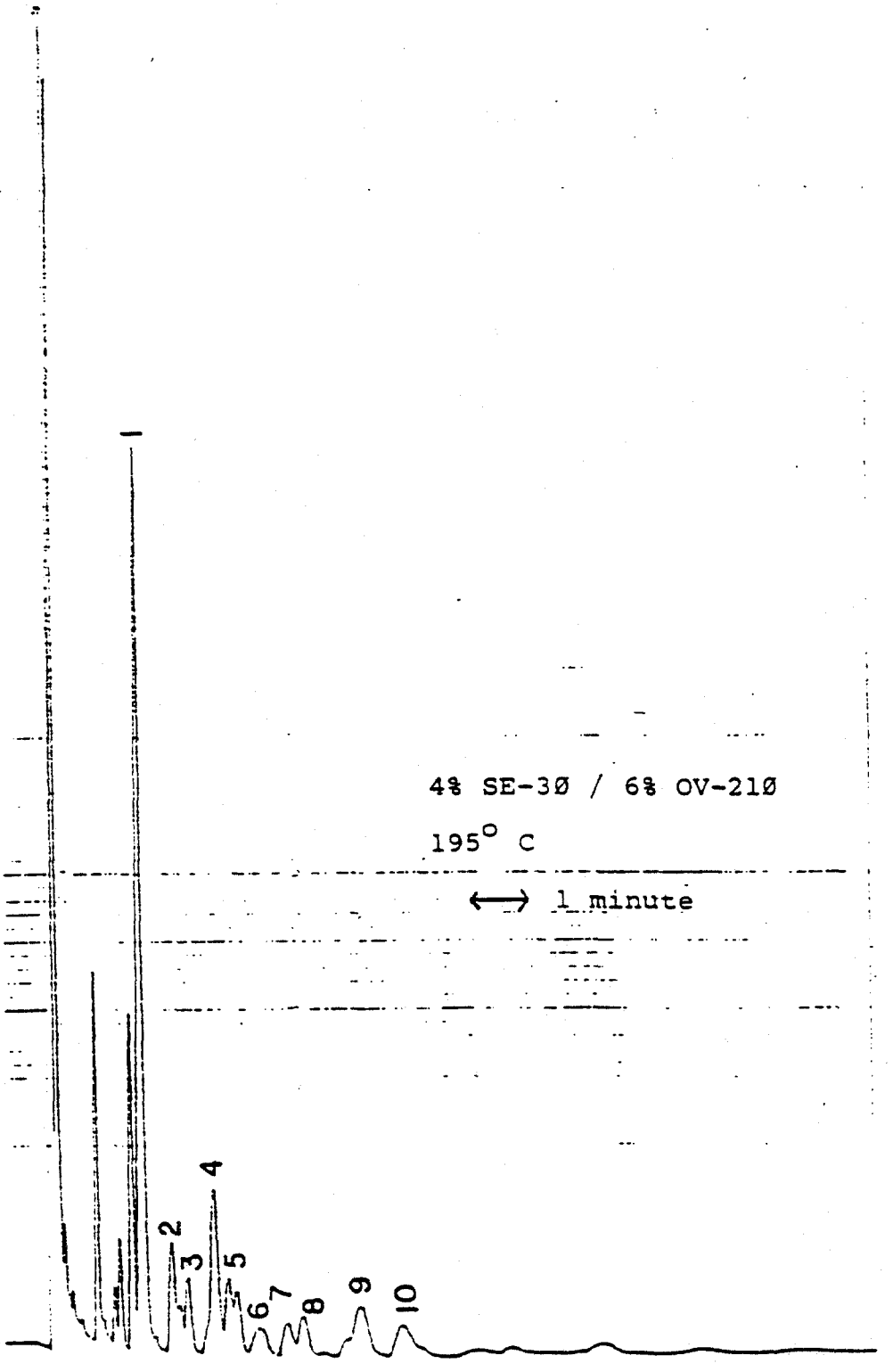

Figure 1. Packed-column chromatogram of Aroclor 1221

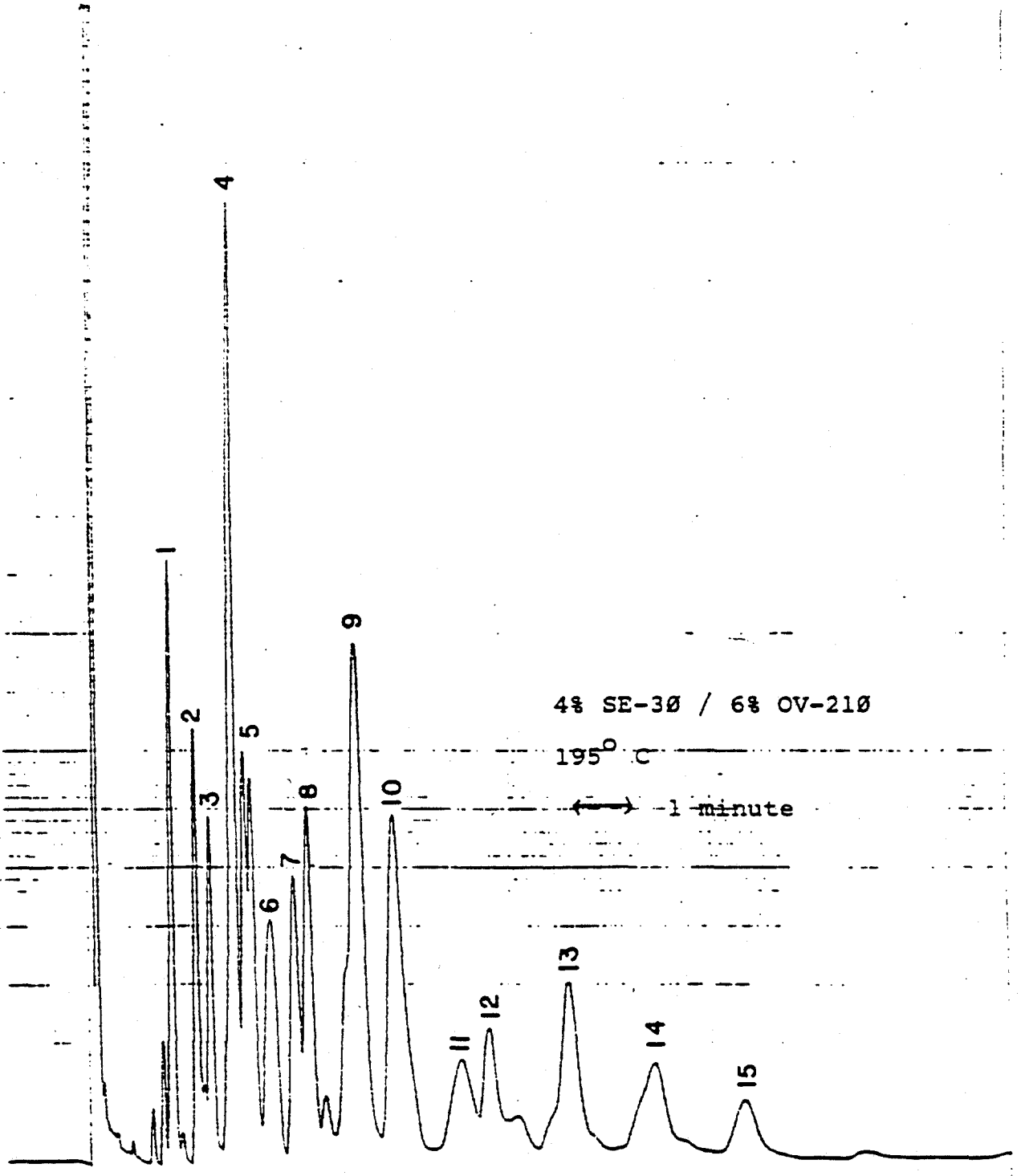

Figure 2. Packed-column chromatogram of Aroclor 1242

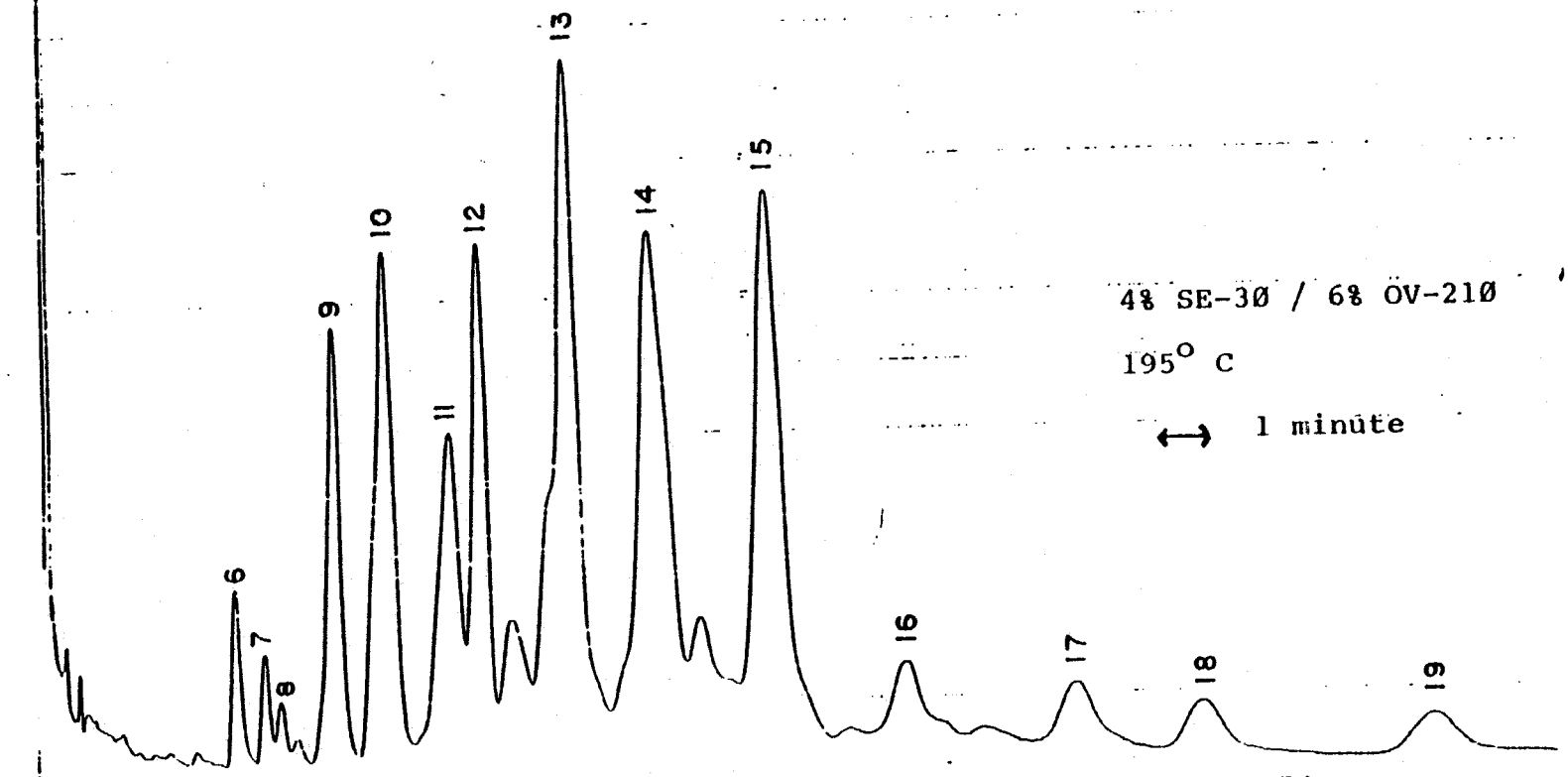

Figure 3. Packed-column chromatogram of Aroclor 1254

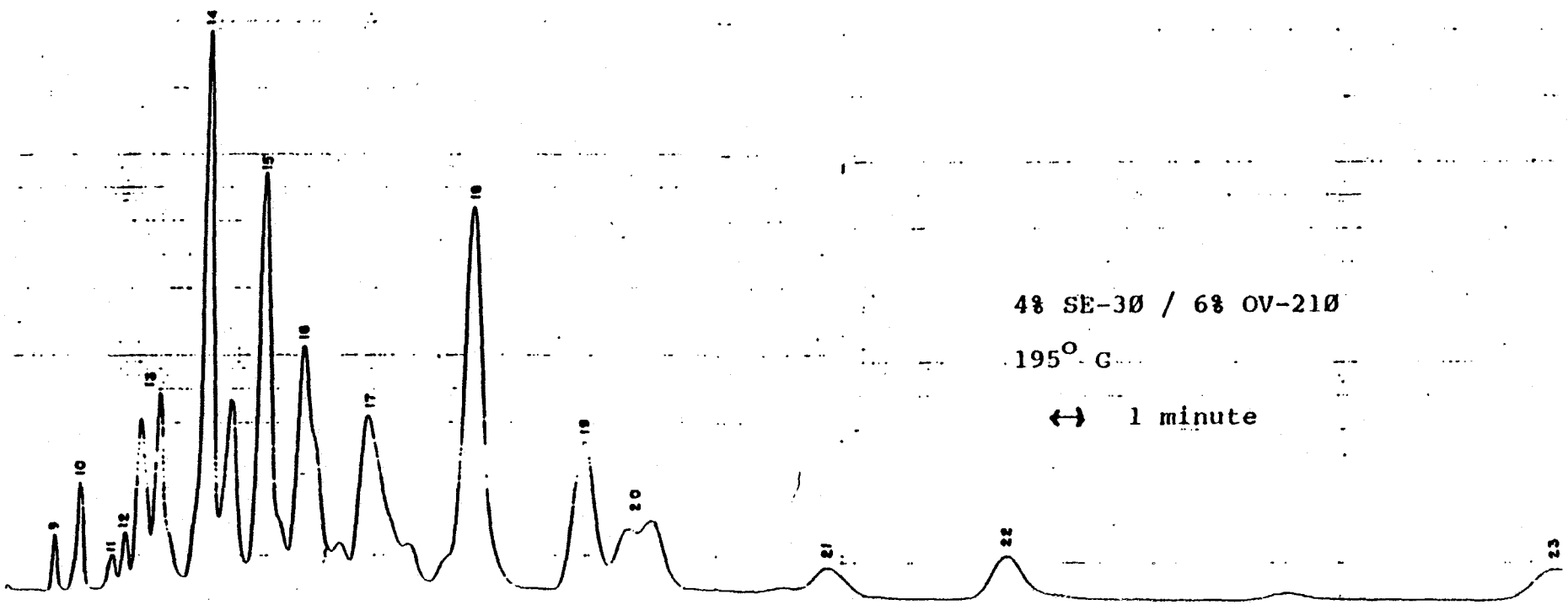

Figure 4. Packed-column chromatogram of Aroclor 1260

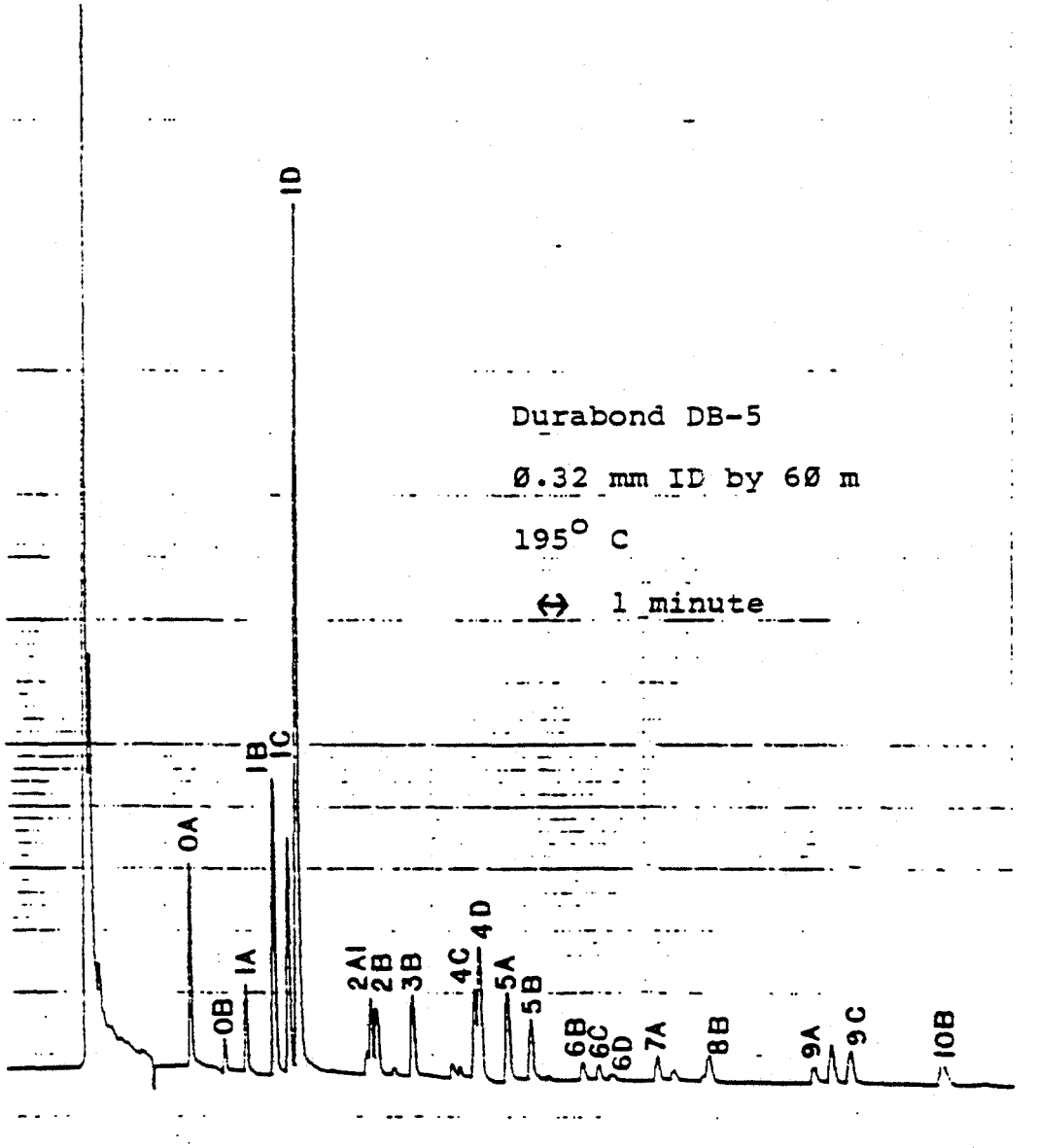

Figure 5. Capillary column chromatogram of Aroclor 1221

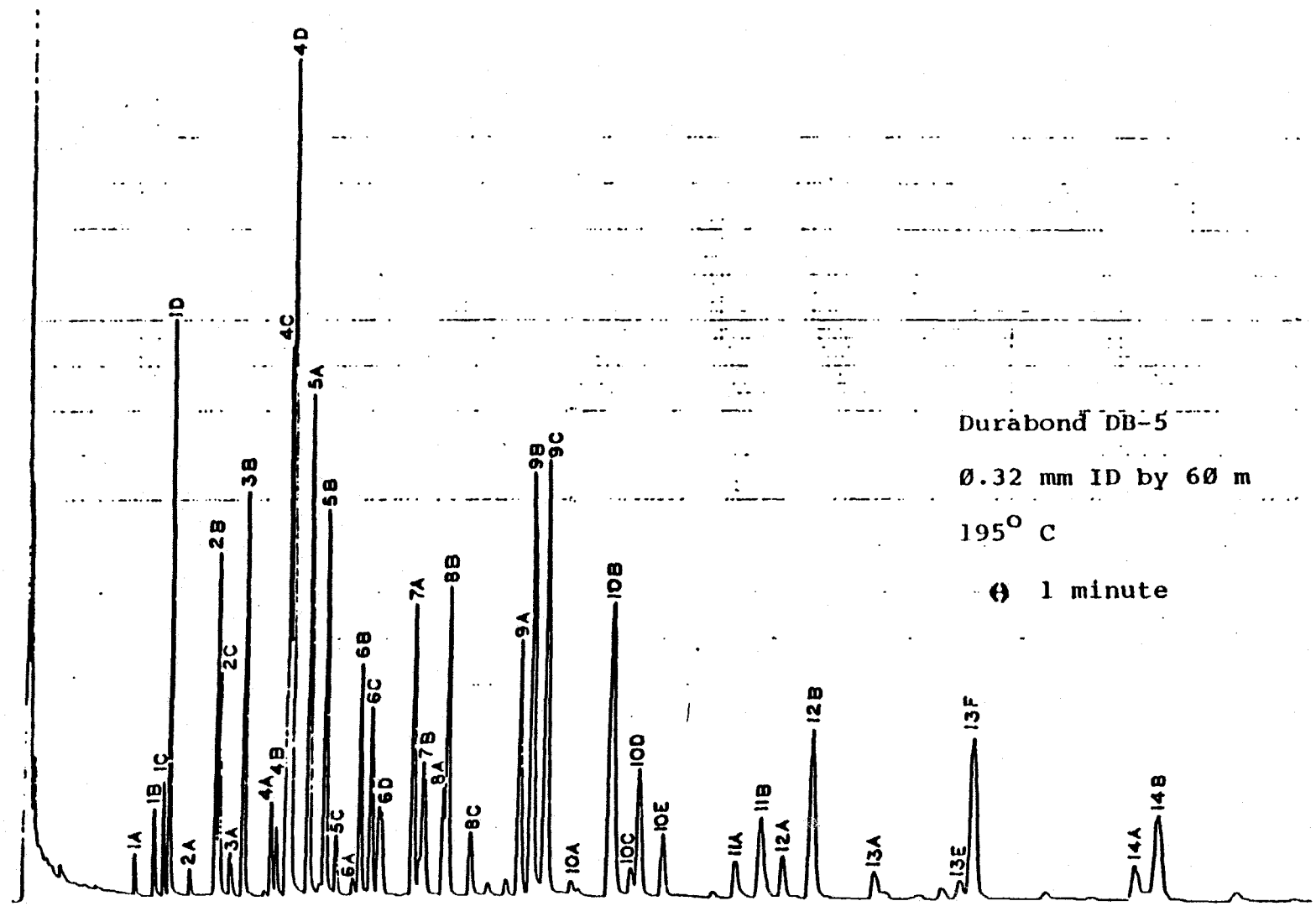

Figure 6. Capillary column chromatogram of Aroclor 1242

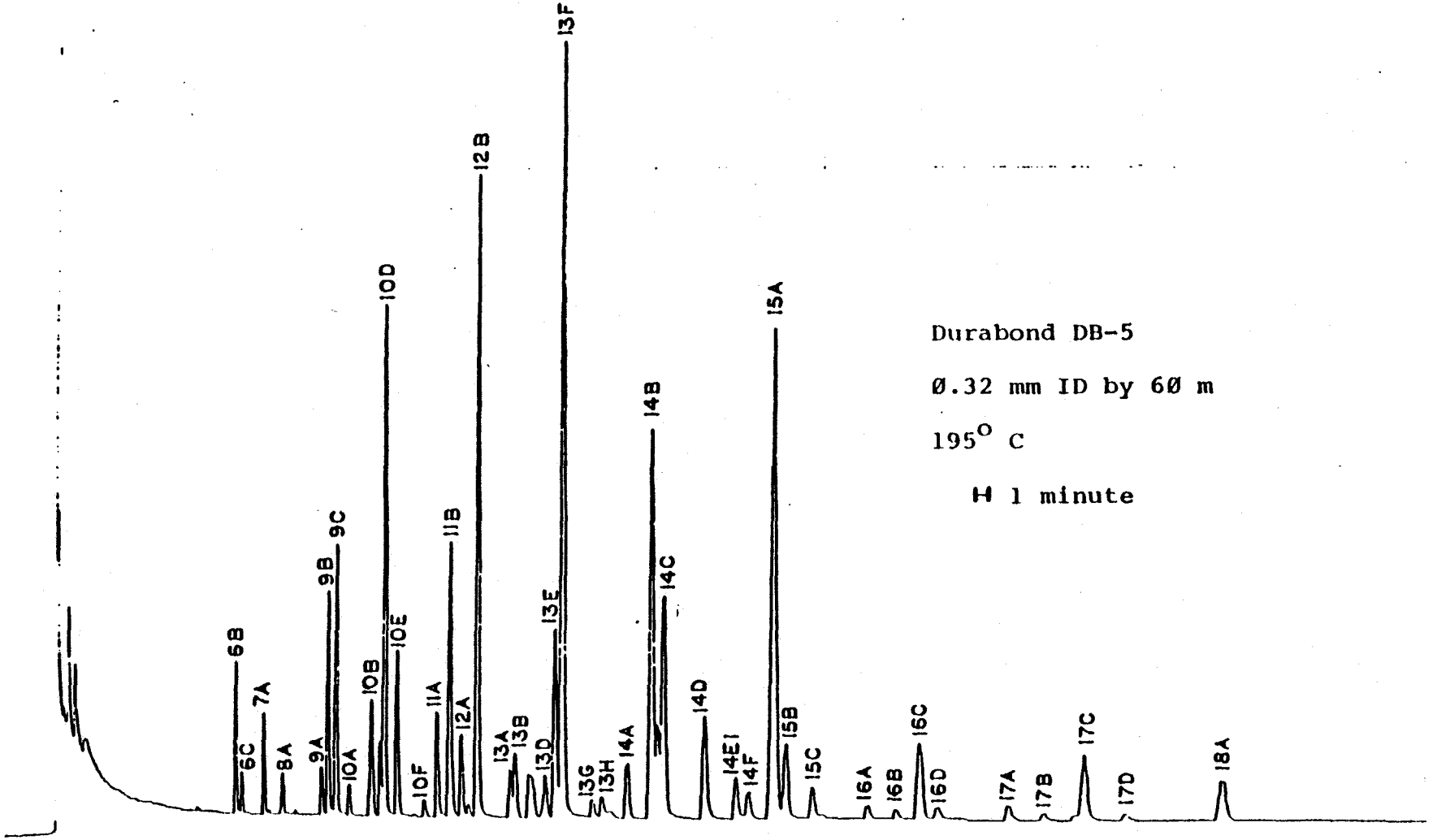

Figure 7. Capillary column chromatogram of Aroclor 1254

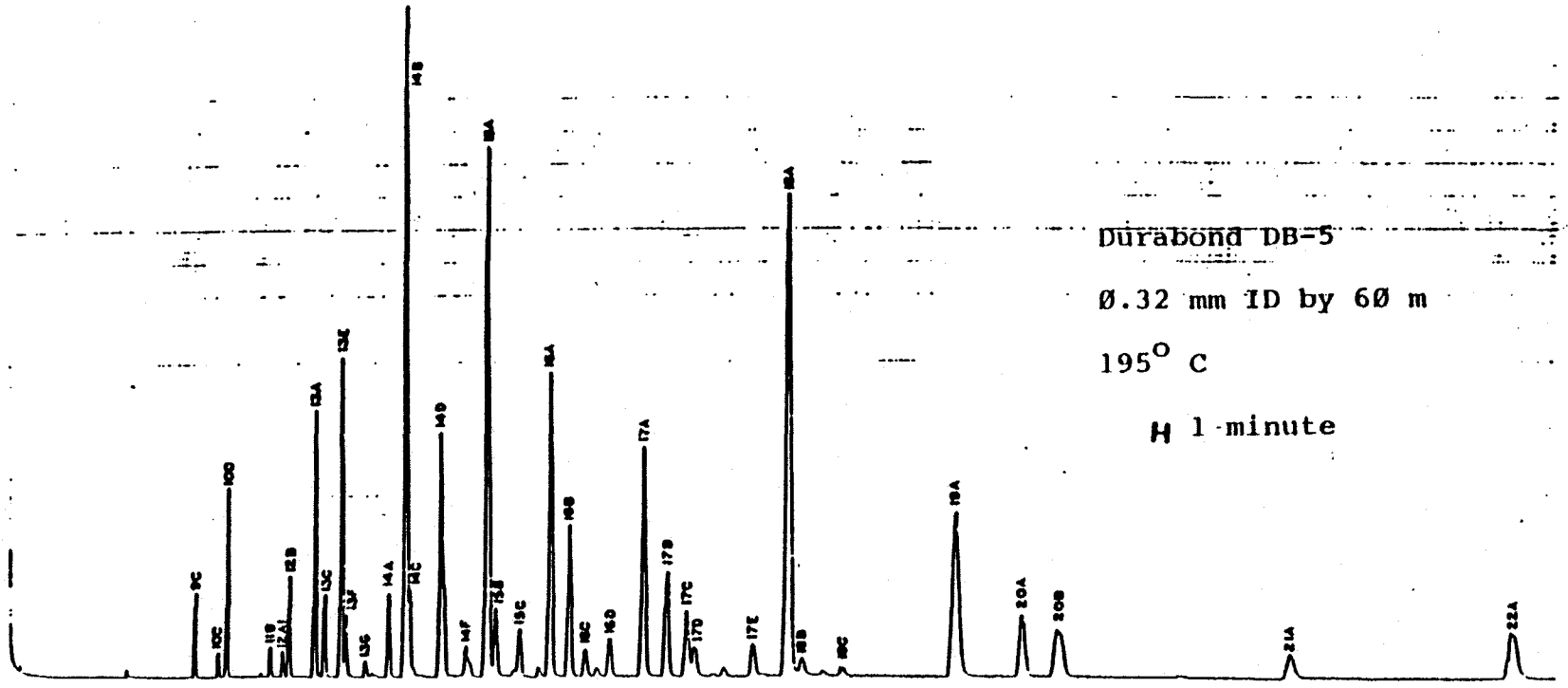

Figure 8. Capillary column chromatogram of Aroclor 126Ø

Number	Structure	Number	Structure
	Monochlorobiphenyls		Trichloropiphenyls
1	2	36	3,3',5
2	3	37	3,4,4'
3	4	38	3,4,5
		39	3,4',5
	Dichlorobiphenyls		
			Tetrachlorobiphenyls
4	2,2'		
5	2,3	4Ø	2,2',3,3'
6	2,3'	41	2,2',3,4
7	2,4	42	2,2',3,4'
8	2,4'	43	2,2',3,5
9	2,5	44	2,2',3,5'
1Ø	2,6	45	2,2',3,6
11	3,3'	46	2,2',3,6'
12	3,4	47	2,2',4,4'
13	3,4'	48	2,2',4,5
14	3,5	49	2,2',4,5'
15	4,4'	5Ø	2,2',4,6
		51	2,2',4,6
	Trichlorobiphenyls	52	2,2',5,5'
		53	2,2',5,6'
16	2,2',3	54	2,2',6,6'
17	2,2',4	55	2,3,3',4
18	2,2',5	56	2,3,3',4'
19	2,2',6	57	2,3,3',5
2Ø	2,3,3'	58	2,3,3',5'
21	2,3,4	59	2,3,3',6
22	2,3,4'	6Ø	2,3,4,4'
23	2,3,5	61	2,3,4,5
24	2,3,6	62	2,3,4,6
25	2,3',4	63	2,3,4',5
26	2,3',5	64	2,3,4',6
27	2,3',6	65	2,3,5,6
28	2,4,4'	66	2,3',4,4'
29	2,4,5	67	2,3',4,5
3Ø	2,4,6	68	2,3',4,5'
31	2,4',5	69	2,3',4,6
32	2,4',6	7Ø	2,3',4',5
33	2',3,4	71	2,3',4',6
34	2',3,5	72	2,3',5,5'
35	3,3',4	73	2,3',5',6

Table I. "Ballschmiter" systematic numbering of PCB compounds.

Number	Structure	Number	Structure
	Tetrachlorobiphenyls		Pentachlorobiphenyls
74	2,4,4',5	105	2,3,3',4,4'
75	2,4,4',6	106	2,3,3',4,5
76	2',3,4,5	107	2,3,3',4',5
77	3,3',4,4'	108	2,3,3',4,5'
78	3,3',4,5	109	2,3,3',4,6
79	3,3',4,5'	110	2,3,3',4',6
80	3,3',5,5'	111	2,3,3',5,5'
81	3,4,4',5	112	2,3,3',5,6
		113	2,3,3',5',6
	Pentachlorobiphenyls	114	2,3,4,4',5
		115	2,3,4,4',6
82	2,2',3,3',4	116	2,3,4,5,6
83	2,2',3,3',5	117	2,3,4',5,6
84	2,2',3,3',6	118	2,3',4,4',5
85	2,2',3,4,4'	119	2,3',4,4',6
86	2,2',3,4,5	120	2,3',4,5,5'
87	2,2',3,4,5'	121	2,3',4,5',6
88	2,2',3,4,6	122	2',3,3',4,5
89	2,2',3,4,6'	123	2',3,4,4',5
90	2,2',3,4',5	124	2',3,4,5,5'
91	2,2',3,4',6	125	2',3,4,5,6'
92	2,2',3,5,5'	126	3,3',4,4',5
93	2,2',3,5,6	127	3,3',4,5,5'
94	2,2',3,5,6'		
95	2,2',3,5',6		Hexachlorobiphenyls
96	2,2',3,6,6'		
97	2,2',3',4,5	128	2,2',3,3',4,4'
98	2,2',3',4,6	129	2,2',3,3',4,5
99	2,2',4,4',5	130	2,2',3,3',4,5'
100	2,2',4,4',6	131	2,2',3,3',4,6
101	2,2',4,5,5'	132	2,2',3,3',4,6'
102	2,2',4,5,6'	133	2,2',3,3',5,5'
103	2,2',4,5',6	134	2,2',3,3',5,6
104	2,2',4,6,6'	135	2,2',3,3',5,6'

Table I. (Continued) "Ballschmiter" systematic numbering of PCB compounds.

Number	Structure	Number	Structure
	Hexachlorobiphenyls		**Heptachlorobiphenyls**
136	2,2',3,3',6,6'	174	2,2',3,3',4,5,6'
137	2,2',3,4,4',5	175	2,2',3,3',4,5',6
138	2,2',3,4,4',5'	176	2,2',3,3',4,6,6'
139	2,2',3,4,4',6	177	2,2',3,3',4',5,6
140	2,2',3,4,4',6'	178	2,2',3,3',5,5',6
141	2,2',3,4,5,5'	179	2,2',3,3',5,6,6'
142	2,2',3,4,5,6	180	2,2',3,4,4',5,5'
143	2,2',3,4,5,6'	181	2,2',3,4,4',5,6
144	2,2',3,4,5',6	182	2,2',3,4,4',5,6'
145	2,2',3,4,6,6'	183	2,2',3,4,4',5',6
146	2,2',3,4',5,5'	184	2,2',3,4,4',6,6'
147	2,2',3,4',5,6	185	2,2',3,4,5,5',6
148	2,2',3,4',5,6'	186	2,2',3,4,5,6,6'
149	2,2',3,4',5',6	187	2,2',3,4',5,5',6
150	2,2',3,4',6,6'	188	2,2',3,4',5,6,6'
151	2,2',3,5,5',6	189	2,3,3',4,4',5,5'
152	2,2',3,5,6,6'	190	2,3,3',4,4',5,6
153	2,2',4,4',5,5'	191	2,3,3',4,4',5',6
154	2,2',4,4',5,6'	192	2,3,3',4,5,5',6
155	2,2',4,4',6,6'	193	2,3,3',4',5,5',6
156	2,3,3',4,4',5		
157	2,3,3',4,4',5'		**Octachlorobiphenyls**
158	2,3,3',4,4',6		
159	2,3,3',4,5,5'	194	2,2',3,3',4,4',5,5'
160	2,3,3',4,5,6	195	2,2',3,3',4,4',5,6
161	2,3,3',4,5',6	196	2,2',3,3',4,4',5',6
162	2,3,3',4',5,5'	197	2,2',3,3',4,4',6,6'
163	2,3,3',4',5,6	198	2,2',3,3',4,5,5',6
164	2,3,3',4',5',6	199	2,2',3,3',4,5,6,6'
165	2,3,3',5,5',6	200	2,2',3,3',4,5',6,6'
166	2,3,4,4',5,6	201	2,2',3,3',4',5,5',6
167	2,3',4,4',5,5'	202	2,2',3,3',5,5',6,6'
168	2,3',4,4',5',6	203	2,2',3,4,4',5,5',6
169	3,3',4,4',5,5'	204	2,2',3,4,4',5,6,6'
		205	2,3,3',4,4',5,5',6
	Heptachlorobiphenyls		
			Nonachlorobiphenyls
170	2,2',3,3',4,4',5		
171	2,2',3,3',4,4',6	206	2,2',3,3',4,4',5,5',6
172	2,2',3,3',4,5,5'	207	2,2',3,3',4,4',5,6,6'
173	2,2',3,3',4,5,6	208	2,2',3,3',4,5,5',6,6'
			Decachlorobiphenyl
		209	2,2',3,3',4,4',5,5',6,6'

Table I. (Continued) "Ballschmiter" systematic numbering of PCB compounds

Peak No.	Congener(s) Present
Øa	2
Øb	4
1a	2,2' - 2,6
1b	2,4 - 2,5
1c	2,3'
1d	2,3 - 2,4'
2a1	3,4 - 3,4'
2b	4,4' - 2,2',5
3a	2,3,6 - 2,3',6
3b	2,2',3 - 2,4',6
4a	2,3',5
4b	2,3',4
4c	2,4',5
4d	2,4,4' - 2,2',4,6
5a	2,3,3' - 2,3,4 - 2',3,4 - 2,2',5,6'
5b	2,3,4' - 2,2',4,6'
6b	2,2',5,5' - 2,3',5',6
6c	2,2',4,5'
6d	2,2',4,4' - 2,2',4,5 - 2,4,4',6
7a	2,2',3,5' - 2,2',4,6,6'
7b	3,4,4' - 2,2',3,4' - 2,3,3',6
8a	2,3',5,5'
8b	2,2',3,4 - 2,3,4',6 - 2,3',4',6
9a	2,4,4',5 - 2,2',3,5,6'
9b	2,3,4,5 - 2,3',4',5 - 2',3,4,5
9c	2,3',4,4' - 2,2',3,5,6 - 2,2',3,5',6
10b	2,3,3',4' - 2,3,4,4'
10d	2,2',3,4',5 - 2,2',4,5,5'

Table II. Congeners in capillary peaks for Aroclor 1221

Peak No.	Congener(s) Present
1a	2,2' - 2,6
1b	2,4 - 2,5
1c	2,3'
1d	2,3 - 2,4'
2a	2,2',6
2b	4,4' - 2,2',5
2c	2,2',4
3a	2,3,6 - 2,3',6
3b	2,2',3 - 2,4',6
4a	2,3',5
4b	2,3',4
4c	2,4',5
4d	2,4,4'
5a	2',3,4 - 2,2',5,6'
5b	2,3,4' - 2,2',4,6'
5c	2,2',3,6
6a	2,2',3,6'
6b	2,2',5,5' - 2,3',5',6
6c	2,2',4,5'
6d	2,2',4,4' - 2,2',4,5 - 2,4,4',6
7a	2,2',3,5' - 2,2',4,6,6'
7b	3,4,4' - 2,2',3,4' - 2,3,3',6
8a	2,3',5,5'
8b	2,2',3,4 - 2,3,4',6 - 2,3',4',6
8c	2,2',3,3'
9a	2,4,4',5 - 2,2',3,5,6'
9b	2,3,4,5 - 2,3',4',5 - 2',3,4,5
9c	2,3',4,4' - 2,2',3,5,6 - 2,2',3,5',6
10a	2,2',3,4',6 - 2,2',3',4,6
10b	2,3,3',4' - 2,3,4,4'
10c	2,2',3,3',6 - 2,2',3,5,5' - 2,2',4,4',6,6'
10d	2,2',3,4',5 - 2,2',4,5,5'
10e	2,2',4,4',5
11a	2,2',3,4,5 - 2,2',3',4,5 - 2,2',3,5,6,6'
11b	2,2',3,4,5' - 2,3,3',5,5' - 2,3,4,4',6
12a	2,2',3,4,4' - 2,3,4,5,6
12b	3,3',4,4' - 2,3,3',4',6
13a	2,2',3,3',4
13e	2,3,3',4',5 - 2,3,3',4,5' - 2,2',3,4',5,6
13f	2,3,3',4,5 - 2,3',4,4',5 - 2,2',3,4',5',6
14a	2,2',3,4',5,5' - 2,3,3',4,5',6
14b	2,3,3',4,4' - 2,2',3,3',4,6'
15a	2,2',3,4,4',5'

Table III. Congeners in capillary peaks for Aroclor 1242

Peak No.	Congener(s) Present
6b	2,2',5,5' - 2,3',5',6
6c	2,2',4,5'
6d	2,2',4,5 - 2,4,4',6
7a	2,2',3,5' - 2,2',4,6,6'
7b	3,4,4' - 2,2',3,4'
8b	2,2',3,4 - 2,3,4',6 - 2,3',4',6
8c	2,2',3,3'
9a	2,4,4',5 - 2,2',3,5,6'
9b	2,3',4',5 - 2',3,4,5
9c	2,3',4,4' - 2,2',3,5,6 - 2,2',3,5',6
10a	2,2',3,4',6 - 2,2',3',4,6
10b	2,3,3',4' - 2,3,4,4'
10c	2,2',3,3',6 - 2,2',3,5,5'
10d	2,2',3,4',5 - 2,2',4,5,5'
10e	2,2',4,4',5
10f	2,2',3,3',5 - 2,3,3',4,6
11a	2,2',3,4,5 - 2,2',3',4,5
11b	2,2',3,4,5' - 2,3,3',5,5' - 2,3,4,4',6
12a	2,2',3,4,4'
12a1	2,2',3,3',6,6'
12b	2,3,3',4',6
13a	2,2',3,3',4
13b	unknown
13c	2,2',3,5,5',6
13d	2',3,4,5,5' - 2,2',3,3',5,6' - 2,2',3,4,5',6
13e	2,3,3',4',5 - 2,3,3',4,5' - 2,2',3,4',5,6
13f	2,3,3',4,5 - 2,3',4,4',5 - 2,2',3,4',5',6
13g	2,3,4,4',5 - 2,2',3,3',5,6 - 2,2',3,4,5,6'
13h	2',3,3',4,5 - 2,2',3,3',4,6 - 2,2',3,4,5,6
14a	2,2',3,4',5,5' - 2,3,3',4,5',6
14b	2,3,3',4,4' - 2,2',3,3',4,6'
14c	2,2',4,4',5,5'
14d	2,2',3,4,5,5'
14e1	2,2',3,3',4,5'
14f	2,2',3,4,4',5
15a	2,2',3,4,4',5' - 2,3,3',4,5,6 - 2,3,3',4',5,6
15b	2,3,3',4,4',6
15c	2,2',3,3',4,5

Table IV. Congeners in capillary peaks for Aroclor 1254

Peak No.	Congener(s) Present
16a	2,3,4,4',5,6
16b	2,2',3,4,4',5,6' - 2,2',3,4',5,5',6
16c	2,2',3,3',4,4'
16d	2,3',4,4',5,5'
17a	2,2',3,3',4,5,6' - 2,2',3,4,4',5,6
17b	2,2',3,3',4',5,6
17b1	unknown
17c	2,3,3',4,4',5 - 2,2',3,3',4,4',6
17d	2,2',3,3',4,5,5' - 2,3,3',4,5,5',6
18a	2,2',3,4,4',5,5'
19a	2,2',3,3',4,4',5

Table IV. (continued). Congeners in capillary peaks for Aroclor 1254

Peak No.	Congener(s) Present
9c	2,2',3,5,6 - 2,2',3,5',6
10c	2,2',3,3',6 - 2,2',3,5,5'
10d	2,2',3,4',5 - 2,2',4,5,5'
11b	2,2',3,4,5' - 2,3,3',5,5' - 2,3,4,4',6
12a1	2,2',3,3',6,6'
12b	2,3,3',4',6
13a	2,2',3,3',4
13c	2,2',3,5,5',6
13e	2,3,3',4',5 - 2,3,3',4,5' - 2,2',3,4',5,6
13f	2,3,3',4,5 - 2,3',4,4',5 - 2,2',3,4',5',6
13g	2,2',3,3',5,6 - 2,2',3,4,5,6'
14a	2,2',3,4',5,5' - 2,3,3',4,5',6
14b	2,3,3',4,4' - 2,2',3,3',4,6'
14c	2,2',4,4',5,5'
14d	2,2',3,4,5,5'
14e	2,2',3,3',5,6,6'
14f	2,2',3,4,4',5 - 2,2',3,3',4,6,6'
15a	2,2',3,3',4',5' - 2,3,3',4,5,6
15b	2,3,3',4,4',6
15c	2,2',3,3',5,5',6
16a	2,3,4,4',5,6
16b	2,2',3,4,4',5,6' - 2,2',3,4',5,5',6
16c	2,2',3,3',4,4'
16d	2,3',4,4',5,5' - 2,2',3,4,5,5',6
17a	2,2',3,3',4,5,6' - 2,2',3,4,4',5,6
17b	2,2',3,3',4',5,6
17c	2,3,3',4,4',5 - 2,2',3,3',4,4',6
17d	2,2',3,3',5,5',6,6'
17e	2,2',3,3',4,5,5' - 2,3,3',4,5,5',6
18a	2,2',3,4,4',5,5'
18b	2,3,3',4',5,5',6
18c	2,3,3',4,4',5',6
18d	2,2',3,3',4,5,6,6'
19a	2,2',3,3',4,4',5 - 2,3,3',4,4',5,6
20a	2,2',3,3',4',5,5',6
20b	2,2',3,3',4,4',5',6 - 2,2',3,4,4',5,5',6
21a	2,2',3,3',4,4',5,6
22a	2,2',3,3',4,4',5,5'
23a	2,2',3,3',4,4',5,5',6

Table V. Congeners in capillary peaks for Aroclor 1260

One Day Equilibration

3.Ø l "Milli Q" water

0.600 g Slosh III 1ØØØB (200 mg/l suspended solids)

equilibrated 24 hours at 2Ø °C.

sediment recovered 97.Ø%

Peak No.	Water[1]	Blank%	Solids[2]	Blank%	Kp
2	83	3	2.11	1	$2.5x1Ø^4$
3	115	2	2.36	1	$2.1x1Ø^4$
4	12Ø	6	7.82	1	$6.5x1Ø^4$
5	9Ø	6	3.89	1	$4.3x1Ø^4$
6	18Ø	4	6.66	1	$3.7x1Ø^4$
7	175	4	6.ØØ	1	$3.4x1Ø^4$
8	177	4	7.68	1	$4.3x1Ø^4$
9	92	6	8.Ø4	1	$8.7x1Ø^4$
1Ø	77	12	6.19	1	$8.Øx1Ø^4$
12	21	1Ø	1.5Ø	1	$7.1x1Ø^4$

1- water values in ng/l (as 1242)

2- solids values in ug/g (as 1242)

Table VI. One day equilibration test

One Week Equilibration

3.Ø l "Milli Q" water

0.600 g Slosh III 1ØØØB (200 mg/l suspended solids)

equilibrated one week at 2Ø °C.

sediment recovered 96.Ø%

Peak No.	Water[1]	Blank%	Solids[2]	Blank%	Kp
2	89	3	1.97	1	$2.2x1Ø^4$
3	116	3	2.18	1	$1.9x1Ø^4$
4	124	7	7.27	1	$5.9x1Ø^4$
5	89	7	3.54	2	$4.Øx1Ø^4$
6	198	4	6.11	1	$3.1x1Ø^4$
7	189	4	4.79	1	$2.5x1Ø^4$
8	194	4	6.86	1	$3.5x1Ø^4$
9	95	7	7.11	1	$7.5x1Ø^4$
1Ø	81	13	5.56	1	$6.9x1Ø^4$
12	22	11	1.18	1	$5.4x1Ø^4$

1- water values in ng/l (as 1242)

2- solids values in ug/g (as 1242)

Table VII. One week equilibration test

Two Week Equilibration

3.Ø l "Milli Q" water

0.600 g Slosh III 1ØØØB (200 mg/l suspended solids)

equilibrated two weeks at 2Ø °C.

sediment recovered 95.3%

Peak No.	Water[1]	Blank%	Solids[2]	Blank%	Kp
2	1Ø4	3	2.6Ø	1	$2.5x1Ø^4$
3	128	3	2.92	1	$2.3x1Ø^4$
4	132	7	9.36	1	$7.1x1Ø^4$
5	72	9	4.41	1	$6.1x1Ø^4$
6	222	4	7.76	1	$3.5x1Ø^4$
7	212	4	6.41	1	$3.Øx1Ø^4$
8	2Ø6	4	8.75	1	$3.5x1Ø^4$
9	113	6	9.73	1	$8.6x1Ø^4$
1Ø	99	11	7.75	1	$7.8x1Ø^4$
12	27	1Ø	2.Ø9	1	$7.7x1Ø^4$

1- water values in ng/l (as 1242)

2- solids values in ug/g (as 1242)

Table VIII. Two week equilibration test

Results from replicate samples containing 20 mg/l of suspended particles from core 91.8, 4-8 cm are shown in tables IX-XI. Accurate quantification was possible only for peaks 2-12 as a result of the small total amount of suspended matter (60 milligrams total) and low concentrations of the post peak 12 components. The results are quite acceptable. Other duplicate samples discussed later in the report show even better reproducibility. As indicated in tables VI-XI all quantifications have been corrected for procedural blanks. Conditions of the experiments were chosen so that such corrections were kept small, generally less than 10%. The replicate samples of tables IX-XI were also checked for PCB recovery. Based on previously determined sediment PCB concentrations in core 91.8, 4-8 cm, the recoveries in the these three distribution coefficient experiments were 101±7%, 96±6% and 96±11% for peak 4,6 and 8 components respectively.

b) Variations of K_p with Suspended Matter Concentration and Dissolved Organic Carbon (DOC). The data in table XII shows an apparent inverse relationship of K_p to suspended matter concentration. The effect is quite large, averaging about a factor of five between 3.8 and 100 mg/l for packed-column peak 2-10 components. Subsequent experiments demonstrated that this effect was caused primarily by changes in DOC concentrations. For the three samples in table XII, DOC concentrations were the result of desorption of organic matter from the sediment into the milli-Q water (distilled water circulated through two high-purity ion exchange columns and a charcoal column and filtered through a 0.22 micron membrane). Values ranged from non-detectable in the 3.8 mg/l sample, to 0.15 mg/l DOC in the 20 mg/l solids sample to 0.54 mg/l in the sample with 100 mg/l solids. Results of a similar experiment using filtered Hudson River water are shown in table XIII. When the DOC concentrations are held

Bottle Equilibration I

3.Ø l "Milli Q" water

Ø.Ø6Ø g 91.8 4-8 (2Ø mg/l suspended solids)

equilibrated 48 hours at 2Ø °C.

sediment recovered 94.2%

unrecorded DOC

Peak No.	Water[1]	Blank%	Solids[2]	Blank%	Kp
2	276	1	7.45	4	$2.7x1Ø^4$
3	25Ø	2	6.26	5	$2.5x1Ø^4$
4	146	6	18.99	2	$1.3x1Ø^5$
5	52	12	6.29	9	$1.2x1Ø^5$
6	3Ø1	3	16.53	2	$5.5x1Ø^4$
7	1Ø4	8	6.45	6	$6.2x1Ø^4$
8	133	7	1Ø.92	4	$8.2x1Ø^4$
9	45	14	9.Ø9	5	$2.Øx1Ø^5$
1Ø	39	22	6.3Ø	9	$1.6x1Ø^5$
12	17	14	2.9Ø	5	$1.7x1Ø^5$

1- water values in ng/l (as 1242)

2- solids values in ug/g (as 1242)

Table IX. Packed-column Kps for Bottle Equilibration I

Bottle Equilibration II

3.Ø l "Milli Q" water

Ø.Ø6Ø g 91.8 4-8 (2Ø mg/l suspended solids)

equilibrated 48 hours at 2Ø °C.

sediment recovered 93.7%

unrecorded DOC

Peak No.	Water[1]	Blank%	Solids[2]	Blank%	Kp
2	271	1	8.39	3	$3.1x1Ø^4$
3	258	2	5.68	5	$2.2x1Ø^4$
4	155	3	2Ø.15	2	$1.3x1Ø^5$
5	65	1Ø	6.47	11	$1.Øx1Ø^5$
6	366	1	17.93	2	$4.9x1Ø^4$
7	122	5	5.96	8	$4.9x1Ø^4$
8	149	4	11.91	4	$8.Øx1Ø^4$
9	6Ø	7	1Ø.73	4	$1.8x1Ø^5$
1Ø	52	1Ø	6.82	9	$1.3x1Ø^5$
12	14	8	3.1Ø	5	$2.2x1Ø^5$

1- water values in ng/l (as 1242)

2- solids values in ug/g (as 1242)

Table x. Packed-column Kps for Bottle Equilibration II

Bottle Equilibrated Partition Coefficients

"Milli Q" water and sediment 91.8 4-8 cm were used to make three liter samples of the three suspended solids concentrations

	Partition Coefficients		
Peak No.	3.8 mg/l[1]	20 mg/l[2]	100 mg/l
2	9.0×10^4	2.9×10^4	1.8×10^4
3	8.7×10^4	2.4×10^4	1.9×10^4
4	3.6×10^5	1.3×10^5	7.6×10^4
5	3.4×10^5	1.1×10^5	8.1×10^4
6	1.2×10^5	5.2×10^4	3.1×10^4
7	2.2×10^5	5.6×10^4	3.7×10^4
8	2.0×10^5	8.1×10^4	7.3×10^4
9	3.9×10^5	1.9×10^5	9.8×10^4
10	2.7×10^5	1.5×10^5	1.1×10^5
12	2.7×10^5	2.0×10^5	1.1×10^5
DOC (mg/L)	< 0.10	0.15	0.54

Table XII. Bottle equilibrated partition coefficients with 91.8 4-8 versus suspended solids concentration
The same trend is evident in the lower distribution coefficients of the 200 mg/l samples (SLOSH III) of Tables VI - VIII compared to the 20 mg/l samples (91.8, 4-8cm) of Tables IX -XI.

1. This sample was prepared in 19 liters of water.

2. Note the excellent agreement between this 20 mg/l sample and the previous three (Tables IX - XI).

Bottle Equilibration III

3.Ø l "Milli Q" water

Ø.Ø6Ø g 91.8 4-8 (2Ø mg/l suspended solids)

equilibrated 48 hours at 2Ø °C.

sediment recovered 94.4%

unrecorded DOC

Peak No.	Water[1]	Blank%	Solids[2]	Blank%	Kp	Ave.[3]
2	28Ø	1	8.41	3	$3.Øx1Ø^4$	2.9±Ø.2
3	258	2	5.67	5	$2.2x1Ø^4$	2.3±Ø.2
4	164	3	19.68	2	$1.2x1Ø^5$	1.3±Ø.1
5	49	14	6.36	11	$1.3x1Ø^5$	1.2±Ø.2
6	4Ø6	1	13.41	3	$3.3x1Ø^4$	4.6±1.3
7	139	4	6.12	8	$4.4x1Ø^4$	5.2±1.Ø
8	185	3	11.48	4	$6.2x1Ø^4$	7.5±1.3
9	51	9	9.1Ø	5	$1.8x1Ø^5$	1.8±Ø.2
1Ø	55	1Ø	6.Ø1	11	$1.1x1Ø^5$	1.3±Ø.3
12	12	9	2.69	6	$2.3x1Ø^5$	2.1±Ø.4

1- water values in ng/l (as 1242)

2- solids values in ug/g (as 1242)

3- average and range of distribution coefficients reported in Tables 2-11 through 2-13, the values are reported here deleting the factor of ten reported in the Kp column

Table XI. Packed-column Kps for Bottle Equilibration III

Bottle Equilibrated Partition Coefficients

Filtered Hudson River water and sediment 91.8 4-8 cm were used to make three liter samples of the three suspended solids concentrations

	Partition Coefficients		
	3.21 mg/l DOC	3.29 mg/l DOC	3.66 mg/l DOC
Peak No.	20 mg/l solids	50 mg/l solids	100 mg/l solids
2	1.7×10^4	1.4×10^4	1.8×10^4
3	1.4×10^4	1.2×10^4	1.7×10^4
4	4.2×10^4	3.9×10^4	4.6×10^4
5	8.7×10^4	8.5×10^4	1.1×10^5
6	7.3×10^4	6.8×10^4	8.2×10^4
7	8.6×10^4	7.9×10^4	1.3×10^5
8	1.6×10^5	1.7×10^5	1.5×10^5
9	2.1×10^5	2.3×10^5	1.9×10^5
10	2.5×10^5	2.1×10^5	2.7×10^5
12	3.1×10^5	2.9×10^5	3.3×10^5

Table XIII. Bottle equilibrated partition coefficients with controlled DOC concentrations

fairly constant, the consistent inverse relationship between K_p and suspended matter concentration is not observed. Results of additional experiments using SLOSH III at 100 mg/l and varying the DOC by using water from a small swamp on the Lamont grounds are shown in table XIV. A consistent inverse relationship between K_p and DOC concentration was observed. Finally, very similar values of K_p were obtained for a sample prepared with milli-Q water and 1000 mg/l SLOSH III which had a post-equilibration DOC of 9.61 mg/l and the sample with 100 mg/l SLOSH III with a DOC adjusted to 8.6 with Lamont swamp water (table XV) again indicating minimal dependence of K_p on suspended matter concentration and suggesting that DOC is the controlling variable.

c) Variation of K_p with Temperature. Table XVI shows the results of packed column analysis of distribution coefficient experiments at four temperatures between 0 & 35°C using 200 mg/l of suspended solids from the 4-8 cm sample of core 91.8. The fairly high suspended matter concentration which yields a correspondingly high PCB spike permits quantification of PCB components through decachlorobiphenyl. Values of K_p show a consistent decrease with temperature between 0 & 35°C ranging from about twenty-five percent to a factor of 3-4. Table XVII shows the results of capillary column analyses of the same samples. Tables XVIII and XIX show results of similar replicate experiments using sediment from core 190.9. Agreement between these duplicates and the experiments employing the sediment from core 91.8 is excellent.

IV. Henry's Law Constants

a) System Parameters. The apparatus used for these determinations consisted of a 19 liter glass bottle which contained three liters of

Bottle Equilibrated Partition Coefficients

All samples were 100 mg/l suspended solids made with SLOSH III 1000B

Peak No.	Partition Coefficient 1.86 mg/l DOC	4.33 mg/l DOC	8.63 mg/l DOC	11.04 mg/l DOC
2	2.7×10^4	2.2×10^4	1.8×10^4	1.6×10^4
3	2.6×10^4	2.7×10^4	1.6×10^4	1.5×10^4
4	7.1×10^4	6.6×10^4	5.6×10^4	4.4×10^4
5	5.2×10^4	5.1×10^4	3.3×10^4	3.1×10^4
6	4.3×10^4	3.8×10^4	2.7×10^4	2.2×10^4
7	4.1×10^4	3.9×10^4	2.5×10^4	1.8×10^4
8	5.2×10^4	4.7×10^4	3.5×10^4	2.9×10^4
9	8.2×10^4	6.8×10^4	5.7×10^4	5.6×10^4
10	8.7×10^4	7.3×10^4	4.9×10^4	5.1×10^4
12	8.1×10^4	7.0×10^4	4.6×10^4	4.3×10^4
13	1.3×10^5	1.2×10^5	8.6×10^4	7.7×10^4
14	1.2×10^5	1.0×10^5	7.1×10^4	6.8×10^4
15	1.0×10^5	9.3×10^4	6.6×10^4	5.3×10^4

Table XIV. Bottle equilibrated partition coefficients versus DOC

Bottle Equilibrated Partition Coefficients

Both samples were made with SLOSH III 1000B

	Partition Coefficients	
	8.63 mg/L[1] DOC	9.61 mg/L[2] DOC
Peak No.	100 mg/l solids	1000 mg/l solids
2	1.8×10^4	1.8×10^4
3	1.6×10^4	1.5×10^4
4	5.6×10^4	5.4×10^4
5	3.3×10^4	3.5×10^4
6	2.7×10^4	3.0×10^4
7	2.5×10^4	2.3×10^4
8	3.5×10^4	3.2×10^4
9	5.7×10^4	6.0×10^4
10	4.9×10^4	5.6×10^4
12	4.6×10^4	4.8×10^4
13	8.6×10^4	8.5×10^4
14	7.1×10^4	6.6×10^4
15	6.6×10^4	6.9×10^4

1- made from SLOSH III 1000B and Lamont Swamp water

2- made from SLOSH III 1000B and "Milli Q" water

Table XV. Bottle equilibrated partition coefficients with large DOC concentrations

Bottle Equilibrated Partition Coefficients

All samples were 200 mg/l suspended solids made from sediment 91.8 4-8 and "Milli Q" water

Peak No.	0 °C	12 °C	25 °C	35 °C
2	2.6×10^4	2.5×10^4	8.2×10^3	6.3×10^3
3	2.7×10^4	2.6×10^4	9.7×10^3	6.4×10^3
4	5.2×10^4	4.6×10^4	2.3×10^4	1.8×10^4
5	8.3×10^4	8.0×10^4	4.2×10^4	2.9×10^4
6	4.6×10^4	3.9×10^4	2.2×10^4	2.3×10^4
7	5.6×10^4	5.2×10^4	1.6×10^4	1.1×10^4
8	5.6×10^4	5.0×10^4	3.0×10^4	2.1×10^4
9	1.1×10^5	1.1×10^5	4.6×10^4	4.8×10^4
10	9.8×10^4	1.2×10^5	5.8×10^4	4.0×10^4
11	1.0×10^4	9.1×10^4	5.3×10^4	4.0×10^4
12	1.1×10^4	9.8×10^4	5.9×10^4	4.3×10^4
13	3.0×10^5	3.0×10^5	1.3×10^5	1.2×10^5
14	2.0×10^5	2.0×10^5	1.1×10^5	1.1×10^5
15	2.4×10^5	2.3×10^5	1.3×10^5	1.2×10^5
16	3.8×10^5	3.6×10^5	1.6×10^5	1.5×10^5
17	3.6×10^5	3.4×10^5	1.3×10^5	1.2×10^5
18	3.0×10^5	2.8×10^5	2.3×10^5	2.1×10^5
19	4.0×10^5	3.9×10^5	3.1×10^5	3.0×10^5
20	3.7×10^5	3.7×10^5	2.9×10^5	2.8×10^5
21	5.6×10^5	5.4×10^5	4.9×10^5	4.9×10^5

Table XVI. Packed-column Kps versus temperature for sediment 91.8 4-8

Bottle Equilibrated Partition Coefficients

Peak No.	Ø °C	12 °C	25 °C	35 °C
22	$6.6x10^5$	$6.4x10^5$	$5.1x10^5$	$4.9x10^5$
23	$1.0x10^6$	$9.8x10^5$	$6.5x10^5$	$6.3x10^5$
deca[1]			$1.4x10^6$	$1.6x10^6$

1- decachlorobiphenyl, too little to detect in the water phase at Ø and 12 degrees

Table XVI. (Continued) Packed-column Kps versus temperature for sediment 91.8 4-8

Bottle Equilibrated Partition Coefficients

All samples were 200 mg/l suspended solids made from sediment 91.8 4-8 and "Milli Q" water

Peak No.	0 °C	12 °C	25 °C	35 °C
1a	2.3×10^4	2.1×10^4	7.0×10^3	7.0×10^3
2a	1.9×10^4	2.0×10^4	7.0×10^3	6.0×10^3
2b	3.2×10^4	2.9×10^4	1.2×10^4	1.0×10^4
3a	2.1×10^4	1.8×10^4	1.0×10^4	7.0×10^3
3b	2.8×10^4	2.8×10^4	1.1×10^4	7.0×10^3
4a	4.8×10^4	4.1×10^4	2.0×10^4	1.6×10^4
4b	7.8×10^4	7.1×10^4	2.5×10^4	2.5×10^4
4c	5.8×10^4	5.6×10^4	2.2×10^4	2.1×10^4
4d	1.2×10^5	1.1×10^5	5.1×10^4	5.9×10^4
5a	2.9×10^4	2.7×10^4	2.0×10^4	1.2×10^4
5b2	6.5×10^4	6.2×10^4	2.7×10^4	3.1×10^4
5c	1.2×10^5	1.2×10^5	4.4×10^4	4.7×10^4
6a	4.5×10^4	4.6×10^4	1.9×10^4	1.6×10^4
6b	5.1×10^4	4.7×10^4	2.1×10^4	2.2×10^4
6c	6.4×10^4	6.0×10^4	2.2×10^4	2.4×10^4
7a	5.0×10^4	4.1×10^4	1.7×10^4	1.7×10^4
7b	1.2×10^5	1.1×10^5	4.1×10^4	4.4×10^4
8a	5.1×10^4	4.9×10^4	1.5×10^4	1.7×10^4
8b	6.5×10^4	6.0×10^4	3.1×10^4	3.8×10^4

Table XVII. Capillary column Kps versus temperature for sediment 91.8 4-8

Bottle Equilibrated Partition Coefficients

Peak No.	0 °C	12 °C	25 °C	35 °C
8c	$5.0x10^4$	$4.3x10^4$	$1.9x10^4$	$1.5x10^4$
9a	$1.4x10^5$	$1.3x10^5$	$6.1x10^4$	$5.00x10^4$
9b	$1.5x10^5$	$1.4x10^5$	$4.8x10^4$	$5.2x10^4$
9c	$1.4x10^5$	$1.3x10^5$	$5.1x10^4$	$6.0x10^4$
10a	$1.3x10^5$	$1.3x10^5$	$5.1x10^4$	$6.0x10^4$
10b	$1.4x10^5$	$1.2x10^5$	$3.9x10^4$	$3.7x10^4$
10c	$1.2x10^5$	$1.1x10^5$	$3.6x10^4$	$4.0x10^4$
11a	$1.2x10^5$	$1.2x10^5$	$3.6x10^4$	$4.1x10^4$
11b	$1.6x10^5$	$1.4x10^5$	$4.4x10^4$	$4.7x10^4$
12a	$8.6x10^4$	$8.1x10^4$	$3.0x10^4$	$3.3x10^4$
12b	$2.5x10^5$	$2.4x10^5$	$1.3x10^5$	$1.2x10^5$
12c	$2.6x10^5$	$2.5x10^5$	$9.6x10^4$	$1.0x10^5$
13a	$1.9x10^5$	$1.9x10^5$	$1.1x10^5$	$1.0x10^5$
13b	$3.1x10^5$	$2.9x10^5$	$1.5x10^5$	$1.4x10^5$
14a	$1.3x10^5$	$1.2x10^5$	$1.1x10^5$	$9.3x10^4$
14c	$2.8x10^5$	$2.6x10^5$	$1.3x10^5$	$1.1x10^5$
15a	$4.1x10^5$	$3.9x10^5$	$1.2x10^5$	$1.1x10^5$
16a	$3.8x10^5$	$3.5x10^5$	$1.8x10^5$	$1.6x10^5$
17a	$3.5x10^5$	$3.4x10^5$	$1.4x10^5$	$1.2x10^5$
18a	$3.1x10^5$	$2.9x10^5$	$2.0x10^5$	$2.0x10^5$
19a	$3.5x10^5$	$3.5x10^5$	$3.0x10^5$	$2.9x10^5$

Table XVII. (Continued) Capillary column Kps versus temperature for sediment 91.8 4-8

Bottle Equilibrated Partition Coefficients

All samples were 200 mg/l suspended solids made from sediment 190.9 16-20 plus 24-29

Peak No.	0 °C	12 °C	25 °C	35 °C
2-chloro	($3.9x10^3$)	($3.7x10^3$)	($1.9x10^3$)	($1.6x10^3$)
1b	$2.4x10^4$	$2.0x10^4$	$8.0x10^3$	$8.0x10^3$
2a	$2.3x10^4$	$2.1x10^4$	$9.0x10^3$	$1.0x10^4$
2b	$3.9x10^4$	$3.3x10^4$	$1.5x10^4$	$1.6x10^4$
3a	$2.3x10^4$	$2.0x10^4$	$8.0x10^3$	$9.0x10^3$
3b	$3.1x10^4$	$2.6x10^4$	$1.4x10^4$	$1.0x10^4$
4a	$4.7x10^4$	$3.9x10^4$	$1.7x10^4$	$1.8x10^4$
4c	$5.7x10^4$	$4.3x10^4$	$1.9x10^4$	$1.8x10^4$
5a	$3.1x10^4$	$3.4x10^4$	$1.3x10^4$	$1.0x10^4$
5b1	$3.4x10^4$	$3.6x10^4$	$1.5x10^4$	$1.1x10^4$
5b2	$5.9x10^4$	$6.0x10^4$	$2.9x10^4$	$3.0x10^4$
6a	$5.0x10^4$	$4.6x10^4$	$2.3x10^4$	$2.0x10^4$
6b	$5.4x10^4$	$5.3x10^4$	$2.1x10^4$	$2.4x10^4$
6c	$6.1x10^4$	$6.3x10^4$	$2.7x10^4$	$2.7x10^4$
7a	$5.9x10^4$	$5.0x10^4$	$3.0x10^4$	$2.4x10^4$
7c	$6.7x10^4$	$6.1x10^4$	$4.0x10^4$	$3.5x10^4$
8b	$7.3x10^4$	$5.3x10^4$	$3.0x10^4$	$3.0x10^4$
9c	$1.3x10^5$	$7.1x10^4$	$4.6x10^4$	$4.0x10^4$
10a	$1.4x10^5$	$1.2x10^5$	$6.0x10^4$	$4.8x10^4$
10b	$1.5x10^5$	$1.3x10^5$	$5.7x10^4$	$5.9x10^4$
11b	$1.7x10^5$	$1.5x10^5$	$4.1x10^4$	$4.1x10^4$
12b	$2.6x10^5$	$2.1x10^5$	$1.5x10^5$	$1.3x10^5$
12c	$2.8x10^5$	$2.3x10^5$	$6.3x10^4$	$5.4x10^4$

Table XVIII. Capillary column Kps versus temperature for sediment 190.9 16-20 and 24-29
Values for 2-chlorobiphenyl are highly uncertain as a result of the low ECD sensitivity for this compound.

Bottle Equilibrated Partition Coefficients

All samples were 200 mg/l suspended solids made from sediment 190.9 16-20 plus 24-29

Peak No.	0 °C	12 °C	25 °C	35 °C
2-chloro	$(3.6x10^3)$	$(3.5x10^3)$	$(1.5x10^3)$	$(1.3x10^3)$
1b	$2.5x10^4$	$1.7x10^4$	$1.0x10^4$	$8.0x10^3$
2a	$2.6x10^4$	$2.1x10^4$	$1.4x10^4$	$8.0x10^3$
2b	$3.5x10^4$	$3.3x10^4$	$2.2x10^4$	$1.4x10^4$
3a	$1.9x10^4$	$2.0x10^4$	$1.0x10^4$	$8.0x10^3$
3b	$2.7x10^4$	$2.4x10^4$	$1.4x10^4$	$1.1x10^4$
4a	$5.0x10^4$	$4.0x10^4$	$2.0x10^4$	$1.8x10^4$
4c	$5.9x10^4$	$4.3x10^4$	$2.4x10^4$	$1.9x10^4$
5a	$3.6x10^4$	$3.3x10^4$	$1.4x10^4$	$1.1x10^4$
5b1	$4.1x10^4$	$3.9x10^4$	$1.4x10^4$	$1.3x10^4$
5b2	$6.4x10^4$	$6.3x10^4$	$3.6x10^4$	$2.7x10^4$
6a	$5.1x10^4$	$4.9x10^4$	$2.2x10^4$	$1.5x10^4$
6b	$5.5x10^4$	$5.1x10^4$	$2.9x10^4$	$1.7x10^4$
6c	$6.9x10^4$	$6.2x10^4$	$3.1x10^4$	$2.1x10^4$
7a	$5.7x10^4$	$4.7x10^4$	$2.2x10^4$	$1.9x10^4$
7c	$7.0x10^4$	$5.9x10^4$	$3.5x10^4$	$2.8x10^4$
8b	$6.9x10^4$	$5.8x10^4$	$3.3x10^4$	$2.7x10^4$
9c	$1.3x10^5$	$8.2x10^4$	$5.1x10^4$	3.7x104
10a	$1.3x10^5$	$1.1x10^5$	$7.0x10^4$	$4.5x10^4$
10b	$1.4x10^5$	$1.1x10^5$	$6.9x10^4$	$4.9x10^4$
11b	$1.7x10^5$	$1.3x10^5$	$5.1x10^4$	$4.4x10^4$
12b	$2.4x10^5$	$2.0x10^5$	$1.3x10^5$	$9.1x10^4$
12c	$2.8x10^5$	$2.1x10^5$	$8.9x10^4$	$5.7x10^4$

Table XIX. Capillary column Kps versus temperature for sediment 190.9 16-20 and 24-29 (duplicate sample)
Values for 2-chlorobiphenyl are highly uncertain as a result of the low ECD sensitivity for this compound.

milli-Q water and a predetermined amount of PCB contaminated sediment. A magnetic stirrer was used continuously during equilibration. The glass bottle was immersed in a temperature controlled water bath in which the water level was kept several inches above the water level inside the bottle. The top of the bottle was plugged with a two-hole silicone stopper lined with hexane-washed aluminum foil. In each hole was a glass tube, the "inlet" tube went about two inches into the bottle and the "outlet" tube about twelve. During equilibration the tops of the tubes were sealed with glass plugs. During stripping of PCBs from the air, the stirrer was turned off and the tubes were topped with florisil columns, one column on the inlet and two in series on the outlet. The column on the inlet side was used to strip PCBs from incoming ambient air. The first column on the outlet side collected PCBs vaporized in the bottle during equilibration and the second outlet column was used as a blank. Stripping was accomplished by attaching a vacuum pump to the outlet side.

An experiment was performed with CO_2 to determine the efficiency of the air flow system. Three liters of milli-Q water and a small amount of dry ice were added to a 19 l bottle which was then sealed. After 24 hours at 25°C, the stripping procedure was begun and CO_2 measurements were made every minute on the air phase at the outlet. The results are shown in figure 9. The concentration of CO_2 dropped exponentially with a half time of about 110 seconds. Based on these results a 15 minute stripping time was adopted.

The time required to reach equilibrium between the water and vapor phase was determined in two experiments that measured water vapor and CO_2

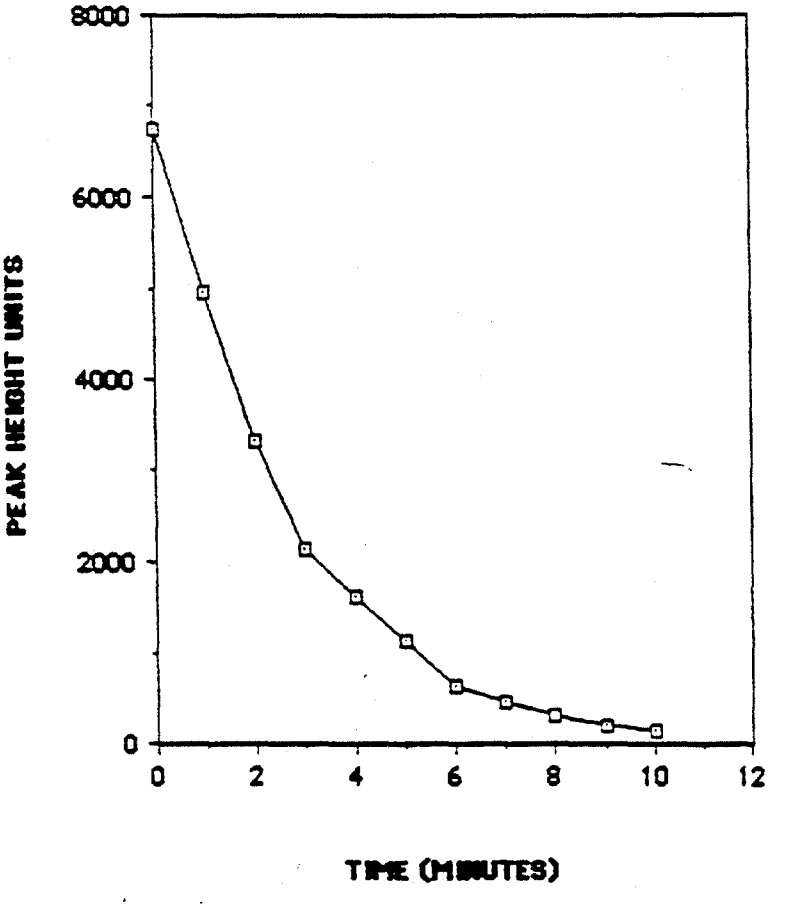

Figure 9. CO_2 versus time for determination of stripping efficiency

transport. From the water experiment, an air boundary layer thickness of 2.3 cm was determined. The CO_2 experiment gave a liquid boundary layer of 7.4×10^{-3} cm. These values were applied to estimate PCB fluxes using the model of Liss and Slater (1974). Applying diffusion coefficients from Bopp (1979 & 1983) it was determined that PCB equilibration would be essentially complete in a few hours. Model results for a typical hexachlorobiphenyl are shown in figure 10. Based on these results, an equilibration time of twenty-four hours was chosen. This would allow for complete suspended matter/water/air equilibration.

To produce an easily quantifiable signal in the vapor phase PCBs, each experiment was run for ten days (ten equilibration/stripping cycles resulting in the extraction of 160 liters of air). Henry's law constants were calculated from measured final water, air and suspended matter concentrations. Measured final K_D values (concentration of suspended matter divided by concentration in the water) were assumed to apply to each individual equilibration and a Henry's law was determined that produced the final observed concentrations when applied to ten sequential equilibrations.

Results of replicate experiments using 200 mg/l suspended matter from the 4-8 cm section of core 91.8 equilibrated at 25°C are shown in table XX. The reproducibility demonstrated in the two runs is quite acceptable, generally 10-20%. Mass balances based on peak 4 components accounted for 92% of the PCBs added in run 1 and 94% in run 2. Table XXI shows results for similar replicate experiments using suspended matter from core 190.9.

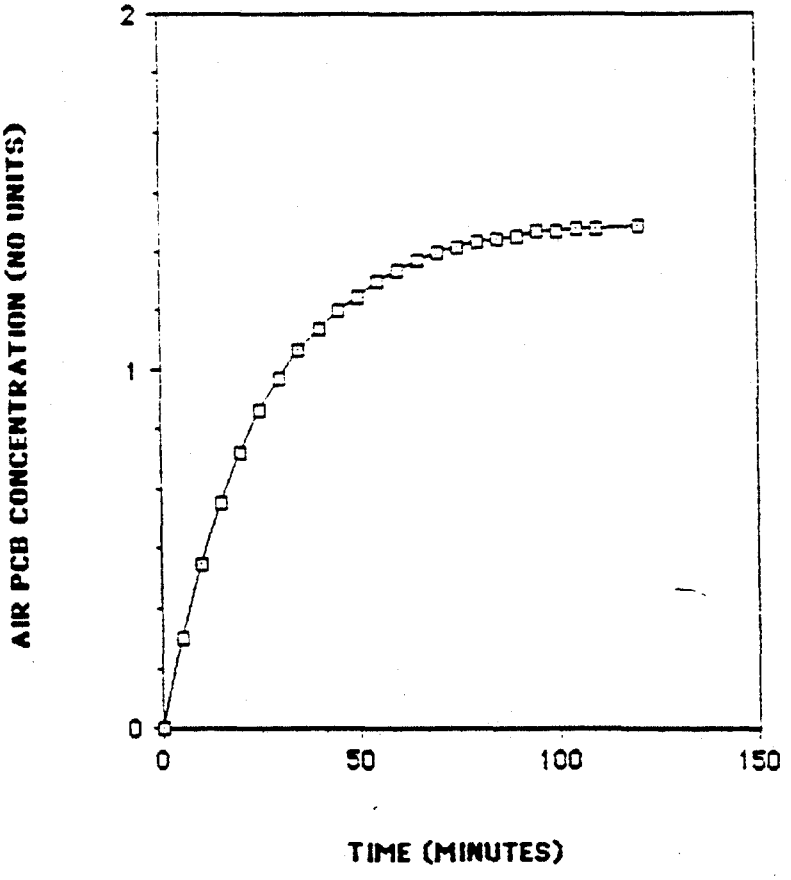

Figure 10. Calculated PCB fluxes for estimating equilibration time

Model inputs were typical physiochemical constants for a hexachlorobiphenyl.

Bottle Equilibrated Henry's Law Constants

All samples were 200 mg/l suspended solids made from sediment 91.8 4-8 and "Milli Q" water

Peak No.	Run 1	Run 2
1a	2.3×10^{-2}	2.7×10^{-2}
2a	4.9×10^{-2}	5.2×10^{-2}
2b	4.1×10^{-2}	4.6×10^{-2}
3a	4.5×10^{-2}	4.6×10^{-2}
3b	3.9×10^{-2}	4.3×10^{-2}
4a	5.1×10^{-2}	5.6×10^{-2}
4b	3.7×10^{-2}	3.6×10^{-2}
4c	4.2×10^{-2}	4.6×10^{-2}
4d	3.1×10^{-2}	3.5×10^{-2}
5a	4.3×10^{-2}	4.4×10^{-2}
5c	3.1×10^{-2}	3.3×10^{-2}
6a	2.4×10^{-2}	3.3×10^{-2}
6b	1.8×10^{-2}	2.6×10^{-2}
7a	1.7×10^{-2}	2.1×10^{-2}
7b	1.3×10^{-2}	1.9×10^{-2}
8a	8.5×10^{-3}	8.2×10^{-3}
8b	6.2×10^{-3}	6.6×10^{-3}
8c	5.2×10^{-3}	5.7×10^{-3}
9a	1.7×10^{-2}	1.9×10^{-2}

Table xx. Reproducibility of capillary column Henry's law constants

Bottle Equilibrated Henry's Law Constants

Peak No.	Run 1	Run 2
9b	$1.1x10^{-2}$	$1.4x10^{-2}$
9c	$8.9x10^{-3}$	$1.0x10^{-2}$
10a	$1.2x10^{-2}$	$1.4x10^{-2}$
10b	$9.6x10^{-3}$	$1.1x10^{-2}$
10c	$9.0x10^{-3}$	$9.2x10^{-3}$
11a	$7.8x10^{-3}$	$7.6x10^{-3}$
11b	$7.1x10^{-3}$	$8.3x10^{-3}$
12a	$8.2x10^{-3}$	$8.7x10^{-3}$

Table XX. (Continued) Reproducibility of capillary column Henry's law constants

Bottle Equilibrated Henry's Law Constants

All samples were 200 mg/l suspended solids made from sediment 190.0 16-20 plus 24-24 and "Milli Q" water

Peak No.	Run 1	Run 2
2-chloro[1]	(2.3×10^{-2})	(2.9×10^{-2})
1b	1.9×10^{-2}	2.6×10^{-2}
2a	4.2×10^{-2}	5.3×10^{-2}
2b	6.2×10^{-2}	5.4×10^{-2}
3a	4.1×10^{-2}	5.5×10^{-2}
3b	4.7×10^{-2}	5.2×10^{-2}
4a	5.9×10^{-2}	6.7×10^{-2}
4c	5.7×10^{-2}	4.9×10^{-2}
5a	6.2×10^{-2}	7.3×10^{-2}
5b1	6.6×10^{-2}	6.3×10^{-2}
5b2	8.2×10^{-2}	7.6×10^{-2}
6a	3.3×10^{-2}	3.9×10^{-2}
6b	3.2×10^{-2}	4.6×10^{-2}
6c	4.3×10^{-2}	5.2×10^{-2}
7a	1.1×10^{-2}	1.9×10^{-2}
7c	3.3×10^{-2}	4.2×10^{-2}
8b	6.6×10^{-3}	7.8×10^{-3}

1. Values for 2-chlorobiphenyl in this table and in Table XXII are highly uncertain as a result of the low ECD sensitivity for this compound.

Table XXI. Capillary column Henry's law constants for sediment 190.9 16-20 plus 24-29

b) Temperature Dependence of Measured Henry's Law Constants. A set of experiments were run at 0, 12, 25 & 35°C using sediment from core 190.9 (16-20 plus 24-29 cm) to determine the temperature dependence of the Henry's law constants. The results are shown in table XXII. Analyses of the data yields a general pattern shown in figure 11. For each component, the Henry's law constant was normalized to the value measured at 25°C. Zero degree values ranged from 7 to 16 percent of the 25°C value. Twelve degree values all were between 19 and 30 percent of the 25°C value. Thirty-five degree values ranged from 1.77 to 2.59 times as large as the twenty-five degree values. There is no apparent regular variation of this pattern with degree of chlorination.

c) Partitioning from wet sediment. An experiment was run to determine the partitioning of PCB components between wet sediment and air. The bottom of a 19 l bottle was covered with about 1 cm of wet sediment from core 190.9 (16-20 + 24-29 cm). The mixture contained 60% water (4g dry sediment + 6g water). The wet sediment was allowed to equilibrate with air at 25°C for 24 hours and then the PCBs were stripped from the air. As above, ten equilibration/stripping cycles were performed. PCB components were measured in the air and, using the total concentrations on the original sediment and the distribution coefficients from the 25°C experiment of table XVII, calculated for the water. The Henry's law constants derived via this procedure are shown in table XXIII. These values are in close agreement with the 25°C values reported in table XXI. This indicates that modeling the transport of PCBs from wet sediment to air can be reasonably accomplished from a knowledge of the total PCB concentration on the sediment and application of the distribution coefficients and Henry's law constants reported here.

Bottle Equilibrated Henry's Law Constants

All samples were 200 mg/l suspended solids made from sediment 190.9 16-20 plus 24-29 and "Milli Q" water

Peak No.	0 °C	12 °C	25 °C [1]	35 °C
2-chloro	(2.8×10^{-3})	(5.3×10^{-3})	(2.6×10^{-2})	(4.8×10^{-2})
1	2.4×10^{-3}	5.1×10^{-3}	2.3×10^{-2}	4.8×10^{-2}
2a	4.2×10^{-3}	1.0×10^{-2}	4.7×10^{-2}	9.2×10^{-2}
2b	8.7×10^{-3}	1.8×10^{-2}	6.7×10^{-2}	1.3×10^{-1}
3a	5.1×10^{-3}	1.0×10^{-2}	4.6×10^{-2}	1.0×10^{-1}
3b	8.4×10^{-3}	1.2×10^{-2}	5.6×10^{-2}	1.0×10^{-1}
4a	4.3×10^{-3}	1.4×10^{-2}	6.2×10^{-2}	1.4×10^{-1}
4c	4.2×10^{-3}	1.2×10^{-2}	5.3×10^{-2}	1.3×10^{-1}
5a	9.2×10^{-3}	1.3×10^{-2}	6.6×10^{-2}	1.7×10^{-1}
5b1	5.7×10^{-3}	1.9×10^{-2}	7.1×10^{-2}	1.4×10^{-1}
5b2	7.3×10^{-3}	1.9×10^{-2}	8.1×10^{-2}	2.1×10^{-1}
6a	5.9×10^{-3}	1.1×10^{-2}	3.7×10^{-2}	6.7×10^{-2}
6b	3.4×10^{-3}	9.0×10^{-3}	4.3×10^{-2}	9.0×10^{-2}
6c	6.2×10^{-3}	1.6×10^{-2}	6.2×10^{-2}	1.1×10^{-1}
7a	3.7×10^{-3}	5.1×10^{-3}	2.3×10^{-2}	5.5×10^{-2}
7c	3.5×10^{-3}	8.6×10^{-3}	3.9×10^{-2}	7.4×10^{-2}
8b	7.9×10^{-4}	1.5×10^{-3}	7.2×10^{-3}	1.7×10^{-2}

1. Note the agreement between this 25 degree sample and the other two replicate samples of Table XXI.

Table XXII. Capillary column Henry's law constants versus temperature

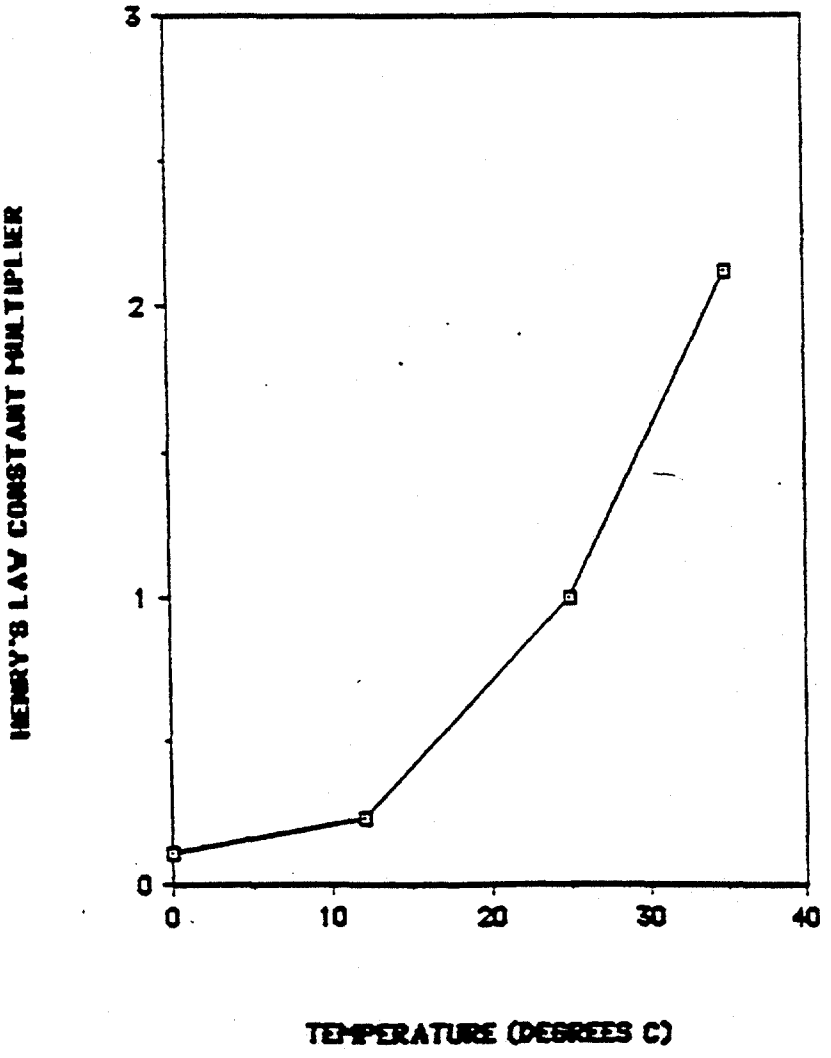

Figure 11. Average trend of Henry's law constants versus temperature

Bottle Equilibrated Wet Sediment - Air Partition Coefficients

All samples were made from sediment 190.0 16-20 plus 24-24 and "Milli Q" water.

Peak No.	Partition Coefficient
2-chloro	2.7×10^{-2}
1b	3.0×10^{-2}
2a	5.1×10^{-2}
2b	5.2×10^{-2}
3a	5.3×10^{-2}
3b	5.1×10^{-2}
4a	6.6×10^{-2}
4c	5.9×10^{-2}
5a	6.9×10^{-2}
5b1	6.8×10^{-2}
5b2	7.2×10^{-2}
6a	3.7×10^{-2}
6b	4.8×10^{-2}
6c	5.4×10^{-2}
7a	2.6×10^{-2}
7c	3.7×10^{-2}
8b	7.3×10^{-3}

1. The value for 2-chlorobiphenyl is highly uncertain as a result of the low ECD sensitivity for this compound.

Table XXII. Capillary column wet sediment - air partition coefficients for sediment 190.9 16-20 plus 24-29

IV. Conclusions

This work has provided values for distribution coefficients and Henry's law constants of PCB components on Hudson River sediments as a function of temperature. The importance of dissolved organic carbon concentrations on controlling distribution coefficients was clearly demonstrated. When DOC concentrations were taken into account, no dependence of distribution coefficients on suspended matter concentration could be detected. The experiments were designed to produce values appropriate for use as inputs to models of PCB transport from contaminated Hudson River sediment that would be a result of the Hudson River PCB Reclamation Project. Future work in this area should be directed toward better quantification of the effect of DOC on distribution coefficients and toward investigating the effect of this important parameter on Henry's law constants.

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