



Characterization of polyurethane foam (PUF) and sorbent impregnated PUF (SIP) disk passive air samplers for measuring organophosphate flame retardants



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HIGHLIGHTS

- Organophosphate esters (OPEs) are measured in urban air.
- PUF disk and SIP disk samplers are calibrated for OPEs.
- Sampling rates (R) for PUF and SIP disks are close to default value of 4 m³/day.
- COSMO-RS solvation theory was used to estimate $K_{\text{PUF-Air}}$ for the OPEs.

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ABSTRACT

This study aimed to characterize the uptake of organophosphate esters (OPEs) by polyurethane foam (PUF) and sorbent-impregnated polyurethane foam (SIP) disk passive air samplers (PAS). Atmospheric OPE concentrations were monitored with high-volume active air samplers (HV-AAS) that were co-deployed with passive air samplers. Samples were analyzed for tris(2-chloroisopropyl) phosphate (TCIPP), tri(phenyl) phosphate (TPhP), tris(2-chloroethyl) phosphate (TCEP), and tris(2,3-dichloropropyl) phosphate (TDCIPP). The mean concentration of \sum OPEs in air was 2650 pg/m³ for the HV-AAS. Sampling rates and the passive sampler medium (PSM)-air partition coefficient ($K_{\text{PSM-Air}}$) were calculated for individual OPEs. The average calculated sampling rates (R) for the four OPEs were 3.6 ± 1.2 and 4.2 ± 2.0 m³/day for the PUF and SIP disks, respectively, and within the range of the recommended default value of 4 ± 2 m³/day. Since most of the OPEs remained in the linear uptake phase during the study, COSMO-RS solvation theory and an oligomer-based model were used to estimate $K_{\text{PUF-Air}}$ for the OPEs. The estimated values of $\log K_{\text{PUF-Air}}$ were 7.45 (TCIPP), 9.35 (TPhP), 8.44 (TCEP), and 9.67 (TDCIPP). Finally, four configurations of the PUF and SIP disks were tested by adjusting the distance of the gap opening between the upper and lower domes of the sampler housing: i.e. 2 cm, 1 cm, no gap and 1 cm overlap. The sampling rate did not differ significantly between these four configurations ($p < 0.05$).

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1. Introduction

Organophosphate esters (OPEs) are used for a variety of industrial purposes, including flame retardants, plasticizers, stabilizers, antifoaming and wetting agents and additives (Marklund et al.,

2003). Recently, since the ban of some brominated flame retardants (BFRs) (EU, 2003; Betts, 2008; UNEP, 2009; BSEF, 2012), the use of OPEs as replacements has increased. Despite these increases in the use of OPEs, some of them have been reported to be persistent and to bioaccumulate in biota (Van den Eede et al., 2011; Van der Veen and Boer, 2012). In addition, OPEs are known to be potentially carcinogenic and toxic to aquatic organisms and animals and to cause skin irritation for humans (WHO, 2000; Pakalin et al.,

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2007; Reemtsma et al., 2008; Liu et al., 2014; Zhang et al., 2016).

Since OPEs are mostly used as additives, and not chemically bonded to the polymeric structure, they have the potential to migrate from products into the environment through dissolution, abrasion and volatilization (Van der Veen and Boer, 2012). These chemicals have been observed in high concentrations in air and water, even in remote areas (Marklund et al., 2003; Mihajlović et al., 2011; Möller et al., 2011, 2012; Salamova et al., 2013; Shoeib et al., 2014; Hoffman et al., 2015, Sühling et al., 2016). Thus, there is an incentive to study and better understand their environmental mobility, fate and effects.

Passive air samplers (PAS) and especially polyurethane foam (PUF) disk type PAS are being increasingly used for studies on flame retardants (FRs) and other persistent organic pollutants (POPs) in air. Their simplicity and low cost makes them popular, especially for spatial studies and for sampling in remote areas where electricity is not available to operate active air samplers (Melymuk et al., 2011, 2014; Möller et al., 2011, 2012; Tuduri et al., 2012; Salamova et al., 2013; Ahrens et al., 2013; Shoeib et al., 2014; Hoffman et al., 2015). The PUF-PAS have been used under the Global Atmospheric Passive Sampling (GAPS) Network since 2005 to provide comparable global-scale data for assessing air burdens and long-range transport of POPs and emerging contaminants (Poza et al., 2006). The applicability of the PUF-PAS to more volatile compounds was made possible by the development of the sorbent impregnated polyurethane foam (SIP) or SIP-disk sampler (Ahrens et al., 2013; Shoeib et al., 2008). However, in order to utilize PUF-PAS and SIP-PAS for providing accurate measurements of emerging chemicals in air they must first be calibrated; this typically involves an uptake study where active air samplers are deployed alongside the passive air samplers to derive a linear phase sampling rate (R) (Shoeib and Harner, 2002). Under typical sampling conditions and for most POP-like chemicals, R-values for the GAPS-type sampler are shown to be about 4 m³/day for both gas-phase and particle-phase chemicals, although elevated sampling rates have been observed at sites characterized by high winds (Shoeib and Harner, 2002; Shoeib et al., 2008; Chaemfa et al., 2008; Klanova et al., 2008; Petrich et al., 2013). The uptake study results can also be used, in some cases, to estimate the passive sampler medium (PSM)-air partition coefficient ($K_{\text{PSM-Air}}$) for chemicals that come to equilibrium during the time-course of the uptake study (Shoeib and Harner, 2002). Another option for estimating $K_{\text{PSM-Air}}$ is by using computational methods. For instance Parnis et al. (2015, 2016) applied COSMO-RS, a quantum chemical-based solvation theory estimation method to estimate PUF-air partition coefficients ($K_{\text{PUF-Air}}$) for polycyclic aromatic hydrocarbons (PAHs). A key benefit of COSMO-RS is that it does not require training data as other estimation methods do.

In this study we characterize the PUF and SIP disk samplers for the uptake of OPEs based on a field uptake study carried out in Toronto during 2010 against conventional high volume air samplers. The specific objectives include:

- (i) to report the concentrations of OPEs in urban outdoor air in Toronto over a period of several months in 2010 using high-volume active air samplers (HV-AAS)
- (ii) to use these air measurements to assess the sampling rates (R-values) and $K_{\text{PSM-Air}}$ values for OPEs for PUF and SIP disks that were co-deployed over the same time period
- (iii) to compare the experimental estimates for $K_{\text{PUF-Air}}$ to computed values derived from COSMO-RS
- (iv) to compare performance of four different configurations of the PUF and SIP disk samplers

2. Materials and methods

2.1. Sampling

The calibration of the PAS was performed at a semi-urban meteorological station in Toronto (Environment and Climate Change Canada field site, 43°46' N, 79°28' W) from March 30 to October 13, 2010. HV-AAS were collected one to two times a week, with approximately 330 m³ of air collected over each 24 h sampling period (PS-1 type sampler, Tisch Environmental, Cleves, OH, USA). The OPEs were collected on a glass-fiber filter (GFF) (Type A/E Glass, 102 mm diameter, 1 μm pore size, Pall Corporation) that traps the particle phase, followed by a PUF/XAD-2 cartridge (the PUF/XAD-2 cartridge consisted of 15 g of XAD-2 resin (SupelpakTM-2, precleaned from Supelco) sandwiched between a PUF plug (76 mm diameter and 60 mm thick, precleaned from Supelco) that was cut in half) for trapping gas-phase compounds. Previous studies have shown that OPEs are present in ambient air almost entirely on particles (Carlsson et al., 1997; Melymuk et al., 2011; Möller et al., 2011, 2012) and similarly here, the OPEs on the HV-AAS PUF were below detection (Shoeib et al., 2014). However, some studies have also reported OPEs in the gas-phase, which are likely attributed to ultrafine particles that are not captured efficiently by GFF, depending on the pore size (Sühling et al., 2016; Wolschke et al., 2016). Parallel samples were collected using two different PAS media (i.e., PUF and SIP disks), which were deployed for 7, 21, 28, 42, 56, 84, 112, 140, 168, and 197 days. Duplicate PUF and SIP disks were collected on days 28, 84, and 197 to verify reproducibility. PUF disks (14 cm diameter × 1.35 cm thick; surface area 365 cm², mass 4.40 g, volume 207 cm³, Tisch Environmental, Cleves, OH, USA) were pre-cleaned before sampling and SIP-PAS were impregnated with finely ground XAD-4 resin (Supelco, Bellefonte, PA) (approximately 0.5 g per PUF disk) and prepared according to the protocol from Shoeib et al. (2008) (for details, see supporting information (SI)). During field deployment, the SIP and PUF disks were housed inside pre-cleaned stainless steel chambers (with spacing between the domes following the “GAPS default” design, Model TE-200-PAS, Tisch Environmental) and deployed approximately 2 m above the ground. Details regarding the passive and active air sample collection, including quality assurance/quality control (QA/QC) aspects are discussed in the SI and have been reported previously (Shoeib et al., 2014; Ahrens et al., 2013). Field blanks (n = 6 for both PUF and SIP) were collected intermittently by exposing the sampling media for a few seconds and then treating it as a collected sample.

In addition, four configurations of the PUF and SIP disks were tested by adjusting the distance of the gap opening between the upper and lower domes of the sampler housing (i.e., “GAPS default” with 1 cm overlap, “flush chamber” with no overlap, “1 cm gap chamber”, and a “2 cm gap chamber”) (Fig. S1). The PUF and SIP disks were co-deployed in the different chamber configurations for 28 days. All samples were stored at −20 °C until extraction within four weeks. Details of the sampling, dates, air volume, and meteorological data are presented in the SI (Tables S1 and S2, Fig. S2). The samples were screened for the following compounds: TDCIPP, TDBPP, TCEP, TCPP (isomers TCiPP, TCPP2 and TCPP3), TPhP, EHDPP, TBEP, TEHP, TCP (isomers o, p, and m), TPPP, TDMPP and TTBP (see Table S3 in the SI for all names and CAS numbers), but only tris(2-chloroisopropyl) phosphate (TCIPP), tris(2-chloroethyl) phosphate (TCEP), tri(phenyl) phosphate (TPhP) and tris(2,3-dichloropropyl) phosphate (TDCIPP) were detectable and above the method detection limit (MDL) (for details, see SI).

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