Supplementary Information for

Assessing Human Exposure to Chemicals in Materials, Products and Articles:

A Modular Mechanistic Framework

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1) <u>Nomenclature</u>

Acontact	Contact area between skin and sink surface (m ²)					
A_{exp}	Exposed body surface area (m ²)					
$A_{mouthing}$	Mouthed object surface area (m ²)					
A_s	Surface area of sink (non-source) surfaces (m ²)					
A_{ss}	Surface area of source surfaces (m ²)					
АСН	Air change rate; $ACH = Q/V(1/h)$					
AR _{source}	Application rate of source (µg/h)					
bw	Body weight (kg)					
C_0	Material-phase SVOC concentration (µg/m ³)					
$C_{\rm a,sat}$	Saturation concentration in air ($\mu g/m^3$)					
Cm	SVOC concentration in clothing material ($\mu g/m^3$)					
$C_{o,sat}$	Saturation concentration in octanol (µg/m ³)					
C_{pm}	Gas-phase SVOC concentration in porous material (µg/m ³)					
C_s	Concentration of SVOCs on sink surfaces (µg/m ²)					
C _{ssl}	Concentration of SVOCs associated with skin-surface lipids (μ g/m ³)					
C_t	Particle- and gas-phase SVOC concentration in the gas phase (μ g/m ³)					
CR_s	Rate of contact with sink surfaces (m ² /h)					
d	Exposure duration (h)					
Da	Diffusion coefficient of the SVOC in air (m ² /h)					
D_m	Diffusion coefficient of the SVOC in clothing material (m ² /h)					
DI	Daily intake (μg/kg)					
Ε	Emission rate of SVOCs from source materials (µg/(m ² ·h))					
EF	Exposure frequency (1/h)					
Ex_{cloth_d}	Dermal exposure rate to clothing (μg/h)					
Ex _{dust_ing}	Dust ingestion exposure rate (µg/h)					
Ex _{gas_d}	Transdermal exposure rate from the gas phase (μ g/h)					
Exinh	Inhalation exposure rate (µg/h)					
Exmouthing	Mouthing exposure rate for mouthing of source (μ g/h)					
$Ex_{mouthing_other}$	Mouthing exposure rate for mouthing of objects with sink surfaces (µg)					
Ex _{part_d}	Transdermal exposure rate for particles adhered to exposed skin (μg/h)					
Ex_{source_d}	Exposure rate for direct contact of source with the skin (μ g/h)					
Ex _{source_ing}	Source ingestion exposure rate (µg/h)					
Ex _{surf_d}	Transdermal exposure rate for dermal contact with sink surfaces (μg/h)					
F	Particle-phase concentration of SVOCs in indoor environments (µg/m ³)					
Fout	Outdoor particle-phase concentration of SVOCs (µg/m ³)					
f_A	Fraction of chemical available for uptake (-)					
fom_dust	Fraction of organic matter in dust (-)					
fom_part	Fraction of organic matter associated with airborne particles (-)					
fret	Retention fraction of a source (-)					
Н	Henry's law constant (m³·Pa/mol)					
h _{m,s}	Mass transfer coefficient for the sink (non-source) surface (m/h)					
h_m	Mass transfer coefficient for the surface of a source (m/h)					

IR _{dust}	Dust intake rate (g/h)					
IR _{inh}	Inhalation intake rate (m ³ /h)					
IR _{source}	Source intake rate (g/h)					
i	Represents a specific SVOC out of N SVOCs (-)					
source_ssl	Flux from source to skin-surface lipids $(\mu g/(m^2 \cdot h))$					
ssl_c	Flux from skin-surface lipids to dermal capillaries ($\mu g/(m^2 \cdot h)$)					
k_{p_g}	Transdermal permeability coefficient from the gas phase (m/h)					
k_{p_ssl}	Transdermal permeability coefficient from the skin-surface lipids to dermal capillaries (m/h)					
K _{dust}	Dust/gas partition coefficient (m^3/g)					
Kaw	Air/water partition coefficient (-)					
K _{ca}	Clothing/gas partition coefficient (-)					
Km	Dust/material partition coefficient (m^3/g)					
Koa	Octanol/air partition coefficient (-)					
Kow	Octanol/water partition coefficient (-)					
Kp	Gas/particle partition coefficient of SVOCs $(m^2/\mu g)$					
Ks	Sink surface/gas partition coefficient (m)					
K _{ssl}	Partition coefficient between skin-surface lipids (SSL) and clothing (-)					
L	Thickness of the porous material (m)					
Lc	Characteristic length (m)					
L_m	Thickness of clothing material (m)					
Ms	Mass loading of settled dust on sink (non-source) surfaces ($\mu g/m^2$)					
M_{ss}	Mass loading of settled dust on source surface ($\mu g/m^2$)					
MR	Migration rate during mouthing $(g/(m^2 \cdot h))$					
m _x	Dust mass concentration at the depth of x ($\mu g/m^3$)					
n	Freundlich constant (-)					
Ν	Number of SVOCs considered (-)					
$P_{dust.s}$	Concentration of SVOCs in the dust settled on the sink (non-source)					
	surfaces (ug/g)					
P _{dust}	Concentration of SVOCs in the dust settled on the source surface(ug/g)					
P_{p}	Size-dependent particle penetration factor (-)					
p_s	Saturation vapor pressure of pure SVOCs (Pa: mmHg)					
0	Ventilation rate (m^3/h)					
€ Q nart_skin	Transfer rate from particles adhered to skin (m/h)					
R	Universal gas constant (m ³ ·Pa/(K·T))					
R_{p}	Size-dependent particle resuspension rate (1/h)					
Re	Revnolds number					
r _{uptake}	Chemical uptake rate (1/h)					
S	Generation rate of particles from indoor sources (ug/h)					
Sc	Schmidt Number					
Sh	Sherwood Number					
t	Time (h)					
- T	Temperature (K)					
- TSP	Mass concentration of total suspended particles in the room (ug/m^3)					
TSPout	Mass concentration of total suspended particles outdoors ($\mu g/m^3$)					
V	Volume of the room (m^3)					
-						

	<i>v_{dd}</i> depending on the orientation of the surface.				
V_{dv}	Size-dependent particle deposition velocity to a vertical wall (m/h)				
Vdu	Size-dependent particle deposition velocity to an upward-facing				
	horizontal surface (m/h)				
Vdd	Size-dependent particle deposition velocity to a downward-facing				
	horizontal surface (m/h)				
W_0	SVOC mass fraction in the source $(\mu g/g)$				
W _{dust}	SVOC mass fraction in dust settled on source surfaces (µg/g)				
Wdust,s	SVOC mass fraction in dust settled on sink (non-source) surfaces				
	(μg/g)				
X	Depth from the surface of the material (m)				
y (or C_g)	Gas-phase concentration of SVOCs in indoor environments ($\mu g/m^3$)				
y_0	Gas-phase concentration of SVOCs in the layer immediately adjacent				
	to the source (μg/m³)				
Yout	Outdoor gas-phase concentration of SVOCs (μg/m ³)				
y_s	Gas-phase concentration of SVOCs in the layer immediately adjacent				
	to the non-source surfaces (μg/m³)				
δ	Thickness of the organic film (m)				
δο	Critical film thickness at which adsorption transforms to absorption				
00	(m)				
ε	Porosity of material (-)				
$ ho_{dust}$	Density of dust (μg/m³)				
$ ho_{\it part}$	Density of airborne particles (µg/m³)				
$ ho_{source}$	Density of source (µg/m³)				

2) List of Consensus Points

<u>Consensus Point 1:</u> To address challenges posed by exposure modeling, mechanistic models are preferred. Mechanistic models are based on physicochemical principles and are thus more generalizable in contrast to empirical models. They can be selected and varied in their level of complexity based on the application. Diverse data sets and the estimation of key input parameters using structure-based or other predictive relationships can be included in mechanistic modeling approaches. It is clear that mechanistic models have to be validated, and input parameter development and validation still require good data, which often does not exist.

<u>Consensus Point 2</u>: The environmental compartments relevant to modeling chemical exposure indoors are the gas phase, airborne particles, settled dust and exposed indoor surfaces, including those of the occupants. Additionally, clothing exposed to indoor air can serve as exposure mediator potentially increasing or decreasing dermal uptake.

<u>Consensus Point 3</u>: The assumption of equilibrium between gas phase, particle phase, dust and surfaces is a prerequisite for simpler SVOC models. However, this assumption has to be treated with caution. The greater the capacity of an environmental compartment, the longer it will take for that compartment to reach equilibrium with other compartments.

<u>Consensus Point 4</u>: SVOC emissions are assumed to be externally controlled, thus internal diffusion is neglected and the source is considered as non-depleting. Clothing is a special case due to differences in time scales, thus internal diffusion and source depletion may be relevant.

<u>Consensus Point 5</u>: It is assumed that the air in the indoor environment is well-mixed. An exception might be indoor air inside closed spaces such as closets and cabinets, which should be considered separately as needed.

<u>Consensus Point 6</u>: For some SVOCs emitted by indoor sources, outdoor air concentrations are low and can thus be neglected in exposure assessments. In other cases, indoor and outdoor concentrations may

be comparable, thus the question of the relevance of outdoor contributions has to be taken into account and concentrations of SVOCs in the infiltrating air may have to be considered.

<u>Consensus Point 7</u>: Exposure can occur immediately via dermal contact with or ingestion of the source (Direct Exposure). Alternatively, emission from the source to environmental compartments occurs first, followed by transport and chemical transformations, resulting in the SVOC's presence in one or more compartments from which exposure occurs (Indirect Exposure).

<u>Consensus Point 8</u>: Mechanistically consistent source emission categories, derived from a continuum of sources, serve as the starting point for modeling exposure to SVOCs emitted by sources in the indoor environment. These categories are: solid, soft, frequent contact, applied, sprayed and high temperature. <u>Consensus Point 9</u>: Stationary non-porous sources that are not frequently handled or touched (e.g., furniture, TVs, or vinyl flooring) have large emitting surface areas relative to the volume of most indoor environments or to the area that might come in contact with an exposed person. Exposure to SVOCs present in these solid sources mainly occurs by Indirect Exposure.

<u>Consensus Point 10</u>: Soft sources include cushions, mattresses, foams, carpets and clothing. Exposure to soft sources can occur both via Direct Exposure due to frequent close contact of a person to these sources and via Indirect Exposure due to their often large emitting surface areas.

<u>Consensus Point 11</u>: Exposure to certain SVOCs in sources that are frequently handled (e.g., electronic devices, toys) or mouthed by children (e.g., teethers) is more likely to occur via Direct Exposure. The emission category for this type of source is frequent contact.

<u>Consensus Point 12</u>: A liquid source that is directly applied to the body (e.g., body lotion, shampoo) is mainly linked to Direct Exposure. If the source is applied to a surface or is exposed to the indoor air (e.g., paint or detergent), Indirect Exposure dominates. Applied sources have to be considered pulse emission sources and thus require dynamic modeling approaches.

<u>Consensus Point 13</u>: A source that is sprayed towards the body can cause both Direct and Indirect Exposure (e.g., insect repellant). If the source is sprayed away from a person (e.g., air freshener), Indirect

Exposure contributes more. Both cases are pulse emissions and thus dynamic equations to model emission, transport and exposure are necessary.

<u>Consensus Point 14</u>: Combustion or heating processes such as burning a candle or cooking contribute mostly to Indirect Exposure. The relevant emission category is high temperature. This type of emission is a pulse emission that needs to include dynamic emission and chemical reactions.

<u>Consensus Point 15</u>: For modeling SVOC behavior in indoor environments, chemical transformations (e.g., oxidation, hydrolysis) should be discussed, even if they are not addressed quantitatively._

<u>Consensus Point 16</u>: Transport, partitioning and reactivity of SVOCs indoors are highly complex processes and not completely understood.



3) Mechanistic Modeling Framework to Predict Exposure to SVOCs

Figure S1: Dominant exposure pathways for SVOCs in indoor environments.

The red numbers refer to the equations listed below.

4) Emission and Transport Modeling Equations

General Note: Not all aspects of the framework have been modeled to date in a way that is appropriate

for the purpose of this framework. In these cases, the need for further model development is stated.

1. Emission into the gas phase

a. From solid sources, soft sources, and dried liquid sources:

$$E = h_m \cdot (y_0 - y)$$

Note: It is assumed that internal diffusion is negligible.

b. From applied sources (pulse emission):

Dynamic model, research needed

c. From sprayed sources (pulse emission):

Model development needed

d. From high temperature sources (pulse emission):

Model development needed

2. Emission to airborne particles

a. From sprayed sources (pulse emission):

Model development needed

b. From high temperature sources (pulse emission):

Model development needed

3. Emission to settled dust

From both solid and soft sources and including emission into the gas phase:

$$E = h_m \cdot (y_0 - y) + v_d \cdot TSP \cdot P_{dust} - v_d \cdot F$$

4. Gas/particle partitioning

$$F = K_p \cdot TSP \cdot y$$

Note: Instant equilibrium is assumed.

5. Dust/gas partitioning

a. For dust settled on source surfaces:

$$P_{dust} = K_{dust} \cdot y_0$$

Note: Alternatively, partitioning between dust and source material can be described using the

dust/material partition coefficient K_m . See Liu et al. 2016¹ for details.

b. For dust settled on sink surfaces:

$$P_{dust,s} = K_{dust} \cdot y_s$$

- 6. Surface/gas partitioning for sink surfaces
- a. For solid sink surfaces:

$$C_s = K_s \cdot y_s$$

b. For soft sink surfaces:

$$[\varepsilon + (1 - \varepsilon) \cdot K_s + K_{dust} \cdot m_x] \frac{\partial C_{pm}}{\partial t} = \varepsilon \cdot D_t \frac{\partial^2 C_{pm}}{\partial x^2}$$

$$C_{pm} = 0 \text{ for } t = 0, 0 \le x \le L;$$
 $\frac{\partial C_{pm}}{\partial t} = 0 \text{ for } t > 0, x = L;$ $C_{pm} = y_s \text{ for } t > 0, x = 0$

c. In the presence of an organic surface film:

$$\frac{dC_{s,j}}{dt} = h_{m,s,j} \left(y_j - \frac{C_{s,j}}{\delta \cdot K_{oa}} \right) + v_d \cdot F$$
$$\delta = \delta_0 + \sum_{j=1}^N \frac{C_{s,j}}{\rho_j}$$

Note: See Eichler et al. 2019² for further detail.

7. Mass balance for particle transport

$$V\frac{dTSP}{dt} = Q \cdot P_p \cdot TSP_{out} - Q \cdot TSP - v_d \cdot TSP \cdot (A_s + A_{ss}) + R_p \cdot M_s \cdot A_s + R_p \cdot M_{ss} \cdot A_{ss} + S$$

Change in	Particles entering	Particles	Particles depositing	Resuspension of	Resuspension of	Particles
particle mass	from outdoors with	leaving with	on sink and source	dust from sink	dust from source	being
concentration	ventilation	ventilation	surfaces	surfaces	surfaces	generated
over time						indoors

$$\frac{dM_s}{dt} = v_d \cdot TSP - R_p M_s \quad or \quad \frac{dM_s}{dt} = v_d \cdot TSP - R_p M_s$$

8. Mass balance for dust settled on sink surfaces

$$\frac{d(C_{s} + M_{s} \cdot P_{dust,s})}{dt} = h_{m,s} \cdot (y - y_{s}) + v_{d} \cdot F - R_{p} \cdot \bigotimes_{s} \cdot P_{dust,s}$$
Change in SVOC concentration
on sink surface and dust over
time
Emission from the
sink surface into the
gas phase
SVOC concentration
in dust deposited
on sink surface

9. General mass balance for indoor SVOCs

$$V\frac{dy}{dt} + V\frac{dF}{dt} = Q \cdot (y_{out} + F_{out}) - Q \cdot (y + F) + h_m \cdot A_{ss} \cdot (y_0 - y) - h_{m,s} \cdot A_s \cdot (y - y_s)$$
$$-v_d \cdot F \cdot (A_{ss} + A_s) + R_p \cdot M_{ss} \cdot P_{dust} \cdot A_{ss} + R_p \cdot M_s \cdot P_{dust,s} \cdot A_s$$

Note: If outdoor concentrations are assumed to be negligible, *y*_{out} and *F*_{out} equal 0, respectively.

Note: This mass balance does not include clothing-mediated effects.

10. Clothing/gas partitioning

a. General approach:

$$\frac{\partial C_m}{\partial t} = D_m \frac{\partial^2 C_m}{\partial x^2}$$

Boundary condition at clothing surface:

$$-D \frac{\partial C_m}{\partial x}\Big|_{x=L_m} = h \underbrace{(y - C_m)}_{K_{ca}}$$

b. If diffusion in clothing can be ignored:

$$\frac{\partial C_m}{\partial t} = h_m \left(y - \frac{C_m}{L_m \cdot K_{ca}} \right)$$

Note: The diffusivity within the clothing material can be ignored, if the characteristic time required

for clothing to reach equilibrium with the gas phase is much larger than the time required for diffusion to occur: $\frac{K_{ca}L_m}{h_m} \gg \frac{L^2}{D_m}$ (alternatively, if $\frac{h_m \cdot L}{D_m} \gg 1$).

Note: See Cao et al. 2016³ for further detail.

11. Clothing/particle partitioning

Model development needed

5) Exposure Modeling Equations

Note: The exposure modeling equations (Eq. 12-15) listed below do not account for different bioaccessibilities and have thus considered worst case scenarios. However, we recommend applying bioaccessibility factors if these are available.^{4, 5}

General conversion from exposure rate to daily intake:

$$DI = \frac{Ex \cdot d}{bw}$$

12. Direct Exposure

a. Dermal uptake via direct contact with a source:

Transfer from a solid source to skin surface: $Ex_{source_d} = J_{source_ssl} \cdot A_{contact}$

Transfer from liquid source to skin surface: $Ex_{source_d} = w_0 \cdot AR_{source} \cdot f_A \cdot f_{ret}$

Note: See Huang et al. 2017⁶, CHAP 2014⁷ and Wormuth et al. 2006⁸ for example approaches.

- Transfer from skin surface to dermal capillaries: $J_{ssl_c} = C_{ssl} \cdot k_{p_ssl}$
- b. Ingestion of a source:

 $Ex_{source ing} = w_0 \cdot IR_{source}$

c. Mouthing of a source:

$$Ex_{mouthing} = w_0 \cdot A_{mouthing} \cdot MR \cdot EF \cdot f_A \cdot d$$

13. Dermal uptake

a. From the gas phase to dermal capillaries:

$$Ex_{gas_d} = C_g \cdot k_{p_g} \cdot A_{exp}$$

Note: See Weschler and Nazaroff 2014⁹ for the calculation of k_{p_q} .

Note: See Gong et al. 2014¹⁰ and Morrison et al. 2016¹¹ for a dynamic modeling approach.

b. From airborne particles or dust particles:

$$Ex_{part_d} = F \cdot A_{exp} \cdot q_{part_skin} \cdot f_A$$

Note: See Wormuth et al. 2006⁸ and Giovanoulis et al. 2018¹² for values of f_A .

Note: F should be replaced by $P_{dust,s}$ for dust from sink surfaces and by $P_{dust,s}$ for dust from source

surfaces.

c. From sink surfaces:

$$Ex_{surf_d} = C_s \cdot CR_s \cdot f_A$$

d. From clothing:

$$Ex_{cloth_d} = C_{ssl} \cdot k_{p_ssl} \cdot A_{exp}$$
$$C_{ssl} = K_{ssl} \cdot C_m$$

Note: See Morrison et al.¹³ and Cao et al. 2018¹⁴ for more detail. Eq. 13d is based on the assumption that the skin-surface lipids (SSL) are in equilibrium with the clothing. This is likely not the case for

many SVOCs because the timescale for reaching equilibrium¹⁵ is often longer than the duration of contact between clothing and the skin-surface lipids. Thus, this equation describes a worst case scenario.

14. Inhalation

Inhalation of gas phase and airborne particles:

$$Ex_{inh} = C_t \cdot IR_{inh}$$

with $C_t = C_a + F$

15. Ingestion

a. Ingestion of dust:

$$Ex_{dust_ing} = w_{dust} \cdot IR_{dust}$$

Note: For dust from sink surfaces, w_{dust} should be replaced by $w_{dust,s}$.

Note: w_{dust} can be approximated with f_{om_dust} .

b. Mouthing of objects/exposed clothing and hand-to-mouth:

See 13c. f_A might vary.

Note: Empirical equations available in Isaacs et al. 2014¹⁶ and Huang et al. 2017⁶.

6) Estimation Approaches for Model Parameters

I. Saturation vapor pressure (*p_s*)

Antoine equation (A, B, C are substance-specific coefficients)¹⁷:

$$\log(p_s) = A - \frac{B}{C+T}$$

Note: See Vyazovkin, Koga, and Schick 2018¹⁸ for an overview of experimental methods to determine the vapor pressure of chemicals with different volatilities. Wu et al. 2016¹⁹ developed a method to measure vapor pressure for SVOCs.

II. Octanol/air partition coefficient (K_{oa})

$$K_{oa} = \frac{K_{ow}}{K_{aw}} = \frac{K_{ow} \cdot R \cdot T}{H}$$

Relationship between p_s and K_{oa} :



Figure S2: Comparison of K_{oa} values calculated by SPARC (ARChem) and the poly-parameter Linear-Free-Energy-Relationship (pp-LFER)²⁰ (LSER Database). The compounds in ascending order of K_{oa} (SPARC) values are DMP, DiBA, DnBA, DEP, DiBP, DnBP, TPP, DPP, DEHA, BBzP, TEHP, DINA, DEHTP, DINCH, DEHP, DINP, DPHP, and TOTM.

III. Gas-phase concentration immediately adjacent to the source (y_0)

General relationship between y_0 , p_s , and C_0 :

$$y_0 = \gamma \cdot w_0 \cdot p_s$$

with $w_0 = \frac{c_0}{\rho_{product}}$

For phthalates and phthalates alternatives (Eichler et al. 2018²¹):

$$y_0 = 3.70 \cdot w_0 \cdot p_s$$

For phthalates and organophosphate flame retardants (Liang et al. 2018²²):

$$y_0 = 3.405 \cdot w_0 \cdot p_s$$

IV. Mass-transfer coefficient (*h_m*)

$$h_m \text{ or } h_{m_F} = Sh \cdot \frac{D_a}{L_c}$$

 $Sh = 0.664 \cdot Re^{\frac{1}{2}} Sc^{1/3}$

Note: This estimation of h_m and $h_{m,s}$ uses the correlations in Axley 1991²³. Typically, the average air velocity across interior surfaces is in the range of 0.01-0.16 m/s as reported by Huang et al. 2004²⁴. This value could be an underestimation, thus specific air velocity and characteristic lengths should be selected when estimating the mass transfer coefficient for particular indoor cases.

V. Gas/particle partition coefficient (*K*_p)

Definition (Pankow 1994²⁵):

$$K_p = \frac{F/TSP}{C_g}$$

Extended by Finizio et al. 1997²⁶:

$$K_p = \frac{f_{om_part} \times K_{oa}}{\rho_{part}}$$

$$\log(K_p) = \log(K_{oa}) + \log(f_{om_part}) - 11.91$$

Another method (Naumova et al. 2003²⁷, regression based on PAH data in atmosphere with PM_{2.5}):

$$\log(K_p) = -0.860 \log(p_s) - 4.67$$

See Salthammer and Schripp 2015²⁸ and Salthammer and Goss 2019²⁰ for more information on the determination of K_p .

VI. Dust/gas partition coefficient (K_{dust})

$$K_{dust} = \frac{P_{dust}}{C_g} = \frac{f_{om_dust} \times K_{oa}}{\rho_{dust}}$$

VII. Non-source surface/gas partition coefficient (K_s)

a. Wood floors, ceiling and walls, and furniture (Xu et al. 2009²⁹, regression for phthalates):

$$\log(K_s) = -0.779 \log(p_s) - 1.93$$

b. Windows, mirrors, tile and ceramic fixtures:

Freundlich isotherm fitted by Xu and Little (2006)³⁰ for DEHP: K_s = 3800, n = 1.5

c. Carpet (Xu et al. 2009²⁹, regression for phthalates):

$$\log(K_s) = -0.627 \log(p_s) - 1.08$$

d. Stainless steel (Liang et al. 2018³¹):

Freundlich isotherm fitted for TCEP: K_s = 31.6, n = 0.24

Freundlich isotherm fitted for TCPP: K_s = 67.1, n = 0.26

e. Polyurethane foam (Liang et al. 2019³²) depending on the temperature:

For TCEP: $K_{\rm s}$ = 2 · 10⁻¹⁸ · T^{0.5} · e^{17335/T}

For TCIPP:
$$K_s = 2 \cdot 10^{-16} \cdot T^{0.5} \cdot e^{15468/T}$$

f. See also Liu et al. 2014³³ and Liu et al. 2016³⁴ for K_s values for polychlorinated biphenyls (PCBs) and organophosphorus flame retardants (OPFRs) for a variety of materials.

VIII. Gas/clothing partition coefficient (*K*_{ca})

- a. See Morrison et al. 2018³⁵ for gas/clothing partition coefficients for PCBs in cotton and polyester, and in blends of polyester, cotton, viscose/rayon, and/or elastane.
- b. See Cao et al. 2016³ for gas/clothing partition coefficients for diisobutyl phthalate (DiBP), di-n-butyl phthalate (DnBP), and bis(2-ethylhexyl) phthalate (DEHP) in cotton clothing.
- c. See Morrison et al. 2015³⁶ for gas/clothing partition coefficients for diethyl phthalate (DEP) and DnBP in cotton clothing.

7) Decision Tree



Figure S3: Decision tree for exposure mechanism selection based on source emission category.

<u>References</u>

1. Liu, X.; Guo, Z.; Krebs, K. A.; Greenwell, D. J.; Roache, N. F.; Stinson, R. A.; Nardin, J. A.; Pope, R. H., Laboratory Study of PCB Transport from Primary Sources to Settled Dust. *Chemosphere* **2016**, *149*, 62-69.

2. Eichler, C. M. A.; Cao, J.; Isaacman-VanWertz, G.; Little, J. C., Modeling the Formation and Growth of Organic Films on Indoor Surfaces. *Indoor Air* **2019**, *29*, 17-29.

3. Cao, J.; Weschler, C. J.; Luo, J.; Zhang, Y., Cm-History Method, a Novel Approach to Simultaneously Measure Source and Sink Parameters Important for Estimating Indoor Exposures to Phthalates. *Environ. Sci. Technol.* **2016**, *50*, (2), 825-834.

4. Wei, W.; Bonvallot, N.; Gustafsson, Å.; Raffy, G.; Glorennec, P.; Krais, A.; Ramalho, O.; Le Bot, B.; Mandin, C., Bioaccessibility and bioavailability of environmental semi-volatile organic compounds via inhalation: A review of methods and models. *Environ. Int.* **2018**, *113*, 202-213.

5. Raffy, G.; Mercier, F.; Glorennec, P.; Mandin, C.; Le Bot, B., Oral bioaccessibility of semi-volatile organic compounds (SVOCs) in settled dust: A review of measurement methods, data and influencing factors. *J. Hazard. Mater.* **2018**, *352*, 215-227.

6. Huang, L.; Ernstoff, A. S.; Fantke, P.; Csiszar, S. A.; Jolliet, O., A review of models for near-field exposure pathways of chemicals in consumer products. *Sci. Total Environ.* **2017**, *574*, 1182-1208.

7. CHAP *Chronic Hazard Advisory Panel on Phthalates and Phthalate Alternatives*; U.S. Consumer Product Safety Commission: Bethesda, MD, 2014.

Wormuth, M.; Scheringer, M.; Vollenweider, M.; Hungerbühler, K., What are the sources of exposure to eight frequently used phthalic acid esters in Europeans? *Risk Anal.* 2006, *26*, (3),803-824.
 Weschler, C. J.; Nazaroff, W. W., Dermal Uptake of Organic Vapors Commonly Found in Indoor

Air. Environ. Sci. Technol. 2014, 48, 1230-1237.

10. Gong, M.; Zhang, Y.; Weschler, C. J., Predicting dermal absorption of gas-phase chemicals: transient model development, evaluation, and application. *Indoor Air* **2014**, *24*, 292-306.

11. Morrison, G. C.; Weschler, C. J.; Bekö, G., Dermal uptake directly from air under transient conditions: advances in modeling and comparisons with experimental results for human subjects. *Indoor Air* **2016**, *26*, (6), 913-924.

12. Giovanoulis, G.; Bui, T. T.; Xu, F.; Papadopoulou, E.; Padilla-Sanchez, J. A.; Covaci, A.; Haug, L. S.; Cousins, A. P.; Magnér, J.; Cousins, I. T.; de Wit, C. A., Multi-pathway human exposure assessment of phthalate esters and DINCH. *Environ. Int.* **2018**, *112*, 115-126.

13. Morrison, G. C.; Weschler, C. J.; Bekö, G., Dermal uptake of phthalates from clothing: Comparison of model to human participant results. *Indoor Air* **2017**, *27*, (3), 642-649.

14. Cao, J.; Zhang, X.; Zhang, Y., Predicting dermal exposure to gas-phase semi-volatile organic compounds (SVOCs): an improved description of SVOC mass transfer between clothing and skin surface lipids. *Environ. Sci. Technol.* **2018**, *52*, 4676-4683.

15. Weschler, C. J.; Nazaroff, W. W., Semivolatile organic compounds in indoor environments. *Atmos. Environ.* **2008**, *42*, (40), 9018-9040.

16. Isaacs, K. K.; Glen, W. G.; Egeghy, P.; Goldsmith, M.-R.; Smith, L.; Vallero, D.; Brooks, R.; Grulke, C. M.; Özkaynak, H., SHEDS-HT: An Integrated Probabilistic Exposure Model for Prioritizing Exposures to Chemicals with Near-Field and Dietary Sources. *Environ. Sci. Technol.* **2014**, *48*, (21), 12750-12759.

17. Schwarzenbach, R. P.; Gschwend, P. M.; Imboden, D. M., *Environmental Organic Chemistry*. 2nd Edition ed.; John Wiley & Sons, Inc.: Hoboken, NJ, 2003.

18. *Handbook of Thermal Analysis and Calorimetry: Recent Advances, Techniques and Applications.* 2nd Edition ed.; Elsevier: Amsterdam, NL, 2018; Vol. 6.

19. Wu, Y.; Eichler, C. M. A.; Chen, S.; Little, J. C., Simple Method To Measure the Vapor Pressure of Phthalates and Their Alternatives. *Environ. Sci. Technol.* **2016**, *50*, 10082-10088.

20. Salthammer, T.; Goss, K.-U., Predicting the Gas/Particle Distribution of SVOCs in the Indoor Environment Using Poly Parameter Linear Free Energy Relationships. *Environ. Sci. Technol.* **2019**, *53*, 2491-2499.

21. Eichler, C. M. A.; Wu, Y.; Cao, J.; Shi, S.; Little, J. C., Equilibrium relationship between SVOCs in PVC products and the air in contact with the product. *Environ. Sci. Technol.* **2018**, *52*, (5), 2918-2925.

22. Liang, Y.; Liu, X.; Allen, M. R., Measurements of Parameters Controlling the Emissions of Organophosphate Flame Retardants in Indoor Environments. *Environ. Sci. Technol.* **2018**, *52*, (10), 5821-5829.

23. Axley, J. W., Adsorption Modelling for Building Contaminant Dispersal Analysis. *Indoor Air* **1991**, *2*, 147-171.

24. Huang, J. M.; Chen, Q.; Ribot, B.; Rivoalen, H., Modelling Contaminant Exposure in a Single-family House. *Indoor and Built Environment* **2004**, *13*, (1), 5-19.

25. Pankow, J. F., An Absorption Model of Gas/particle Partitioning of Organic Compounds in the Atmosphere. *Atmos. Environ.* **1994**, *28*, (2), 185-188.

26. Finizio, A.; Mackay, D.; Bidleman, T.; Harner, T., Octanol-air partition coefficient as a predictor of partitioning of semi-volatile organic chemicals to aerosols. *Atmos. Environ.* **1997**, *31*, (15), 2289-2296.

27. Naumova, Y. Y.; Offenberg, J. H.; Eisenreich, S. J.; Meng, Q.; Polidori, A.; Turpin, B. J.; Weisel, C. P.; Morandi, M. T.; Colome, S. D.; Stock, T. H.; Winer, A. M.; Alimokhtari, S.; Kwon, J.; Maberti, S.;

Shendell, D.; Jones, J. W.; Farrar, C., Gas/particle distribution of polycyclic aromatic hydrocarbons in coupled outdoor/indoor atmospheres. *Atmos. Environ.* **2003**, *37*, (5), 703-719.

28. Salthammer, T.; Schripp, T., Application of the Junge- and Pankow-equation for estimating indoor gas/particle distribution and exposure to SVOCs. *Atmos. Environ.* **2015**, *106*, 467-476.

29. Xu, Y.; Cohen Hubal, E. A.; Clausen, P. A.; Little, J. C., Predicting Residential Exposure to Phthalate Plasticizer Emitted from Vinyl Flooring: A Mechanistic Analysis. *Environ. Sci. Technol.* **2009**, *43*, (7), 2374-2380.

30. Xu, Y.; Little, J. C., Predicting emissions of SVOCs from polymeric materials and their interaction with airborne particles. *Environ. Sci. Technol.* **2006**, *40*, (2), 456-461.

31. Liang, Y.; Liu, X.; Allen, M. R., Measuring and modeling surface sorption dynamics of organophosphate flame retardants on impervious surfaces. *Chemosphere* **2018**, *193*, (754-762), 754.

32. Liang, Y.; Liu, X.; Allen, M. R., The influence of temperature on the emissions of organophosphate ester flame retardants from polyisocyanurate foam: Measurement and modeling (supporting information). *Chemosphere* **2019**, *In press*.

33. Liu, X.; Guo, Z.; Roache, N. F., Experimental method development for estimating solid-phase diffusion coefficients and material/air partition coefficients of SVOCs. *Atmos. Environ.* **2014**, *89*, 76-84.

34. Liu, X.; Allen, M. R.; Roache, N. F., Characterization of organophosphorus flame retardants' sorption on building materials and consumer products. *Atmos. Environ.* **2016**, *140*, 333-341.

35. Morrison, G.; Andersen, H. V.; Gunnarsen, L.; Voral, D.; Uhde, E.; Kolarik, B., Partitioning of PCBs from air to clothing materials in a Danish apartment. *Indoor Air* **2018**, *28*, (1), 188-197.

36. Morrison, G. C.; Li, H.; Mishra, S.; Buechlein, M., Airborne phthalate partitioning to cotton clothing. *Atmos. Environ.* **2015**, *115*, 149-152.