Determination of silicone-air partition coefficients for passive air sampling of SVOCs

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Introduction

Semivolatile organic compounds (SVOCs) are omnipresent in the indoor environment. They originate from common indoor equipment and processes. Physical properties of SVOCs cause them distribute from a source to both the gaseous and the particulate phase (dust particles). Passive sampling is a powerful tool of determination of inhalation exposure to these potentially harmful compounds in the indoor environment. Silicone rubber, a non-porous polymer that has been routinely used for passive sampling of water, could be employed as a suitable sampler of SVOCs also in air. One of important parameters of a passive sampler is a partition coefficient *K* between the sampler, e.g. silicone rubber (SR) and the sampled environment, e.g. air (A). It serves as an indicator of duration of linear phase of the compound sorption to the sampler and also describes the capacity of the sampler for gas-phase uptake. The duration of linear phase is important for determination of air concentration - assuming air-side controlled uptake, the use of a generic sampling rate R_s for calculation of air concentration is justifiable for a broad range of SVOCs. In this study, we determined K_{SR-A} for selected polyaromatic hydrocarbons (PAHs), polychlorinated biphenyls

Methods

Preparation of silicone rubber:

 cutting of SR sheets (Altesil, 0.5 mm) into 4 pieces of 7×28 cm and Soxhlet-extraction (PCBs) and organochlorinated pesticides (OCPs) using a chamber design with a passive doser of SVOCs (Fig. 1), which enables creating controllable conditions.

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- for 40 hours in ethylacetate to remove oligomers and impurities
- gradual spiking of target SVOCs (PAHs, PCBs, OCPs) in MeOH:water solution (final MeOH concentration 35 % (v/v))

Preparation of Tenax TA tubes:

 soxhlet-extraction in hexane after each analysis and drying in vacuum rotary evaporator

Equilibration experiment

- flow rate set to 200 cm³/min
- air volume: 12 I, 60 I, 300 I, 1500 I, 7200 I
- temperature 25 °C

Determination of concentration:

- c_A: Tenax TA tubes were analysed on GC-MS with thermal desorption unit (TDU).
 Compounds were desorbed at 300 °C, cryotrapped and transferred to GC column.
- c_{SR}: approximately 60 mg of dosing sheet was cut and extracted in 10 ml hexane for 3 hours on a shaker. The extract was removed and stored and the procedure was repeated with fresh solvent. Both extracts were combined and reduced to final volume of 1 ml. 10 µl of the extract was spiked to a clean Tenax TA tube



Fig. 1 Scheme of chamber apparatus used in the equilibration experiment. Pink arrows indicate direction of air flow, while blue area shows a doser consisting of silicone rubber with surface area of approximately 1570 cm².



 $K_{SR-A} =$ (1)

Conclusions

- ✓ K_{SR-A} values measured in this study corresponds well with the values reported in the literature
- ✓ sampling of more volatile compounds needs to be done at low volumes and repeatedly
- Iess volatile SVOCs tend to stay in SR and it is challenging to mobilise them to gas phase even when a great volume of air is pumped, which indicates high capacity of SR for such compounds

