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Effects of Room Airflow on Accurate Determination of PUF-PAS Sampling Rates in the Indoor Environment

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Abstract

Accurate and precise interpretation of concentrations from polyurethane passive samplers (PUF-PAS) is important as more studies show elevated concentrations of PCBs and other semivolatile air toxics in indoor air of schools and homes. If sufficiently reliable, these samplers may be used to identify local sources and human health risks. Here we report indoor air sampling rates (R_s) for polychlorinated biphenyl congeners (PCBs) predicted for frequently used double-dome and a half-dome PUF-PAS designs. Both our experimentally calibrated ($1.10 \pm 0.23 \text{ m}^3 \text{ d}^{-1}$) and modeled ($1.08 \pm 0.04 \text{ m}^3 \text{ d}^{-1}$) R_s for the double-dome samplers compare well with literature reports for similar rooms. We determined that variability of wind speeds throughout the room significantly ($P < 0.001$) effected uptake rate. We examined this effect using computational fluid dynamic modeling and 3-D sonic anemometer measurements and found the airflow dynamics to have a significant but small impact on the precision of calculated airborne concentrations. The PUF-PAS concentration measurements were within 27% and 10% of the active sampling concentration measurements for the double-dome and half-dome designs, respectively. While the half-dome samplers produced more consistent concentration measurements, we find both designs to perform well indoors.

Environmental Significance

The presence of airborne polychlorinated biphenyls (PCBs) in residential homes and schools is compelling justification for the development of inexpensive, non-intrusive, and accurate sampling methods. The polyurethane equipped passive air sampler (PUF-PAS) presents a powerful opportunity to more easily identify and quantify airborne PCBs in these environments. Challenges in using PUF-PAS indoors include determination of an accurate sampling rate (R_s) and accounting for variable air flow within a room. Here we present a practical and accurate method for determining an indoor R_s , as a function of wind speed in a room. We found both double-dome and half-dome PUF-PAS designs to provide accurate measures of airborne concentrations of PCBs using modeled sampling rates.

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Conflicts of Interest

The authors declare no competing financial interest.

†Supporting Information

Electronic supplementary information (ESI) available: Details of the methods and additional figures.

Introduction

Polyurethane equipped passive air samplers (PUF-PAS) are frequently used to examine semivolatile organic compounds (SVOC) in the atmosphere.^{1–16} They are used to directly measure urban air concentrations^{1, 6–16}, track atmospheric fate and transport^{2–4, 17–19}, characterize atmospheric sources,^{1, 3, 5, 7, 10, 14} and assess human exposure^{1, 20–23} in the outdoor environment, but have yet to be widely adopted for use in the indoor environment. With the growing concern of SVOCs in residential homes and schools, validating PUF-PAS methods in the indoor environment is of critical importance.^{20, 24–27} PCBs in particular are becoming an increasingly important issue due to their widespread presence in schools.^{20, 21, 27–32} Recent research has shown that inhalation exposure to PCBs may be equal to or greater than dietary exposure for children.^{20, 21} The growing concern about elevated concentrations of airborne PCBs in schools is a compelling justification for the development of inexpensive, non-intrusive, and accurate sampling methods. PUF-PAS methods are an attractive approach for this because, contrarily to the energy intensive nature of active sampling methods, PUF-PAS methods are inexpensive and require minimal labor. They also allow for simultaneous sampling in separate areas of the building and provided time-average airborne concentrations useful for estimating exposures.

The reason PUF-PAS methods have not been more widely utilized in the indoor environment is the uncertainty in the determination of sampling rates (R_s).^{20, 24, 33, 34} The standard method for determining sampling rates for PUF-PAS samplers relies on the loss of depuration compounds.^{1, 3, 4, 7, 12–14, 17, 35} Unfortunately, these compounds are inappropriate for indoor use due to the human exposure potential. In the absence of depuration compounds, a constant value ($4 \text{ m}^3 \text{ d}^{-1}$ outdoors or $0.8 \text{ m}^3 \text{ d}^{-1}$ indoors for PCBs, for example) is often assumed for the R_s .^{2, 5, 8, 10, 13, 20, 22, 23, 25, 26, 36–38} While this approach has been shown to provide a reasonable estimate, it fails to account for all environmental variability. We have previously shown that sampling rates of gas-phase PCB congeners for a PUF-PAS sample in the outdoor environment is a predictable diffusive mass transfer process. Using widely available meteorological measurements and chemical characteristics, we developed a predictive model for R_s and sampling volumes.^{39–41} In outdoor environments, the primary meteorological driver for R_s is wind speed ($R^2 = 0.91$).⁴⁰

The central goal of this study was to determine an accurate indoor PUF-PAS R_s for gas-phase PCBs and describe how the airflow in a room effects the interpretation of PUF-PAS results. PCBs are an ideal chemical for this type of work because of the extensive

characterization that has already been done for these compounds. We hypothesized the same predictive model framework used in outdoors environment would apply to indoor environments, if an accurate estimate of wind speed were available. We further hypothesized that simple parameterization of a room's airflow can lead to more consistent and reliable PUF-PAS use in the indoor environment. The specific objectives of this study were to 1) Determine an accurate PUF-PAS sampling rate in the indoor environment; 2) Evaluate and modify an outdoor sampling rate model for PCBs in the indoor environment; 3) Examine the effects of room airflow dynamics on sampling rates; and 4) Develop recommendations for standard operating procedures for using PUF-PAS samplers indoors.

Methods and Materials

Study Design

Our study was performed with two passive sampler designs and a low-volume active sampler. The double-dome (DB-dome) PUF-PAS sampler design (with a 24 cm top bowl and 19.5 cm bottom bowl) is based on a commonly used PUF-PAS design.^{6, 12, 14, 15, 35, 42, 43} The half-dome (HF-dome) PUF-PAS design consists of only the top bowl of the DB-dome design with the PUF disk suspended below it.^{44, 45} The PUF disk used in the passive air samplers were purchased from Tisch Environmental. The PUF tubes used in the low-volume air sampler were purchased from SKC (Eighty Four, PA).

The uptake of gas-phase PCBs, or more generally semi-volatile organic compounds (SVOCs), on a PUF disk is a function of a diffusive sampling rate and the concentration gradient between the air and PUF sample,

$$\frac{dM_{PUF}}{dt} = R_s \left(C_{air} - \frac{C_{PUF}}{K_{PUF}} \right) \quad (1)$$

where M_{PUF} is the mass of the target compound measured on the PUF sample, C_{air} is the concentration in the air (ng m^{-3}), C_{PUF} is the concentration on the PUF (ng m^{-3}), and K_{PUF} is the PUF-air partition coefficient.^{14, 39, 41, 42, 46–48} The sampling rate is a product of an air-side resistance dominated mass transfer coefficient (k_v , m s^{-1}) and the surface area of the PUF sample (A_s). Previously we calibrated the predictive model for R_s using the mathematical model based on laminar flow along a flat plate to determine the mass transfer coefficient,

$$\frac{k_v l}{D} = \gamma \left(\frac{V_i l}{\nu} \right)^{1/2} \left(\frac{\nu}{D} \right)^{1/3} \quad (2)$$

where γ is a dimensionless empirically calibrated constant, D is the molecular diffusivity for each compound ($\text{m}^2 \text{s}^{-1}$), V_i is the wind speed inside the PAS chamber (m s^{-1}), ν is the kinematic viscosity of the air ($\text{m}^2 \text{s}^{-1}$), and l is the PUF diameter (m).^{39–41} If the kinetics

were truly described by laminar flow along a flat plate, γ would equal 0.646.⁴⁹ In the outdoor environment we found it to be about 0.3.⁴⁰ In the indoor environment we suspect the kinetics to be much closer to laminar flow than the outdoor environment and therefore chose to use 0.646. Our experiments were designed to test this assumption in a typical indoor environment. The sampling rate is calculated from the mass transfer coefficient and the surface area of the PUF disk (365 cm²).

$$R_s = k_v A_s \quad (3)$$

Previously, we applied an empirical calibration based on lab measurements presented by Tuduri et al (2006) to convert air velocity from outside to inside the DB-dome sampler.⁴³ To model the HF-dome design, this relation was omitted in the calculation of R_s .⁴⁰

The study was designed to examine primarily gas-phase compounds, i.e. PCBs. Our modeling framework has been designed and developed around gas-phase compounds and thus does not account for particle-phase compounds. Previous work suggests that particle-phase compounds are sampled at similar rates to gas-phase compounds, suggesting the viability of PUF-PAS methods in this type of analysis.^{37, 50} However, the current study assumes the effect of particle-associated PCBs to be negligible.

This study was conducted in two phases in an occupied office (1131 SC) at the Seaman's Center for the Engineering Arts and Sciences at the University of Iowa. The purpose of Phase-1 was to measure R_s from chemical uptake on a series of passive samplers. We then compared the empirical R_s with the predictive model and literature. Phase-1 consisted of 18 double-dome PUF-PAS samples deployed at the same time. We collected a set of triplicates after each week over 6 consecutive weeks (Figure S5).

The purpose of the second phase of the study was to analyze the spatial variability of R_s throughout the room. Phase-2 consisted of twelve double-dome PUF-PAS samples and twelve half-dome PUF-PAS samples deployed consecutively in triplicate. We deployed and collected a set of double-dome and a set of half-dome triplicates each week over 4 consecutive weeks. Each deployment was in a different location of the room (Figure S7). Wind speed and temperature, were measured with a 3-D sonic anemometer at each location in the room for week long intervals during the study period. The 3-D sonic anemometer collected the three wind vector components and the temperature at a one hertz frequency.

Throughout both phases of the study, we operated a low-volume active air sampler equipped with polyurethane foam plug (Universal PCXR4 Sample Pump from SKC, Eighty Four, PA) at a flow rate 5 L min⁻¹ oriented upward at a 45° angle. Active samples were taken at approximately 50–65 hour intervals to ensure continuous coverage. Active samples were exchanged 3 times a week on Mondays at 8 a.m., Wednesdays at 12 p.m., and Fridays at 5 p.m. A breakthrough test of the active sampling showed efficient retention of PCBs for this sampling length (Figure S1). During Phase-2, we operated the low-volume sampler and the 3-D sonic anemometer in different room locations for weeklong intervals.

Chemical Analysis

The samples were analyzed for all 209 PCB congeners as described elsewhere.^{39, 48, 51, 52} Briefly, the PUF sample media was precleaned using a pressurized solution of 1:1 acetone:hexane (Dionex ASE 350) and stored in aluminum foil and sealed plastic bags. Samples were spiked with 50 ng of surrogate standards (PCB14 (3,5-dichlorobiphenyl), PCB65-d5 (2,3,5,6-tetrachlorobiphenyl-d5, deuterated), and PCB166 (2,3,4,4',5,6-hexachlorobiphenyl)), extracted with a 1:1 hexane-acetone in the ASE 350, cleaned on a column of acidified silica, and analyzed by the internal standard method on GC-MS/MS (Agilent 7890A GC system, Agilent 7000 Triple Quad, Agilent 7693 autosampler). The quality of the chemical measurements was assessed using surrogate recoveries, blanks, replicate sampling, and breakthrough studies. Average surrogate recoveries for all samples and blanks were $74 \pm 16\%$, $77 \pm 14\%$, and $98 \pm 13\%$ for PCB14, PCB65-d5, and PCB166, respectively. There was no statistical difference in recoveries between samples/blanks, Phase-1/Phase-2 samples, and low-volume/PUF-PAS samples. The average sum PCB level in all blanks was 1.85 ± 1.18 ng. Likewise, there was no statistical difference in blank levels between Phase-1/Phase-2 blanks, and low-volume/PUF-PAS samples. As mentioned above, a breakthrough test of the active sampling showed efficient retention of PCBs. See supporting information for further details.

Room Air Flow

A computational fluid dynamics (CFD) model of the room was constructed with the STAR-CCM+ software and simulations were run as steady state with the k- ω Reynolds averaged Navier Stokes (RANS) turbulence model as the physics model.^{53–67} The mesh numbers for our two simulations were 886,763 and 1,990,485, respectively. The CFD model included two inflows to the room; a 6" diameter HVAC inlet at a set point of 140 cfm and the door. The residuals from our model simulations demonstrating convergence can be found in the supporting information (Figure S8). We compared the CFD prediction to the measured wind speed using a CSAT3 3-D sonic anemometer (Campbell Scientific) placed at different positions within the room. We found the CFD model, at an HVAC set point of 140 cfm, and anemometer data to be within 1 standard deviation of each other for all four of our sampling locations within the room (Figure S4).

Results and Discussion

Phase-1: Experimental and Predicted DB-Dome Uptake Curves

An empirical R_s was calculated for each congener by dividing the slope of the uptake curve (ng d^{-1}) by the low-volume determined concentration (ng m^{-3}). The average low-volume concentration ($n=4$) during Phase 1 was 12 ± 4 ng m^{-3} (Figure S2). The average R_s ($n=38$ congeners) for this study was 1.10 ± 0.23 $\text{m}^3 \text{d}^{-1}$ (Figure 2). This is comparable to what is reported by others. For example, Bohlin and colleagues estimated an average indoor PUF-PAS R_s for PCBs of 1.2 $\text{m}^3 \text{d}^{-1}$ and Hazrati and Harrad estimated an R_s of 0.8 $\text{m}^3 \text{d}^{-1}$. The uptake remained linear ($R^2=0.973$) throughout the experiment for congeners consistently measured at levels above the LOQ and did not approach saturation (Figure 1, Figure 3).

We modeled the R_s from room-averaged wind speeds measured with the 3-D sonic anemometer as inputs. The samplers were deployed from one to six weeks during this period. The wind speed was highest when the building ventilation system was on during weekdays ($0.19 \pm 0.07 \text{ m s}^{-1}$) and lowest when the ventilation system was off during nights and weekends ($0.07 \pm 0.02 \text{ m s}^{-1}$). The predicted R_s values for each DB-dome sampler ranged from 1.0 to $1.3 \text{ m}^3 \text{ d}^{-1}$; a difference from the empirically determined R_s of less than a 25% (excluding PCB105) for the 38 congeners that contributed more than 1% of the sum of all PCBs (Figure 2). The difference was more variable for congeners that were present at low concentrations. The flowrate model also accurately predicted the expected uptake curves for many of the most dominate congeners (Figure 3). With the exception of PCB1, no PCB congeners showed signs of approaching saturation within the 6 week uptake study. We conclude that our assumption for the theoretical γ value of 0.646 is appropriate in this indoor environment. We postulate that with accurate wind speed inputs the sampling rate model can determine an sampling rate in any room. Resulting concentrations can be expected within 25% of the average of a series of low-volume measurements) in any room.

Phase-2: The Effects of Sampler Location and Variable Airflow

The PUF-PAS sampler is designed for long-term integration of concentrations. This makes it useful for identifying continuous sources, or for calculating human exposure. But this also requires placement that is representative of the intended environmental conditions. In a room, the location of the sampler may be important. We designed Phase-2 of our study to examine this hypothesis. While the dynamics of flow within a room has been examined using computational fluid dynamic (CFD) modeling,^{53–67} we know of no studies of room air flow variability and its effect on PUF-PAS sampling.

The location of the PUF-PAS in the room did matter. The PCB accumulation (ng day^{-1}) at each location varied significantly ($P < 0.001$) for both sampler designs. The HF-dome samplers placed at location 3 had the highest PCB accumulation for that sampler design. The DB-dome sampler placed at location 1 had the highest PCB accumulation rate and shortest deployment period for that sampler design. The samplers placed at location 4 had the lowest mass uptake rate of PCBs, for both sampler designs (Table S1). Empirical sampling rates were calculated for every congener at each location for both sampler designs used in Phase-2 as the PCB mass collected divided by the low-volume determined PCB concentration and deployment time.^{24, 38, 42, 47, 48, 68} The DB-dome design was particularly affected by the position in the room, and varied by almost a factor of 3 between the maximum and minimum. The HF-dome sampler design was less affected by room position and only varied by a factor of 1.4 between maximum and minimum (Table S1).

There are two possible reasons for variability of PCB accumulation with room location: the concentrations of airborne PCBs vary within the room; or the actual sampling rates vary within the room. Although the concentrations of PCBs vary over time, there are no known point sources of PCBs in the room. There was no window or window caulking; there was carpet throughout the room; the walls were painted the same off-white color. The ΣPCB airborne concentration was $7.7 \pm 1.7 \text{ ng m}^{-3}$ (Figure S2) and there was no significant difference ($P = 0.311$) between the four different locations sampled by low-volume.

Therefore, it is more likely that R_s varies for each sampler, and this variability is caused by the variability in wind speed at each location. This conclusion is supported by position-specific wind speed estimates from the CFD model (Figure 4). Both sampler designs showed small but significant ($P < 0.01$) linear correlations with wind speed, with the exception of the DB-dome triplicate at location one. Wind speed does not sufficiently explain the high accumulation rates exhibited by the DB-dome triplicates deployed for one week at location 1. These samples were deployed for only one week – the shortest period we used. Other studies have reported high accumulation rates for short deployments of this design in the outdoor environment.^{68–70}

We use our model to predict a room-averaged R_s of 1.08 and 2.69 $\text{m}^3 \text{d}^{-1}$ for the DB-dome and HF-dome designs, respectively, using the average wind speed parameters from the 3-D sonic anemometer. This estimate is not statistically different ($P > 0.05$) from empirically calibrated R_s for either sampler designs. However, the HF-dome design was better predicted (mean residual = 13%), than the DB-dome design (mean residual = 38%). We also modeled an R_s for each PUF-PAS at its specific placement within the room (Figure 5). Using these estimates and omitting the DB-dome outliers discussed above, the mean R_s residual between predicted and measured was slightly reduced (~2%) for both sampler designs, further demonstrating the influences of room airflow on sampling rate determination (Table S1). Overall we find that windspeed is the most important predictor. Nevertheless, we are unable to account for all the variability, particularly for the DB-dome sampler design. Because our analytical variability is small, other factors such as minor airborne concentration gradients or temporal concentration changes may be contributing factors. This is evidenced by the low-volume concentration estimates which ranged from 5.9 to 12.3 ng m^{-3} and had a relative standard deviation of 24% during Phase-2 of this study.

Ultimately the goal of implementing PUF-PAS methods is to determine a time averaged airborne concentration. In this context, the differences between using a room-averaged or location specific R_s has little affect on the PUF-PAS airborne concentration measurements. Using the room-averaged wind speeds to determine the R_s , the PUF-PAS determined concentrations were within 32% and 15% of the low-volume determined concentrations for the DB-dome and HF-dome designs, respectively. When incorporating the effects of room position, the PUF-PAS determined concentrations were within 27% and 10% of the low-volume determined concentrations for the DB-dome and HF-dome designs, respectively (Figure 6). This minor improvement demonstrates that room-averaged R_s predictions are nearly as accurate as position specific R_s predictions when determining airborne concentrations. As stated previously, the low-volume concentration estimates had a relative standard deviation of 24% during Phase-2 of this study. This indicates the low-volume and passive sampling methods are producing estimates with similar degree of variability.

Phase-2: Examining Airflow Variability throughout The Simulated Room

It is important to fully understand what constitutes room-averaged conditions with the assumptions that room-averaged wind speeds provide accurate airborne concentrations. We examined the variability of wind speed in our study room using the CFD model. We found

several instances of airflow characteristics not being described well by room-averaged parameters, in both the vertical and horizontal directions.

The lowest wind speeds were found during the nights and weekends when the building ventilation system was shut down. The highest wind speeds were found in the vertical downward direction against a wall and closest to the ventilation diffuser on the ceiling. Due to this airflow pattern and boundary layer mixing, the area closest to the walls experienced elevated air flow. Therefore, any sampler placed near the wall (~30 cm) would experience wind parameters that are not representative of the room-averaged parameters (Figure 7). Similarly, near the ceiling and near surfaces (such as tops of bookcases), there are elevated average wind speeds. Since the air diffuser is the primary driver of ventilation within the room, we expect turbulent zones near the diffuser that dissipate with distance. Along the easternmost and westernmost wall (~1.2 m from diffuser), we found zones of increased turbulence approximately 1 m wide where the air stream from the diffuser perpendicularly intersect the wall.

We also examined the airflow profiles near the doorway and the effects of having the door open or closed on the air profile. The effects were minimal and most pronounced near the ground. This is likely because the gap under the door was producing a stream of air into the room when the door was closed but this influence is more diffused once the door has been opened. We were also able to observe a noticeable effect within approximately the first meter from the door into the room. Our test room had only one door so there is no chance of experiencing a cross draft through the room that may exist if a room had two doors open or another similar scenario with multiple large openings. Additional findings and images from the CFD modeling of the room can be found in the SI.

Implications for PUF-PAS use Indoors

The use of PUF-PAS in the indoor environment is challenging due to an accurate determination of R_s . However it presents a powerful opportunity to more easily identify and quantify airborne SVOCs, including PCBs, in homes, schools, and workplaces. This study has shown that it is possible to accurately determine an indoor R_s where an accurate understanding of the airflow is available. Although this study is focused on PCBs it is applicable to other SVOCs with similar physical chemical properties (such as PAHs, PBDEs, OCPs, PFCs, etc). From a practical standpoint the average airflow parameters within a room should provide a reasonably accurate estimate of R_s for any position in the room that is not experiencing large eddies. We recommend samplers be placed at least 30 cm from the wall, ceiling, or any surface; at least 50 cm from the direct line of the HVAC air diffuser, and at least 1 m away from the door to avoid the effects of turbulent mixing. Equation 4 may be used to calculate a sampling rate for a given room from a known room averaged wind speed (WS , $m\ s^{-1}$), molecular weight, temperature ($^{\circ}C$), and an empirical constant, c , of 1.326 for DB-dome or 1.723 for HF-dome. In environments like our study room it is important to account for both when the HVAC system is on and off, by taking a time weighted average. In our study the HVAC system was on 36% (f_{on}) of the time, and off 64% of the time (f_{off}).

$$R_s = (f_{on}\sqrt{WS_{on}} + f_{off}\sqrt{WS_{off}}) \left(\frac{1}{\sqrt[2]{MW}} \right) 10^{[0.0012 * T + c]} \quad (4)$$

Equation 5 is adapted from Harner et al. (2004) and may be used to calculate an effective sampling volume from the deployment time (t , days), the volume of the PUF disk (V_{PUF} , m^3), the PUF-air partition coefficient (K_{PUF}), and the R_s ($m^3 d^{-1}$) calculated from equation 4.¹⁴ The K_{PUF} parameters can be calculated from the empirical relation presented by Shoeib and Harner (2002).⁴²

$$V_{eff} = (V_{PUF}K_{PUF}) \left[1 - e^{-\left(\frac{R_s}{V_{PUF}K_{PUF}} \right) t} \right] \quad (5)$$

Although the effective sampling volume equation corrects compounds approaching saturation, these equations can be applied to estimate when saturation might occur prior to deployment to determine an appropriate deployment length. Within our study room, several PCBs will reach half saturation (t_{50}) in a 6 week period. PCB 1 reaches t_{50} in 2 weeks; PCBs 2 and 3 reach t_{50} in 4 weeks; PCBs 4 and 10 reach t_{50} in 6 weeks. For room styles similar to the one in this study we would recommend a PUF-PAS deployment of 4–8 weeks.

In practice it may be difficult to measure or approximate the room averaged air flow parameters due to cost or access. In these instances assuming a sample rate of $1.0 m^3 d^{-1}$ ($k_v = 27.4 m^3 d^{-1} m^{-2}$) for the double dome sampler or $2.6 m^3 d^{-1}$ ($k_v = 27.4 m^3 d^{-1} m^{-2}$) for the half dome sampler may be appropriate for most room styles as the ventilation is typically designed to have similar values of wind speed and air turnover regardless of room size. While the ranges of R_s reported for similar studies overlap, we suspect the differences in the reported average indoor PUF-PAS R_s can be attributed to different air ventilation rates for the different room styles or position in the room (Table 1).^{24, 34, 42, 44, 45, 48} Much of the differences between the studies conducted in similar room styles for PCBs may be attributed to differences of sampler placement within the room.^{24, 34} Our study has shown that adjustments of less than 30 cm of sampler placement may effect interpretation of the sample.

In rooms where significantly different wind speeds are expected, such as a scientific laboratory, assuming a value of 1.0 or $2.6 m^3 d^{-1}$ for the DB-dome and HF-dome, respectively, would under-predict the airborne concentration. According to ANSI/ASHRAE Standard 62 (Ventilation for Acceptable Indoor Air Quality) the required minimum ventilation rate for science laboratories (0.18 cfm/ft^2) is three times higher than the minimum ventilation rate for lecture rooms and office spaces (0.06 cfm/ft^2) and may explain the higher R_s values reported by Persoon and Hornbuckle and Shoeib and Harner from studies conducted in scientific labs.^{42, 48, 71}

It is important to note that the conclusions of this study are based upon the commonly used PAS design with a 24 cm top bowl, a 19.5 cm bottom bowl, a 2.5 cm gap between the bowls, a 1.5 cm overlap, and holes in the bottom to aid airflow. We suspect many of the conclusion in this paper to apply to other similar sampler designs. However, caution should be exercised when variations on the common design are used. If a PUF disk other than Tisch Environmental PUF are used, sampling rates can be corrected by adjusting by PUF surface area.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.
Measured uptake of the 6 most prevalent congeners (or congener coelution).

Figure 2. Experimental R_s values and predicted R_s values for 38 congeners that contributed more than 1% of the sum of all PCBs.

Figure 3. Predicted and experimentally determined uptake curves for PCB 11, 52, 95, and 110. The experimental effective volume was calculated as the mass collected divided by the low-volume determined concentration.

Figure 4. Correlations between ΣPCB accumulation rates and location specific wind speeds from the CFD model. The colored DB-dome markers represent the outlier samplers collected at location 1.

Figure 5. Correlations between experimental determined and predicted R_s values based on position specific wind speed parameters from the CFD model for both sampler designs.

Figure 6.

Comparison between PCB congener concentrations determined by active sampling and passive sampling for 38 congeners that contributed more than 1% of the sum of all PCBs. For the room averaged PUF-PAS estimates, an R_s of 1.08 and 2.69 $\text{m}^3 \text{d}^{-1}$ for the DB-dome and HF-dome designs, respectively, was used to determine an airborne concentration.

Figure 7.

Horizontal profile showing the effects of elevated wind speeds along the wall and the convergence of airflow to room average parameters at increasing distances from the wall generated from the CFD model in our study zone. The anemometer data that corresponds with this location was also included to show the general agreement between the 3-D sonic anemometer data and the CFD.

Table 1

Comparison to other studies determining indoor PUF-PAS sampling rates.^{24, 34, 42, 44, 45, 48}

Average (m ³ d ⁻¹)	Range (m ³ d ⁻¹)	Compound	Room Style	Study
<i>Double-Dome</i>				
1.1	0.4 – 2.8	PCBs	Occupied Office	This Study (Phase-1)
1.3	0.6 – 2.9	PCBs	Occupied Office	This Study (Phase-2)
1.2	0.9 – 1.7	PCBs	Lecture Hall	Bohlin et al (2014)
0.8	0.6 – 1.6	PCBs	Vacant Office	Hazrati and Harrad (2007)
2.6	2.0 – 3.5	PCBs	Scientific Lab	Persoon and Hornbuckle (2009)
1.5	0.9 – 2.9	PBDEs	Lecture Hall	Bohlin et al (2014)
1.2	<0.1 – 5.5	PAHs	Lecture Hall	Bohlin et al (2014)
2.3	na	PAHs	Factory	Bohlin et al (2010)
<i>Half-Dome or Exposed PUF Sampler</i>				
2.7	1.9 – 4.4	PCBs	Occupied Office	This Study (Phase-2)
3.4	1.8 – 8.3	PCBs	Scientific Lab	Shoeib and Harner (2002)
2.5	na	PAHs	Factory	Bohlin et al (2010)
2.5	na	PBDEs	Residential Home	Wilford et al (2004)