

SUPPLEMENTARY MATERIAL

Dermal absorption of semivolatile organic compounds from the gas phase: sensitivity of exposure assessment to key parameters

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Contents

Intermediate equations used to derive the SVOC transdermal permeability coefficient and to estimate the gas phase concentration from its concentration in total indoor air.

Transdermal permeability coefficient

The transdermal permeability coefficient, k_{p-g} (m/h), is calculated using a resistors-in-series approach proposed by Weschler and Nazaroff (2012):

$$\frac{1}{k_{p-g}} = \frac{1}{\gamma_d} + \frac{1}{k_{p-b}} \quad (1)$$

Where γ_d is the coefficient that describes the external transport of an SVOC from the gas phase in the core of a room through the boundary layer adjacent to the skin (m/h) and k_{p-b} is the compound's permeability coefficient which describes the SVOC's transport from the gas phase at the skin surface through the epidermis to the dermal capillaries (m/h) and is estimated as follows:

$$k_{p-b} = \frac{k_{p-w}}{K_{gw}} \quad (2)$$

Where K_{gw} is the equilibrium partition coefficient for the SVOC between the gas phase and water and can be estimated as follows (Meylan and Howard, 1991):

$$K_{gw} = \frac{H}{RT} \quad (3)$$

Where H is the Henry's law constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$), R is the gas constant ($8.314 \text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}$) and T is temperature (K).

In Equation 2, k_{p-w} is the compound's permeability coefficient through the stratum corneum/viable epidermis when the vehicle in contact with skin is water (cm/h) and is estimated as follows:

$$k_{p-w} = \frac{k_{p-cw}}{1 + B} \quad (4)$$

Where k_{p-cw} is the compound's permeability coefficient through the stratum corneum when the vehicle in contact with the skin is water (cm/s) and is estimated using Equation 5 (Mitragotri, 2002):

$$\log(k_{p-cw}) = 0.7 \times \log(K_{ow}) - 0.0722 \times MW^{\frac{2}{3}} - 5.252 \quad (5)$$

Where K_{ow} is the species octanol-water partition coefficient and MW is the molecular weight of the compound (g/mol). However, this may lead to greater uncertainty when $MW > 400$ (Mitragotri, 2002).

In Equation 4, B is the ratio of the stratum corneum permeability (k_{p-cw}) to the viable epidermis permeability for the selected compound and is estimated using Equation 6 (Bunge et al., 1995):

$$B = \frac{k_{p-cw} \times MW^{0.5}}{2.6} \quad (6)$$

Where k_{p-cw} is expressed in cm/h.

SVOC gas phase concentration

SVOC gas phase concentration (C_g) can be estimated from its concentration in total indoor air (C_a) using a partitioning model proposed by Weschler and Nazaroff (2010):

$$C_g = \frac{C_a}{1 + ([TSP] \times K_p)} \quad (7)$$

Where $[TSP]$ is the total suspended particle concentration ($\mu\text{g}/\text{m}^3$) and K_p is the gas/particle distribution coefficient ($\text{m}^3/\mu\text{g}$). K_p can be estimated according to Equation 8 (Weschler and Nazaroff, 2010):

$$K_p = \frac{f_{om-part} \times K_{oa}}{\rho_{part} \times 10^6} \quad (8)$$

Where $f_{om-part}$ is the volume fraction of organic matter associated with airborne particles, ρ_{part} is the density of airborne particles (g/m^3) and K_{oa} is the octanol/air partition coefficient. K_{oa} can be estimated according to Equation 9:

$$K_{oa} = \frac{K_{ow} \times R \times T}{H} \quad (9)$$

Where K_{ow} is the octanol/water distribution coefficient, H is the Henry's law constant ($\text{Pa}\cdot\text{m}^3/\text{mol}$), R is the gas constant ($8.314 \text{ Pa}\cdot\text{m}^3/\text{mol}\cdot\text{K}$) and T is temperature (K).

We combined these equations to express and estimate C_g from C_a as follows:

$$C_g = \frac{C_a}{1 + ([TSP] \times \frac{f_{om-part} \times K_{ow} \times R \times T}{\rho_{part} \times 10^6 \times H})} \quad (10)$$

When using these models we made the implicit assumption that SVOC are in equilibrium between gas and particulate phases.

References

Bunge, A.L. Cleek, R.L and Vecchia, B.E. (1995) A new method for estimating dermal absorption from chemical exposure. 3. Compared with steady-state methods for prediction and data analysis, *Pharm. Res.*, 12, 972-982.

Meylan, W. and Howard, P. (1991) Bond contribution method for estimating Henry's law constants, *Environ. Toxicol. Chem.*, 10, 1283-1293.

Mitragotri, S. (2002) A theoretical analysis of permeation of small hydrophobic solutes across the stratum corneum based on scaled particle theory, *J. Pharm. Sci.*, 91, 744-752.

Weschler, C.J. and Nazaroff, W.W. (2012) SVOC exposure indoors: fresh look at dermal pathways, *Indoor Air*, 22, 356-377.

Weschler, C.J. and Nazaroff, W.W. (2010) SVOC partitioning between the gas phase and settled dust indoors, *Atmos. Environ.*, 44, 3609-3620.