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Measurements of Octanol−Air Partition Coefficients (K_{OA}) for Polybrominated Diphenyl Ethers (PBDEs): Predicting Partitioning in the Environment

Tom Harner* and Mahiba Shoeib

Meteorological Service of Canada, Environment Canada, 4905 Dufferin Street,
Toronto, Ontario, Canada M3H 5T4

Octanol−air partition coefficients (K_{OA}) are reported for 13 polybrominated diphenyl ethers (PBDEs) over the temperature range (15−45) °C. K_{OA} exhibited a log−linear relationship with inverse absolute temperature, and values at 25 °C range from 9.3 (PBDE-17) to 12.0 (PBDE-126). These are approximately 1 to 2 orders of magnitude greater than those measured for the counterpart polychlorinated biphenyls (PCBs). PBDEs also showed a strong temperature dependence. The enthalpy of phase change from octanol to air, ΔH_{OA}, was ($\approx$70 to $\approx$120) kJ mol^{-1}. This corresponds to a 20−100 times higher K_{OA} value at 5 °C versus 35 °C. A method is presented for estimating K_{OA} at any temperature for additional PBDEs using relative retention times. Log K_{OA} values were compared against two sets of recently published subcooled liquid vapor pressures (p^o_L) that show significant discrepancies. Activity coefficients in octanol (γ_O) for PBDEs ranged from 1 to 10 when one set of vapor pressures was used. This was consistent with other classes of SOCs and indicated near ideal solution behavior. When the second set of values was used, calculated activity coefficients were in the range 10−100, suggesting that these vapor pressure values were inaccurate. Application of K_{OA} for describing partitioning of PBDEs to aerosols and soils was also examined. The predicted percentages (at 25 °C) on aerosols ranged from 1.2% for PBDE-17 to 85% for PBDE-183 and agreed well with measured data, confirming that surface−air partitioning is an important process for the distribution and fate of PBDEs in the environment. Results of illustrative calculations for air−soil partitioning suggest that, because of their high K_{OA} values, PBDEs will exhibit similar background soil concentrations as the PCBs despite having much lower air concentrations.

Introduction

Polybrominated diphenyl ethers (PBDEs) are added to numerous products because of their ability to retard fire. In 1992 global production of PBDEs was estimated at 40 000 tons.[1] Technical formulations contain numerous congeners, and their numbering is analogous to that of the polychlorinated biphenyls (PCBs). Decabromodiphenyl ether (PBDE-209) is the most widely produced formulation, accounting for ≈75% of global production of PBDEs and consisting almost entirely of PBDE-209. The "pentabromodiphenyl ether" product consists mainly of congeners 47, 99, and 100. This formulation has been phased out in Japan and will also be phased out in Europe. However, its use in North America continues without any restriction or regulation.

PBDEs are ubiquitous environmental pollutants and have been detected in biotic and abiotic matrixes that include fish, birds, sediment, marine mammals, and human plasma and milk. It is of great concern that PBDEs are on the rise; levels in Swedish human milk have increased exponentially over the period 1972−1997[2] with a doubling time of approximately five years. PBDEs have also been reported in arctic air[3] and air from several background and urban sites in the Great Lakes region[4] where ΣPBDE ranged from ≈5 pg m^{-3} at background sites near the Great Lakes to as high as ≈50 pg m^{-3} in urban Chicago. The Great Lakes study also highlighted partitioning to aerosols as a relevant process for PBDEs. It is important therefore to assess the volatility of PBDEs and to describe and predict their partitioning to terrestrial organic phases and aerosols. International agreements (UN-ECE and UNEP protocols) on POPs call for reliable partitioning data that can be used to screen and assess chemicals of concern.[5,6]

Recently reported subcooled liquid vapor pressures (p^o_L) by Wong et al.[7] and Tittlemier and Tomy[8] are the first data that allow us to assess the volatility and long-range transport potential of PBDEs. Unfortunately, however, the data from these two studies disagree with discrepancies of more than an order of magnitude for some congeners.

The octanol−air partition coefficient, K_{OA}, is the ratio of the solute concentration in air versus octanol when the octanol−air system is at equilibrium. It is a useful descriptor of a chemical's mobility in the atmospheric environment and thought to be the key descriptor of the absorptive partitioning of semivolatile compounds between the atmosphere and organic phases found in soil, in vegetation, and on aerosols. Numerous models employed to screen and rank chemicals for persistence and long-range transport potential have incorporated K_{OA}.[5,6,9] Measurements of K_{OA} and its temperature dependence have now been made for a range of semivolatile organic chemicals (SOCs) including chlorobenzenes,[10−12] PAHs and PCNs,[13] dioxins and furans,[14] and organochlorine (OC) pesticides.[15] In general, log K_{OA} varies linearly with inverse absolute temperature. Partitioning into octanol (organic phases) increases by a factor of ≈2.5 to ≈3.5 for every 10 °C decrease in temperature.

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* To whom correspondence should be addressed. E-mail: tom.harner@ec.gc.ca. Fax: 416 739 5708.

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Table 1. K_{OA} Values for PBDEs over the Temperature Range (15 to 45) °C

PBDE congener	log K_{OA}	A^a	B^a	ΔH_{OA}	$\Delta_{vap}H^b$	$\gamma_O{}^c$	aerosol %^{d}	aerosol %^{d}	$C_{soil}{}^d$/(ng g^{-1} dw)
	(25 °C)			kJ mol^{-1}	kJ mol^{-1}		(25 °C)	(0 °C)	(predicted)
17 (2,2′,4)	9.30	−3.45	3803	72.8		3.6	1.2	15.6	
28 (2,4,4′)	9.50	−3.54	3889	74.5		3.1	1.9	23.7	
47 (2,2′,4,4′)	10.53	−6.47	5068	97	92	1.5	17	88.4	4.2
66 (2,3′,4,4′)	10.82	−7.88	5576	107	93.5	1.0	29	95.6	
77 (3,3′,4,4′)	10.87	−5.69	4936	94.5	95.3	1.4	32	93.9	
100 (2,2′4,4′,6)	11.13	−7.18	5459	105			45	97.6	0.85
99 (2,2′4,4′5)	11.31	−4.64	4757	91.1	100.3	1.1	56	97.4	7.76
85 (2,2′,3,4,4′)	11.66	−6.22	5331	102		1.2	74	99.2	
126 (3,3′,4,4′,5)	11.97	−8.41	6077	116			85	99.8	
154 (2,2′,4,4′,5,6′)	11.92	−4.62	4931	94.4			84	99.4	0.32
153 (2,2′,4,4′,5,5′)	11.82	−5.39	5131	98.2	107.6	2.8	80	99.4	0.45
156 (2,3,3′,4,4′,5)	11.97	−5.80	5298	101			85	99.6	
183 (2,2′,3,4,5,5′,6)	11.96	−3.71	4672	89.5			85	99.4	

[a] Regression coefficients (A and B) are for eq 1 (i.e. log $K_{OA} = A + B/T$). [b] From Wong et al.[7] [c] Based on p°$_L$ data from Wong et al.[7] [d] The percentages on aerosols and equilibrium soil concentrations were predicted at 25 °C using eqs 4−6 and the parameters listed in the text. The mean air concentrations (pg m^{-3}) at (20 ± 3) °C from Strandberg et al.[4] are as follows: PBDE-47, 10.8; PBDE-100, 0.87; PBDE-99, 6.6; PBDE-154, 0.19; PBDE-153, 0.28. Note: these total air concentrations were corrected to gas-phase concentrations using eqs 4 and 5.

This study reports K_{OA} values as a function of temperature for 13 PBDE congeners. K_{OA}-based models describing aerosol−air[16] and soil−air[17,18] partitioning of SOCs are briefly reviewed and used to predict environmental partitioning of individual PBDEs to aerosols and soil.

Experimental Section

Chemicals. Solid PBDE standards (≈1 mg; PBDEs-17, -28, -47, -66, -77, -85, -99, -100, -126, -153, -154, -156, and -183; see Table 1 for substitution patterns) were obtained from Wellington Laboratories (Guelph, Ontario). Octanol solutions were prepared by adding 1 mL of octanol (EM Science, Merck) to about 1 mg of solid chemical. Saturated or near-saturated solutions were produced by sonicating for several hours. Undissolved chemical was allowed to settle, and a known volume of each solution (≈10 to ≈20 μL) was combined and diluted to 1 mL in octanol. Solute concentrations in this mixture were approximately 1% of their saturation value, and thus interactions between PBDE molecules should be minimal.

Method. A detailed description of the apparatus is presented in ref 14/ Briefly, nitrogen from a compressed cylinder at a controlled flow rate of (200 to 400 mL min^{-1}) was saturated with octanol by sparging through a column about 20 cm in height. The octanol-saturated gas stream was cooled to the measurement temperature and excess octanol collected in a trap. The gas stream was then directed to the generator column that consisted of glass beads coated with 300 μL of the mixed octanol solution. Equilibrated gas-phase chemicals in the gas stream exiting the generator column were collected on an adsorbent trap which contained about 20 g of C_{18}-bonded silica (IST Ltd, Mid Glamoragn, U.K.). Flow rates were measured at the exit of the trap to determine total sample volumes. Traps were extracted with 15 mL of 50:50 hexane/dichloromethane, and the resulting solutions were then reduced in volume to ≈500 μL with a gentle stream of nitrogen. The cooling coil, octanol trap, and generator column were submerged in a thermostat-controlled (±0.1 °C) water bath that was kept at least 10 °C cooler than the octanol used to saturate the gas stream. As with earlier studies,[14] the system operates under a slight positive pressure. This results in a very minor adjustment to the flow rate measured at the outlet.

Concentrated extracts were analyzed for PBDEs using a Hewlett-Packard 5890 gas chromatograph (GC) equipped with split/splitless injection and an electron capture detector (ECD). The injector and detector temperatures were (250 and 300) °C, respectively. A 60 m DB-5 column (J&W Scientific) with 0.25 mm i.d. and 0.25 μm film thickness operated with hydrogen carrier gas was used for separation using the following GC oven temperature program: initial at 170 °C, hold for 0.5 min, 2 °C min^{-1} to 270 °C, hold for 15 min. Mirex and ^{13}C-PCB105 were used as internal standards for the volume correction. Calibration standards for quantification were made from serial dilutions of the mixed octanol solution used in the generator column. Determined concentrations are expected to have an uncertainty of approximately ±10%.

Results and Discussion

Quality Control. Two octanol solutions were made; the first consisted of the lower molecular weight PBDEs (congeners 17, 28, and 47) and two reference compounds (PCB congeners 95 and 153) that were measured in a previous study.[11] The second solution consisted of higher molecular weight PBDEs (congeners 47, 66, 77, 100, 99, 85, 126, 154, 153, 156, and 183) and PCB-95. Inclusion of reference compounds from previous measurements helped to ensure consistency with previously reported K_{OA} data. PBDE-47 and PCB-95 were also added to the second octanol solution to ensure consistency between the two sets of measurements in this study.

The log K_{OA} values at 25 °C for PCB-95 and PCB-153 in the first experiment were 8.82 and 9.70, respectively, within 10% of previous data by Harner and Bidleman.[11] The value for PCB-95 in the second experiment (8.71) was consistent with the first value, and the same was true for PBDE-47 (10.39 in the first experiment and 10.50 in the second). These results indicate that the measurements conducted in this study were consistent internally and also with previous measurements of K_{OA} for other compound classes.

The possibility of chemical breakthrough in the absorbent trap was checked by periodically connecting a second trap in series with the first. No breakthrough was observed. Complete extraction of compounds from the traps was tested by spiking with a known quantity of the standard mixture and collecting two sequential extracts of the trap. None of the test chemicals was detected in the second extract of the trap, and recoveries in the first extract were better than 70% for all except three congeners. A correction

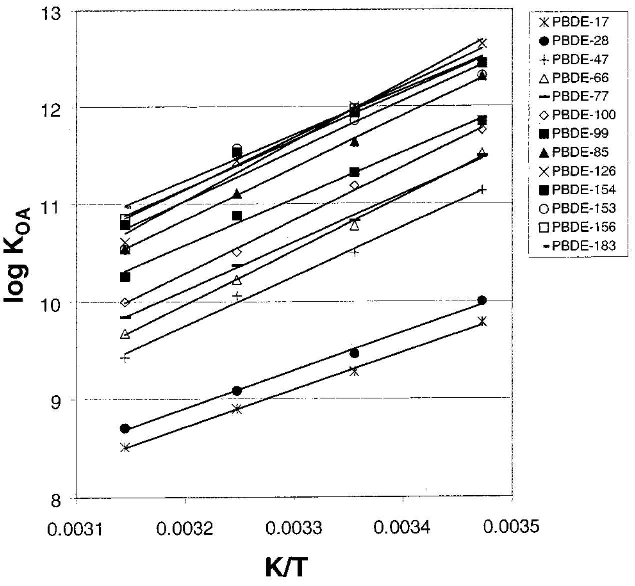

Figure 1. Measurements of K_{OA} for 13 PBDEs over the temperature range +15 to +45 °C.

was necessary for congeners 153, 156, and 183 that had recoveries in the range (40 to 55)%.

Temperature Dependence of K_{OA}. The octanol−air partition coefficient K_{OA} was correlated against $1/T$ over the temperature range (15 to 45) °C and showed a log−linear relationship according to the equation

$$\log K_{OA} = A + B/T \tag{1}$$

Results for 13 PBDEs are presented in Figure 1. Regression parameters for eq 1 are included in Table 1, and interpolated K_{OA} values at 25 °C are listed. In general K_{OA} values for PBDEs were 1 to 2 orders of magnitude greater than those previously observed for the counterpart PCBs.[11] For instance, at 25 °C the log K_{OA} value is 9.02[11] for PCB-66 and 10.82 for PBDE-66—a factor of 60 greater. This can be extended to the real environment, where it is expected that PBDEs will partition from the atmosphere to soils, vegetation, and aerosols more strongly than their PCB counterparts. Comparisons for other PBDE and PCB congeners have similar results: PBDE-77 and PCB-77, factor of 14; PBDE-126 and PCB-126, factor of 41; PBDE-153 and PCB-153, factor of 122.

The temperature coefficient for octanol−air transfer, ΔH_{OA} (derived from the slope of Figure 1, i.e., $\Delta H_{OA} = 2.3BR$, where $R = 8.314$), is also shown in Table 1. Values ranged from ($\approx$70 to $\approx$120) kJ mol^{-1} and are in good agreement with enthalpies of vaporization, $\Delta_{vap}H$, recently reported for selected congeners.[7] To elaborate on this temperature effect, log K_{OA} for PBDE-47 is 9.47 at 45 °C and 11.13 at 15 °C, corresponding to an almost 50-fold increase in K_{OA} over this 30 deg drop in temperature. It follows that, at colder temperatures, PBDE-47 will partition more strongly to soil, aerosols, and other terrestrial organic phases. It is this temperature-dependent partitioning of PBDEs that controls their cycling in the environment and determines air concentrations that adjust to diurnal and seasonal variations in air and surface temperature. It also governs how they are fractionated latitudinally from warm source regions to colder climate regions.

Estimating K_{OA} for Additional PBDEs. In this study we have measured K_{OA} values for 13 of the more relevant PBDE congeners that are detected in the environment. However, it may be useful to predict temperature-dependent K_{OA} values for other congeners.

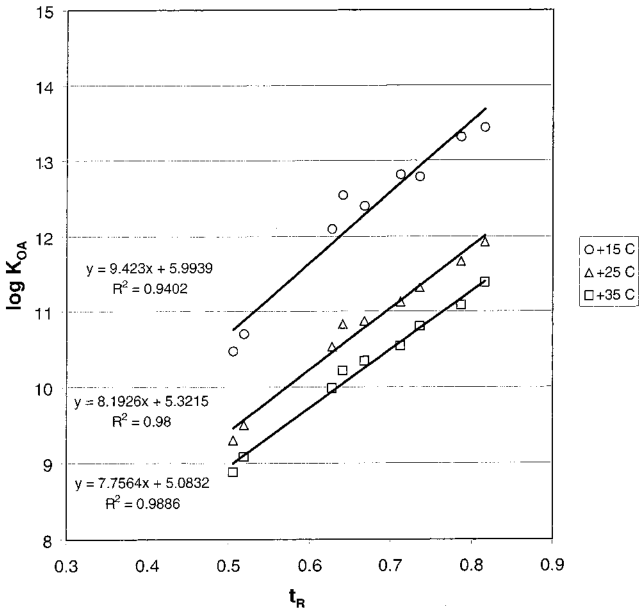

Figure 2. Correlation of log K_{OA} versus relative retention time (RRT) at +15, +25, and +35 °C. RRTs were reported by Sjödin et al.[19] and measured against Dechlorane 603 on a CPSil-8 column.

Figure 2 correlates log K_{OA} versus relative retention time (t_R) values reported by Sjödin et al.[19] at (15, 25, and 35) °C. Values of t_R were measured against Dechlorane 603 on several columns of different polarity. The results on a CPSil-8 column were used here. To improve the predictive ability of this method, K_{OA} values for PBDEs-153, -156, and -183 were excluded, since a significant recovery factor was applied to the measured K_{OA} data. At each temperature, K_{OA} is related to t_R by

$$\log K_{OA} = a' + b' t_R \tag{2}$$

To account for differences in temperature, a' and b' values from the regression equations in Figure 2 were plotted against $1/T$. The resulting regression coefficients were

$$a' = 2187.9/(T/\mathrm{K}) - 2.020 \quad \text{and} \quad b' = 4003.7/(T/\mathrm{K}) - 5.2425$$

Thus, for PBDE congeners not measured directly in this study, it is possible to estimate, semiempercially, the log K_{OA} value at any temperature using eq 2, the t_R values reported by Sjödin et al.,[19] and the expressions for the regression coefficients a' and b' (above).

Comparison to $p°_L$ Values. Recently, Tittlemier and Tomy[8] and Wong et al.[7] reported subcooled liquid vapor pressures ($p°_L$) for PBDE congeners that were determined by the GC retention method. However, the results from these two studies were not consistent, and in some cases discrepancies were more than an order of magnitude. Figure 3a is a plot of log K_{OA} versus log $p°_L$, comparing the results of this study to the two published data sets for $p°_L$. In both cases there appears to be a near 1:1 relationship between log K_{OA} and log $p°_L$. This comparison does not allow us to determine which $p°_L$ data are more correct. However, when results from other SOC classes (PCBs, PCNs, PCDD/Fs) are added (Figure 3b), it appears that the data from ref 7 are more consistent.

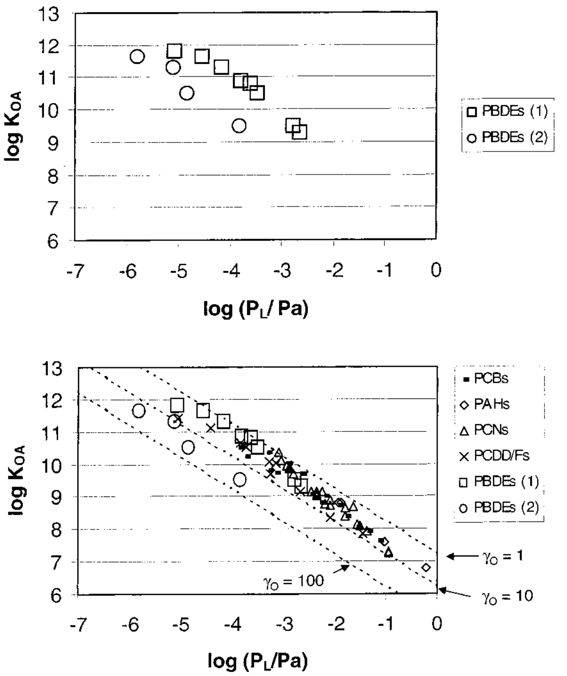

Figure 3. Log K_{OA} versus log $p^o{}_L$ (Pa) at 25 °C for selected semivolatile organic chemicals: PBDEs (1) = $p^o{}_L$ data from Wong et al.[7]; PBDEs (2) = $p^o{}_L$ data from Tittlemier and Tomy.[8]

The octanol−air partition coefficient can be defined as

$$K_{OA} = C_O/C_A = RT/(\gamma_O V_O p^o{}_L) \tag{3}$$

where C_O and C_A are the equilibrium concentrations of the solute in octanol and air, respectively, R is the universal gas constant, T is the absolute temperature, γ_O is the activity coefficient in octanol, V_O is the molar volume of octanol (157 m^3 mol^{-1}), and $p^o{}_L$ is the subcooled liquid vapor pressure in pascal. According to Raoult's law, γ_O approaches unity for an ideal solution. In other words, γ_O is a measure of nonideal behavior resulting from interactions between PBDE molecules and octanol molecules, that is, a measure of how "active" the PBDE molecules are in octanol solution compared to their pure liquid reference states. In general, activities are greater for molecules that have dissimilar properties.

Equation 3 can be rearranged to calculate γ_O for any combination of K_{OA} and $p^o{}_L$, or alternatively, theoretical lines can be determined for different values of γ_O, as was done in Figure 3b. The results presented in Figure 3b show that for several classes of semivolatile organic compounds (SOCs) γ_O values are similar and fall within unity and a value of ten, indicating near ideal behavior. This result is expected, since PBDE molecules and octanol molecules are both slightly polar. The suspect $p^o{}_L$ values reported by Tittlemier and Tomy[8] result in γ_O values in the range 10 to 100.

Partitioning to Aerosols. Expressions have been developed that can relate concentrations of SOCs in air to their respective equilibrium values on aerosols[16] and soil.[17,18] For aerosols,

$$\log K_P = \log K_{OA} + \log f_{om} - 11.91 \tag{4}$$

where K_P is the particle gas partition coefficient which relates the portion of chemical on the particles to its gas-phase concentration and f_{om} is the fraction of organic matter on the aerosol that is free to exchange chemical.

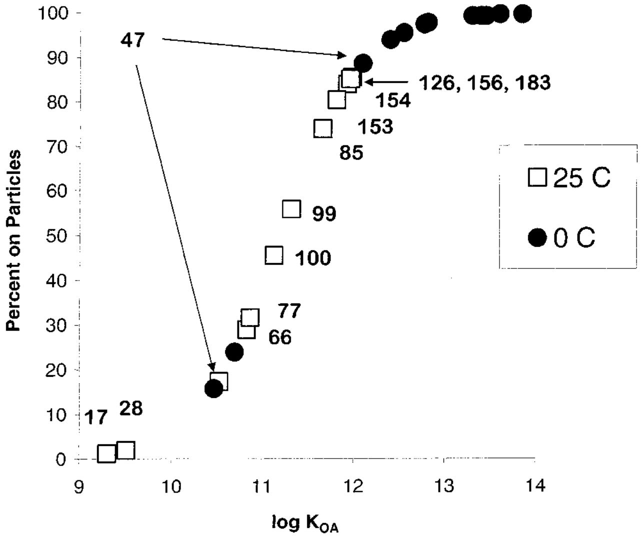

Figure 4. Percent of PBDEs on particles at 25 °C and 0 °C calculated using eqs 4−6 and parameters listed in the text. Results for 25 °C are labeled with PBDE congener numbers. PBDE-47 is labeled at 25 °C and 0 °C (see Table 1 footnote for details).

The fraction on particles, ϕ, is calculated as

$$\phi = K_P\ \mathrm{TSP}/(K_P\ \mathrm{TSP} + 1) \tag{5}$$

TSP is the concentration of suspended particulate matter in air. Typical values for f_{om} and TSP are 0.2 and 25 $\mu g\ m^{-3}$, respectively. On the basis of eqs 4 and 5, predicted percentages on aerosols were determined at 25 °C for all PBDE congeners (Table 1 and Figure 4) with the following approximate ranges: tetra-PBDEs, (20 to 30)%; penta-PBDEs, (40 to 70)%; hexa-PBDEs, 80%+. These results agree well with recent measurements by Strandberg et al.[4] at (20 ± 3) °C of gaseous and particulate PBDEs in the Great Lakes atmosphere. Calculations at 0 °C are also included and show the strong influence of temperature on the partitioning behavior of PBDEs. For instance, at 25 °C PBDE-47 is mostly in the gas-phase with only ≈17% associated with the particle phase whereas at 0 °C it is almost entirely (≈88.4%) on particles.

Partitioning to Soils. Hippelein and McLachlan[17,18] measured the dimensionless soil−air partition coefficient (K_{SA}) for several classes of SOCs (chlorobenzenes, polychlorinated biphenyls, and polycyclic aromatic hydrocarbons). They were able to relate this partitioning to the octanol−air partition coefficient using the relationship

$$K_{SA} \approx 2 f_{oc} K_{OA} \tag{6}$$

where f_{oc} is the fraction of organic carbon in the soil. On the basis of the K_{OA} values at 25 °C determined in this study, an equilibrium soil−air partition coefficient was calculated using eq 6. Calculations were based on a typical soil having a soil solids density of 2500 kg m^{-3} and f_{oc} = 0.02. Converting these to realistic equilibrium soil concentrations required knowledge of the measured gas-phase air concentrations of selected PBDEs.

Strandberg et al.[4] reported air concentrations of individual PBDE congeners at three background sites and one urban site. The samples were collected as part of the Integrated Atmospheric Deposition Network (IADN) monitoring network that is operated jointly by Canada and the United States. To minimize variability in the data, only samples collected in the temperature range (+20 ± 3) °C over the period 1997−1999 were included in the study. In general ΣPBDE was 20 to 70 times lower than ΣPCB and similar to concentrations of several OC pesticides. Total PBDE concentrations were converted to gas-phase concentrations using eqs 4 and 5 as discussed above, and a mean (pg m^{-3}) value representing the four sites was calculated: PBDE-47, 10.8; PBDE-100, 0.87; PBDE-99, 6.6; PBDE-154, 0.19; PBDE-153, 0.28. These air concentrations were used to convert K_{SA} values to soil concentrations (i.e. $C_{soil} = C_{air}/K_{SA}$; C_{air} is the gas-phase air concentration) that are listed in Table 1.

Predicted soil concentrations (as ng g^{-1} dry wt) ranged from 0.32 (PBDE-154) to 7.8 (PBDE-99). These concentrations are approximately in the range observed for PCBs in continental background soils.[20] Thus, despite much lower air concentrations of PBDEs compared to PCBs, soil concentrations may be similar as a result of greater K_{OA} values that drive the transfer of PBDEs from the atmosphere to terrestrial organic phases.

In conclusion, the availability of physical chemical data for PBDEs puts us in a unique and interesting position where we can model the partitioning and predict concentrations of PBDEs in various compartments in-step with or ahead of actual measurements. Our predictions based on measured K_{OA} values suggest that PBDEs will strongly partition to soil and other terrestrial organic phases and that particle−gas partitioning will play a key role in the transport and fate of PBDEs in the environment.

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