

Limitations of modelling tools for calculating the gas-particle distribution of organic pollutants in the indoor environment

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In environmental sciences, the physical and chemical properties of compounds are frequently applied for modelling their distribution between air, soil and water. A similar approach is used in indoor sciences for estimating their distribution and dynamics between gas phase, particle phase and settled dust for estimating human exposure. This, however, requires a detailed understanding of the environmentally important compound parameters, their interrelation and of the algorithms for calculating kinetic and partitioning coefficients.

The gas/particle partitioning of semi volatile organic compounds with relevance for the indoor environment is usually estimated on basis of physico-chemical models (see equation 1 with C_p = concentration in the particle phase, C_g = concentration in the gas phase, [TSP] = concentration of the total suspended particles, K_p = gas/particle distribution coefficient). The parameters of major concern for the determination of K_p are the saturation vapor pressure (p_0), the Henry's law constant (H), the octanol/water partition coefficient (K_{OW}), the octanol/air partition coefficient (K_{OA}) and the air/water partition coefficient (K_{AW}).

$$\frac{C_p}{C_p + C_g} = \frac{[TSP] \cdot K_p}{1 + [TSP] \cdot K_p} \quad (1)$$

For the partitioning between the gas phase and settled house dust, equation (2) can be applied with $f_{om,dust}$ = volume fraction of organic matter, ρ_{dust} = density of settled dust (Weschler and Nazaroff, 2010).

$$X_{dust,pred} = \frac{f_{om,dust} \cdot K_{OA} \cdot C_g}{\rho_{dust}} \quad (2)$$

For most of the relevant organic compounds reliable experimental data are not available. Therefore, calculated gas/particle distributions and fractions can widely differ due to the uncertainties in predicted p_0 and K_{OA} values. This is not a serious problem if the target compound is of very low ($< 10^{-6}$ Pa) or very high ($> 10^{-2}$ Pa) volatility, but in the intermediate region even small changes in p_0 or K_{OA} will have a strong impact on the expected partition behaviour.

The precision in prediction can be strongly affected by a superposition of model uncertainties and uncertainties in the physical parameters. The different algorithms (EPIWIN, SPARC) and extrapolation methods lead to partially significant deviations in the predicted values (Schossler et al., 2011). Moreover many algorithms do not distinguish between structural isomers. This is of high relevance since some compounds are applied as isomeric mixtures.

As shown in Figure 1, the indoor particle concentration [TSP], which is often assumed as $20 \mu\text{g}/\text{m}^3$, also has a strong influence on the particle associated fraction.

The K_{OA} value can only be used for particle absorption from the gas phase if the organic portion of the particle is high. The same is true for absorption in settled house dust. The octanol-air distribution coefficient K_{OA} is commonly derived from the octanol-water (K_{OW}) and the air-water (K_{AW}) coefficient by $K_{OA} = K_{OW}/K_{AW}$. Moreover, K_{AW} and p_0 are fundamentally related to Henry's law constant (H).

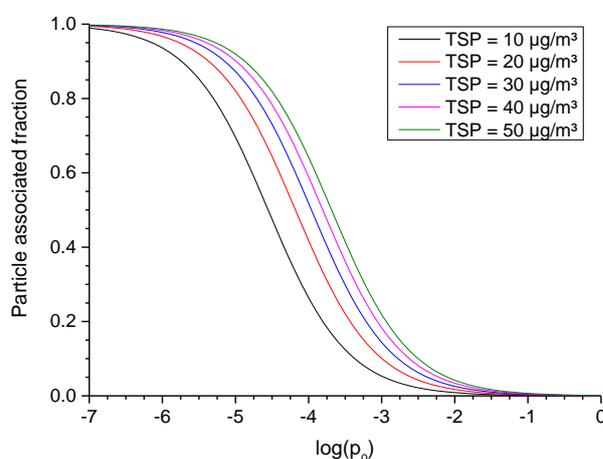


Figure 1. : The particle associated fraction of an organic compound in dependence of vapour pressure p_0 and TSP concentration.

In this work it is shown, how parameter uncertainties and variations of indoor conditions might influence the distribution behaviour of compounds in the indoor environment. A problem might occur for compounds of medium volatility. The description of their gas-/particle distribution behaviour is due to large errors (Salthammer and Schripp, 2015). Good estimates for the distribution of SVOCs between gas and particle phase are only possible when the great majority of SVOCs ($> 90\%$) can be expected in the gas phase or particle phase, respectively.

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