



# Calibration of polydimethylsiloxane and polyurethane foam passive air samplers for measuring semi volatile organic compounds using a novel exposure chamber design

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## HIGHLIGHTS

- Rs and Ksampler-air measured for PDMS and PUF using an exposure chamber with passive release source for SVOCs.
- Similar Rs irrespective of chemical and sampler type supporting the use of a single generic Rs for gas-phase SVOCs.
- Relationship between Rs and windspeed demonstrated that allows estimation of Rs for specific deployment conditions.
- Ksampler-air for PDMS 10 times higher than for PUF indicating longer deployment periods per volume of sampler for PDMS.
- Strong relationship between Ksampler-air and Koa demonstrated and equations derived for Kpdms-air and Kpuf-air with Koa.

## ARTICLE INFO

### Article history:

Received 13 February 2019

Received in revised form

4 April 2019

Accepted 6 April 2019

Available online 8 April 2019

Handling Editor: J. de Boer

### Keywords:

Passive air sampling

Calibration

PDMS

PUF

SVOCs

Partition coefficients

## ABSTRACT

Passive air sampling is increasingly used for air quality monitoring and for personal sampling. In a novel experimental exposure chamber study, 3 types of polydimethylsiloxane (PDMS, including sheet and wristband) and 1 type of polyurethane foam (PUF) passive air samplers were tested for gas-phase uptake of 200 semi volatile organic compounds (SVOCs) during six months. For 155 SVOCs including PAH, PCB, phthalates, organophosphate esters, musk compounds, organochlorine- and other pesticides, a normalized generic uptake rate (Rs) of  $7.6 \pm 1.3 \text{ m}^3 \text{ d}^{-1} \text{ dm}^{-2}$  and a generic mass transfer coefficient (MTC) of  $0.87 \pm 0.15 \text{ cm s}^{-1}$  at a wind speed of  $1.3 \text{ m s}^{-1}$  were determined. Variability of sampling rates within and between passive sampling media and analyte groups was not statistically significant, supporting the hypothesis of air-side controlled uptake regardless of sampling material. A statistical relationship was developed between the sampling rate and windspeed which can be used to obtain a sampling rate applicable to specific deployment conditions. For 98 SVOCs, partition coefficients (Ksampler-air) for PUF and PDMS were obtained, which determine the duration of linear uptake and capacity of the sampler for gas-phase uptake. Ksampler-air for PDMS were approximately 10 times higher than for PUF, suggesting that PDMS can be deployed for longer time per volume of sampler, while uptake remains in the linear phase. Statistical relationships were developed to estimate Kpuf-air and Kpdms-air from Koa. These results improve the understanding of the performance of PDMS and PUF passive samplers and contribute to the development of PDMS for the use as a promising personal sampler.

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## 1. Introduction

Environmental exposure to chemicals has been shown to contribute to adverse health outcomes of the general population,

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especially during prenatal and early postnatal life (Grandjean et al., 2008). As such, there is a need for efficient and cost-effective quantitative methods for assessing exposure. Passive sampling technologies can potentially provide insight into the presence and concentrations of a wide range of chemicals over a longer time period than active samplers. For these reasons, passive air samplers are being increasingly used as an alternative to active samplers. Polyurethane foam (PUF) disks are popular for monitoring concentrations of semi-volatile organic compounds (SVOCs) outdoors and indoors (e.g., Okeme et al., 2016a; Shoeib and Harner, 2002a, 2002b; Wania et al., 2003; Saini et al., 2015). Silicone rubber (polydimethyl siloxane or PDMS) is now seeing widespread adoption as a passive sampler for stationary air (Okeme et al., 2018a, 2018b) or as a personal brooch (Okeme et al., 2018a, 2018b) and as a wristband (O'Connell et al., 2014; Hammel et al., 2016; Nicole, 2018; Aerts et al., 2018; Donald et al., 2016; Bergmann et al., 2017; Hammel et al., 2018; Anderson et al., 2017) for capturing personal (chronic) exposures.

Passive air samplers are inexpensive and easy to deploy, do not need electricity and maintenance and are noise-free and therefore can be used on a large scale (Markovic et al., 2015). However, the accuracy of passive samplers is limited due to variability in published uptake rates ( $R_s$ ) (Okeme et al., 2018a, 2018b; Chaemfa et al., 2009; Bohlin et al., 2014). To use passive samplers for environmental and health studies, their uptake rates and capacities need to be better characterized to produce results that are comparable study-to-study.

Passive air samplers capture gas- and particle-phase compounds. The uptake of gas-phase chemicals is based on molecular diffusion; particle-associated chemicals are captured by particle impaction. In practice, the factors influencing the uptake rate  $R_s$  of chemicals are not fully understood and measured values of  $R_s$  vary according to study and chemical group (Okeme et al., 2018a, 2018b). In theory the use of a generic  $R_s$  for gas-phase uptake of a broad range of SVOCs rather than compound or group-specific  $R_s$  is justifiable for sampling in the linear phase assuming air-side controlled uptake which is independent of physico-chemical properties for those chemicals found in the gas phase (Hazrati and Harrad, 2007; Saini et al., 2015; Okeme et al., 2018a, 2018b; Bartkow et al., 2005). However many of the reported studies still recommend a group-, homolog- or compound-specific  $R_s$  to increase precision of air concentration estimates (Melymuk et al., 2011; Bohlin et al., 2014).

The use of PUF and PDMS passive samplers and  $R_s$  to translate between the mass accumulated by the sampler and the corresponding air concentration assumes that the sampler is in the linear uptake phase. Knowledge of the partition coefficient of a chemical between sampler and air ( $K_{\text{sampler-air}}$ ) is required to estimate the duration of the linear uptake phase and the capacity of the passive sampler for gas-phase uptake (Shoeib and Harner, 2002a, 2002b; Okeme et al., 2016b). The  $R_s$  and  $K_{\text{sampler-air}}$  can be measured in a calibration study in which chemical uptake by a passive air sampler is characterized by comparing gas-phase concentrations with active air sampling techniques (Okeme et al., 2016b; Shoeib and Harner, 2002a, 2002b; Wania et al., 2003; Saini et al., 2015; Newton et al., 2016). These values can also be estimated by a calibration study (Okeme et al., 2018a, 2018b) or can be estimated using the relationship between  $K_{\text{sampler-air}}$  and octanol-air partition ratio ( $K_{\text{oa}}$ ) (Shoeib and Harner, 2002a, 2002b).

While useful, calibration studies to estimate  $R_s$  and  $K_{\text{sampler-air}}$  have several limitations. Values obtained from a calibration study are subject to time and site-specific variability, which may hinder the applicability of the data under different circumstances (Genualdi and Harner, 2012). This is especially true for outdoor studies considering factors like wind speed, air temperature, air

concentrations and gas-phase/particle-bound ratio are not exactly known or vary during deployment. Additionally,  $K_{\text{sampler-air}}$  measurements are generally limited to compounds that reach equilibrium within the sampling duration. Low volatile compounds are unlikely to reach equilibrium with air and sampler within the typical duration of calibrations studies (Okeme et al., 2016b).

Most calibration studies have been conducted on PUF passive samplers; few studies have calibrated the uptake characteristics of PDMS. This study aims to further characterize the uptake characteristics of PDMS as a passive air sampler, along with PUF in the context of environmental monitoring and personal exposure measurement. To overcome the mentioned limitations of other calibration studies, in this study a novel exposure chamber design was developed with a passive release source of gas-phase SVOCs, to measure their uptake rates and uptake capacities. A large number of 200 SVOCs was included with a variety of physical-chemical properties, such as polychlorobiphenyls (PCB), polycyclic aromatic hydrocarbons (PAH), musk compounds, phthalates, pesticides and organophosphate esters (See Table S5 for full list of compounds). We tested the hypothesis that  $R_s$  for gas-phase compounds is uniform across compound groups. In addition, the study assessed the variability of uptake rates and uptake capacities amongst three types of PDMS, including the commercially available silicone wristbands, and PUF. Furthermore, the study derived a relationship for estimating sampling rates for passive samplers deployed in field studies. Determining sampling rates and partition coefficients for a wide range of SVOCs under well defined conditions will make an essential contribution to the knowledge base on the interpretation of exposure data with passive sampling.

## 2. Experimental section

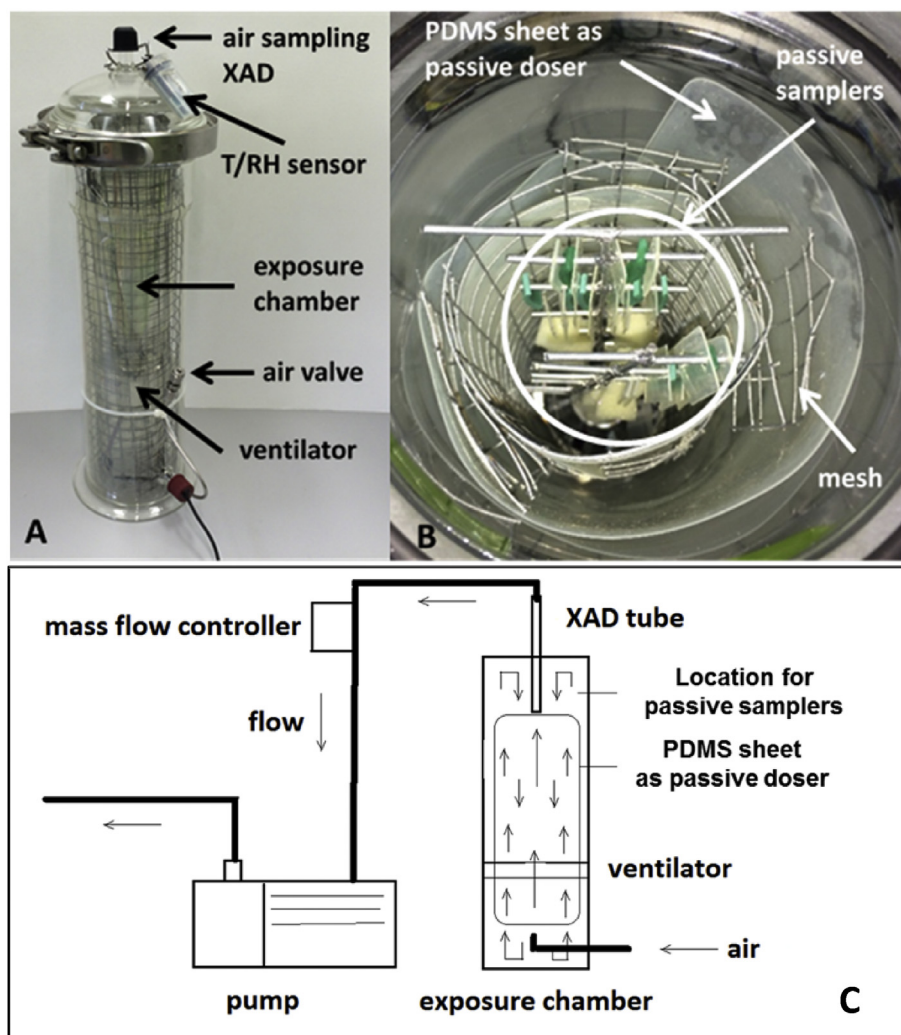
Two studies were performed: a preliminary study in 2013 with the use of pre-spiked PDMS samplers to test the exposure chamber (See supplementary data) and the main study in 2017 with PDMS and PUF where both uptake and release of SVOCs were measured.

### 2.1. Exposure chamber description

Calibration experiments were performed during a period of six months in a glass exposure chamber (length 40 cm, internal diameter 10 cm) (See Fig. 1). As a release source (passive doser) of SVOCs, a  $300 \times 300 \times 0.5$  mm pre-spiked PDMS sheet (AlteSil™ Silicone Laboratory Sheet, Altec Extrusions Limited, UK) was placed around a wire-netting. Passive samplers were hung inside the wire-netting to prevent contact with the PDMS passive doser. A small ventilator (cooling fan, model TFD-6025L12X, Titan Technology Ltd., Taiwan) operating at an airspeed of  $1.3 \text{ m s}^{-1}$  was mounted at the bottom of the exposure chamber for circulation of air. Adsorption tubes for measuring active air concentrations were connected to an outlet vent at the top of the chamber. Air was drawn into the chamber via an inlet vent at the bottom of the chamber. During the study, the average temperature and relative humidity inside the chamber were  $20.7 \pm 0.2$  °C and  $44.0 \pm 3.0\%$ , respectively.

### 2.2. Passive and active sampling

Four types of passive sampling materials were tested: PDMS AlteSil™ (sampler dimensions:  $25 \times 15 \times 0.5$  mm, surface area:  $790 \text{ mm}^2$ , mass: 0.2 g, density:  $1.08 \text{ g cm}^{-3}$ ), PDMS SSP-M823 (sampler dimensions:  $20 \times 11 \times 1.0$  mm, surface area:  $520 \text{ mm}^2$ , mass: 0.2 g, density  $1.09 \text{ g cm}^{-3}$ , Specialty Silicone Products, Inc., USA), green, brown and black coloured silicone wristbands (sampler dimensions:  $21 \times 5.7 \times 1.7$  mm, surface area:  $330 \text{ mm}^2$ ,



**Fig. 1.** Picture of the outside of the exposure chamber (A), top view of the inside of the exposure chamber (B) and schematic presentation of exposure chamber experimental set-up (C).

mass: 0.2 g, density  $1.08 \text{ g cm}^{-3}$ , [24hourwristband.com](http://24hourwristband.com), USA), and PUF (sampler dimensions:  $29 \times 14 \times 14 \text{ mm}$ , surface area:  $2050 \text{ mm}^2$ , mass: 0.1 g, density:  $0.022 \text{ g cm}^{-3}$ , Tisch Environmental, Inc., USA). After 1, 4, 10, 30, 50, 71, 91 and 161 exposure days, triplicate samplers of each type of PDMS and PUF were retrieved from the exposure chamber. In addition one pre-spiked sampler of each type of PDMS was retrieved to monitor the decrease in concentration of SVOCs. These pre-spiked samplers were prepared in the same way as the PDMS sheet used as a release source. During the exposure periods, the air in the chamber was sampled with a low volume pump (Laboport, KNF Neuberger, Germany) through two XAD-2 adsorption tubes connected in series (ODxlength:  $8 \times 110 \text{ mm}$ , 400/200 mg sorbent, cat. no. 226-30-06, SKC Inc., USA) to prevent breakthrough of SVOCs. A low flow rate of  $0.5 \text{ L min}^{-1}$  was achieved with a mass flow controller (HI-TEC series F-100/200, Inacom Instruments, the Netherlands). The adsorption tubes were changed at the same time as the passive samples were retrieved (See [Table S1](#) and [Table S2](#) for detailed measurement schedules). All samples were stored in the freezer at  $-20^\circ \text{C}$  until extraction and chemical analysis.

### 2.3. Loading of PDMS sheets with SVOCs

PDMS sheets, used as a passive release source, were spiked with

200 SVOCs (See [Table S4](#) for full list of compounds) ([Booij et al., 2002](#); [Smedes, 2018](#)). First, the chemical compounds were pipetted into a 5 L jar filled with a methanol/water (9:1) solution and PDMS sheets, creating a concentration between  $1.8$  and  $7.1 \text{ mg L}^{-1}$  for of each compound. The solution was gently shaken for 56 days in a rotary shaker, to allow the compounds to equilibrate between the solvent and PDMS. In order to encourage the hydrophobic components to sorb into the PDMS, the polarity of the solution was increased gradually during this period by adding water to ultimately create a 7% methanol solution (See [Table S3](#) for the detailed loading procedure). During and after the spiking procedure, small pieces of the PDMS sheets were analyzed, to determine the concentration of SVOCs in the loaded PDMS sheets.

### 2.4. Pre-cleaning and extraction

All PDMS and PUF materials were pre-cleaned in ethyl acetate using Soxhlet extraction for two weeks. All samples were cold extracted twice with 20 mL of Acetonitrile at room temperature on a rotation shaker for two days ([Smedes et al., 2017](#); [Smedes, 2018](#)). After each cold extraction the PUF samples were ultrasonic extracted for 15 min. Extracts were reduced to 2–3 mL using a rotary film evaporator (Rotavapor R-210, Buchi, Switzerland). In order to exchange solvent, 50 mL of methanol was added and the total

extract was concentrated once again to 2–3 mL with a rotary film evaporator. The extracts were gently blown down to precisely 1 mL using nitrogen. For GC analysis, 50% of the extracts were reconstituted into 0.5 mL hexane. Both XAD-2 tubes (including backup tube) were extracted separately in methanol/acetonitrile (20:80) using an Accelerated Solvent Extractor (ASE) (Dionex ASE-350, Dionex Corporation, USA).

## 2.5. Analysis

Extracts were analyzed using either GC-MS, GC-MS-MS or LC-MS-MS (ESI-NEG/ESI-POS) (See Table S4 and S5) (Smedes et al., 2017; Smedes, 2018). Briefly, 16 polycyclic aromatic hydrocarbons (PAH), 28 polychlorobiphenyls (PCB), 4 methylated naphthalenes, 24 organochlorine pesticides (OCP), and 11 additional hydrophobic pesticides were analyzed using an Agilent 7890 A Series gas chromatograph (GC) with MMI injector (Agilent, USA) and Agilent 7000 tandem mass selective detector (MSD) using multiple reaction monitoring (MRM) with two ion transitions for each compound. 11 musk-compounds, 23 phthalates and 24 organophosphate esters (OPE) were analyzed on an Agilent 6890 gas chromatograph and Agilent 5973 N mass selective detector operated in selected ion mode (SIM) using electron impact ionization. GC separation was performed on an MS-DB5 UI capillary column (length 30 m x diameter 0.25 mm x film thickness 0.25  $\mu\text{m}$ , Agilent J&W, USA), with 1–2  $\mu\text{L}$  injected in splitless mode using He as the carrier gas (see Table S6 for details). 60 hydrophobic pesticides and 7 other hydrophobic compounds were analyzed in the ESI-Jetstream mode by an Agilent 6460 high-performance liquid chromatography and tandem mass spectrometry (HPLC-MSMS) using a biphenyl reversed phase column (Kinetex 2.6  $\mu\text{m}$ , Biphenyl 100 A, 2.1 mm i. d. x 100 mm, Phenomenex, USA). The identification of target compounds was accomplished by comparing the retention time and two optimized ion pairs with corresponding standard compounds.

## 2.6. Quality assurance and quality control (QA/QC)

Prior to extraction, PDMS, PUF, XAD-2 and blank samples of each sampler type were spiked with 16  $^{13}\text{C}$ -PCBs, 16 deuterated PAHs, two deuterated musk-compounds, three  $^{13}\text{C}$ -OCPs, two deuterated OPEs and 15 deuterated pesticides as recovery internal standards to determine extraction efficiencies (See Table S5 for complete list of internal standards). 1,2,3,4-Tetrachloro-naphthalene (TCN), used as an internal injection standard for quantification, was added to the final volume of extracts prior to GC analysis. Recoveries of the deuterated and  $^{13}\text{C}$ -labeled internal standards ranged from 60 to 120%, with an average recovery of  $87.6 \pm 11.2$ . (See Table S7 for individual internal standard recoveries). Results for individual samples were corrected based on the recoveries of the internal standards. All results were blank corrected except where concentrations of analytes in field blanks were <5% of those in samples.

The variability of the passive sampling measurements in the exposure chamber were assessed by comparing results of triplicate samples for each type of PDMS and PUF from each sampling period. Within sampler type, the arithmetic mean of coefficient of variation (CV) was 20% for all chemical compounds. No significant difference in CV was observed amongst the four sampler types. However, CV differed according to chemical group and analytical method with arithmetic mean values of 15% for GCMS/MS and 34% for LCMS/MS, mainly due to the difference in chemical concentration in the passive samplers. The arithmetic mean CV was 11% for high concentrations of >100 ng per sampler and 38% for low concentrations of <0.1 ng per sampler (See Table S8 for CV details).

The collection efficiency of the XAD-2 adsorption tubes for the different chemical compounds was assessed by comparing results

of the two adsorption tubes connected together. The concentration in the second (backup) tube was <3% of the concentration in the first adsorption tube for most chemicals. For pesticides, hydrophilic compounds and OPEs, concentrations in the backup tube were average 11%, 16% and 46% lower compared with the first tube. Assuming that the backup tube has a maximum breakthrough of 46%, then for OPE at least 80% of the compounds were captured with XAD-2 with the two connected tubes.

The analysis of phthalates was associated with high and variable background levels as a result of contamination from laboratory products and air. As such, in addition to performing a blank correction, deuterated phthalates were used to compare with native phthalates. No significant differences were found between Rs and log K for native and deuterated phthalates (*t*-test,  $p > 0.1$ ). The variability (CV) between native and deuterated phthalates was 14% for Rs and 4% for logK. Thus, blank correction was sufficient and the data of the native and deuterated phthalates were used to calculate Rs.

## 3. Results

Passive sampling rates ( $\text{m}^3 \text{d}^{-1} \text{dm}^{-2}$ ) and partition coefficients (K<sub>sampler-air</sub>, in volume units  $\text{m}^3 \text{air m}^{-3} \text{sampler}$ ) were derived from the masses (ng) of SVOCs on the PDMS and PUF passive samplers over time and the concentration of SVOCs in air ( $\text{ng m}^{-3}$ ) of the exposure chamber obtained by active sampling. The exchange of chemicals between the passive sampler and air can be presented in three stages: the linear or kinetic region, the curvilinear region, and the equilibrium region (Shoeib and Harner, 2002a, 2002b; Wania et al., 2003; Bartkow et al., 2005) (see Figure S2). The linear uptake phase of the chamber experiment was used to calculate the Rs of 155 out of 200 SVOCs. The equilibrium phase was used to derive the K<sub>sampler-air</sub> for 98 chemicals that reached equilibrium in the 161 days exposure period. Rs and K<sub>sampler-air</sub> were not derived for 16 pesticides that were too hydrophobic to be sorbed into the PDMS sheet during the spiking procedure (See S5 for list of compounds with Rs and K<sub>sampler-air</sub>).

### 3.1. Sampling rates

We assumed that the sampling rate was constant over time when sampling in the linear uptake phase because the experimental temperature and wind speed were stable in the exposure chamber (Bohlin et al., 2014). Therefore, values of Rs ( $\text{m}^3 \text{d}^{-1} \text{dm}^{-2}$ ) and mass transfer coefficients MTC ( $\text{cm sec}^{-1}$ ) were determined for each type of PDMS/PUF passive sampler using the time-integrated method (Shoeib and Harner, 2002a, 2002b; Okeme et al., 2016a) (see supporting data). Average Rs and MTC per sampler type and chemical group are presented in Table 1 and Figure S1. Rs for individual compounds were normalized to a surface area of 1  $\text{dm}^2$  to assess variability of Rs between sampler types. CV's of Rs ranged from 12 to 19% within sampler type and 10–15% between sampler type. For chemical groups, CV's of Rs ranged from 5 to 20% within group and 4–11% between group. Similar CVs of  $\leq 20\%$  were obtained for the comparison of MTCs. Differences in CV's were not systematic or statistically significant (*t*-test,  $p > 0.1$ ). CV's findings were consistent with the theory that uptake rates should not depend on the physical and chemical properties of target chemical or sampling medium, where the chemical uptake for gas-phase compounds is air-side controlled during the linear uptake phase (Bartkow et al., 2005). As such, the results presented here for 155 compounds from 8 chemical groups with varying physical and chemical properties support the approach of using a single generic Rs for gas-phase compounds. Moreover, the analytical reproducibility (CV) of the triplicate samples was of the same order of magnitude as the within/in between group variability, which

**Table 1**

Arithmetic means of normalized sampling rates (Rs, in  $\text{m}^3 \text{d}^{-1} \text{dm}^2$ ) and mass transfer coefficients (MTC, in  $\text{cm sec}^{-1}$ ) per chemical group including standard deviation ( $\pm$ SD) and range, average correlation coefficients ( $r^2$ ) for the uptake curves per chemical group, normalized for PDMS and PUF passive samplers.

Chemical group	AlteSil PDMS (1 $\text{dm}^2$ )			Silicone wristband (1 $\text{dm}^2$ )			SSP-M823 PDMS (1 $\text{dm}^2$ )			PUF (1 $\text{dm}^2$ )		
	Rs $\pm$ SD	Range	$r^2$	Rs $\pm$ SD	range	$r^2$	Rs $\pm$ SD	Range	$r^2$	Rs $\pm$ SD	range	$r^2$
PAH (11)	7.8 $\pm$ 0.6	6.9–8.8	0.95	8.8 $\pm$ 1.1	7.4–11	0.96	8.0 $\pm$ 0.6	7.3–9.5	0.95	8.1 $\pm$ 1.1	6.7–9.5	0.99
Musk (11)	7.4 $\pm$ 0.5	6.4–8.2	0.96	6.4 $\pm$ 0.9	5.3–7.4	0.91	7.8 $\pm$ 0.4	7.4–8.6	0.91	7.0 $\pm$ 0.5	6.3–7.7	0.95
Phthalates (23)	7.7 $\pm$ 1.4	5.7–10.5	0.89	7.2 $\pm$ 1.5	4.4–10.8	0.87	7.1 $\pm$ 1.3	4.3–9.4	0.90	7.4 $\pm$ 0.9	5.9–8.6	0.88
OCF (20)	6.9 $\pm$ 0.4	5.8–7.6	0.97	6.9 $\pm$ 0.5	5.4–7.6	0.97	6.0 $\pm$ 0.2	5.5–6.5	0.96	7.9 $\pm$ 0.6	6.8–9.1	0.98
OPE (26)	7.5 $\pm$ 1.5	4.5–9.3	0.83	7.3 $\pm$ 2.1	3.9–11.6	0.80	7.6 $\pm$ 2.7	4.3–16	0.77	7.4 $\pm$ 1.2	5.5–9.4	0.79
PCB (14)	7.2 $\pm$ 0.3	6.7–7.6	0.97	7.5 $\pm$ 0.5	6.7–8.4	0.98	6.4 $\pm$ 0.3	5.8–6.9	0.95	7.1 $\pm$ 0.2	6.9–7.6	0.97
Pesticides (45)	8.8 $\pm$ 1.4	5.5–10.9	0.83	9.2 $\pm$ 1.3	6.1–11.5	0.76	7.9 $\pm$ 1.3	4–10.2	0.76	7.6 $\pm$ 1.5	5.3–11.5	0.87
Miscellaneous (5)	7.8 $\pm$ 1.6	5.2–11.4	0.87	7.6 $\pm$ 1.4	5.6–10.4	0.88	8.3 $\pm$ 1.6	6.7–11.4	0.86	7.6 $\pm$ 1.2	5.5–9.6	0.89
total mean (155)	7.7 $\pm$ 1.3	4.5–11.4	0.90	7.7 $\pm$ 1.6	3.9–11.6	0.90	7.4 $\pm$ 1.6	4.0–11.4	0.87	7.5 $\pm$ 1.0	5.3–11.5	0.90
total median	7.4		0.96	7.3		0.94	7.4		0.95	7.3		0.96
	MTC $\pm$ SD	Range	$r^2$	MTC $\pm$ SD	range	$r^2$	MTC $\pm$ SD	Range	$r^2$	MTC $\pm$ SD	range	$r^2$
PAH (11)	0.93 $\pm$ 0.07	0.83–1.04	0.95	1.00 $\pm$ 0.11	0.85–1.21	0.96	0.93 $\pm$ 0.06	0.84–1.09	0.95	0.93 $\pm$ 0.12	0.77–1.09	0.99
Musk (11)	0.86 $\pm$ 0.05	0.73–0.94	0.96	0.74 $\pm$ 0.09	0.62–0.84	0.91	0.86 $\pm$ 0.04	0.78–0.92	0.93	0.80 $\pm$ 0.06	0.73–0.89	0.95
Phthalates (23)	0.90 $\pm$ 0.16	0.64–1.23	0.92	0.84 $\pm$ 0.17	0.53–1.26	0.88	0.82 $\pm$ 0.15	0.48–1.07	0.89	0.85 $\pm$ 0.1	0.68–0.99	0.88
OCF (20)	0.82 $\pm$ 0.04	0.69–0.89	0.98	0.79 $\pm$ 0.06	0.63–0.89	0.98	0.70 $\pm$ 0.02	0.66–0.75	0.96	0.90 $\pm$ 0.07	0.79–1.05	0.98
OPE (26)	0.87 $\pm$ 0.17	0.52–1.09	0.82	0.81 $\pm$ 0.16	0.54–1.14	0.85	0.85 $\pm$ 0.17	0.48–1.09	0.84	0.84 $\pm$ 0.13	0.63–1.09	0.79
PCB (14)	0.84 $\pm$ 0.03	0.79–0.90	0.97	0.86 $\pm$ 0.06	0.78–0.95	0.98	0.75 $\pm$ 0.03	0.69–0.80	0.94	0.83 $\pm$ 0.03	0.80–0.92	0.97
Pesticides (45)	1.05 $\pm$ 0.16	0.66–1.34	0.84	1.06 $\pm$ 0.14	0.72–1.29	0.76	0.91 $\pm$ 0.15	0.47–1.17	0.77	0.86 $\pm$ 0.14	0.61–1.12	0.84
Miscellaneous (5)	0.93 $\pm$ 0.19	0.62–1.35	0.87	0.90 $\pm$ 0.19	0.64–1.25	0.87	0.96 $\pm$ 0.17	0.76–1.29	0.86	0.89 $\pm$ 0.12	0.74–1.11	0.90
total mean (155)	0.91 $\pm$ 0.15	0.52–1.35	0.90	0.88 $\pm$ 0.17	0.53–1.29	0.88	0.84 $\pm$ 0.15	0.47–1.29	0.88	0.87 $\pm$ 0.11	0.61–1.12	0.90
total median	0.87		0.96	0.85		0.95	0.84		0.95	0.85		0.96

means that the differences were likely related to analytical variability. A normalized generic Rs of  $7.6 \pm 1.3 \text{ m}^3 \text{d}^{-1} \text{dm}^{-2}$  and a generic MTC of  $0.87 \pm 0.15 \text{ cm s}^{-1}$  were derived from the individually determined values of Rs and MTC of the chemical compounds and passive sampling materials.

### 3.2. Partition coefficients, $K_{\text{sampler-air}}$

Values of  $K_{\text{sampler-air}}$  were determined for 98 of the more volatile SVOC that reached equilibrium between the passive samplers and chamber air during the experiment (Table 2 and Table S11).  $K_{\text{sampler-air}}$  values were determined by dividing the concentration of a chemical compound in the sampler ( $\text{ng m}^{-3}$ ) by the concentration of the chemical compound in air ( $\text{ng m}^{-3}$ ). For each chemical, the equilibrium phase was determined with the calculated EAVs over time; until no increase in EAV was observed. For the PDMS samplers the equilibrium phase was confirmed by the use of additional pre-spiked samplers; equilibrium was reached when the EAV of a chemical compound in both non-spiked and pre-spiked samplers were equal (see Fig. S2).

$K_{\text{sampler-air}}$  derived for the three different types of PDMS (AlteSil™, SSP-M823 and silicone wristband) were comparable (see Fig. S3), with CV's  $\leq 2.9\%$ . Overall,  $K_{\text{sampler-air}}$  (in  $\text{m}^3 \text{air m}^{-3}$  sampler) for PUF was a factor 10 lower than  $K_{\text{sampler-air}}$  for PDMS (see Fig. 3). This is mainly due to the lower density of PUF compared to PDMS (see Fig. S6 for  $K_{\text{sampler-air}}$  in  $\text{m}^3 \text{air kg}^{-1}$  sampler). The result demonstrates that, per volume of sampler, PDMS has a higher sorptive capacity than PUF and consequently PDMS can be deployed for longer duration than PUF while remaining in the linear uptake phase (Okeme et al., 2016b). The factor 10 higher  $K_{\text{sampler-air}}$  for PDMS compared to PUF agreed well with experimental and calculated values for PUF and PDMS in literature (Okeme et al., 2017; Sprunger et al., 2007; Kamprad and Goss, 2007; Francisco et al., 2017; Parnis et al., 2016).

## 4. Discussion

### 4.1. Sampling rates versus air velocity

Sampling rates depend on the air velocity (wind speed). A

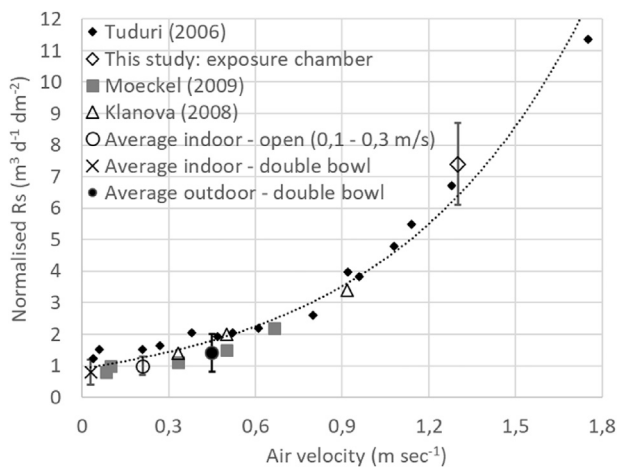
higher air velocity increases the sampling rate by decreasing the air-side boundary layer surrounding the passive sampling material (Tuduri et al., 2006; Bartkow et al., 2005; Klanova et al., 2008; Moeckel et al., 2009). Consequently, because of the high air velocity of  $1.3 \text{ m s}^{-1}$  in the exposure chamber experiments, the generic Rs of  $7.6 \pm 1.3 \text{ m}^3 \text{d}^{-1} \text{dm}^{-2}$  was higher than the (normalized) values from published field experiment studies. The average normalized Rs from 18 field experiment studies was  $0.8 \pm 0.4$  and  $1.0 \pm 0.8 \text{ m}^3 \text{d}^{-1} \text{dm}^{-2}$  for passive samplers used indoors with and without a housing (double bowl), respectively (e.g. Shoeib and Harner, 2002; Hazrati and Harrad, 2007; Saini et al., 2015; Okeme et al., 2016a) and  $1.4 \pm 0.6 \text{ m}^3 \text{d}^{-1} \text{dm}^{-2}$  for deployment outdoors with a double bowl housing (e.g., Chaemfa et al., 2008; Okeme et al., 2018a, 2018b; Persoon and Hornbuckle, 2009; Harner et al., 2013; He and Balasubramanian, 2010; Liu et al., 2016; Melymuk et al., 2011; Bohlin et al., 2014; Abdollahi et al., 2017; Holt et al., 2017; Strandberg et al., 2018; Tuduri et al., 2006).

We plotted sampling rates against wind speed for studies that monitored the air velocities during sampler deployment (Tuduri et al., 2006; Moeckel et al., 2009; Klanova et al., 2008). Since Moeckel et al. and Klanova et al. only measured the windspeed outside the double bowl housing during deployment, we applied a wind dampening factor of 5 to derive the air velocities inside the sampler housing used in these studies. This factor was taken from Tuduri et al. (2006) who measured wind dampening factors of approximately 4–6 for double-bowl sampler housing. The generic Rs of  $7.6 \pm 1.3 \text{ m}^3 \text{d}^{-1} \text{dm}^{-2}$  derived in this exposure chamber study fitted the exponential relationship generated here using literature data (see Fig. 2). To assess whether the average normalized Rs calculated from 18 studies lacking windspeed data also fitted the exponential relationship, we assumed that average air velocities were  $0.1\text{--}0.3 \text{ m s}^{-1}$  and  $2\text{--}4 \text{ m s}^{-1}$  for indoors and outdoors, respectively, being typical values reported for these situations. The response of sampling rate to increased wind speed is consistent with an air-side controlled uptake mechanism and supports the use of a generic Rs. If the wind speed is known, equation (1) may be used for estimating gas-phase sampling rates to apply to field measurements.

**Table 2**  
Partition coefficients  $\log K_{\text{PDMS-air}}$  and  $\log K_{\text{PUF-air}}$  with standard deviation ( $\pm$ SD) for three types of PDMS and PUF.

Compound	PUF	Altesil	Wristband	SSP-M823	Compound	PUF	Altesil	Wristband	SSP-M823
DMP-d4	5.58 ± 1.01	7.51 ± 1.93	6.83 ± 1.32	7.40 ± 1.34	PCBz	4.79 ± 1.17	5.91 ± 1.21	5.88 ± 1.35	5.95 ± 1.10
DMP	5.64 ± 1.08	7.50 ± 1.20	6.85 ± 0.82	7.43 ± 1.09	PCBz (2)	4.77 ± 1.12	5.90 ± 0.95	5.84 ± 1.60	5.92 ± 1.19
DEP-d4	5.58 ± 1.00	7.03 ± 1.64	6.49 ± 1.22	6.97 ± 1.47	HCBz	5.40 ± 1.14	6.45 ± 1.34	6.44 ± 1.22	6.47 ± 1.08
DEP	5.93 ± 2.75	7.83 ± 2.22	7.15 ± 2.55	7.76 ± 2.14	HCBz (2)	5.39 ± 0.77	6.43 ± 1.23	6.40 ± 1.48	6.45 ± 1.31
DIBP-d4	6.81 ± 0.53	8.41 ± 0.31	7.81 ± 0.52	8.20 ± 0.09	alfa-HCH	6.04 ± 1.33	6.57 ± 1.36	6.38 ± 1.85	6.60 ± 0.96
DiBP	6.84 ± 0.32	8.38 ± 2.83	7.83 ± 2.42	8.18 ± 2.61	beta-HCH	7.27 ± 1.34	6.64 ± 1.36	6.52 ± 2.25	6.58 ± 1.45
chlorpropham	6.93 ± 2.85	7.83 ± 3.85	7.65 ± 4.46	7.71 ± 4.99	gamma-HCH	6.41 ± 1.78	6.90 ± 1.39	6.60 ± 1.41	6.88 ± 1.05
fluopyram-benzamide	6.77 ± 0.93	7.88 ± 3.62	7.66 ± 2.36	7.95 ± 2.56	delta-HCH	7.30 ± 4.17	6.95 ± 2.25	6.78 ± 3.93	6.95 ± 1.13
pendimethalin	7.10 ± 0.77	8.15 ± 1.19	8.06 ± 2.05	8.04 ± 2.09	heptachlor	6.24 ± 0.93	7.13 ± 1.15	7.11 ± 1.35	7.13 ± 1.32
toclofos-methyl	7.26 ± 1.72	7.99 ± 3.47	7.98 ± 4.15	7.94 ± 3.35	Aldrin	6.40 ± 1.92	7.43 ± 1.64	7.45 ± 1.28	7.45 ± 1.14
BP-d10	4.60 ± 3.06	5.64 ± 2.43	5.55 ± 2.70	5.68 ± 2.51	telodrin	6.54 ± 0.17	7.50 ± 0.55	7.49 ± 0.69	7.50 ± 0.52
BP-d10 (2)	4.54 ± 1.46	5.6 ± 1.140	5.50 ± 1.85	5.62 ± 1.36	isodrine	6.73 ± 2.11	7.59 ± 2.27	7.61 ± 2.41	7.61 ± 2.27
PCB 1 (PRC)	5.00 ± 1.13	5.96 ± 1.32	5.92 ± 1.52	6.00 ± 1.27	heptachlor-epoxide	6.93 ± 0.52	7.72 ± 0.75	7.61 ± 1.04	7.69 ± 0.91
PCB-2 (PRC)	5.35 ± 0.84	6.20 ± 1.30	6.15 ± 1.55	6.22 ± 1.35	chlordan-trans	7.06 ± 0.47	7.85 ± 0.77	7.79 ± 0.98	7.83 ± 1.11
PCB-3 (PRC)	5.39 ± 0.86	6.22 ± 1.39	6.17 ± 1.78	6.23 ± 1.48	44DDE	7.22 ± 0.63	8.12 ± 2.68	8.14 ± 3.00	8.12 ± 3.42
PCB-10 (PRC)	5.49 ± 0.80	6.33 ± 1.31	6.30 ± 1.35	6.35 ± 1.31	alpha-endosulfan	6.92 ± 0.11	7.81 ± 1.86	7.59 ± 0.01	7.82 ± 2.69
PCB-14 (PRC)	5.87 ± 0.73	6.71 ± 1.27	6.66 ± 1.35	6.72 ± 1.17	chlordan-cis	7.10 ± 0.54	7.76 ± 0.53	7.75 ± 0.49	7.74 ± 0.51
PCB-30 (PRC)	5.85 ± 0.70	6.77 ± 1.30	6.73 ± 1.17	6.77 ± 1.24	24DDE	7.24 ± 1.17	8.28 ± 0.15		
PCB-50 (PRC)	6.34 ± 0.30	7.13 ± 0.80	7.12 ± 1.05	7.14 ± 0.95	dieldrin	7.03 ± 0.24	8.05 ± 1.16	7.86 ± 0.67	7.99
PCB-28	6.44 ± 0.37	7.18 ± 0.84	7.13 ± 1.19	7.18 ± 1.02	24DDD		8.30 ± 0.58		
PCB-21 (PRC)	6.45 ± 0.40	7.19 ± 0.78	7.17 ± 1.05	7.20 ± 0.93	endrin	7.15 ± 0.30	8.22 ± 0.56	8.02 ± 1.22	
PCB-52	6.75 ± 0.44	7.44 ± 0.83	7.40 ± 0.76	7.44 ± 0.69	cashmeron	5.05 ± 1.11	7.18 ± 2.36	6.61 ± 1.37	6.93 ± 0.46
PCB-104 (PRC)	6.72 ± 0.41	7.48 ± 0.80	7.47 ± 0.73	7.49 ± 0.74	celestolide	5.85 ± 0.67	7.69 ± 1.33	7.35 ± 1.41	7.67 ± 0.67
PCB-55 (PRC)	7.11 ± 0.62	7.83 ± 0.47	7.80 ± 0.55	7.83 ± 0.65	phantolide	5.99 ± 0.62	7.64 ± 1.27	7.33 ± 0.84	7.64 ± 0.58
PCB-101	7.18 ± 0.81	8.01 ± 0.41	7.98 ± 1.17	8.00 ± 1.13	musk-ambrette	6.48 ± 0.52	7.44 ± 0.91	7.13 ± 0.71	7.39 ± 0.81
PCB-78 (PRC)	7.28 ± 0.55	8.07 ± 0.29	8.01 ± 1.20	8.04 ± 1.07	traseolide	6.54 ± 0.51	8.12 ± 2.04	7.85 ± 1.46	8.22 ± 0.72
PCB-145 (PRC)	7.22 ± 0.86	8.11 ± 0.44	8.09	8.05	galaxolide	6.30 ± 0.44	7.97 ± 1.67	7.72 ± 1.28	8.02 ± 1.20
1,6-dimethyl naphthalene	4.52 ± 2.15	5.64 ± 1.64	5.56 ± 1.98	5.67 ± 1.63	tonalide	6.37 ± 0.77	7.97 ± 1.46	7.70 ± 1.15	8.01 ± 0.32
1-methyl naphthalene	4.10 ± 2.47	5.28 ± 1.32	5.18 ± 2.23	5.28 ± 2.18	musk-xyleen	6.44 ± 0.19	7.30 ± 0.45	7.21 ± 0.73	7.30 ± 0.54
2,6-dimethyl naphthalene	4.44 ± 2.06	5.57 ± 1.62	5.50 ± 1.91	5.61 ± 1.60	musk-moskeen	6.52 ± 0.31	7.50 ± 0.57	7.33 ± 1.05	7.50 ± 0.72
2-methyl naphthalene	4.04 ± 1.53	5.20 ± 1.04	5.12 ± 1.42	5.21 ± 1.56	musk-tibeteen	6.81 ± 0.89	7.55 ± 0.89	7.51 ± 0.77	7.60 ± 0.39
naphthalene	3.81 ± 3.80	4.78 ± 3.55	4.96 ± 7.67	4.65 ± 1.42	musk-ke-ton	7.19 ± 0.27	8.16 ± 0.60	7.93 ± 0.01	8.14 ± 0.01
acenaphthylene	5.09 ± 1.43	5.71 ± 1.66	5.66 ± 1.57	5.70 ± 1.89	carvone R + S	4.31 ± 1.06	6.53 ± 2.50	5.70 ± 1.98	6.47 ± 2.71
acenaphthene	5.07 ± 0.34	5.87 ± 1.44	5.80 ± 1.34	5.86 ± 1.45	thymol	6.10 ± 2.76	6.32 ± 8.92	6.15 ± 9.59	6.09 ± 5.79
fluorene	5.61 ± 0.64	6.27 ± 1.49	6.22 ± 1.41	6.27 ± 1.50	4-chloro-3-methylphenol	6.29 ± 0.71	5.86 ± 1.04	5.74 ± 2.05	5.82 ± 1.09
phenanthrene	6.22 ± 0.61	6.73 ± 0.88	6.69 ± 0.46	6.74 ± 0.54	eugenol	5.52 ± 3.47	6.59 ± 5.55	6.08 ± 2.56	6.23 ± 2.63
anthracene	6.59 ± 0.79	7.04 ± 1.98	7.02 ± 1.62	7.07 ± 1.51	2-phenylphenol	6.63 ± 0.80	6.25 ± 1.24	6.19 ± 7.04	6.22 ± 1.44
fluoranthene	7.08 ± 0.25	7.55 ± 0.35	7.53 ± 0.34	7.57 ± 0.33	diphenylamine	7.59 ± 2.56	6.77 ± 1.17	6.63 ± 4.03	6.75 ± 0.81
Pyrene	7.19 ± 0.38	7.66 ± 0.37	7.65 ± 0.27	7.67 ± 0.35	diphenylamine (duplicate)	7.19 ± 2.38	7.35 ± 7.76	7.32 ± 6.16	7.38 ± 7.38
TEP	5.32 ± 1.32	7.90 ± 2.56	7.18 ± 2.52	7.80 ± 1.82	benzylbenzoate	6.42 ± 1.36	7.66 ± 1.00	7.20 ± 2.11	7.60 ± 0.98
TIPP	4.58 ± 2.78	8.09 ± 7.67	6.96 ± 4.53	7.91 ± 7.97	benzophenone	5.85 ± 0.86	7.24 ± 2.29	6.96 ± 5.69	7.20 ± 1.45
TPP	5.48 ± 2.45	8.67 ± 2.50	7.75 ± 2.35		caffeine	6.62 ± 4.23			
TMPP	6.66 ± 3.12	7.13 ± 4.22	7.02 ± 2.81	7.14 ± 3.42	DEET	6.38 ± 1.40			
HCBD	3.39 ± 0.8	4.94 ± 1.32	4.80 ± 2.03	4.94 ± 1.37					
HCBD (2)	3.39 ± 0.76	4.88 ± 1.29	4.81 ± 2.25	4.91 ± 1.21					

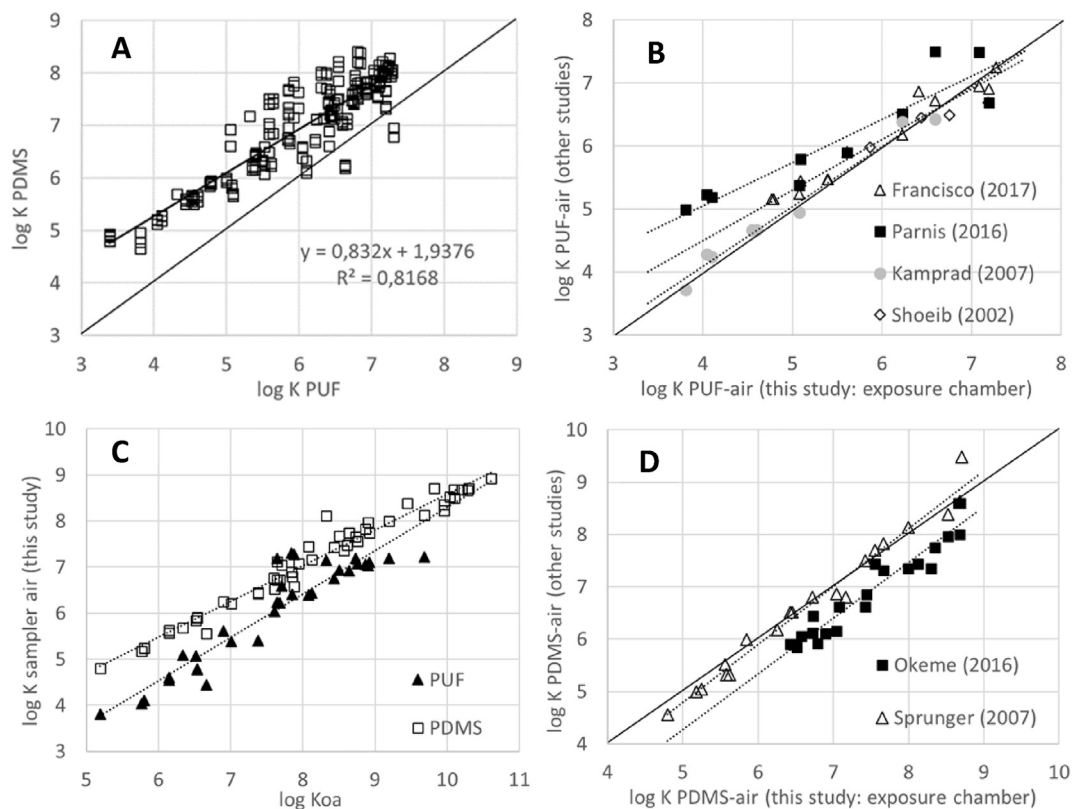
$$R_s (\text{m}^3 \text{d}^{-1} \text{dm}^{-2}) = 0.922 \exp(1.489 * \text{air velocity} (\text{m sec}^{-1})) \quad (1)$$



**Fig. 2.** The exponential relationship between air velocity ( $\text{m sec}^{-1}$ ) and sampling rate ( $\text{m}^3 \text{d}^{-1} \text{dm}^{-2}$ ) derived from three wind effect studies (Tuduri et al., 2006; Moeckel et al., 2009; Klanova et al., 2008), including the generic  $R_s$  derived in this study.

#### 4.2. Partition coefficients

The derived Ksampl-air values for PDMS and PUF in the exposure chamber experiments were compared with partition coefficients determined experimentally in other studies (Sprunger et al., 2007; Okeme et al., 2016a; Francisco et al., 2017; Parnis et al., 2016; Kamprad and Goss, 2007; Shoeib and Harner, 2002a, 2002b) (see Fig. 3). In these studies,  $\log K_{\text{sampl-air}}$  values were determined for a range of SVOCs such as PAH, OCP and PCB at temperatures between 15 and 25 °C. Okeme et al. (2016a) and Kamprad and Goss (2007) used a gas chromatographic retention method (GC-RT) at 25 °C and 15 °C to derive  $K_{\text{sampl-air}}$ . Sprunger et al. (2007) listed values from different research groups for which the temperature was not exactly known but, as stated, was near 25 °C. Parnis et al. (2016), Francisco et al. (2017) and Shoeib and Harner (2002a, 2002b) derived values in exposure chamber



**Fig. 3.** The relationship between log K PDMS (this study: combined values of the 3 types of PDMS) and log K PUF (this study) (A), the relationship between log K sampler-air in this study and log K sampler-air experimentally determined in other studies for PUF (B) and PDMS (D) for selected PAH, PCB and OCP at 15–25 °C and the relationship between log K sampler-air in this study and log Koa experimentally determined in other studies for PDMS and PUF for selected PAH, PCB and OCP at 20–25 °C (C).

experiments at 22–23 °C.

In general, the log K sampler-air values derived in this study agreed well with the values from other studies. Our log K pdms-air values were similar to the values reported by Sprunger et al. (2007), with a good correlation ( $r^2 = 0.98$ ) and a root mean square error (RMSE) of 0.24. Our K pdms-air values and the K pdms-air values derived with the GC-RT method agreed well ( $r^2 = 0.93$ ) over the entire range of K pdms-air, however the GC-RT values were 0.5 log units (8%) lower than the values from this study. This systematic difference can partly be explained by the difference in experimental temperature of approximately 5 °C between both studies. In accordance with literature (Shoeib and Harner, 2002a, 2002b; Parnis et al., 2016), a temperature increase of 5 °C corresponds with a lower log K sampler-air of approximately 0.2 log units and vice versa. Log K puf-air values derived in this study also corresponded well to the values reported by Kamprad and Goss (2007), Francisco et al. (2017) and Shoeib and Harner (2002a, 2002b), with good correlations ( $r^2 > 0.95$ ) and RMSE between 0.15 and 0.28. The measured K puf-air values reported by Parnis et al. (2016) deviated significantly from our values (RMSE = 0.77), especially for the lower log K puf-air values < 5.

While we and others have measured K sampler-air for many compounds, finding an empirical relationship with the octanol air partition coefficient Koa, would allow extrapolation beyond the measured values. Several approaches for estimating K puf-air for SVOCs from Koa have been reported in literature (Okeme et al., 2017; Zhao et al., 2004; Zhang et al., 2009). Log K sampler-air values for both PUF and PDMS from this study and those in the literature were compared with log Koa values at temperatures between 20 and 25 °C (e.g., Okeme et al., 2017; Shoeib and Harner, 2002a, 2002b; Harner and Bidleman, 1998) (see Fig. 3). K sampler-

air values were compared with Koa values for SVOCs including PAH, OCP and PCB.

For both PUF and PDMS, log K pdms-air was linearly related to log Koa according to the following equations:

$$\log K_{\text{pdms-air}} = 0.778 \log K_{\text{oa}} + 0.813 \quad (2)$$

$$\log K_{\text{puf-air}} = 0.940 \log K_{\text{oa}} - 1.105 \quad (3)$$

A strong correlation was shown between log K sampler-air and log Koa for PDMS ( $r^2 = 0.97$ ) and PUF ( $r^2 = 0.86$ ), however there was greater scatter for PUF, especially for 4 OCPs, which resulted in a lower correlation. The relationship between log Koa and log K puf-air was strongly correlated for the three estimation methods reported by Zhang et al. (2009) and (see Fig. S5). Also, results were consistent with Okeme et al. (2017) who showed that both log Koa and sub-cooled vapor pressure were strongly correlated for many compounds and can be used for estimating K puf-air.

## 5. Conclusions

This study determined overall passive sampling rates for gas-phase chemicals. A generic  $R_s$  of  $7.6 \pm 1.3 \text{ m}^3 \text{ d}^{-1} \text{ dm}^{-2}$  and a generic MTC of  $0.87 \pm 0.15 \text{ cm s}^{-1}$  were derived for PUF and PDMS, as a sheet and as a wristband, using a novel exposure chamber experiment in which we tested 200 chemicals, including PCBs, PAHs, musk compounds, phthalates, pesticides and organophosphate esters, at an air velocity of  $1.3 \text{ cm s}^{-1}$ . It is important to emphasize that differences in  $R_s$  for gas-phase compounds were not found according to passive sampling material, e.g., PUF and PDMS as a sheet vs wristband. Further, we derived a relationship

between sampling rate and windspeed that allows estimation of Rs for a wide range of conditions indoors and outdoors. We have demonstrated that sampling rates for a wide range of gas-phase SVOCs, with PUF and PDMS as sampling media, are similar, without statistically significant differences in Rs and MTC between passive sampler types and chemical groups, supporting the contention that uptake is air-side controlled, regardless of sampling material. This supports the use of a single generic sampling rate for gas-phase compounds depending on air velocity.

Partition coefficients K<sub>sampler-air</sub> for 98 chemicals were determined for PUF and PDMS. In general, K<sub>sampler-air</sub> for PDMS were 10 times higher than for PUF which implies that linear uptake will occur over a longer duration for PDMS than PUF, per volume of sampler. It should be noted that only gas-phase uptake was studied; because of the porosity/structure of PUF, this sampler can have advantages when sampling particle associated chemicals. The values of K<sub>sampler-air</sub> also can be used to estimate the time period over which linear uptake is expected for a specific chemical. The derived partition coefficients in this study corresponded well with the values reported in the literature. Further, equations were derived to estimate K<sub>sampler-air</sub> from K<sub>oa</sub> for gas-phase SVOCs in air and PUF and PDMS. The derived correlation equations in this study for PUF and PDMS can be used for estimating K<sub>sampler-air</sub>. The results show that K<sub>pdms-air</sub> can also be experimentally derived using the GC-RT method, especially for chemicals that will not reach equilibrium over the duration of a typical uptake study.

The results of this study can guide passive sampling strategies. They provide an overview of chemicals that can be assessed with passive sampling, methods for obtaining optimal sampling durations, and methods for interpretation of passive sampler concentrations into gas-phase air concentrations. Finally, the results can be used to estimate gas-phase air concentrations from personal wristband measurements. To do that, further investigation of the air velocity dependence of Rs and the air velocity along wristbands during deployment would be a recommendation for future work.

## Acknowledgments

We thank Foppe Smedes (Masaryk University, Faculty of Science, Research Centre for Toxic Compounds in the Environment) for assisting in the development of the exposure chamber experiments.

## Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.chemosphere.2019.04.043>.

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