Supporting Information: A model for risk-based screening and prioritization of human exposure to chemicals from near-field sources

Authors: Li Li[1], John N. Westgate[2,#], Lauren Hughes[2], Xianming Zhang[1,2], Babak Givehchi[1], Liisa Toose[2], James M. Armitage[3], Frank Wania[1], Peter Egeghy[4], Jon A. Arnot[1,2,5*]

1. Department of Physical and Environmental Sciences, University of Toronto Scarborough, Toronto, ON, Canada, M1C 1A4

2. ARC Arnot Research and Consulting, Toronto, ON, Canada, M4M 1W4

3. AES Armitage Environmental Sciences, Inc., Ottawa, ON, Canada, K1L 8C3

4. Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, NC, United States, 27709

5. Department of Pharmacology and Toxicology, University of Toronto, ON, Canada, M5S 1A8

Corresponding author: Arnot, J. A., 36 Sproat Avenue, Toronto, Ontario, M4M 1W4, Tel: +1 (647)-225-3771; Email: jon@arnotresearch.com

(J. N. W.) Current affiliation: Pest Management Regulatory Agency, Health Canada, Ottawa, ON, Canada

The Supporting Information contains 23 pages, 5 tables, 2 texts, and 3 figures.

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Table S1 Summary of Z values (mol m^{-3} Pa^{-1}) and relevant parameters exposure model.

Media	Z value	Parameters and Units
Gaseous phase	$Z_{\mathrm{G}} = \frac{1}{R \cdot T}$	R: Ideal Gas Law constant (8.314 Pa·m^3 mol^{-1}·K^{-1}); T: Temperature (298.15 K);
Particulate / dust phase	$Z_{\mathrm{P},i} = K_{\mathrm{PA},i} \cdot Z_{\mathrm{G}}$	$K_{\mathrm{PA},i}$: Dimensionless equilibrium particle-gas partition coefficient for particles of size fraction i. $K_{\mathrm{PA},i} = K_{\mathrm{P},i} \times \rho_{\mathrm{P}}$, where $K_{\mathrm{P},i}$ (m^3 μg^{-1}) describes the ratio of concentration in particulates of size fraction i to that in gaseous phase, which can be calculated according to ref.[1], and ρ_{P} is the density of particle (μg m^{-3}).
Water phase	$Z_{\mathrm{W}} = \frac{Z_{\mathrm{G}}}{K_{\mathrm{AW}}}$	K_{AW}: Dimensionless equilibrium air-water partition coefficient.
Lipid phase	$Z_{\mathrm{L}} = Z_{\mathrm{W}} \cdot K_{\mathrm{OW}}$	K_{OW}: Dimensionless equilibrium octanol-water partition coefficient.
Non-lipid organic matter	$Z_{\mathrm{NLOM}} = 0.035 \cdot Z_{\mathrm{W}} \cdot K_{\mathrm{OW}}$	0.035: proportionality constant for non-lipid organic matter
Air	$Z_{\mathrm{A}} = \left(1 - \sum_i v_{\mathrm{P,A},i}\right) \cdot Z_{\mathrm{G}} + \sum_i \left(v_{\mathrm{P,A},i} \cdot Z_{\mathrm{P},i}\right)$	$v_{\mathrm{P,A},i}$: Volume fraction of particles of size fraction i in the bulk indoor air;
Carpet	$Z_{\mathrm{C}} = v_{\mathrm{A,C}} \cdot Z_{\mathrm{G}} + \left(1 - v_{\mathrm{A,C}} - \sum_i v_{\mathrm{P,C},i}\right) \cdot K_{\mathrm{CA}} \cdot Z_{\mathrm{G}} + \sum_i \left(v_{\mathrm{P,C},i} \cdot Z_{\mathrm{P},i}\right)$	$v_{\mathrm{A,C}}$: Volume fraction of air in the bulk carpet (0.89); $v_{\mathrm{P,C},i}$: Volume fraction of particles of size fraction i in the bulk carpet; K_{CA}: Dimensionless partition coefficient between carpet and air;
PUF	$Z_{\mathrm{U}} = v_{\mathrm{A,U}} \cdot Z_{\mathrm{G}} + \left(1 - v_{\mathrm{A,U}} - \sum_i v_{\mathrm{P,U},i}\right) \cdot K_{\mathrm{UA}} \cdot Z_{\mathrm{G}} + \sum_i \left(v_{\mathrm{P,U},i} \cdot Z_{\mathrm{P},i}\right)$	$v_{\mathrm{A,U}}$: Volume fraction of air in the PUF(0.98); $v_{\mathrm{P,U},i}$: Volume fraction of particles of size fraction i in the bulk PUF; K_{UA}: Dimensionless partition coefficient between PUF and air;

Vinyl floor	$Z_F = \left(1 - \sum_i v_{P,F,i}\right) \cdot K_{FA} \cdot Z_G + \sum_i \left(v_{P,F,i} \cdot Z_{P,i}\right)$	$v_{P,F,i}$: Volume fraction of particles of size fraction i in the bulk vinyl floor; K_{FA}: Dimensionless partition coefficient between vinyl floor and air;
Organic Film (j = vertical, down-facing, or up-facing surfaces)	$Z_{M,j} = \left(1 - \sum_i v_{P,M,i,j}\right) \cdot K_{MA} \cdot Z_G + \sum_i \left(v_{P,M,i,j} \cdot Z_{P,i}\right)$	$v_{P,M,i,j}$: Volume fraction of particles of size fraction i in the bulk organic film j; K_{MA}: Dimensionless partition coefficient between organic film and air; Calculated according to ref.[2]
Human body	$Z_H = Z_L \cdot v_{L,H} + Z_{NLOM} \cdot v_{NLOM,H} + Z_W \cdot v_{W,H}$	$v_{L,H}$, $v_{NLOM,H}$, $v_{W,H}$: Volume fractions of lipid, non-lipid organic matter, and water, respectively, in human body.
Hands	$Z_{Ha} = Z_L \cdot v_{L,Ha} + Z_W \cdot v_{W,Ha}$	$v_{L,Ha}$, $v_{W,Ha}$: Volume fractions of lipid and water, respectively, in hands.
Rest of skin	$Z_S = Z_L \cdot v_{L,S} + Z_W \cdot v_{W,S}$	$v_{L,S}$, $v_{W,S}$: Volume fractions of lipid and water, respectively, in skin.

Table S2 Summary of D values (mol Pa^{-1} h^{-1}) and relevant parameters in the direct exposure model.

Process	Equation	Parameter definition
Inhalation of indoor air to human body	$D_{\mathrm{ihH}} = G_{\mathrm{V}} \cdot \tau \cdot \left(Z_{\mathrm{G}} \cdot E_{\mathrm{R}} + \sum_i \left(Z_{\mathrm{P},i} \cdot v_{\mathrm{P,A},i} \cdot d_{\mathrm{P},i} \right) \right)$	G_{V}: Gross flow rate for exchange with the environment (m^3 h^{-1}); τ: Fraction of time spent indoors (unitless); E_{R}: Absorption efficiency via respiratory tract (unitless); E_{R}=100% in Tier 0 mode and E_{R}=70% in Tier 1 mode. $v_{\mathrm{P,A},i}$: Volume fraction of particles of size fraction i in the indoor air (unitless); $d_{\mathrm{P},i}$: Deposition fraction of particles of size fraction i in the human respiratory system (unitless).
Dermal permeation into human body	$D_{\mathrm{YH}} = A_{\mathrm{Y}} \cdot K_{\mathrm{P}} \cdot Z_{\mathrm{W}}$ (Y = hand, rest of skin)	A_{Y}: Surface area of Y (hand or rest of skin) (m^2); K_{P}: Aqueous skin permeation coefficient, i.e., measured in water (m h^{-1}); Calculated using the method by ten Berge.[3] For skin permeation coefficients measured in the bulk skin, K_{P} should be multiplied with Z value of the bulk skin (Z_{S}).
Non-dietary ingestion into human body	$D_{\mathrm{moH}} = n \cdot A_{\mathrm{lip}} \cdot d_{\mathrm{Ha}} \cdot TE_{\mathrm{moH}} \cdot Z_{\mathrm{Ha}}$	n: Frequency of hand-to-mouth contact events per hour (h^{-1}); A_{lip}: Area of lip (m^2); d_{Ha}: Thickness of the lipid layer on the hand (m); TE_{moH}: Transfer efficiency from hand to mouth (unitless).
Contact between surface and hands	$D_{\mathrm{X\text{-}Ha}} = n \cdot A_{\mathrm{palm}} \cdot d_{\mathrm{X}} \cdot TE_{\mathrm{X\text{-}Ha}} \cdot Z_{\mathrm{X}}$ (X = carpet, PUF, vinyl floor, organic film)	n: Frequency of surface-to hand contact events per hour (h^{-1}); A_{palm}: Area of palms (m^2); d_{X}: Thickness of surface X (m); $TE_{\mathrm{X\text{-}Ha}}$: Transfer efficiency from X to hand (unitless).
Air diffusion to skin	$D_{\mathrm{diS}} = MTC_{\mathrm{A}} \cdot A_{\mathrm{S}} \cdot Z_{\mathrm{G}}$	MTC_{A}: Mass transfer coefficient of the chemical in air (m h^{-1}); A_{S}: Area of skin (m^2).
Fecal egestion from	$D_{\mathrm{eH}} = \frac{E_{\mathrm{D}} \cdot G_{\mathrm{D}} \cdot Z_{\mathrm{D}}}{Q}$	E_{D}: Absorption efficiency via gastrointestinal tract (unitless);

Process	Equation	Parameter definition
human body		G_D: Ingestion rate ($m^3\ h^{-1}$) Z_D: Weighted sum of Z values of all ingestion items ($mol\ m^{-3}\ Pa^{-1}$) Q: Theoretical maximum biomagnification factor (unitless)
Growth dilution in human body	$D_{gH} = G_G \cdot Z_H$	G_G: Growth rate ($m^3\ h^{-1}$)
Biotransformation in human body	$D_{mH} = V_B \cdot Z_H \cdot \ln 2 / HL_{human}$	V_B: Volume of human (0.07 m^3); HL_{human}: Biotransformation half-life in human body (h)
Urinary excretion from human body	$D_{urH} = E_U \cdot G_U \cdot Z_W$	E_U: Absorption efficiency during urinary excretion (unitless); Assumed to be 100%; G_U: Urinary excretion rate ($m^3\ h^{-1}$); Assumed to equal the drinking rate used in RAIDAR.
Exhalation excretion from human body	$D_{reH} = G_V \cdot Z_G \cdot E_R$	
Elimination via handwashing and bathing	$D_{wH} = F_{wH} \cdot RE \cdot V_L \cdot Z_L$	F_{wH}: Frequency of handwashing or bathing per hour (h^{-1}); RE: Removal efficiency by handwashing or bathing; V_L: Volume of lipids in hands/skin;
Elimination via skin cell loss in hand and skin	$D_{clY} = F_R \cdot V_L \cdot Z_L$ (Y= hand, rest of skin)	F_R: Frequency of cell regeneration per hour (h^{-1}).

Table S3 Information on 37 chemicals in Case 1

CAS#	Name	Usage category[1]	Chemical properties[2]				Emission rate[3]	Application rate	
			MW ($g\ mol^{-1}$)	$\log K_{OW}$	$\log K_{OA}$	HL_{Air} (h)	ER_{Air} ($g\ h^{-1}$)	Apparent AR ($ng\ h^{-1}$)	t_{exp} (min)
90-15-3	1-Naphthol	chemicals in PCPs	144.2	2.9	8.5	2.1	N.A.	4.3×10^{4}	30
131-57-7	2-Hydroxy-4-methoxybenzophenone	chemicals in PCPs	228.3	3.8	10.0	71.2	N.A.	9.0×10^{4}	1440
91-20-3	Naphthalene	chemicals in PCPs	128.2	3.3	5.2	52.4	N.A.	7.5×10^{2}	30
94-13-3	Propyl paraben	chemicals in PCPs	180.2	3.0	9.6	60.9	N.A.	6.0×10^{4}	1440
120-47-8	Ethyl paraben	chemicals in PCPs	166.2	2.5	9.2	106.8	N.A.	6.0×10^{3}	1440
99-76-3	Methyl paraben	chemicals in PCPs	152.2	2.0	8.6	101.1	N.A.	1.6×10^{5}	1440
94-26-8	Butyl paraben	chemicals in PCPs	194.2	3.6	10.0	64.4	N.A.	3.9×10^{4}	2
62-73-7	Dichlorvos	pesticide/antimicro	221.0	1.4	6.1	31.4	N.A.	2.2×10^{4}	30
134-62-3	N,N-Diethyl-3-methyl-benzamide	pesticide/antimicro	191.3	2.2	8.3	67	N.A.	3.0×10^{4}	30
56-72-4	Coumaphos	pesticide/antimicro	362.8	4.1	10.0	42.4	N.A.	1.2×10^{2}	30
56-38-2	Parathion	pesticide/antimicro	291.3	3.8	8.7	71.2	N.A.	1.2×10^{2}	30
3380-34-5	Triclosan	pesticide/antimicro	289.6	4.8	11.5	65.1	N.A.	4.1×10^{5}	2
106-46-7	1,4-Dichlorobenzene	pesticide/antimicro	147.0	3.4	4.5	3539.4	N.A.	8.7×10^{3}	30
121-75-5	Malathion	pesticide/antimicro	330.4	2.4	9.6	146.3	N.A.	8.7×10^{3}	30
333-41-5	Diazinon	pesticide/antimicro	304.4	3.8	9.1	64.4	N.A.	1.2×10^{2}	30
298-00-0	Parathion-methyl	pesticide/antimicro	263.2	2.9	8.2	90.6	N.A.	1.2×10^{2}	30
68359-37-5	Cyfluthrin	pesticide/antimicro	434.3	6.0	11.9	33.4	N.A.	1.4×10^{3}	30
52918-63-5	Deltamethrin	pesticide/antimicro	505.2	6.2	9.9	33.1	N.A.	5.8×10^{2}	30
1912-24-9	Atrazine	pesticide/antimicro	215.7	2.6	9.6	68.6	N.A.	6.4×10^{2}	30
3383-96-8	Temephos	pesticide/antimicro	466.5	6.0	13.1	48.4	N.A.	1.2×10^{2}	30
60-51-5	Dimethoate	pesticide/antimicro	229.3	0.8	8.8	79.2	N.A.	1.2×10^{2}	30
52645-53-1	Permethrin	pesticide/antimicro	391.3	6.5	10.6	34	N.A.	2.6×10^{4}	30

CAS#	Name	Usage category[1]	Chemical properties[2]				Emission rate[3]	Application rate	
			MW ($g\ mol^{-1}$)	$\log K_{OW}$	$\log K_{OA}$	HL_{Air} (h)	ER_{Air} ($g\ h^{-1}$)	Apparent AR ($ng\ h^{-1}$)	t_{exp} (min)
100-02-7	4-Nitrophenol	pesticide/antimicro	139.1	1.9	9.7	976.4	N.A.	1.2×10^{2}	30
1563-66-2	Carbofuran	pesticide/antimicro	221.3	2.3	9.2	77	N.A.	1.2×10^{2}	30
52315-07-8	Cypermethrin	pesticide/antimicro	416.3	6.6	11.7	33.2	N.A.	1.5×10^{4}	30
141-66-2	Dicrotophos	pesticide/antimicro	237.2	0.0	8.7	40.4	N.A.	1.2×10^{2}	30
94-75-7	2,4-Dichlorophenoxyacetic acid	pesticide/antimicro	221	2.8	8.6	133.1	N.A.	4.3×10^{3}	30
85-68-7	Butyl benzyl phthalate	plasticizer	312.4	4.7	9.0	80.9	5.3×10^{5}	0	0
84-61-7	Dicyclohexyl phthalate	plasticizer	330.4	6.2	11.6	80.9	7.0×10^{3}	0	0
84-69-5	Diisobutyl phthalate	plasticizer	278.4	4.1	8.4	78.7	2.0×10^{4}	0	0
117-84-0	Dioctyl phthalate	plasticizer	390.6	8.1	11.7	65.5	9.1×10^{5}	0	0
84-66-2	Diethyl phthalate	plasticizer	222.2	2.4	7.0	126	1.6×10^{5}	0	0
131-11-3	Dimethyl phthalate	plasticizer	194.2	1.6	6.7	18.9	5.5×10^{4}	0	0
84-74-2	Dibutyl phthalate	plasticizer	278.4	4.5	8.6	78.7	8.9×10^{4}	0	0
131-70-4	Monobutyl phthalate	plasticizer	222.2	2.8	10.0	122.3	88	0	0
117-81-7	Di(2-ethylhexyl) phthalate	plasticizer	390.6	7.6	12.6	55.8	2.0×10^{8}	0	0
80-05-7	Bisphenol A	plasticizer	228.3	3.3	12.7	69.1	8.9×10^{4}	0	0

MW: molar mass; K_{OW}: octanol-water partition coefficient; K_{OA}: octanol-air partition coefficient, HL_{Air}: degradation half-life in air; ER_{Air}: emission rate to air; AR: application rate onto skin; t_{exp}: application duration.

Notes: (i) According to product categories defined in Isaacs et al.[4];

(2) Calculated by the USEPA Estimation Program Interface (EPI) Suite.

(3) Calculated using a method modified from Litter et al.[5]

$$ER = A_{material} \cdot MTC_{A} \cdot \left(Z_{gas} + v_{particle} \cdot Z_{particle}\right) \cdot f_{0}$$

Where, $A_{material}$ is the area of plastic material (in m^2; assumed to be the area of vinyl floor in this study);

MTC_A is the air-side mass transfer coefficient of a chemical (in m h^{-1}), which is simply calculated using an empirical equation:

$$MTC_A = \frac{0.558}{MW^{0.65}} \cdot \frac{1}{\delta},$$

in which δ is the thickness of air boundary layer (0.005 m)

Z_{gas} is Z-value of a chemical in gaseous phase (in mol m^{-3} Pa^{-1}), $Z_{gas} = 1/(R \cdot T)$;

$v_{particle}$ is volumetric fraction of total suspended particles in the indoor air, converted from the mass concentration of total suspended particles;

$Z_{particle}$ is Z-value of a chemical in particulate phase (in mol m^{-3} Pa^{-1}), $Z_{particle} = K_{PG}/(R \cdot T)$, in which the particle-gas partition coefficient K_{PG} is calculated in accordance with Harner and Bidleman;[1]

f_0 is the fugacity in the air immediately adjacent to product surface (in Pa), which is given by

$f_0 = \min\left(\frac{C_{material}}{Z_{material}}, VP\right)$, in which $C_{material}$ is chemical concentration in product material (in mol m^{-3}; converted from the chemical weight fraction), $Z_{material}$ is fugacity capacity of article material (in mol m^{-3} Pa^{-1}; calculated based on the material-air partition coefficient) and VP is vapor pressure of the chemical (in Pa).

Table S4 Sensitivities of modeled uptake rates of chemicals in personal care products to selected input parameters

Sensitivity (S) is defined as the percentage change of a model output, $\partial Y/Y$, with respect to the percentage perturbation in an input parameter, $\partial X/X$, near its baseline value of X_0 (10% above and below the baseline value) with other parameters fixed, i.e.,

$$S = \left.\frac{\partial Y/Y}{\partial X/X}\right|_{X=X_0} = \frac{1}{20\%} \cdot \frac{Y_{X=X_0 \cdot 110\%} - Y_{X=X_0 \cdot 90\%}}{Y_{X=X_0}}.$$

CAS#	Sensitivity						
	90-15-3	131-57-7	91-20-3	94-13-3	120-47-8	99-76-3	94-26-8
K_{OW}	-0.12	-0.62	-0.76	-0.25	-0.21	-0.43	-0.22
K_{OA}	0.057	0.004	0.93	0.014	0.015	0.016	0.006
HL_{Air}	7.3×10^{-4}	4.7×10^{-6}	6.0×10^{-4}	4.5×10^{-5}	2.5×10^{-5}	1.2×10^{-5}	1.3×10^{-5}
ER_{Air}	0	0	0	0	0	0	0
Apparent AR	1	1	1	1	1	1	1

K_{OW}: octanol-water partition coefficient; K_{OA}: octanol-air partition coefficient, HL_{Air}: degradation half-life in air; ER_{Air}: emission rate to air; AR: application rate onto skin.

Table S5 Information on 131 chemicals in Cases 2 and 3

No.	CAS#	Name	MW ($g\ mol^{-1}$)	$\log K_{OW}$	$\log K_{OA}$	HL_{Air} (h)	HL_{Human} (h)	*OED* ($mg\ kg^{-1}\ d^{-1}$)
1	92-87-5	Benzidine	184.2	1.3	10.0	11.4	3.2	3.3
2	10605-21-7	methyl 1H-benzimidazol-2-ylcarbamate	191.2	1.5	10.6	8.7	1.6	11.4
3	101-80-4	4,4'-Oxydianiline	200.2	1.4	10.6	8.8	51.1	0.4
4	101-54-2	N-Phenyl-1,4-benzenediamine	184.2	1.8	9.6	8.8	8.5	2.9
5	119-93-7	o-Tolidine	212.3	2.3	10.9	9.3	7.1	0.04
6	94-13-3	Propylparaben	180.2	3.0	9.6	124.4	2.5	27.3
7	99-59-2	2-methoxy-5-nitroaniline	168.2	1.5	9.2	195.2	18.3	0.6
8	1912-24-9	Atrazine	215.7	2.6	9.6	64	31.6	0.4
9	60-09-3	4-Aminoazobenzene	197.2	3.4	10.1	40.3	7.2	1.1
10	120-47-8	Ethylparaben	166.2	2.5	9.2	139.2	2.5	48.2
11	63-25-2	Carbaryl	201.2	2.4	9.2	67.3	3.5	62.7
12	94-26-8	Butylparaben	194.2	3.6	10.0	113.1	2.5	51.1
13	119515-38-7	Icaridin	229.3	2.6	11.5	31.2	1.6	69.7
14	1563-66-2	Carbofuran	221.3	2.3	9.2	67.3	1.8	0.1
15	120-32-1	Clorophene	218.7	3.6	10.6	98.5	4.4	0.2
16	21725-46-2	Cyanazine	240.7	2.2	12.2	188.1	134.4	0.7
17	99-76-3	Methylparaben	152.2	2.0	8.8	158.2	1.8	4
18	102-06-7	1,3-Diphenylguanidine	211.3	2.9	12.4	20.5	16.5	0.2
19	119-90-4	3,3'-Dimethoxybenzidine	244.3	1.8	12.9	13	7.1	1
20	23103-98-2	Pirimicarb	238.3	1.7	9.2	11.6	1.2	3.4
21	97-54-1	Isoeugenol	164.2	3.0	9.0	20.7	0.5	1.6
22	110235-47-7	Mepanipyrim	223.3	3.3	9.5	8.9	14.4	0.8
23	838-88-0	4,4'-Methylene bis(2-methylaniline)	226.3	3.3	11.8	8.7	12.3	4
24	17804-35-2	Benomyl	290.3	2.1	11.8	8.2	4	4.7

No.	CAS#	Name	MW (g mol^{-1})	logK_{OW}	logK_{OA}	HL_{Air} (h)	HL_{Human} (h)	*OED* (mg kg^{-1} d^{-1})
25	1401-55-4	Tannic acid	636.5	-0.2	17.7	6.5	6.3	0.001
26	121-00-6	2-tert-Butyl-4-methoxy-phenol	180.3	3.5	9.0	48.5	0.5	5.3
27	77-09-8	Phenolphthalein	318.3	2.4	15.8	20.8	7.7	0.6
28	533-74-4	Dazomet	162.3	0.6	8.3	6.1	12.3	7.8
29	25606-41-1	Propamocarb hydrochloride	188.3	1.1	8.3	17.7	2.8	27.3
30	548-62-9	Hexamethyl-p-rosaniline chloride	408.0	0.5	14.4	3.9	7.9	0.001
31	26530-20-1	Octhilinone	213.3	2.5	8.5	44.5	4.6	0.4
32	35554-44-0	Imazalil	297.2	3.8	10.8	20.6	33.5	0.00001
33	134-62-3	DEET	191.3	2.2	8.3	69.2	1.7	22.9
34	732-11-6	Phosmet	317.3	2.8	9.2	11.5	8.6	1.8
35	91-59-8	2-Naphthylamine	143.2	2.3	7.8	8.8	1.9	2
36	107534-96-3	Tebuconazole	307.8	3.7	11.9	152.5	62.3	0.02
37	121-14-2	2,4-Dinitrotoluene	182.1	2.0	7.6	8122	2	0.1
38	2634-33-5	1,2-Benzisothiazolin-3-one	151.2	0.6	7.2	103.2	2.9	0.1
39	34590-94-8	Propanol, 1 (or 2)-(2-methoxymethylethyoxy)-	148.2	-0.4	7.0	45.8	2.7	7.4
40	91-53-2	Ethoxyquin	217.3	3.9	8.9	13.6	14.5	1.2
41	122-99-6	Phenoxyethanol	138.2	1.2	6.9	53.6	3.3	0.2
42	120-71-8	p-Cresidine	137.2	1.7	7.0	8.7	2.6	26.7
43	98-54-4	4-tert-Butylphenol	150.2	3.3	7.6	43.1	4.7	11.2
44	77-40-7	Bisphenol B	242.3	4.1	13.4	21.4	9.6	0.3
45	91-64-5	Coumarin	146.2	1.4	6.8	132.9	3.1	8.6
46	110-26-9	N,N'-Methylenebis(acrylamide)	154.2	-1.5	5.8	38.8	1.7	94.3
47	99-71-8	4-(Butan-2-yl)phenol	150.2	3.1	7.3	39.7	5.6	8.9
48	106-44-5	4-Methylphenol	108.1	1.9	6.3	37.2	3.6	30.6
49	95-48-7	2-Methylphenol	108.1	2.0	6.3	41.7	0.6	30.7

No.	CAS#	Name	MW ($g\ mol^{-1}$)	$\log K_{OW}$	$\log K_{OA}$	HL_{Air} (h)	HL_{Human} (h)	*OED* ($mg\ kg^{-1}\ d^{-1}$)
50	156052-68-5	Zoxamide	336.7	3.8	12.6	163	167.1	0.00005
51	101-61-1	4,4'-methylenebis(N,N-dimethylaniline)	254.4	4.4	9.7	8.5	0.4	0.2
52	88-85-7	Dinoseb	240.2	3.6	8.3	433.9	28.4	0.001
53	131-17-9	Diallyl phthalate	246.3	3.2	8.0	31.4	1.3	0.03
54	67747-09-5	Prochloraz	376.7	4.1	10.3	22.4	507.5	0.04
55	86-30-6	N-nitrosodiphenylamine	198.2	3.1	7.4	70.5	7.4	1.7
56	80-46-6	4-(2-methylbutan-2-yl)phenol	164.3	3.9	8.0	41.9	6.3	0.2
57	119-61-9	Benzophenone	182.2	3.2	7.3	492.4	3	0.5
58	148-24-3	8-Hydroxyquinoline	145.2	1.9	6.5	8.8	4	1.2
59	91-22-5	Quinoline	129.2	2.0	6.2	150.9	3.1	161.5
60	606-20-2	2,6-Dinitrotoluene	182.1	2.1	6.6	8122	4.3	1
61	13674-87-8	TDCPP	430.9	3.7	10.6	96.8	3796.5	0.05
62	56-38-2	Parathion	291.3	3.8	8.7	19	27.4	0.02
63	97-53-0	Eugenol	164.2	2.3	6.4	26.9	0.4	44.1
64	576-26-1	2,6-Dimethylphenol	122.2	2.4	5.9	26.6	2.1	18.1
65	87-62-7	2,6-Dimethylaniline	121.2	1.8	5.8	10.8	2.1	0.03
66	93-15-2	Methyleugenol	178.2	3.0	6.7	23.3	1.4	39
67	94-59-7	Safrole	162.2	3.5	6.9	23.1	7.4	6.1
68	72490-01-8	Fenoxycarb	301.4	4.3	12.1	26.8	60.8	0.02
69	90-04-0	2-Anisidine	123.2	1.2	5.6	18.6	3.7	0.8
70	126-73-8	Tributyl phosphate	266.3	4.0	8.2	22.2	8.4	0.02
71	584-79-2	d-cis,trans-Allethrin	302.4	4.8	10.2	7.9	4.8	0.3
71	28434-00-6	S-Bioallethrin	302.4	4.8	10.2	7.9	4.8	0.1
73	76-87-9	Fentin hydroxide	367.0	3.5	8.3	292.2	10.4	0.00002
74	924-16-3	N-nitrosodi-n-butylamine	158.3	2.6	5.9	65.2	5.5	185.1

No.	CAS#	Name	MW (g mol^{-1})	logK_{OW}	logK_{OA}	HL_{Air} (h)	HL_{Human} (h)	*OED* (mg kg^{-1} d^{-1})
75	298-02-2	Phorate	260.4	3.6	7.3	7	34.7	0.03
76	29091-21-2	Prodiamine	350.3	4.1	8.5	72.9	4.4	0.8
77	83-79-4	Rotenone	394.4	4.1	15.4	5.3	11.2	0.01
78	84-74-2	Di-n-butylphtalate	278.4	4.5	8.6	188.7	1.9	0.05
79	105-99-7	Dibutyl hexanedioate	258.4	4.3	8.0	138.1	1.1	1659.3
80	58-89-9	Hexachlorocyclohexane (gamma isomer)	290.8	4.1	7.8	9212.5	21	0.01
81	128-39-2	2,6-Di-tert-butylphenol	206.3	4.9	8.7	35.6	3.5	19.4
82	1861-32-1	Chlorthal-dimethyl	332.0	4.3	8.3	3968.7	136.5	31.7
83	1119-40-0	Dimethyl glutarate	160.2	0.6	5.2	530.4	0.6	1
84	129-00-0	Pyrene	202.3	4.9	8.2	35	8.3	16.5
85	101-86-0	2-Benzylideneoctanal	216.3	4.8	8.2	31.8	17.1	3
86	120-12-7	Anthracene	178.2	4.5	7.1	43.8	5.1	2.1
87	98-95-3	Nitrobenzene	123.1	1.9	4.9	12502.7	26.8	36.2
88	115-86-6	Triphenyl phosphate	326.3	4.6	8.5	161.4	13.1	0.001
89	72-43-5	Methoxychlor	345.7	5.1	10.2	32.7	285.5	9.5
90	206-44-0	Fluoranthene	202.3	5.2	8.6	59.9	3.1	0.9
91	140-66-9	4-(1,1,3,3-Tetramethylbutyl)phenol	206.3	5.3	9	41.3	6	1.2
92	7696-12-0	Tetramethrin	331.4	4.7	8.9	13.7	2.7	84.4
93	208-96-8	Acenaphthylene	152.2	3.9	6.3	15.9	5.3	5.1
94	87-86-5	Pentachlorophenol	266.3	5.1	11.1	3179.7	31.6	1.1
95	1806-26-4	4-Octylphenol	206.3	5.5	9.2	34.8	4.9	1.6
96	2921-88-2	Chlorpyrifos	350.6	5.0	8.9	19.1	206.3	1.8
97	92-52-4	Biphenyl	154.2	4.0	5.9	243.1	1.9	66.9
98	91-20-3	Naphthalene	128.2	3.3	5.0	81	3.1	12.5
99	7173-51-5	Didecyl dimethyl ammonium chloride	362.1	4.7	12.2	37.8	5.6	0.004

No.	CAS#	Name	MW ($g\ mol^{-1}$)	$\log K_{OW}$	$\log K_{OA}$	HL_{Air} (h)	HL_{Human} (h)	*OED* ($mg\ kg^{-1}\ d^{-1}$)
100	7378-99-6	N,N-Dimethyloctylamine	157.3	3.5	5.4	20	3.7	119.1
101	1024-57-3	Heptachlor epoxide, isomer B	389.3	5.0	8.0	288.9	10293.3	0.02
102	56-55-3	Benz[a]anthracene	228.3	5.8	9.1	35	8.3	0.04
103	29420-49-3	Potassium nonafluoro-1-butanesulfonate	300.1	1.8	5.1	12502.7	752.9	0.2
104	106-46-7	1,4-Dichlorobenzene	147.0	3.4	4.4	5469.9	37.7	3.2
105	127-51-5	3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	206.3	4.8	6.8	10.3	10.1	9.5
106	307-24-4	Perfluorohexanoic acid	314.1	3.5	4.4	3366.1	602.6	0.3
107	111-82-0	Methyl laurate	214.4	5.4	6.3	132.7	1.6	10181.1
108	2795-39-3	Heptadecafluorooctanesulfonic acid potassium salt	500.1	4.5	4.8	12502.7	41686.9	0.0001
108	1763-23-1	Perfluorooctane sulfonic acid	500.1	4.5	4.8	12502.7	41686.9	0.0001
110	375-85-9	Perfluoroheptanoic acid	364.1	4.2	4.3	3366.1	2082.4	0.02
111	754-91-6	Perfluorooctanesulfonamide	499.1	5.8	3.9	10000	147107.9	0.03
112	3825-26-1	Pentadecafluorooctanoic acid	414.1	4.8	4.2	3366.1	47863	0.0007
112	335-67-1	Perfluorooctanoic acid	414.1	4.8	4.2	3366.1	47863	0.01
114	375-95-1	Perfluorononanoic acid	464.1	5.5	4.2	3366.1	29108.2	0.002
115	2058-94-8	Perfluoroundecanoic acid	564.1	6.8	4.1	3366.1	406885.3	0.01
116	335-76-2	Perfluorodecanoic acid	514.1	6.2	4.1	3366.1	108828.8	0.004
117	76-44-8	Heptachlor	373.3	5.5	7.4	28.2	10293.3	17
118	97886-45-8	Dithiopyr	401.4	4.8	11.6	245.8	7.3	0.3
119	205-99-2	Benzo[b]fluoranthene	252.3	5.8	10.4	94.3	5.1	0.003
120	72-54-8	p,p'-DDD	320.1	6	9.6	402.9	762.3	0.1
121	309-00-2	Aldrin	364.9	6.5	9.2	26.7	3006.5	0.008
122	789-02-6	o,p'-DDT	354.5	6.8	10.3	509.6	2610	0.1
123	50-29-3	p,p'-DDT	354.5	6.9	10.4	509.6	22908.7	3.1

No.	CAS#	Name	MW (g mol^{-1})	logK_{OW}	logK_{OA}	HL_{Air} (h)	HL_{Human} (h)	*OED* (mg kg^{-1} d^{-1})
124	60-57-1	Dieldrin	380.9	5.5	11	213.8	9772.4	0.02
124	72-20-8	Endrin	380.9	5.5	11	213.8	9772.4	0.001
126	94-28-0	Tri(ethylene glycol) bis(2-ethylhexanoate)	402.6	5.6	12.4	39.4	0.6	37.7
127	2385-85-5	Mirex	545.6	7.4	11.6	10000	4842403.8	0.0002
128	117-84-0	Di-n-octyl phthalate	390.6	8.1	12.1	85	1.9	0.1
129	1843-05-6	2-Hydroxy-4-(octyloxy)benzophenone	326.4	7	12.3	8	5.8	8.9
130	71751-41-2	Abamectin	873.1	4.4	9.6	2.7	215.7	0.3
131	103-23-1	Di(2-ethylhexyl)adipate	370.6	8.1	12.9	69	2.6	15.4

MW: Molar mass; K_{OW}: Octanol-water partition coefficient; K_{OA}: octanol-air partition coefficient, HL_{Air}: degradation half-life in air; HL_{human}: biotransformation half-life in human body; *OED*: oral equivalent dose.

Text S1 Steady-state mass balance equations for compartments of hand, rest of skin, and human body

Hand:

$$\sum_{\mathrm{X=C,U,F,M}} \left(D_{\mathrm{X\text{-}Ha}} \cdot f_{\mathrm{X}} \right) = \left(D_{\mathrm{clHa}} + D_{\mathrm{moH}} + D_{\mathrm{HaH}} + D_{\mathrm{wH}} \right) \cdot f_{\mathrm{Ha}} \qquad \text{(eq.S1)}$$

Rest of skin:

$$D_{\mathrm{diS}} \cdot f_{\mathrm{A}} = \left(D_{\mathrm{diS}} + D_{\mathrm{clS}} + D_{\mathrm{SH}} + D_{\mathrm{wH}} \right) \cdot f_{\mathrm{S}} \qquad \text{(eq.S2)}$$

Human body:

$$\underbrace{N_{\mathrm{inH}}}_{\text{Ingestion}} + \underbrace{D_{\mathrm{ihH}} \cdot f_{\mathrm{A}}}_{\text{Inhalation}} + \underbrace{\sum_{\mathrm{Y=Ha,S}} \left(D_{\mathrm{YH}} \cdot f_{\mathrm{Y}} \right)}_{\text{Dermal permeation}} + \underbrace{E_{\mathrm{D}} \cdot D_{\mathrm{moH}} \cdot f_{\mathrm{Ha}}}_{\text{Non-dietary ingestion}} = \left(D_{\mathrm{reH}} + D_{\mathrm{eH}} + D_{\mathrm{urH}} + D_{\mathrm{mH}} + D_{\mathrm{gH}} \right) \cdot f_{\mathrm{H}} \qquad \text{(eq.S3)}$$

Text S2 Algorithm for calculating absorption of direct skin application

The rate of chemicals applied being absorbed by human hands/skin (E; ng h^{-1}) is calculated by eq. S4

$$E = AR \cdot SF_{lag} \quad \text{(eq. S4)}$$

whereby,

AR is the rate of a chemical being applied to human hands/skin, i.e., an apparent application rate (ng h^{-1});
SF_{lag} is a unitless scaling factor, which describes the fraction of a chemical that is truly absorbed by human hands/skin before removal due to a time lag in permeation.

Calculation of the apparent application rate

In the real world, the application of a chemical-containing product on human hands or skin is usually an intermittent, as opposite to continuous, process. As a steady-state model, RAIDAR-ICE adopts an "equivalent" application rate, which averages the individual intermittent application rates over a given duration. RAIDAR-ICE considers two types of intermittent applications:

(i) The chemical-containing product is left on after application, such as a moisturizer or a sunscreen. The equivalent application rate is calculated by eq. S5:

$$AR_1 = M \cdot \left(\frac{1+2+3+\cdots Freq}{Freq} \right) \cdot \frac{1}{24}, \quad \text{(eq. S5)}$$

whereby,
M is amount of a chemical being applied to human skin or hands per application (in ng);
$Freq$ is the times of applications per day (in d^{-1}).

(ii) The chemical-containing product is washed off t_{exp} minutes after application, such as a hand soap or a shampoo. The equivalent application rate is calculated by eq. S6:

$$AR_2 = AR_1 \cdot \frac{Freq \cdot t_{exp}}{1440} \quad \text{(eq. S6)}$$

whereby,
t_{exp} is the duration of an application (in min), i.e., the time of exposure to the chemical until wash off.
Note: the model will generate a warning message in a conceptually unlikely scenario of $Fr \times t_{exp} > 1440$.

Calculation of the scaling factor

Not all the chemical in an application can be completely absorbed by human hands/skin because skin permeation can be very slow for certain chemicals. Lag time (t_{lag}) is defined as the minimum duration for a chemical applied to hands/skin to reach full steady-state absorption.[6] The t_{lag} values for hands (including palm and back) and skin are calculated as per Tibaldi et al.[6]

Let us start with a case of single, finite application, in which the amount of a chemical that cumulatively penetrates through skin increases from zero to a maximum (i.e., the steady-state absorption) during the lag-phase. In other words, the total absorbed fraction, which is characterized by a scaling factor SF_{lag}, increases from 0 to 100%. RAIDAR-ICE assumes that the increase in the total absorbed fraction is linear during the lag phase. While the real increase is likely not linear – it is perhaps sigmoidal or logarithmic – the difference in SF_{lag} is not overly large, and thus this simple assumption should be an acceptable first approximation.

In the case of continuous, infinite application, which is assumed by RAIDAR-ICE, the total absorption is an integral of absorptions in individual single, finite applications. Therefore, the total absorbed fraction can be viewed as the area under the curve of SF_{lag} in the case of a single, finite application. When the application duration (t_{exp}) is greater than t_{lag}, the amount of product applied within t_{lag} minutes before removal can only be partially absorbed, while the amount of product applied within a window $t_{exp} - t_{lag}$ can be 100% absorbed (Figure S1, panel a). Therefore, SF_{lag} is calculated as

$$SF_{lag} = \frac{2t_{exp} - t_{lag}}{2t_{exp}}, \text{ when } t_{lag} < t_{exp}$$

When the application duration (t_{exp}) is shorter than t_{lag}, all applied amount can only be partially absorbed (Figure S1, panel b). Therefore, SF_{lag} is calculated as

$$SF_{lag} = \frac{1}{2} \cdot \frac{t_{exp}}{t_{lag}}, \text{ when } t_{lag} > t_{exp}$$

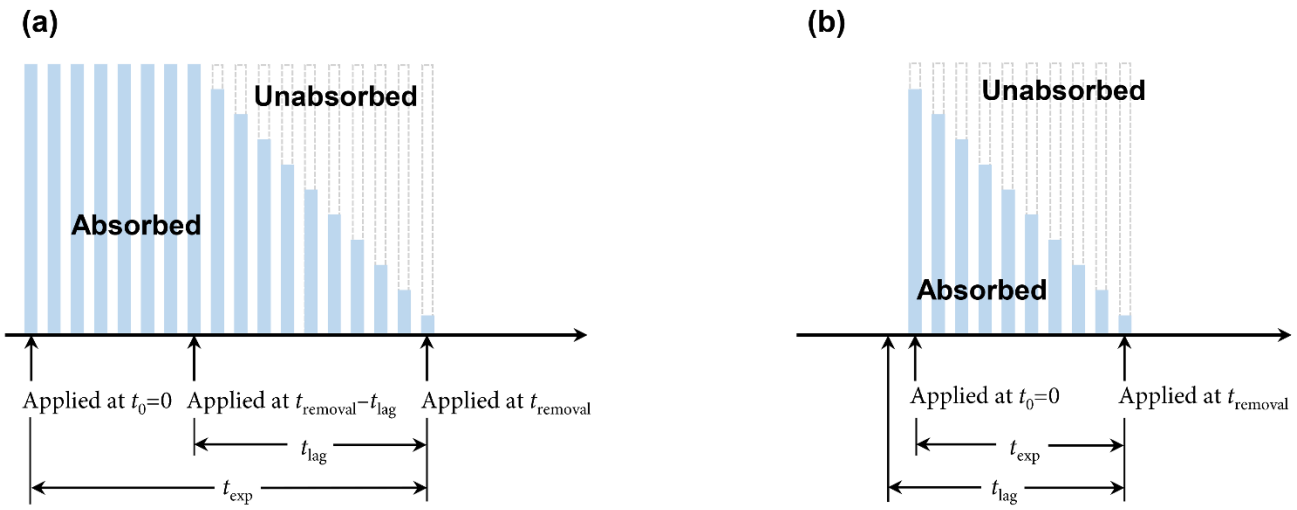


Figure S1 Graphical illustration of the absorbed fraction (blue shadows) in the total applied amount (combined blue and white parts) over the application duration (between the start and the removal) under scenarios of (a) lag time (t_{lag}) being shorter than application duration (t_{exp}), and (b) lag time (t_{lag}) being longer than application duration (t_{exp}). The total applied amount over the application duration is an arbitrary unit.

Figure S2 Relative importance of near-field exposure pathways in intake fractions of 131 chemicals in Case 2

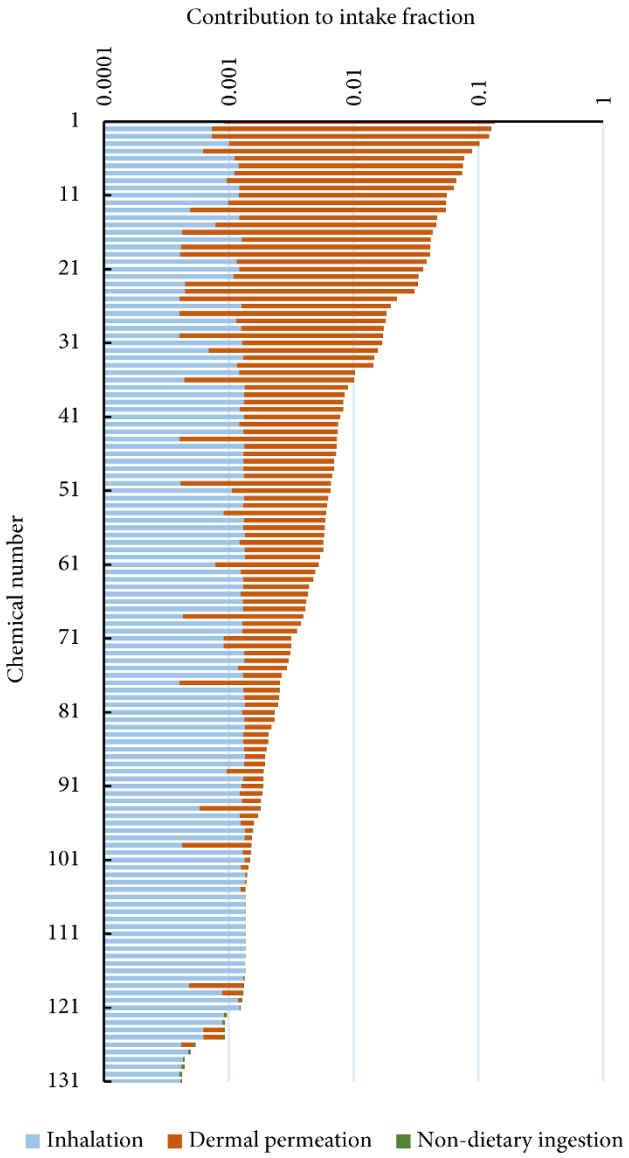


Figure S3 Modeling population intake fraction (Tier 1 *iF*s) on the coupled RAIDAR-ICE and RAIDAR models

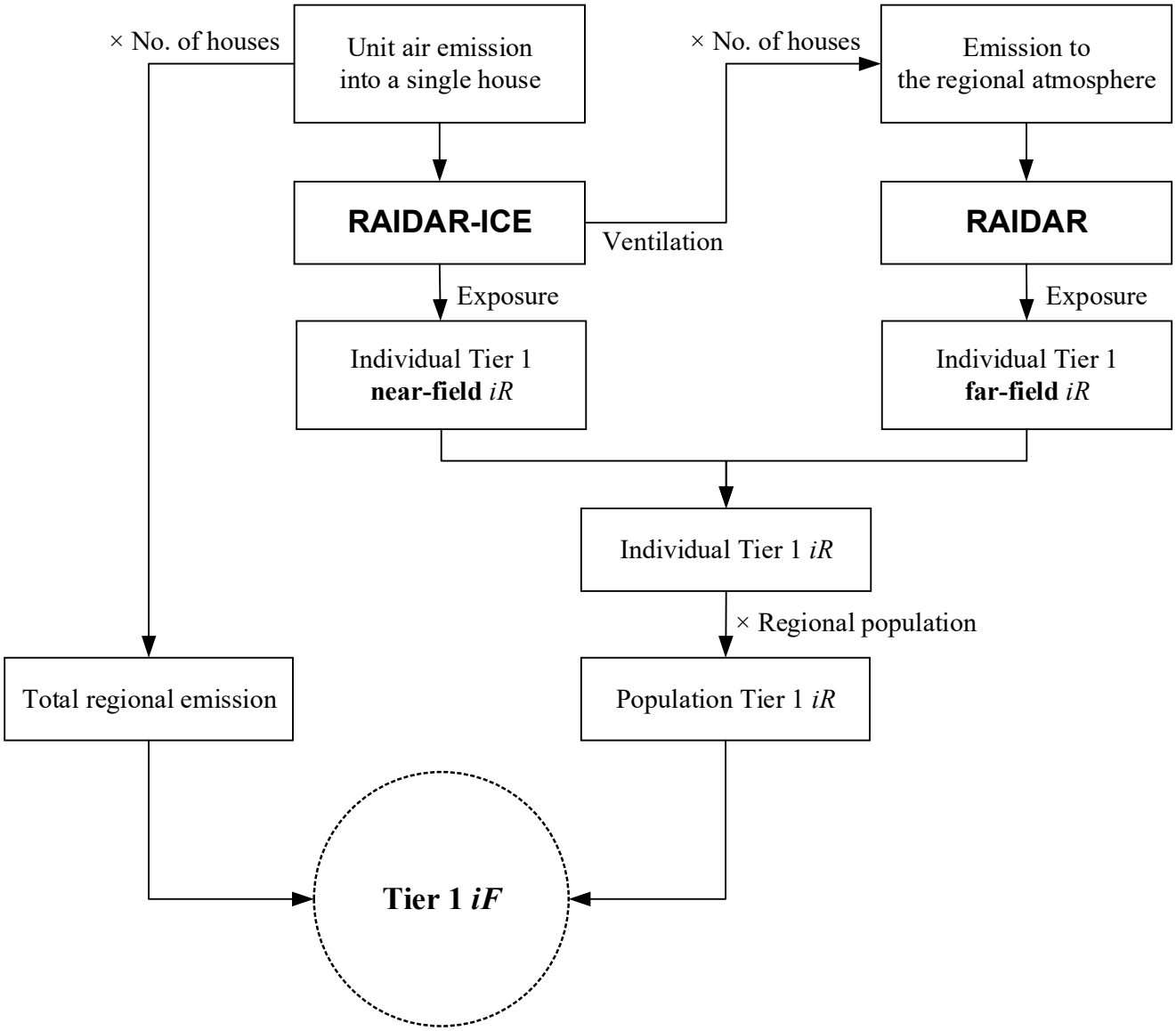
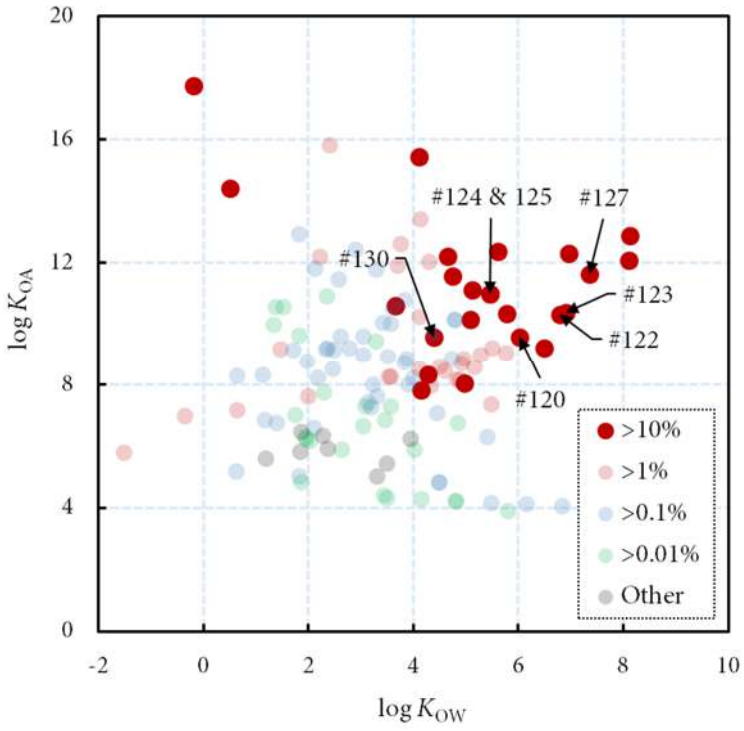


Figure S4 Percentage contribution of diet to the population intake fractions of 131 chemicals in Case 3 Chemicals with a contribution greater than 90% are labeled. For names of the labeled chemicals, please see Table S5.



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