Supporting information

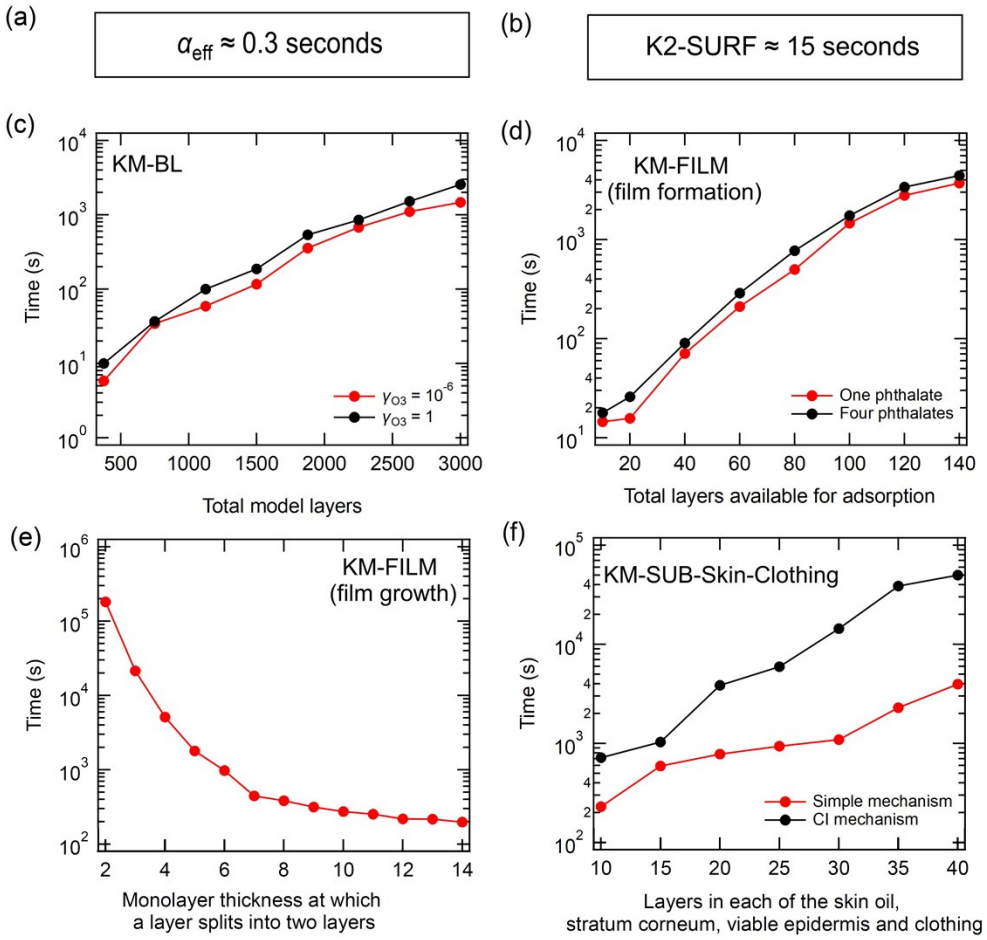

Figure S1: The computational time needed to run a single parameter set for the different models. These were calculated using the 'Run and Time' button in Matlab. The maxNumCompThreads(1) function was used to limit the number of computational threads to one for each simulation and the results were obtained using the following Processor: Intel(R) Core(TM) i7-1065G7 CPU @ 1.30GHz 1.50 GHz. A single value is given for α_{eff} and K2-SURF as these contain a fixed number of layers. For α_{eff} the model was run without outputting a figure. In panel (c) the layer numbers were set to a 1:2 ratio for the layers closest to the surface and further away from the surface. In panel (d) the one phthalate simulation was performed for DEHP adsorbing on aluminum (JJ=1 in the model) and the simulation with four phthalates was performed for DEHP, DEHT, DINP and DINCH adsorbing on steel (JJ=13 in the model). In panels (d) and (e) the number of layers in the boundary layer were set to 10 and 20, respectively. In panel (e) the layers were set to merge if a layer thickness decreased to less than half a monolayer.

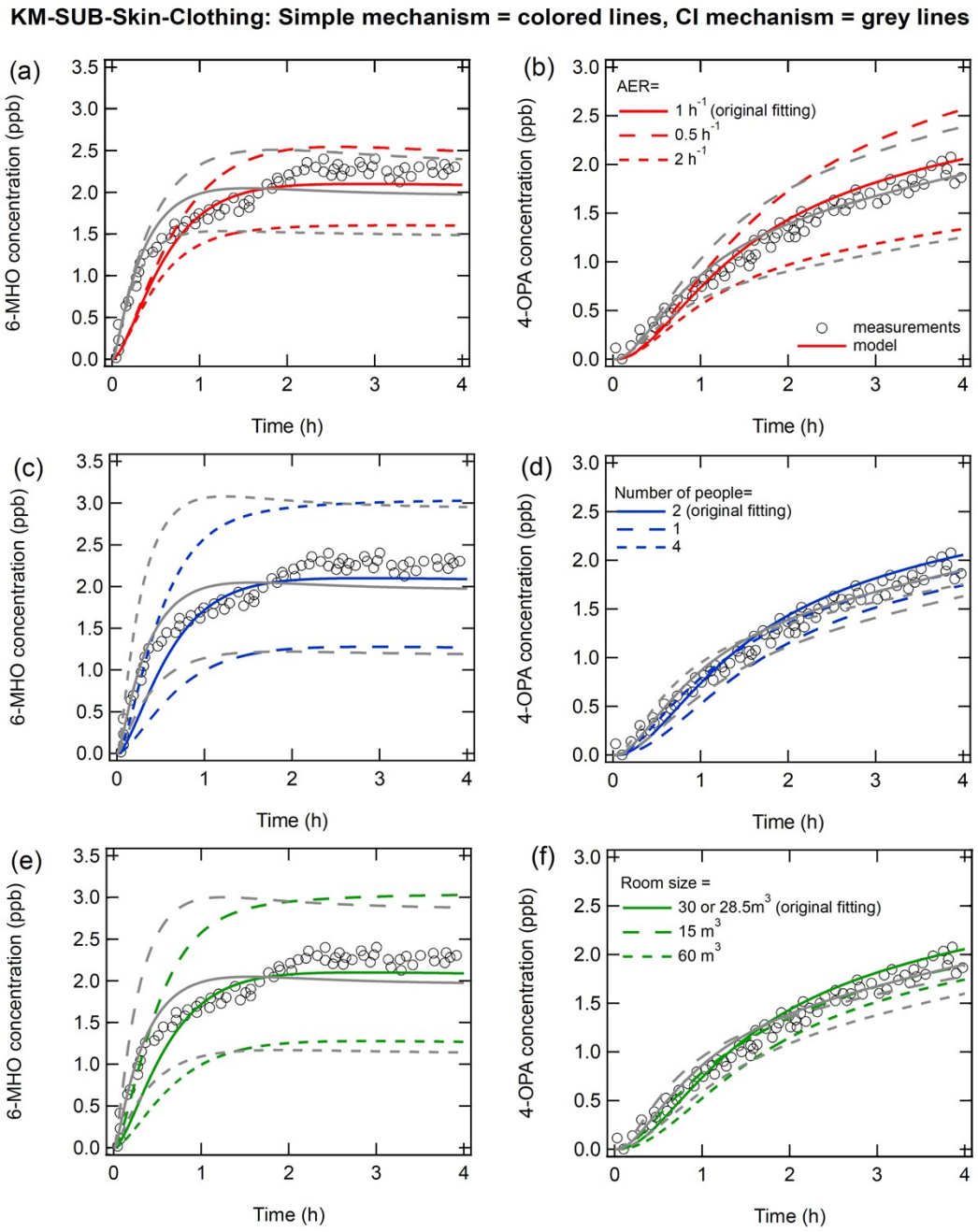

Figure S2: Mixing ratios of 6-MHO and 4-OPA as simulated by the KM-SUB-Skin-Clothing model with the simplified reaction mechanism and more complex CI mechanism. Measurements are from Wisthaler and Weschler (2010)[14] and model parameters can be found in Lakey et al.[62] and Lakey et al. (2023)[63]. Sensitivity tests were performed to investigate the impact of (a-b) air-exchange rate, (c-d) the number of people and (e-f) the room size on the gas-phase concentration of (a, c, e) 6-MHO and (b, d, f) 4-OPA. Note that the reaction rate coefficient of CI with carboxylic acids was reported as 2.7×10^{-20} cm^3 s^{-1} in Lakey et al. (2023)[63] but was actually set to 1.8×10^{-20} cm^3 s^{-1} for Fig. S5 of that publication and is set to that value here. The difference between the rate coefficients makes a small but noticeable difference to the fitting for the CI mechanism.

Table S1: Parameters included in the models.

Symbol	Meaning	Unit
$[X]_{bk}$	Bulk concentration of X in layer *k*	cm^{-3}
$[X]_{bl}$	Concentration of X in the boundary layer	cm^{-3}
$[X]_{bz}$	Concentration of X in bulk layer *z*	cm^{-3}
$[X]_{cl,condensed,j}$	Concentration of X in layer *j* of the condensed-phase clothing	cm^{-3}
$[X]_{cl,gas,j}$	Concentration of X in layer *j* of the gas-phase clothing	cm^{-3}
$[X]_{g}$	Concentration of X in the gas phase	cm^{-3}
$[X]_{g1}$	Concentration of X in layer 1 of the boundary layer	cm^{-3}
$[X]_{gap}$	Concentration of X in the gap between the clothing and the skin	cm^{-3}
$[X]_{gm}$	Concentration of X in layer *m* of the boundary layer	cm^{-3}
$[X]_{gm+1}$	Concentration of X in layer *m* + 1 of the boundary layer	cm^{-3}
$[X]_{gm+n+1}$	Concentration of X in layer *m* + *n* + 1 of the boundary layer	cm^{-3}
$[X]_{gs}$	Concentration of X in the gas phase next to the skin or other surface	cm^{-3}
$[X]_{oil,j}$	Concentration of X in layer *j* of the skin oil	cm^{-3}
$[X]_{s,j}$	Adsorbed surface concentration of *X* in layer *j*	cm^{-2}
$[X]_{s,oil}$	Concentration of X adsorbed to the skin oil surface	cm^{-3}
$[X]_{sc,j}$	Concentration of X in layer *j* of the stratum corneum	cm^{-3}
$[X]_{ve,j}$	Concentration of X in layer *j* of the viable epidermis	cm^{-3}
A	Surface area of a film or surface	cm^2
AER	Air exchange rate	s^{-1}
c_1	Fraction of molecules adsorbed in the C* down configuration	
$C_{g,i}$	Gas-phase concentration of SVOC group *i*	$g\ cm^{-3}$
$C_{p,i}$	Particle-phase concentration of SVOC group *i*	$g\ cm^{-3}$
$C_{t,i}$	Total airborne concentration of SVOC group *i*	$g\ cm^{-3}$
δ	Thickness of a layer	cm
$D_{b,oil,X}$	Diffusion coefficient of *X* in the skin oil	$cm^2\ s^{-1}$
$D_{b,sc,X}$	Diffusion coefficient of *X* in the stratum corneum	$cm^2\ s^{-1}$
$D_{b,ve,X}$	Diffusion coefficient of *X* in the viable epidermis	$cm^2\ s^{-1}$
$D_{b,X}$	Bulk diffusion coefficient of X	$cm^2\ s^{-1}$
$\delta_{clothes}$	Thickness of a clothing layer	cm
$D_{g,eddy,j,X}$	Gas-phase diffusion coefficient of molecule X in layer *j* with turbulence	$cm^2\ s^{-1}$
$D_{g,X}$	Gas-phase diffusion coefficient of molecule X	$cm^2\ s^{-1}$

δ_{oil}	Thickness of a skin oil layer	cm
δ_{sc}	Thickness of a stratum corneum layer	cm
δ_{ve}	Thickness of a viable epidermis layer	cm
δ_{X}	Geometrical diameter of molecule *X*	cm
F_{i}	Net flux of SVOC group *i* to a surface film	g cm^{-2} s^{-1}
F_{net}	Net flux between the gas-phase and gas phase near the clothing	cm^{-2} s^{-1}
f_{om_TSP}	Volume fraction of organic matter in the particles	
γ_{X}	Uptake coefficient of X	
$h_{m,X}$	Mass transfer coefficient of *X* associated with the flux from room air to the clothing	cm s^{-1}
$J_{ads,X}$	Adsorption flux of molecule *X* to a surface	cm^{-2} s^{-1}
$J_{b,s,X}$	Transport flux of *X* from the bulk to the surface	cm^{-2} s^{-1}
$J_{bk,bk-1,X}$	Transport flux of *X* from bulk layer *k* to bulk layer *k*-1	cm^{-2} s^{-1}
$J_{bl,clothes,X}$	Transport flux of *X* from the boundary layer to the gas-phase clothing	cm^{-2} s^{-1}
$J_{clothes,bl,X}$	Transport flux of *X* from the gas-phase clothing to the boundary layer	cm^{-2} s^{-1}
$J_{clothes,gap,X}$	Transport flux of *X* from the gas-phase clothing to the gap between the clothing and skin	cm^{-2} s^{-1}
$J_{clothes,gas,X}$	Transport flux of X from the condensed-phase clothing to the gas-phase clothing	cm^{-2} s^{-1}
$J_{clothes,oil,X}$	Contact transfer flux from the clothing to the skin oil	cm^{-2} s^{-1}
$J_{clothes\_j,clothes\_j-1,X}$	Transport flux of *X* from gas-phase clothing layer *j* to layer *j*-1	cm^{-2} s^{-1}
$J_{coll,X}$	Collision flux of molecule *X* with a surface	cm^{-2} s^{-1}
$J_{des,X}$	Desorption flux of molecule *X* with a surface	cm^{-2} s^{-1}
$J_{gap,clothes,X}$	Transport flux of *X* from the gap between the clothing and skin and the gas-phase clothing	cm^{-2} s^{-1}
$J_{gap,mfp,X}$	Transport flux of *X* from the gap between the clothing and skin and the gas phase next to the skin	cm^{-2} s^{-1}
$J_{gas,clothes,X}$	Transport flux of *X* from the gas-phase clothing to the condensed-phase clothing	cm^{-2} s^{-1}
$J_{mfp,gap,X}$	Transport flux of *X* from the gap between the gas phase next to the skin to the gap between the clothing and skin	cm^{-2} s^{-1}
$J_{oil,clothes,X}$	Contact transfer flux from the skin oil to the clothing	cm^{-2} s^{-1}
$J_{oil,s,X}$	Transport flux of *X* from the skin oil to the surface	cm^{-2} s^{-1}
$J_{oil,sc,X}$	Transport flux of *X* from the skin oil to the stratum corneum	cm^{-2} s^{-1}
$J_{oil\_j,oil\_j-1,X}$	Transport flux of *X* from the skin oil layer *j* to layer *j*-1	cm^{-2} s^{-1}
$J_{s,b,X}$	Transport flux from the surface to the bulk	cm^{-2} s^{-1}
$J_{sc,oil,X}$	Transport flux of *X* from the stratum corneum to the skin oil	cm^{-2} s^{-1}

$J_{sc,ve,X}$	Transport flux of *X* from the stratum corneum to the viable epidermis	$cm^{-2}\ s^{-1}$
$J_{sc\_j,sc\_j-1,X}$	Transport flux of *X* from the stratum corneum layer *j* to layer *j*-1	$cm^{-2}\ s^{-1}$
$J_{ve,blood,X}$	Transport flux of *X* from the viable epidermis into the blood	$cm^{-2}\ s^{-1}$
$J_{ve,sc,X}$	Transport flux of *X* from the viable epidermis to the stratum corneum	$cm^{-2}\ s^{-1}$
$J_{ve\_j,ve\_j-1,X}$	Transport flux of *X* from the viable epidermis layer *j* to layer *j*-1	$cm^{-2}\ s^{-1}$
$k_{a,X}$	Adsorption rate of molecule *X* on an adsorbate free surface	$cm\ s^{-1}$
$k_{b,b,X}$	Transport rate coefficient (velocity) of *X* between bulk layers	$cm\ s^{-1}$
k_{br}	Bulk reaction rate coefficient	s^{-1} or $cm^3\ s^{-1}$
$k_{b,s,X}$	Transport rate coefficient (velocity) of *X* from the bulk to the surface	$cm\ s^{-1}$
$k_{bl,clothes,X}$	Transport rate coefficient (velocity) of *X* between the boundary layer and the gas phase clothing layer	$cm\ s^{-1}$
$k_{clothes,clothes,X}$	Transport rate coefficient (velocity) of *X* between the gas-phase clothing layers	$cm\ s^{-1}$
$k_{clothes,gap,X}$	Transport rate coefficient (velocity) of *X* between the gas-phase clothing and the gap between the clothing and skin	$cm\ s^{-1}$
$k_{clothes,gas,X}$	Transport rate coefficient (velocity) of X from the condensed-phase clothing to the gas-phase clothing	$cm\ s^{-1}$
$k_{clothes,oil,X}$	Contact transfer coefficient (velocity) from the clothing to the skin oil	$cm\ s^{-1}$
$K_{clothes,X}$	Partitioning coefficient of X to substances covering clothing fibres	
$k_{d,X}$	Desorption rate of molecule *X* from the surface	s^{-1}
K_e	Turbulence intensity	s^{-1}
k_{gr}	Gas phase reaction rate coefficient	s^{-1} or $cm^3\ s^{-1}$
$k_{gap,mfp,X}$	Transport rate coefficient (velocity) of *X* between the gap between the clothing and skin and the gas phase next to the skin	$cm\ s^{-1}$
$k_{gas,clothes,X}$	Transport rate coefficient (velocity) of *X* from the gas-phase clothing to the condensed-phase clothing	$cm\ s^{-1}$
$K_{oa,i}$	Octanal-air partitioning coefficient for SVOC group *i*	
$k_{oil,clothes,X}$	Contact transfer coefficient (velocity) from the skin oil to the clothing	$cm\ s^{-1}$
$k_{oil,oil,X}$	Transport rate coefficient (velocity) of *X* between skin oil layers	$cm\ s^{-1}$
$k_{oil,s,X}$	Transport rate coefficient (velocity) of *X* from the surface to the first skin oil bulk layer	$cm\ s^{-1}$
$k_{oil,sc,X}$	Transport rate coefficient (velocity) of *X* between the skin oil and the stratum corneum	$cm\ s^{-1}$
$K_{p,i}$	Particle-air partitioning coefficient of SVOC group *i*	$cm^3\ g^{-1}$
k_{room_bl}	Transport rate coefficient (velocity) of *X* between the gas phase in the room and the gas-phase in the boundary layer	$cm\ s^{-1}$

$k_{s,b,X}$	Transport rate coefficient of X from the surface to the bulk	s^{-1}
$k_{s,oil,X}$	Transport rate coefficient of X from the surface to the skin oil	s^{-1}
$k_{sc,sc,X}$	Transport rate coefficient (velocity) of X between stratum corneum layers	cm s^{-1}
$k_{sc,ve,X}$	Transport rate coefficient (velocity) of X between the stratum corneum and viable epidermis	cm s^{-1}
k_{sr}	Reaction rate coefficient for surface layer reactions	s^{-1} or cm^2 s^{-1}
$k_{ve,blood,X}$	Transport rate coefficient (velocity) of X from the viable epidermis into the blood	cm s^{-1}
$k_{ve,ve,X}$	Transport rate coefficient (velocity) of X between viable epidermis layers	cm s^{-1}
L	Number of layers	
$L_{bl,close}$	Number of layers in the boundary layer close to the surface	
$L_{bl,far}$	Number of layers in the boundary layer further away from the surface	
$L_{clothes}$	Number of layers in the clothing	
L_{oil}	Number of layers in the skin oil	
L_{sc}	Number of layers in the stratum corneum	
L_{ve}	Number of layers in the viable epidermis	
l_X	mean free path of molecule X	cm
p	Clothing porosity	cm^{-2}
$P_{b,j,X}$	Net production rate of species X in layer j of a bulk condensed phase	cm^{-3} s^{-1}
$P_{g,clothes,j,X}$	Net production rate of species X in layer j of the clothing gas phase	cm^{-3} s^{-1}
$P_{g,X}$	Net production rate of species X in the gas phase	cm^{-3} s^{-1}
p_i	Density of the condensed phase SVOC group i	g cm^{-3}
p_{part}	Density of airborne particles	g cm^{-3}
$P_{s,X}$	Net production rate of species X at a surface	cm^{-2} s^{-1}
θ	Surface coverage	
s_j	Surface area of layer j	cm^2
S_j	Surface area of the empty adsorption sites in layer j	cm^2
S_{people}	Surface area of the clothing	cm^2
σ_X	Effective molecular cross section of molecule X	cm^2
T_{BL}	Boundary layer thickness	cm
$T_{clothes}$	Total thickness of the clothing	cm
T_{gap}	Total thickness of the gap between the clothing and the skin	cm
T_o	Initial film thickness	cm
T_{oil}	Total thickness of the skin oil	cm

T_{sc}	Total thickness of the stratum corneum	cm
TSP	Total airborne suspended particle concentration	g cm^{-3}
T_t	Total film thickness	cm
T_{ve}	Total thickness of the viable epidermis	cm
UF_j	Uncovered fraction of molecules in layer j	
$V_{clothes}$	Volume of a layer in the clothing	cm^3
V_j	Volume of layer j	cm^3
V_{oil}	Volume of a layer in the skin oil	cm^3
V_{room}	Volume of the room	cm^3
V_{sc}	Volume of a layer in the stratum corneum	cm^3
V_{ve}	Volume of a layer in the viable epidermis	cm^3
V_X	Volume of one molecule of X	cm^3
x	Penetration depth	cm
$x_{b,i}$	Length that a molecule in SVOC group i must travel to be accommodated in the bulk	cm
x_{eff}	Effective penetration depth	cm
x_{eff}	Effective penetration depth	cm
$\alpha(x)$	Penetration depth dependent mass accommodation coefficient	cm^{-3}
$\alpha_{b,i}$	Bulk accommodation coefficient of a molecule in SVOC group i	
$\alpha_{eff,i}$	Effective mass accommodation coefficient of SVOC group i	
$\alpha_{s,0,X}$	Surface mass accommodation of molecule X on an adsorbate free surface	
$\tau_{d,X}$	Desorption lifetime of molecule X on a surface	s
$\upsilon_{d,i}$	Deposition velocity of SVOC group i	cm s^{-1}
ω_X	Mean thermal velocity of molecule X	cm s^{-1}