

Multimedia Modeling of Polybrominated Diphenyl Ether Emissions and Fate Indoors

XIANMING ZHANG,
MIRIAM L. DIAMOND,*
CATALINA IBARRA, AND STUART HARRAD
*Department of Geography, University of Toronto, Toronto,
Ontario, M5S 3G3, Canada, Division of Environmental Health
and Risk Management, Public Health Building, School of
Geography, Earth, and Environmental Sciences, University of
Birmingham, Birmingham, B15 2TT, United Kingdom*

Received August 02, 2008. Revised manuscript received
January 23, 2009. Accepted January 27, 2009.

We adapted an indoor multimedia fugacity model to consider emissions and fate of polybrominated diphenyl ethers (PBDEs) and to understand the variability of indoor concentrations. The model was applied to an office in which an 80% decrease in PBDE air concentration was observed after an old computer was exchanged with a newer one. PBDE-impregnated polyurethane foam (PUF) and carpet were treated as pseudo-steady-state components with specified fugacities derived from measured concentrations of 173 and 2140 ng·g⁻¹, respectively. Emission rates of 35 and 5.4 ng·h⁻¹, for the old and new computers, respectively, were calculated using the pseudo-steady-state approach. Particle movement (deposition and resuspension) dominates within-room transport processes, and dust removal (vacuuming) and air advection (ventilation) are the main loss processes. The most sensitive parameters to air concentrations and estimated emission rates are room temperature, particle concentrations and deposition velocity, and air exchange rates. The air exchange rates and bouncing on PUF furniture can alter whether the PUF and carpet are sources or sinks of PBDEs. Model results suggest that exposure via air can be reduced by removing dust, having a high air exchange rate, and low indoor temperatures.

Introduction

Polybrominated diphenyl ethers (PBDEs) are a group of brominated compounds commonly used as additive flame retardants in consumer products. The Penta commercial product was primarily used in household furnishings such as polyurethane foam (PUF), vehicle seating and carpet, as well as printed circuit boards and microprocessor packaging in computers. The Octa and Deca commercial products were mainly used for the thermoplastics and the plastic housing for electrical goods (1–3). Concerns exist because of studies documenting the toxicity of Penta and Octa formulations as thyroid active agents that can cause neurological impairments (4). Further, biomonitoring studies have documented the widespread presence of PBDEs in human tissues (5, 6). In response to these concerns, Europe and North America moved to ban production and use of the Penta and Octa formulations in new products (1). For Deca, the European

Union has recently banned its use in electronics and electrical applications (7). These mitigative actions are directed to new uses but not to the existing, in-use stock of products and materials that contain Penta, Octa, and Deca (8, 9).

Recently, Wu et al. (10) found a positive correlation between PBDE concentrations in women's breast milk and dust concentrations in their homes, where dust is the presumed main exposure route (8, 9, 11). Concern also exists for infants, toddlers, and children for whom dust intake is greatest on a per body weight basis (11, 12) and who have been found to have the greatest PBDE concentrations in their blood (13).

PBDE concentrations in air and dust among different homes can vary by as much as 1000-fold (14) and concentrations within a home can also vary across rooms (15). Hazrati and Harrad (2) showed that PBDE concentrations in the air of an office decreased significantly after a computer was replaced with a newer model, which indicated that the computer alone was a major indoor source of PBDEs. Attempts to relate PBDE concentrations in dust to the number or volume of products potentially containing PBDEs has met with limited success (2, 10, 14, 16). Allen et al. (17) improved the ability to predict high PBDE dust concentrations in rooms by assessing the bromine content of products thought to contain PBDEs by using X-ray fluorescence (17). They also noted that the use or presence of TVs and the level of activity in a room contributed to the prediction of PBDE concentrations in dust. While Allen et al. have improved our ability to predict PBDE concentrations in dust, considerable variability remains in the relationship between PBDE in dust and Br content of goods and products.

In addition to activity in a room, the concentrations and fate of PBDE indoors could be affected by factors such as other materials and products found indoors. Followed by emission indoors, semivolatile organic compounds (SVOCs) such as PBDEs can be taken up by indoor materials such as PUF in furniture and carpet and then re-emitted into the air (18, 19). As such, these materials can act as buffers for indoor SVOC concentrations, modulating and/or prolonging their presence and hence exposure (20). As noted above, indoor activities can influence characteristics of the indoor environment such as the dust content: house dust resuspended by normal human activity may contribute 25% of indoor particles in air (21).

Multimedia models have been useful tools for elucidating the behavior of SVOCs (22). Bennett and Furtaw developed and applied a fugacity-based indoor model to study the behavior of pesticides after spraying indoors. Their model considered four environmental media (i.e., air, vinyl floor, carpet, and film on impervious surface) and successfully described fate and transport of pesticides indoors (23). Our goal was to extend and apply the model of Bennett and Furtaw to (1) estimate the emission rate of PBDEs from an indoor source(s); (2) describe the fate and behavior of PBDEs in a multimedia indoor environment and sink/source behavior of indoor goods and materials; and (3) identify factors that influence the fate of PBDEs indoors. We use the example described by Hazrati and Harrad (2) in which PBDE air concentrations in an office decreased by ~80% after a computer was replaced with a newer model. Based on this observation and that of Allen et al. (17), we assume that electronic equipment is the main source of PBDEs to this office.

* Corresponding author phone: 416-978-1586; fax: 416-946-5992; e-mail: miriam.diamond@utoronto.ca.

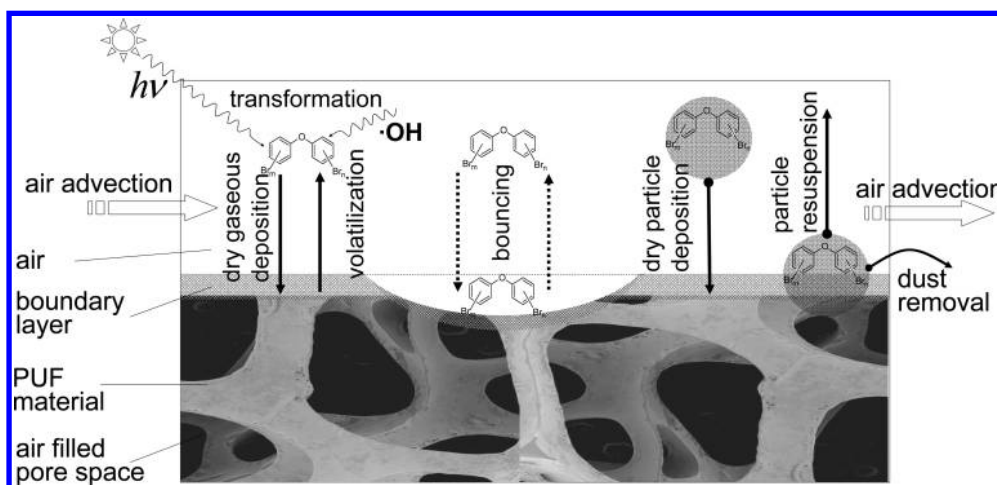


FIGURE 1. PBDE fate processes involved within air and PUF as considered in the indoor environment model. (The micrograph of PUF was taken from DoITPoMS Micrograph Library, University of Cambridge, under the terms of use. The micrograph was contributed by J. A. Curran, Department of Materials Science and Metallurgy, University of Cambridge).

Methods

Multimedia Indoor Environmental Model. Our indoor multimedia fugacity model (Figure S1) builds on that of others (23, 24). We added PUF furniture as another compartment in addition to air, vinyl floor, carpet, and film on impervious surfaces (18, 19).

The model considers gas and particle phases of a chemical with input from chemical impregnated materials such as PUF, carpet and electronic equipment. Losses occur through air advection, dust removal, and chemical transformation. Tables S1 and S2 list equations and parameters used to calculate fugacity capacities or Z values, transport and transformation parameters or D values, respectively.

We consider chemical input from three pathways: (1) air advection from outdoors of gas and particle phases, (2) release from chemical-impregnated PUF and carpets according to a fugacity gradient between the materials and indoor air, and (3) emissions (independent of a fugacity gradient) from indoor sources, e.g., PBDEs from electronic devices such as computers and printers (25). For PBDE-containing PUF furniture and carpets, we adopt a pseudo-steady-state approach whereby we specify the fugacity of these compartments according to measured PBDE concentrations. This approach is analogous to the treatment of “in-place” sediment pollution in lakes (26). Mass balance equations (Table S4) are then used to solve for the unknown fugacities and emissions, assuming that steady-state conditions apply to the air compartment. The model was written in Visual Basic 6.0 on a PC platform.

Modeling PUF Furniture. PUF, to which PBDEs are added up to 10% (27), can act as a source or sink for PBDEs, depending on emissions and the fugacities of the other compartments. PBDEs can exchange between air and PUF through three main processes: (1) gas-phase diffusion, particle-phase deposition and resuspension, and “bouncing” (Figure 1). PUF porosity can be as high as 97.6% (19). Gas-phase exchange is based on three assumptions: (1) the PUF structure is analogous to snow; (2) the bulk phase of PUF is homogeneous and that equilibrium is established instantaneously between the air in the PUF pore space and polymer; (3) gas-phase diffusion of SVOCs is limited from the bulk phase PUF to the overlying air by the PUF–air boundary layer. Particle-phase deposition and resuspension are governed by their respective velocities and gas-particle partitioning. “Bouncing” refers to accelerated gas- and particle-phase exchange between the bulk-phase PUF and air due to compression caused by adults sitting and (some) children bouncing on furniture. This differs from the wind-driven

“pumping” of snow that is parametrized as an increase of the mass transfer coefficient for diffusive air–snow exchange (28). Bouncing is formulated as the product of a compression ratio (the extent of PUF compression), compression frequency, and PUF volume. Compression ratio and frequency presumably vary enormously, and since (to our knowledge) no measurements have quantified this activity, we used default values of 1/3 of the volume being compressed at a frequency of 0.25 h^{-1} .

Model Application to an Office. This case study uses the university office described by Hazrati and Harrad (2). Monitoring of PBDEs in the office air for 9 sequential months showed an ~80% decrease in concentrations after an older computer in the office was replaced with a new one (2). The office was fully carpeted (industrial with thin pile) and contained a computer, printer, plugs and wires for the electrical devices, two PUF chairs, a wooden desk, and a bookshelf. Although there were many books and papers in the office, we did not add paper as a compartment because of its low PBDE concentrations (unpublished data). Detailed characteristics of the office are listed in Table S6.

Measurement of PBDEs in the office. We analyzed two PUF samples from different sections of an office chair >10 years old (PUF samples 2.6 and 2.7 g) and two samples of the 8–9 year old carpet (19.3 and 20.8 cm^2) located next to each other in a corner of the office. The carpet samples were vacuumed to remove the dust. Each sample was Soxhlet-extracted in 300 mL of *n*-hexane at 60 °C for 10 h. The procedures followed are detailed by Harrad et al. (8). Air concentrations that were obtained using passive samplers were reported previously (2) and are summarized in Table S7.

Model Parameterization. The physicochemical properties of PBDEs are listed in Table S8. Temperature corrections were made on values of vapor pressure, K_{OA} , and reaction rates. The thermodynamic and kinetic properties of PBDEs were taken from either the literature or derived from other basic physicochemical properties (Tables S1 and S2). Table 1 lists the measured PBDE concentrations in the PUF and carpet that were used in the pseudo-steady-state modeling of the office. The dimensions of the office are listed in Table S6. Most parameter values were based on the literature; however, some, such as the dust removal and air exchange rates, were our best estimate. Since many parameter values contain considerable uncertainties, we performed a sensitivity analysis (see below).

Emission Estimation. First, PBDE inputs from outdoor air advection were calculated using a median outdoor air

TABLE 1. Concentrations of Selected PBDE Congeners in PUF and Carpet

	concentration($\text{ng} \cdot \text{g}^{-1}$)	
PBDE congener	PUF ^a	carpet ^b
BDE-28	0.34 (0.02)	32 (0.10)
BDE-47	49 (0.13)	912 (0.05)
BDE-66	0.53 (0.17)	31 (0.08)
BDE-100	16 (0.23)	166 (0.05)
BDE-99	90 (0.17)	839 (0.07)
BDE-154	7.4 (0.27)	78 (0.11)
BDE-153	9.8 (0.27)	83 (0.18)
total	173 (0.17)	2140 (0.07)

^a Average of two samples; the value in bracket indicates coefficient of variation (CV). ^b Average of two samples including carpet surface and underlay.

concentration of $0.0085 \text{ ng} \cdot \text{m}^{-3}$ (29) and a presumed air advection (exchange) rate. Second, inputs from the in-place sources of PBDEs in PUF furniture and carpet (if a source) were based on their measured PBDE concentrations and hence fugacities. The final source was the old and new computers and other electronic equipment (e.g., printer and wires) in the office. We considered the old and new computers under two distinct scenarios: the other electronic equipment (printer, wiring, etc.) remained constant in both scenarios as did the remainder of the office's content and other characteristics. Computer emissions were solved according to the mass balance of the air compartment in which the air concentrations were specified as that measured in the office (Table S7). This calculation assumed that the office air was at steady state with respect to emissions which is reasonable given the consistency of measured air concentrations before and after computer replacement (2). We also assumed that concentrations of PBDEs in the in-place sources did not change appreciably with time (hence the pseudo-steady-state formulation). Since the measured air concentrations were obtained using passive samplers, the concentrations were assumed to reflect gas-phase concentrations, from which bulk air concentrations were calculated (see Supporting Information).

Sensitivity Analysis. A sensitivity analysis was conducted on 35 parameters. The model was run by increasing and decreasing individual parameters by 10%. Sensitivity coefficients (SC) were calculated to evaluate the relative changes of model output Y by the changes of input parameters X_i (30):

$$\text{SC}(X_i) = (\Delta Y / Y)(X_i / \Delta X_i) \quad (1)$$

where ΔY and ΔX_i are the absolute change of output and input. Thus, the 10% increase and decrease in each input parameters yields $\Delta X_i / X_i = 0.2$.

Results and Discussion

Concentrations of PBDEs in the University Office. The concentrations of $\Sigma_7\text{BDE}$ were 173 and $2140 \text{ ng} \cdot \text{g}^{-1}$ in the PUF and carpet, respectively (Table 1). BDE-99 and BDE-47 comprised $\sim 80\%$ PBDEs in the PUF and carpet, which is similar to that in TV housings and printed circulated boards (31) and in indoor air concentrations (12, 32). This composition is very close to that of the technical Penta mixture (Figure S2).

Emissions from Computer. After the computer replacement, total PBDE air concentrations decreased by $\sim 80\%$. Model results suggest an 85% decrease in $\Sigma_7\text{BDE}$ emissions from 35 to $5.4 \text{ ng} \cdot \text{h}^{-1}$ before and after computer replacement, respectively (Table S7). These emission rates include those of the computer and a printer, electrical cables, or other

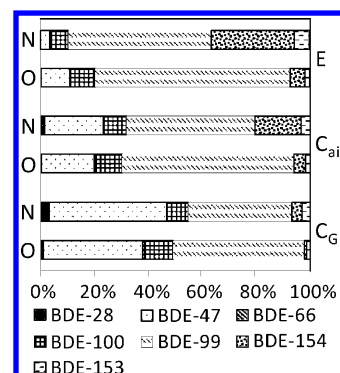


FIGURE 2. PBDE congener profiles of air concentration and emission before and after a computer replacement. N: with new computer; O: with old computer; C_G : gas phase air concentration; C_{air} : bulk air concentration; E: emission;

sources; however, only the computer was replaced. The greater decrease in emissions versus air concentrations could be due to measurement and modeling error or it could be attributable to contributions from the PUF furniture and carpet, as discussed below. The contribution to air concentrations (and the entire system) from air advection was minimal at $0.04 \text{ ng} \cdot \text{h}^{-1}$. The estimated emission from the old computer was comprised of 73% BDE-99 followed by 10, 9.5, and 5.6% of BDE-47, -100, and -154, respectively (Figure 2). Along with the magnitude of emissions, the congener profile changed with the new computer to 53, 3.7, 6.3, and 30% of BDE-99, -47, -100, and -154, respectively.

The estimated emission rates of $\Sigma_7\text{BDEs}$ from the new and old computers in the office of 5.4 and $35 \text{ ng} \cdot \text{h}^{-1}$ equals ~ 25 and $175 \text{ ng} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$ (m^2 of office floor), respectively. These rates are comparable with those measured by Kemmlein et al. (31) of $10.7 \text{ ng} \cdot \text{m}^{-2} \cdot \text{h}^{-1}$ and $21.2 \text{ ng} \cdot \text{unit}^{-1} \cdot \text{h}^{-1}$ $\Sigma_7\text{BDEs}$ from one TV housing (where m^2 refers to the surface area of the TV unit) and one printed circuit board, respectively. The emission rates are also similar to that of Jones-Otazo et al. (11) who estimated aggregate PBDE emissions (10 congeners) from the city of Toronto of $200\text{--}900 \text{ ng} \cdot \text{m}^{-2} \cdot \text{d}^{-1}$ (m^2 of planar surface area) for the early 2000s, which they obtained using a similar method as applied here, but applied at the citywide scale with the Multimedia Urban Model (MUM) (33). Our estimated emissions for BDE-47 and -99 of $0.03\text{--}0.25 \text{ mg} \cdot \text{yr}^{-1}$ from one office (this work) are lower than the $\sim 19\text{--}82 \text{ mg} \cdot \text{capita}^{-1} \cdot \text{yr}^{-1}$ obtained using MUM for Toronto (11) and $7 \text{ mg} \cdot \text{capita}^{-1} \cdot \text{yr}^{-1}$ for Sweden (34) which was obtained by means of a substance flow analysis in the late 1990s. Although the estimates obtained here are for only one computer in one circumstance, we get a sense of emissions from these goods, which is $\sim 8.5\text{--}55 \text{ kg} \cdot \text{yr}^{-1}$ (calculated with new and old computer scenarios, respectively) of $\Sigma_7\text{BDEs}$ from the 180 million computers in use in North America (35).

PBDE Fate in the Office. We illustrate the fate of PBDEs using the base case of the office with the old computer. For comparison, estimates from the new computer scenario are included in brackets.

The old computer was clearly the largest source to the office, with contributions from advection of outdoor air of 3 (2) orders of magnitude less (Figure 3). The PUF furniture acted as a sink for 20% (37%) of the emissions, with inputs mainly from particle deposition. The carpet was the greatest sink, accounting for the loss of $\sim 40\%$ (20%) of emissions (vacuuming was included in these scenarios). Within the office over 90% of total PBDE movement was attributable to the more highly brominated congeners in the particle phase: PBDEs moved from air to carpet and from air to PUF due to dust settling. Air advection to outdoors and intentional dust removal were the two main PBDE loss processes from the

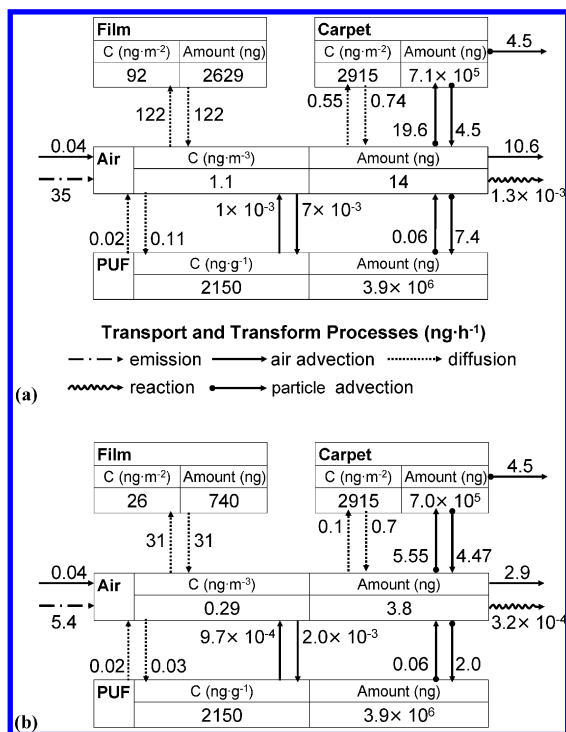


FIGURE 3. Concentrations, amounts, and movement of Σ_7 BDE indoors as estimated by the model: (a) old computer scenario; (b) new computer scenario.

office. These results support the supposition that the indoor environment is a source of PBDEs to outdoor concentrations and the observation of higher urban than rural air concentrations because of high urban building density (29). Since most of the PBDE congeners were in the particle phase, dust removal accounted for 30% (60%) of PBDE output from the office. Therefore, dust removal appears to be a good strategy to reduce PBDE exposure indoors. Indeed, if dust was not removed, then PBDE concentration in air rose from 1.07 (0.23) to 1.58 (0.83) ng·m⁻³. We note that dust removal indoors relocates PBDEs but does not ultimately remove PBDEs from the environment.

PUF bouncing and film–air exchange contributed negligibly to the fate of PBDEs in the office however PUF bouncing could influence air concentrations as discussed below. PBDE movement via air exchange due to bouncing is ~2 orders of magnitude less than that due to particle deposition and resuspension. The minimal net diffusive exchange between PUF–air for the new computer scenario and film–air for both scenarios suggests that these compartments are near equilibrium. However, the high emission rate from the old computer resulted in net diffusive movement from air to PUF, implying that the PUF furniture acted as a sink. Loss due to the reaction of PBDEs in gas-phase air with indoor hydroxyl radicals was negligible.

Expectedly, the fate of BDE-47 was governed more by gas- than particle-phase processes. For example, BDE-47 loss by dust removal was only 26% (54%) whereas it was 66% (67%) for BDE-153. The fate of BDE-47 and -153 was nonetheless governed by the particle phase (e.g., dust) due to the relatively low vapor pressure and high K_{OA} of this class of compounds.

Sensitivity Analysis. A sensitivity analysis using sensitivity coefficients (SCs) of BDE-28, -47, -99, and -153 was conducted to study the influence of individual parameters on estimates of the emission rate and air concentrations. Results indicate that temperature is most influential for emission rates and air concentrations, with its absolute value of SC 1 order of magnitude larger than that for other parameters. Temper-

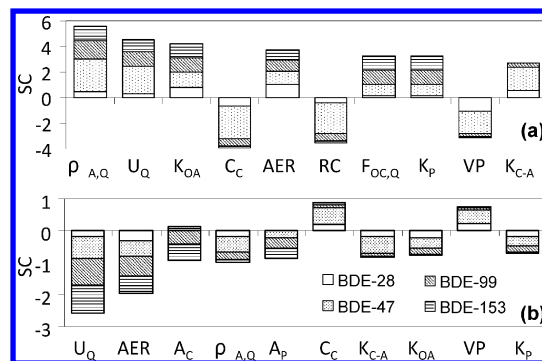


FIGURE 4. Sensitivity coefficients (SCs) to the model input parameters for (a) calculated emission rate and (b) bulk air concentration. Ten most influential parameters other than temperature are presented here. The parameters are arranged in descending order of the sum of SC values for four representative BDE congeners. These parameters are as follows: $\rho_{A,Q}$, particle concentration in air; U_Q , vertical deposition rate of particles in the air; K_{OA} , octanol–air partition coefficient; C_C , PBDE concentration in carpet; AER, air exchange rate; RC, resuspension coefficient; $F_{OC,Q}$, fraction of organic carbon of particles; K_P , particle–air partition coefficient; VP, vapor pressure; K_{C-A} , carpet–air partition coefficient; A_P , area of PUF.

ature is the most influential parameter because it directly affects vapor pressure and K_{OA} , and hence gas–particle partitioning and all related fate processes.

Figure 4 illustrates the SCs of the other 10 most influential parameters which include particle-related parameters, such as particle concentration in air and particle deposition rate. Of the 10 parameters investigated, some are easier to acquire and are less uncertain than others such as the dimensions of PUF furniture and carpet. However, other parameters such as the air exchange rate (AER) and rates of particle movement can be highly uncertain and could be temporally and spatially variable. Yet other parameters such as the carpet–air partition coefficient can and should be measured.

Several of the parameters are important because they can shift the sink/source behavior of the PUF and carpet compartments. If we assume that PBDE emissions from electronic equipment such as a computer or TV occur as a result of movement of the congeners from the impregnated polymers to air or settled dust according to the polymer–air or –dust fugacity gradient, then emission rates could rise if PUF and carpet act as significant sinks, in addition to other loss processes such as dust removal and air advection. Alternatively, emission rates could be independent of the room’s characteristics including sink/source behavior of the other compartments. In that case, air concentrations would respond to emissions only (31).

Effect of Bouncing on PUF Furniture. The indoor environment is highly sensitive to human activities. For instance, walking, sweeping, and vacuuming can increase particle resuspension rates and thus particle concentrations in air (21, 36). We focused on the effect of bouncing on PUF furniture on PBDE fate. We presumed that bouncing would increase the air-to-PUF mass transfer coefficient by decreasing the boundary layer thickness for diffusive exchange and by increasing the particle resuspension rate. As such, we varied these parameters by 1 order of magnitude and noted the change in air concentration and flux between air and PUF for BDE-47 and -153. We also varied the specified PBDE concentration of PUF (C_{PUF}) by a factor of 10 lower and 10 higher than the measured value.

At low C_{PUF} , PUF acted as a sink for BDE-47 and -153 for the base case and increased bouncing scenarios (Figure 5). Bouncing decreased the air concentrations of both congeners since this process increased the net air-to-PUF exchange.

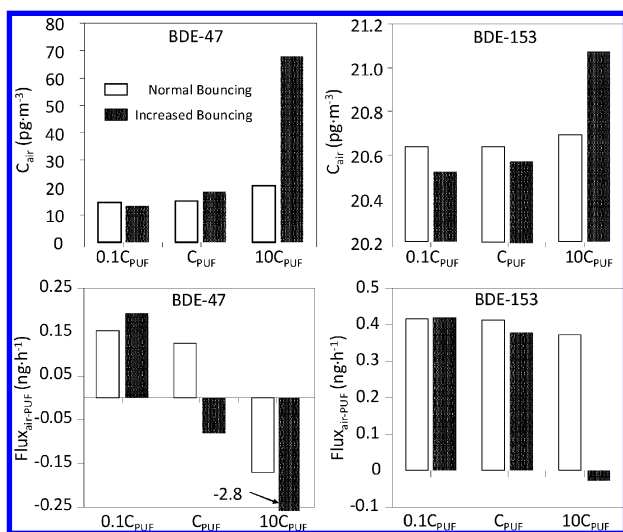


FIGURE 5. Effect of bouncing on PUF furniture on PBDE air concentration and air-PUF flux. Results of BDE-47 and BDE-153 are shown here to illustrate the effect of sink/source behavior as a function of physicochemical properties.

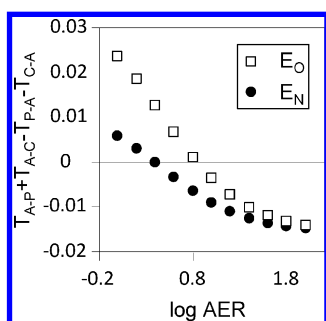


FIGURE 6. Effect of air exchange rate (AER, $\text{m}^3 \cdot \text{h}^{-1}$) on the sink/source behavior of BDE-28 for PUF and carpet. T ($\text{ng} \cdot \text{h}^{-1}$) is the intermedia exchange rate. Subscripts A, P, and C represent air, PUF, and carpet, respectively. The vertical axis represents net chemical exchange from air to PUF and from air to carpet. Positive value signifies that PUF and carpet together act as a sink and negative value means PUF and carpet together act as a source for the emission scenarios E_O , emission rate with the old computer in the room, and E_N , the emission rate with the new computer in the room. ($E_O > E_N$).

With the measured C_{PUF} , PUF acted as a sink for BDE-153 for both bouncing scenarios, but increased bouncing changed the PUF from sink to source of BDE-47. In this case, air concentrations increase from 0.05 to 0.06 $\text{ng} \cdot \text{m}^{-3}$ or 20%. At high C_{PUF} , PUF acted as a source for BDE-47 for both bouncing scenarios—air concentrations increased $\sim 200\%$. For high C_{PUF} , increased bouncing also changed the PUF from a sink to a source of BDE-153. Thus, not surprisingly, bouncing on high C_{PUF} has the greatest impact on air concentrations, particularly of BDE-47 and other lighter congeners.

Effect of Air Exchange Rate (AER). As air concentrations were very sensitive to AER, we explored this effect by changing AER by factors of 0.1 and 10 of the default value (0.75 h^{-1}) and noting net exchange rates of BDE-28 from air to PUF and from air to carpet. A positive net exchange rate signifies that PUF and carpet act as a sink while a negative rate signifies that PUF and carpet act as a source. The simulations were run with emissions from the old and new computers.

Increasing AER decreased air (and dust) concentrations, and consequently decreased the net deposition from air to PUF and from air to carpet (Figure 6). Thus, increasing AER shifted PUF and carpet from being net sinks to sources. In a comparison of the two emission scenarios, this shift in

sink/source behavior was more apparent at the higher emission rate (E_O). With the lower emission rate (E_N), the air concentration was lower, causing a lower net flux from air to PUF and from air to carpet: PUF and carpet were less likely to be sinks or source as AER increased. With the higher emission rate, a higher AER was required to change the PUF and carpet from sink to source. For heavier congeners the PUF and carpet tend to act as sinks because of the high chemical capacity (Z values) of these materials.

These modeling results suggest that the variability observed between Br content in products and materials such as PUF furniture and electronics, and PBDEs in air and/or dust (2, 14, 16, 17), is undoubtedly due to emission source(s), but it also could be mediated by the characteristics of the indoor environment such as temperature, AER, dust deposition and resuspension (which is related to human activity), and dust removal. It is not simple to assess a priori PBDE dynamics in a room based on its contents. Optimistically, the model results showed that PBDE air and dust concentrations were apt to be lowest when AER and dust removal rates were high and temperatures were low. Dusting and/or vacuuming are suggested to lower air and dust concentrations and hence exposure and bouncing on new furniture with high PBDE (or other additive SVOC flame retardant) concentrations could increase one's exposure (and wreck the furniture!).

Acknowledgments

Funding was provided by the Natural Sciences and Engineering Research Council (NSERC), support to Zhang from Department of Geography, University of Toronto and NSERC, and a studentship to Ibarra from the National Council of Science and Technology - Mexico (CONACYT).

Supporting Information Available

Detailed information on model structure, parametrization, mass balance equations, and additional figures and tables showing model results. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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ES802172A

Supporting Information

Multimedia Modeling of PBDE Emissions and Fate Indoors

*Xianming Zhang, Miriam L. Diamond,**

Catalina Ibarra, Stuart Harrad

Department of Geography, University of Toronto, Toronto, Ontario, M5S 3G3,

Canada

Division of Environmental Health and Risk Management, Public Health Building,

School of Geography, Earth, and Environmental Sciences, University of Birmingham,

Birmingham, B15 2TT, United Kingdom

* Corresponding author email: miriam.diamond@utoronto.ca; tel: +1 416 978 1586;

fax: +1 416 978 6729

TABLE S1. Equations Used to Calculate Fugacity Capacities (Z values, mol·m⁻³·Pa⁻¹) of Each Phase and Compartment in the Model

compartment	phase	equation	description and explanation
air	gas	$Z_A = 1/(RT)$	Fugacity capacity of air (gaseous). R (J mol ⁻¹ K ⁻¹) is the ideal gas constant and T (K) is the ambient temperature. ref: (2)
	particle	$Z_{Q,i} = K_{P,i} \cdot \rho_{Q,i} \cdot 10^{-9} \cdot Z_A$	Fugacity capacity of air particles of size fraction i (i=1 to 6). K _P (m ³ /μg) is the ratio of chemical concentration in particle (mol/μg) with chemical concentration in air (mol/m ³). $\log K_{P,i} = \log K_{OA} + \log (f_{OC,i}/0.74) - 11.91$, where K _{OA} is the octanol-air partition coefficient and f _{OC,i} is the organic carbon content of particle in size fraction i (3). Particles in the air were divided into 6 size fractions (0-1μm, 1-2.5μm, 2.5-10μm, 10-65μm, 65-150μm, 150-2000μm) as done by Bennett and Furtaw (2004) (4). Properties of particle of different size fractions were also given in ref. (4). ρ _{Q,i} is particle density (kg/m ³) of size fraction i. The value of 1500 kg/m ³ was used for particle of all size (4).
	bulk	$Z_{B,A} = Z_A + \sum_{i=1}^6 Z_{Q,i} \times \text{Frac}_{Ai}$	Fugacity capacity of bulk air. Since the volume of particles in the air is rather small compared with the bulk phase, the volume of gas phase is approximately equals to that of the bulk phase. Frac _{A,i} is the fraction of particles with size i in the air

Continued in next page

TABLE S1 Continued

compartment	phase	equation	description and explanation
PUF	PUF material	$Z_{\text{PUF}} = K_{\text{PUF-A}} \cdot Z_{\text{A}}$	<p>Fugacity capacity of PUF material. $K_{\text{PUF-A}}$ is the PUF-air partition coefficient.</p> $K_{\text{PUF-A}} = \left(\frac{C_{\text{PUF}}}{C_{\text{Air}}} \right)_{\text{equilibrium}} = \left(\frac{Z_{\text{PUF}} f_{\text{PUF}}}{Z_{\text{Air}} f_{\text{Air}}} \right)_{\text{equilibrium}}.$ <p>At equilibrium, $f_{\text{PUF}} = f_{\text{Air}}$</p> <p>then, $K_{\text{PUF-A}} = \frac{Z_{\text{PUF}}}{Z_{\text{Air}}}$, $Z_{\text{PUF}} = K_{\text{PUF-A}} \cdot Z_{\text{Air}}$</p>
	particle	$Z_{\text{Q},i} = K_{\text{P},i} \cdot \rho_{\text{Q},i} \cdot 10^{-9} \cdot Z_{\text{A}}$	Same as particle in the air compartment
	bulk	$Z_{\text{B,PUF}} = \frac{Z_{\text{PUF}} \cdot \delta_{\text{PUF}} + \sum_{i=1}^6 (Z_{\text{Q},i} \cdot \text{PL}_{\text{PUF},i} / \rho_{\text{Q},i})}{\delta_{\text{PUF}} + \sum_{i=1}^6 \text{PL}_{\text{PUF},i} / \rho_{\text{Q},i}}$	Fugacity capacity of bulk PUF. δ_{PUF} (m) is the thickness of PUF; $\text{PL}_{\text{PUF},i}$ (kg/m^2) is the mass of particles (kg) with size fraction i loaded on 1 m^2 of PUF.

Continued in next page

TABLE S1 *Continued*

compartment	phase	equation	description and explanation
	vinyl	$Z_V = K_{V-A} \cdot Z_A$	Derivation is similar to Z_{PUF} . The values of K_{V-A} were from extrapolation of the regression equation ($\log K_{V-A} = 5.2 - 0.68 \cdot \log VP$) in the study on partition of VOCs between vinyl and air (4,5). VP (Pa) is the vapor pressure of the chemical.
vinyl floor	particle	$Z_{Q,i} = K_{P,i} \cdot \rho_{Q,i} \cdot 10^{-9} \cdot Z_A$	Same as particle in the air compartment
	bulk	$Z_{B,V} = \frac{Z_V \cdot \delta_V + \sum_{i=1}^6 (Z_{Q,i} \cdot PL_{V,i} / \rho_{Q,i})}{\delta_V + PL_{V,i} / \rho_{Q,i}}$	Fugacity capacity of bulk vinyl floor. δ_V (m) is the thickness of vinyl; $PL_{V,i}$ (kg/m ²) is the mass of particles (kg) with size fraction i loaded on 1 m ² of vinyl floor.
	carpet material	$Z_C = K_{C-A} \cdot Z_A$	Derivation is similar to Z_{PUF} . The values of K_{C-A} were from extrapolation of the regression equation ($\log K_{C-A} = 3.82 - 0.62 \cdot \log VP$) in the study on partition of VOCs between carpet and air (4,6).
carpet	particle	$Z_{Q,i} = K_{P,i} \cdot \rho_{Q,i} \cdot 10^{-9} \cdot Z_A$	Same as particle in the air compartment
	bulk	$Z_{B,C} = \frac{Z_C \cdot \delta_C + \sum_{i=1}^6 (Z_{Q,i} \cdot PL_{C,i} / \rho_{Q,i})}{\delta_C + \sum_{i=1}^6 (PL_{C,i} / \rho_{Q,i})}$	Fugacity capacity of bulk carpet. δ_C (m) is the thickness of vinyl; $PL_{C,i}$ (kg/m ²) is the mass of particles (kg) with size fraction i loaded on 1 m ² of carpet.

Continued in next page

TABLE S1 Continued

compartment	phase	equation	description and explanation
film	bulk	$Z_F = 0.48K_{OA} \cdot f_{OC,F} \cdot \rho_F \cdot Z_A / 1000$	Fugacity capacity of organic layer of film. $0.48K_{OA}$ (L/kg) is the organic carbon/air partition coefficient. $f_{OC,F}$ (kg/kg) is the organic carbon fraction of film; ρ_F (kg/m ³) is the density of film; 1000 (L/m ³) is the conversion factor. The values were taken from Diamond et al. (2000) (7)

^a as there are no direct measurement for the partition coefficients for PBDEs between air and PUF cushion, currently for the model, we can only partition coefficients got from indirect approach based on some assumption. One approach assumes the partition behavior of PUF material is the same as octanol. Then, $Z_P = (1 - fr_{P-A})K_{OA}Z_A + fr_{P-A}Z_A \approx (1 - fr_{P-A})K_{OA}Z_A$, $K_{P-A} = Z_P/Z_A = (1 - fr_{P-A})K_{OA} = 0.03K_{OA}$. Another approach bases on extrapolation of the regression equation ($\log K_{P-A} = -0.93 \cdot \log VP + 5.03$) derived from study of partition of VOCs between PUF and air (8). It assumes the relationship between K_{P-A} and VP does not change when performing extrapolation. Values from the two methods are within one order of magnitude difference. Great uncertainties would come from these assumptions for sure. However, for illustrative purpose, the geometric mean of the values from the two methods was used as default value for the model calculation, i.e. $\log K_{P-A} = 0.5[\log(0.03K_{OA}) + (-0.93 \cdot \log VP + 5.03)]$.

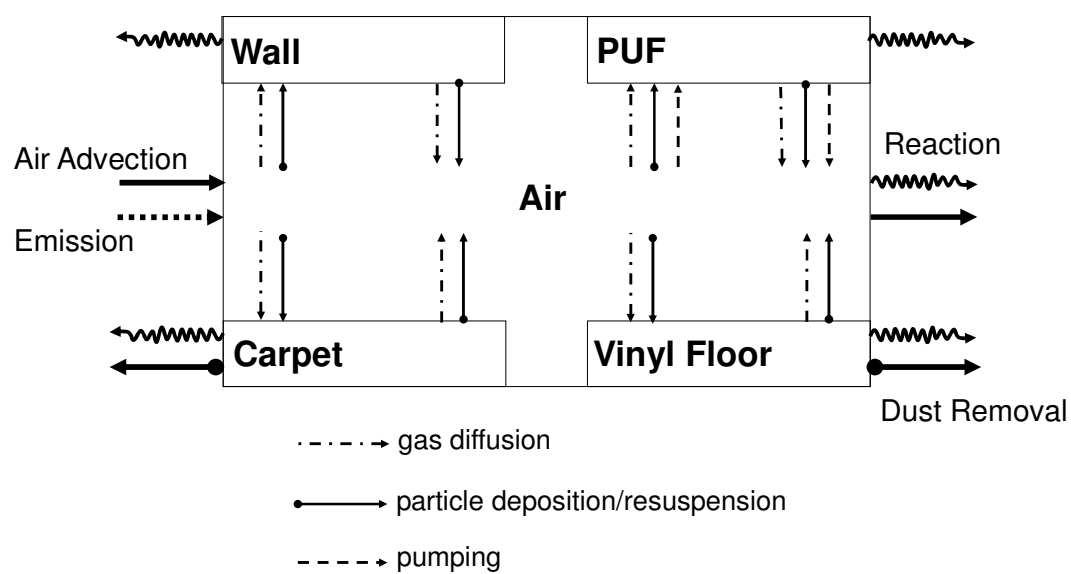


FIGURE S1. Conceptual model for the fate processes of PBDEs in the indoor environment

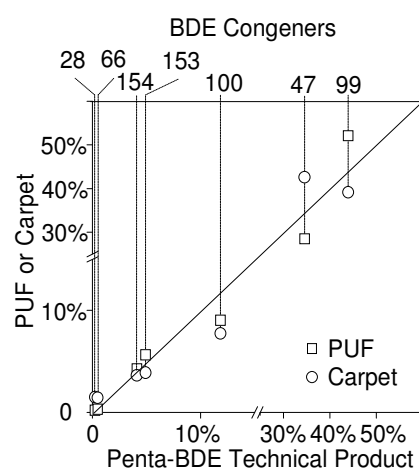


FIGURE S2. Comparison the relative abundance of studied PBDE congeners in Penta technical product (*I*) with those in PUF and carpet measured in this study.

TABLE S2. D values (mol·h⁻¹·Pa⁻¹) associated with PBDE fate processes in the multimedia indoor environmental model

compartment	process	equation	description and explanation
air	gas diffusive transport from air to PUF	$D_{G,A-P} = 1 / \left(\frac{\delta_{bl,P}}{B_A A_{A-P} Z_A} + \frac{h_P \ln 2}{B_A v_{A,P}^{4/3} A_{A-P} Z_A} \right)$	$\delta_{bl,P}$ (m) is boundary layer thickness between air and PUF; B_A (m ² /h) is the molecular diffusivity in air ^a ; A_{A-P} (m ²) is the area between air and PUF; h_P (m) is the thickness of PUF and $h_P \ln 2$ is the average diffusivity length in PUF; $v_{A,P}$ is the volume fraction of air in PUF.
	particle deposition from air to PUF	$D_{Q,A-P} = \sum_{i=1}^6 U_{P,i} A_{A-P} fr_{A,Q,i} Z_{Q,i}$	$U_{P,i}$ (m/h) is the particle deposition rate onto PUF ^b ; $fr_{A,Q,i}$ is the volume fraction of particle in air (4); subscript i indicates the particle size fractions.
	advective transport from air to PUF through bouncing	$D_{adv,A-P} = G_{A-P} Z_A = CR \cdot A_{A-P} \cdot h_P \cdot v_C \cdot Z_A$	CR is the average compression ratio of PUF; v_C (h ⁻¹) is the compress frequency
	gas diffusive transport from air to vinyl	$D_{G,A-V} = 1 / \left(\frac{\delta_{bl,V}}{B_A A_{A-V} Z_A} + \frac{1}{k_F A_{A-V} Z_F} \right)$	$\delta_{bl,V}$ (m) is boundary layer thickness between air and vinyl; A_{A-V} (m ²) is the area between air and vinyl; k_F (m/h) is the mass transfer coefficient in organic film. $\log k_F = 0.704 \log K_{OW} - \log K_{AW} - 11.2$ (9)
	particle deposition from air to vinyl	$D_{Q,A-V} = \sum_{i=1}^6 U_{V,i} A_{A-V} fr_{A,Q,i} Z_{Q,i}$	$U_{V,i}$ (m/h) is the particle deposition rate onto vinyl ^b

Continued in next page

TABLE S2 Continued

compartment	process	equation	description and explanation
air	gas diffusive transport from air to carpet	$D_{G,A-C} = 1 / \left(\frac{\delta_{bl,C}}{B_A A_{A-C} Z_A} + \frac{h_C \ln 2}{B_A V_{A,C}^{4/3} A_{A-C} Z_A} \right)$	$\delta_{bl,C}$ (m) is boundary layer thickness between air and carpet; A_{A-C} (m ²) is the area between air and carpet; h_C (m) is the thickness of carpet
	particle deposition from air to carpet	$D_{Q,A-C} = \sum_{i=1}^6 U_{C,i} A_{A-C} fr_{A,Q,i} Z_{Q,i}$	$U_{C,i}$ (m/h) is the particle deposition rate onto carpet ^b
	gas diffusive transport from air to film	$D_{G,A-F} = 1 / \left(\frac{\delta_{bl,F}}{B_A A_{A-F} Z_A} + \frac{1}{k_F A_{A-F} Z_F} \right)$	$\delta_{bl,v}$ (m) is boundary layer thickness between air and film
	particle deposition from air to film	$D_{Q,A-F} = \sum_{i=1}^6 U_{F,i} A_{A-F} fr_{A,Q,i} Z_{Q,i}$	$U_{F,i}$ (m/h) is the particle deposition rate onto film ^b
	air advection from indoor to outdoor	$D_{adv,A} = G_A Z_A = AER \cdot Z_A$	AER (m ³ ·h ⁻¹) is the air exchange rate; V_A is the volume of air.

Continued in next page

TABLE S2 Continued

compartment	process	equation	description and explanation
air	chemical reaction in the air	$D_{\text{rxn},A} = k_{\text{rxn}} V_A Z_A$	k_{rxn} (h^{-1}) is the pseudo first-order reaction rate constant for reaction of PBDE and OH radical. Since the average indoor OH concentration is 1.1×10^5 molecules/ cm^3 while the outdoor OH concentration is 1.5×10^6 molecules/ cm^3 (4), it is necessary to adjust the rate constant to the indoor environment. Since $k_{\text{rxn}} = k_{\text{OH}}[\text{OH}] = \ln 2/t_{1/2}$, then $k_{\text{rxn, indoor}} = (\ln 2/t_{1/2})([\text{OH}]_{\text{indoor}}/[\text{OH}]_{\text{outdoor}})$
	gas diffusive transport from PUF to air	$D_{G,P-A} = D_{G,A-P}$	conductivity of diffusive transport
PUF	particle resuspension from PUF to air	$D_{Q,P-A} = 0.1 \times D_{Q,A-P} \times \frac{v_C}{v_{C,0}}$	assuming 10% particles trapped by and on PUF are resuspended; $v_{C,0}$ (h^{-1}) is the base case compression frequency; v_C (h^{-1}) is the compression frequency.
	advective transport from PUF to air through bouncing	$D_{\text{adv},P-A} = G_{P-A} Z_P = \text{CR} \cdot A_{P-A} \cdot h_P \cdot v_C \cdot Z_P$	CR is the average compression ratio of PUF

Continued in next page

TABLE S2 Continued

compartment	process	equation	description and explanation
vinyl floor	gas diffusive transport from vinyl to air	$D_{G,V-A} = D_{G,A-V}$	$RC_i (h^{-1})$ is particle resuspension coefficient
	particle resuspension from vinyl to air	$D_{Q,V-A} = \sum_{i=1}^6 (RC_i \cdot A_{A-V} \cdot PL_{V,i} \cdot Z_{Q,i} / \rho_{P,i})$	
	advective transport through dust removal	$D_{adv,V} = \sum_{i=1}^6 PRR_{V,i} \cdot Z_{Q,i} / \rho_{Q,i}$	PRR_V (kg/h) is the particle removal rate from vinyl floor. The default values for this model were assigned by assuming 5% of the dust is removed once a month.
carpet	gas diffusive transport from carpet to air	$D_{G,C-A} = D_{G,A-C}$	as defined and discussed above
	particle resuspension from carpet to air	$D_{Q,V-A} = \sum_{i=1}^6 (RC_i \cdot A_{A-V} \cdot PL_{V,i} \cdot Z_{Q,i} / \rho_{P,i})$	

Continued in next page

TABLE S2 *Continued*

compartment	process	equation	description and explanation
carpet	advective transport through removal	dust $D_{adv,C} = \sum_{i=1}^6 PRR_{C,i} \cdot Z_{Q,i} / \rho_{Q,i}$	PRR_C (kg/h) is the particle removal rate from carpet. Assuming particle loading in carpet is at steady state, PRR_C the difference of particle deposition rate and resuspension rate
film	gas diffusive transport from film to air	$D_{G,F-A} = D_{G,A-F}$	as defined and discussed above
	particle resuspension from film to air	-	negligible compared to diffusive transport

Continued in next page

TABLE S2 Continued

^a molecular diffusivity at 1 atm is estimated using the equation: $B_a = \frac{10^{-3} \cdot T^{1.75} \cdot \sqrt{1/m_{\text{air}} + 1/m}}{(V_{\text{air}}^{1/3} + V^{1/3})^2}$ where T(K) is temperature; m_{air} (28.97g mol⁻¹)

is the molecular mass of air; m(g mol⁻¹) is the molecular mass of the chemical of interest; V_{air} (~20.1cm³mol⁻¹) is the molar volume of gases in air; V(cm³mol⁻¹) is the molar volume of the chemical of interest (10,11).

^b Particle deposition velocity is acquired from Ref (4) and (12). The particle deposition velocities and other particle properties are shown in TABLE S3.

TABLE S3. Properties of Particles in Different Size Fractions

particle size fraction (μm) ^a	fraction of organic carbon ^a	vertical downward deposition velocity ^a ($\text{m}\cdot\text{h}^{-1}$)	horizontal deposition velocity ^b ($\text{m}\cdot\text{h}^{-1}$)	vertical upward deposition velocity ^b ($\text{m}\cdot\text{h}^{-1}$)	resuspension coefficient ^a h^{-1}
0-1	0.35	0.3	3.2×10^{-3}	3.6×10^{-5}	1.1×10^{-7}
1-2.5	0.30	1.2	3.2×10^{-4}	negligible ^c	4.6×10^{-7}
2.5-10	0.30	2.7	3.2×10^{-4}	negligible	6.8×10^{-6}
10-65	0.20	2.7×10^2	1.8×10^{-5}	negligible	2.9×10^{-5}
65-150	0.15	2.7×10^3	3.6×10^{-6}	negligible	4.2×10^{-6}
150-2000	0.05	2.7×10^4	3.6×10^{-8}	negligible	4.2×10^{-6}

^a Ref: Bennett and Furtaw (2004) (4). ^b Ref: Lai and Nazaroff (2000) (12). ^c $<10^{-8}$

TABLE S4. Mass Balance Equations for PBDEs in the Indoor Environment

compartment	equation	description and explanation
air	$\frac{dM_A}{dt} = E + G_A C_O + D_{P-A} f_P + D_{V-A} f_V + D_{C-A} f_C + D_{F-A} f_F - D_A f_A$	<p>M_A (mol) is the amount of chemical in air; t (h) is time; E (mol/h) is emission rate from pure source; G_A (m^3/h) is the flow rate of air from outdoor to indoor. Assuming the only air exchange pathway is between indoor and outdoor, then $G_A = AER$, where AER ($m^3 \cdot h^{-1}$) is the air exchange rate and V_A (m^3) is the volume of indoor air; C_O (mol/m^3) is the PBDE outdoor concentration (13); $D_{P-A} = D_{G,P-A} + D_{Q,P-A} + D_{adv,P-A}$; $D_{V-A} = D_{G,V-A} + D_{Q,V-A}$; $D_{C-A} = D_{G,C-A} + D_{Q,C-A}$; $D_{F-A} = D_{G,F-A} + D_{Q,F-A}$; $D_A = D_{G,A-P} + D_{Q,A-P} + D_{G,A-V} + D_{Q,A-V} + D_{G,A-C} + D_{Q,A-C} + D_{G,A-F} + D_{Q,A-F} + D_{adv,A} + D_{rxn,A}$; f (Pa) is fugacity and the subscript represent the compartments.</p>
PUF	$\frac{dM_P}{dt} = D_{A-P} f_A - D_P f_P$	<p>M_P (mol) is the amount of chemical in PUF; $D_{A-P} = D_{G,A-P} + D_{Q,A-P} + D_{adv,A-P}$; $D_P = D_{G,P-A} + D_{Q,P-A} + D_{adv,P-A}$</p>
vinyl floor	$\frac{dM_V}{dt} = D_{A-V} f_A - D_V f_V$	<p>M_V (mol) is the amount of chemical in vinyl; $D_{A-V} = D_{G,A-V} + D_{Q,A-V}$; $D_V = D_{G,V-A} + D_{Q,V-A} + D_{adv,V}$</p>
carpet	$\frac{dM_C}{dt} = D_{A-C} f_A - D_C f_C$	<p>M_C (mol) is the amount of chemical in carpet; $D_{A-C} = D_{G,A-C} + D_{Q,A-C}$; $D_C = D_{G,C-A} + D_{Q,C-A} + D_{adv,C}$</p>
film	$\frac{dM_F}{dt} = D_{A-F} f_A - D_F f_F$	<p>M_C (mol) is the amount of chemical in carpet; $D_{A-F} = D_{G,A-F} + D_{Q,A-F}$; $D_C = D_{G,F-A} + D_{Q,F-A}$</p>

TABLE S5. Equations Related to PUF Modeling**mass balance equation**

$$dM_P/dt = (D_{G,A-P} + D_{Q,A-P} + D_{adv,A-P})f_A - (D_{G,P-A} + D_{Q,P-A} + D_{adv,P-A})f_P$$

parameter equation**description****D Values (mol·Pa⁻¹· h⁻¹)**

$D_{G,A-P}$	$D_{G,A-P} = 1 / \left(\frac{\delta_{bl,P}}{B_A A_{A-P} Z_A} + \frac{h_p \ln 2}{B_A v_{A,P}^{4/3} A_{A-P} Z_A} \right)$	dry gaseous deposition from air to PUF
$D_{Q,A-P}$	$D_{Q,A-P} = \sum_{i=1}^6 U_{P,i} A_{A-P} fr_{A,Q,i} Z_{Q,i}^a$	dry particle deposition from air to PUF
$D_{adv,A-P}$	$D_{adv,A-P} = CR \cdot A_{A-P} \cdot h_p \cdot v_C \cdot Z_A$	advective transport from air to PUF through bouncing
$D_{G,P-A}$	$D_{G,P-A} = D_{Q,A-P}$	volatization from PUF to air
$D_{Q,P-A}$	$D_{Q,P-A} = \sum_{i=1}^6 (RC_i \cdot A_{A-P} \cdot PL_{P,i} \cdot Z_{Q,i} / \rho_{P,i})$	particle resuspension from PUF to air
$D_{adv,P-A}$	$D_{adv,P-A} = CR \cdot A_{A-P} \cdot h_p \cdot v_C \cdot Z_P$	advective transport from PUF to air through bouncing

Z Values (mol·Pa⁻¹· m³)

Z_A	$Z_A = 1/(RT)$	air (gaseous)
$Z_{Q,i}$	$Z_{Q,i} = K_{P,i} \cdot \rho_{Q,i} \cdot 10^{-9} \cdot Z_A$	particle

parameter description

M_P	amount of PBDE in PUF (mol)
t	time (h)
f_A, f_P	fugacity of air and PUF
$\delta_{bl,P}$	boundary layer thickness between air and PUF (m)
B_A	molecular diffusivity in air (m ² /h)
A_{A-P}	area between air and PUF (m ²)
$h_p \cdot \ln 2$	average diffusivity length in PUF (m)
$v_{A,P}$	volume fraction of air in PUF
U_P	particle deposition velocity onto PUF (m/h)
$fr_{A,Q}$	volume fraction of particle in air
CR	average compression ratio of PUF
v_C	compression frequency (h ⁻¹)
RC	particle resuspension coefficient (h ⁻¹)
$PL_{P,i}$	particle loading on PUF (kg/m ²)
$\rho_{P,i}$	particle density (kg/m ³)
K_P	partition coefficient between particle and air (m ³ /μg)

^a subscript i represent particles with size fraction i

TABLE S6. Characteristics of the university office as input to the model

parameter	value
office dimension, area (m ²)×height (m)	4.84×2.70
PUF, area (m ²)×thickness (m)	1.66×0.05
carpet, area (m ²)×thickness (m)	4.84×0.005
wallboard film, area (m ²)×thickness (m)	28.6×(1×10 ⁻⁸) ^a
PUF density (kg·m ⁻³)	22
carpet density (kg· m ⁻²)	2.84
film density (kg·m ⁻³)	1.2 ^b
air exchange rate (h ⁻¹)	0.75 ^b
dust removal rate (g·h ⁻¹)	0.01 ^c

^a Reference for film thickness: (7). ^b Ref (4). ^c artificially assigned by assuming 15% of the dust on carpet is removed in a month through vacuuming.

TABLE S7. PBDE Air Concentrations and Estimated Emission Rates Before and After Computer Replacement

PBDE congener	gaseous air phase concentration ^a		bulk air concentration ^b		PBDE emission rate ^c	
	(pg·m ⁻³)		(pg·m ⁻³)		(ng·h ⁻¹)	
	old computer	new computer	old computer	new computer	old computer	new computer
BDE-28	4.3	2.5	4.5	2.6	0.04	0.01
BDE-47	153.7	37.8	208.3	51.2	3.63	0.20
BDE-66	3.8	n.d. ^d	4.5	-	0.07	0.01
BDE-100	44.2	7.2	104.0	20.2	3.33	0.34
BDE-99	203.3	33.2	680.9	111.0	25.29	2.84
BDE-154	4.3	3.7	46.9	40.4	1.95	1.64
BDE-153	4.9	2.4	15.9	7.9	0.62	0.30
Σ ₇ BDE	418.0	86.8	1065.0	233.3	34.9	5.4

^a PBDE air concentrations before and after computer replacement in the office come from the work by Hazrati and Harrad (2006) (14). The air was sampled through passive samplers and it is assumed that no particles were sampled. The measured concentrations were treated as gaseous phase air concentrations. ^b bulk air concentrations were calculated by adding the PBDE concentrations of gaseous phase and particulate phase. Particulate PBDE concentrations were derived from gaseous phase concentrations and particle-air partitioning coefficient. The detailed calculation method is listed below. ^c the emission rate here refers to that from pure sources such as computer and printer. ^d no detection.

TABLE S8. Physicochemical Properties of the Studied PBDE Congeners

PBDE congener	molar mass (g/mol)	melting point ^a (°C)	vapor pressure ^{a, b} (Pa)	K _{OA} ^c	t _{1/2, air} ^d (h)
BDE-28	406.9	64.3	$\log p_L^0(T) = 11.30 - 4160/T$	$\log K_{OA}(T) = -3.54 + 3889/T$	181.7
BDE-47	485.8	84.5	$\log p_L^0(T) = 12.85 - 4940/T$	$\log K_{OA}(T) = -6.47 + 5068/T$	255.9
BDE-66	485.8	106.0	$\log p_L^0(T) = 13.23 - 5109/T$	$\log K_{OA}(T) = -7.88 + 5576/T$	253.9
BDE-100	564.7	100.5	$\log p_L^0(T) = 13.37 - 5339/T$	$\log K_{OA}(T) = -7.18 + 5459/T$	356.5
BDE-99	564.7	92.5	$\log p_L^0(T) = 14.13 - 5268/T$	$\log K_{OA}(T) = -4.64 + 4757/T$	466.5
BDE-154	643.6	131.8	$\log p_L^0(T) = 14.38 - 5900/T$	$\log K_{OA}(T) = -4.62 + 4931/T$	693.2
BDE-153	643.6	161.5	$\log p_L^0(T) = 13.66 - 5763/T$	$\log K_{OA}(T) = -5.39 + 5131/T$	1107.9

^a Ref: Tittlemier et al. (2002) (15). ^b subcooled liquid vapor pressure is used because the environment temperature is less than the melting point of the PBDE congeners. ^c Ref: Harner and Shoeib (2002) (16). ^d values from USEPA software EPOWIN v1.92. These values were based on outdoor environment with an average OH concentration of 1.5×10^6 molecules/cm³. In the indoor model, the values were converted using the method listed in TABLE S2. For temperature correction, uniform activation energy of 10 kJ/mol was adopted (17). Then,

$$t_{1/2}(T) = t_{1/2}(298K) \cdot 10^{\frac{10^4}{2.303R} \left(\frac{1}{T} - \frac{1}{298} \right)}$$

Calculation Bulk Air Concentration from Gas Phase Air Concentration

The measured air concentration using passive sampling is assumed to be the gaseous phase concentration. To reflect the total PBDEs in the air, the concentration in the bulk air were calculated using the gaseous phase concentration. The bulk air concentration is the sum of gaseous phase concentration (C_G) and particulate phase concentration ($C_{P,i}$), where subscript i indicates different particle size fractions:

$$C_A \text{ (ng/m}^3\text{)} = C_G \text{ (ng/m}^3\text{)} + \sum C_{P,i} \text{ (ng/m}^3\text{)}$$

The particulate phase concentration C_P can be derived from gaseous phase concentration by using particle-air partition coefficient ($K_{P,i}$), particle mass concentration in air ($\rho_{A,Q,i}$):

$$C_{P,i} \text{ (ng/m}^3\text{)} = C_G \text{ (ng/m}^3\text{)} \times K_{P,i} \text{ (m}^3/\mu\text{g)} \times \rho_{A,Q,i} \text{ (\mu g/m}^3\text{)}$$

Particle-air partition coefficient ($K_{P,i}$) can be derived from:

$$\log K_{P,i} = \log K_{OA} + \log (f_{OC,i}/0.74) - 11.91$$

where K_{OA} is the octanol-air partition coefficient and $f_{OC,i}$ is the organic carbon content of particle i (3).

Particle mass concentration ($\rho_{A,Q,i}$) can be derived from particle volume fraction ($vf_{Q,i}$) and particle density ($\rho_{Q,i}$):

$$\rho_{A,Q,i} \text{ (\mu g/m}^3\text{)} = 10^9 \text{ (\mu g/kg)} \times \rho_{Q,i} \text{ (kg/m}^3\text{)} \times vf_{Q,i}$$

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