USEtox – characterizing human and ecotoxicological impacts of chemicals in LCA

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Main Application Areas of USEtox

Near-field/far-field USEtox framework is suitable for **comparative evaluation of chemicals** emitted along product life cycles and chemicals in various product applications. Primary application areas are (model already tested):

Application area	Product types already covered in our framework (emissions already directly or indirectly included)
Product life cycle assessment (LCA)	Food contact materials
High-throughput exposure screening	Personal care products; food contact materials
High-throughput risk screening	Children toys; building materials; paints
Chemical exposure and risk prioritization	Household products (cleaning, personal care, and home maintenance products)
Chemical alternatives assessment (CAA) / chemical substitution	Building materials; personal care products; agricultural pesticides

http://doi.org/10.1007/s11367-021-01889-y

What is USEtox?

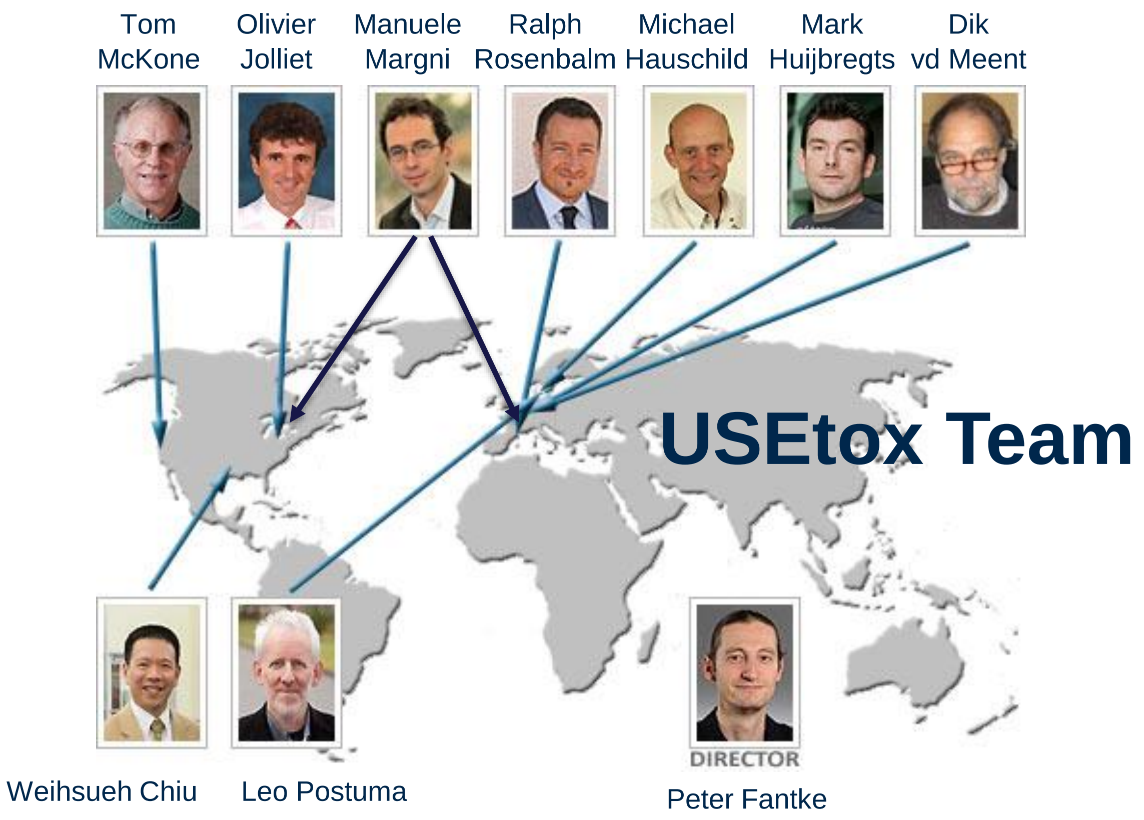
- Global scientific consensus model
- Human toxicity & freshwater ecotoxicity
- Organic chemicals & metal ions

- Initiated by the UNEP-SETAC Life Cycle Initiative
- Used by European Commission and US EPA

http://vimeo.com/usetox/video

USEtox: the UNEP-SETAC toxicity model

USEtox: A parsimonious model to assess toxic impacts of chemicals on humans and ecosystems.
Now extended to chemicals in products



- **Parsimonious** – as simple as possible, as complex as necessary
- **Mimetic** – not differing more from the original models than these differ among themselves
- **Evaluated** – providing a repository of knowledge through evaluation against a broad set of existing models
- **Transparent** – being well documented, including the reasoning for model choices

USEtox characterization factors

- **Quantitatively** determine the impact score per impact category, in Comparative Toxic Unit (CTU): $CTU_{h\ midpoint}$ = cases or incidences
- $CTU_{h\ damage}$ = DALY – Disability Adjusted Life Years

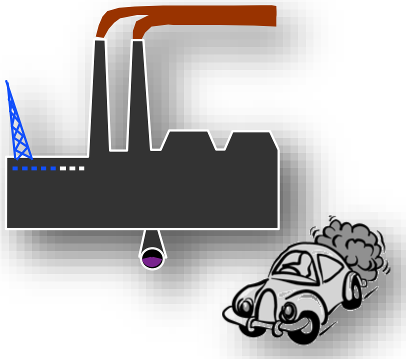
$$IS = \sum_{i}\sum_{x} CF_{x,i} \times m_{x,i}$$

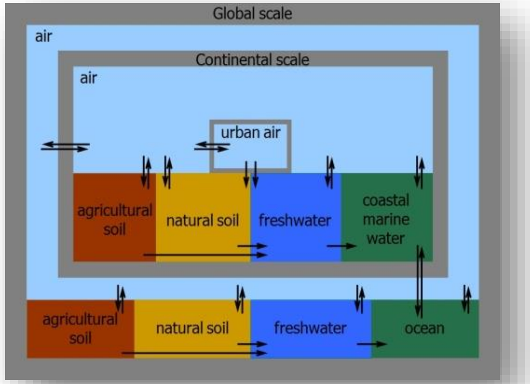
IS : impact score [CTU/functional unit]=[cases/functional unit]
CF : **characterization factor [CTU/kg]**
m : life cycle emission [kg/functional unit]
x : index for substance
i : index for compartment

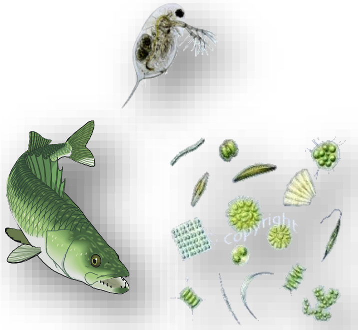
- A **characterization factor** is …
- A quantitative representation of the (relative) hazard potential of a specific emission per kg emitted,
- Expressed as absolute metric or relative to a reference substance.

- *Example:* Human toxicity characterization factor of benzene: 5.5E-07 CTU_h/kg (cases per kg emitted to urban air (comparative toxic units = disease cases)

Impact Pathway: Ecotoxicity Impacts







Emission

Emission flow
[$kg_{emitted}$ /d]

Fate

Mass in environment
[$kg_{in\ compartment}$]

Exposure

Dissolved mass fraction
[$kg_{bioavailable}$]

Effects

Potential effects
[PAF x m³]

Fate factor, FF

[$kg_{in\ compartment}$ per $kg_{emitted}$/d]

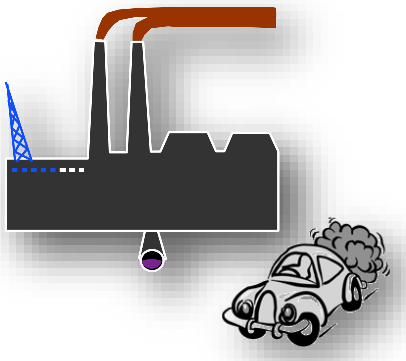
Ecoexposure factor, XF

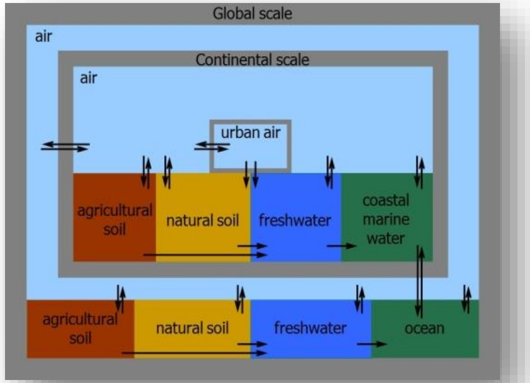
[$kg_{bioavailable}$ per $kg_{in\ compartment}$]

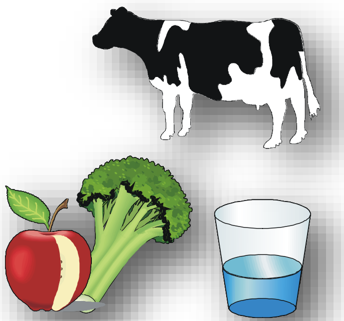
Effect factor, EF

[PAF x m³ per $kg_{bioavailable}$]

Impact Pathway: Human Toxicity Impacts







Emission

Emission flow
[$\text{kg}_{\text{emitted}}$ /d]

Fate

Mass in environment
[$\text{kg}_{\text{in compartment}}$]

Exposure

Human intake
[$\text{kg}_{\text{intake}}$/d]

Effects

Potential effects
[disease cases/d]

Fate factor, FF

[$\text{kg}_{\text{in compartment}}$ per $\text{kg}_{\text{emitted}}$/d]

Human exposure factor, XF

[$\text{kg}_{\text{intake}}$/d per $\text{kg}_{\text{in compartment}}$]

Effect factor, EF

[disease cases/d per $\text{kg}_{\text{intake}}$/d]

Impact Pathway: Characterization Factors in USEtox

Emission → **Fate** → **Exposure** → **Effects** → **Damage**

Fate factor | **Exposure factor** | **Effect factor** | **Damage factor**

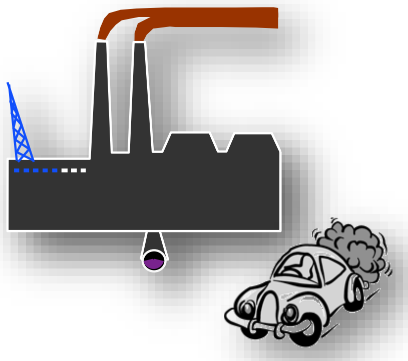
[e.g. DALY/case]

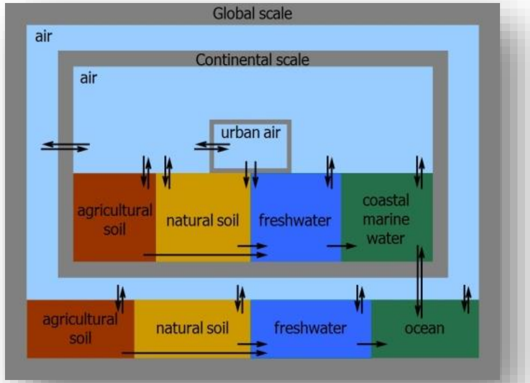
Midpoint characterization factor , CF_{midpoint} [impacts/kg$_{\text{emitted}}$]

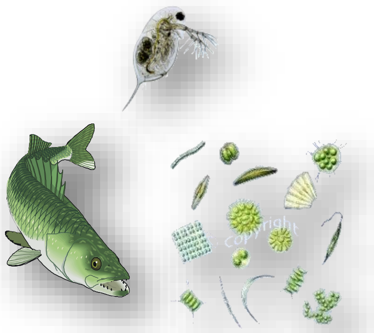
Damage characterization factor , $CF_{\text{damage}} = XF \times FF \times ERF \times SF$ [damage/kg$_{\text{emitted}}$]

USEtox far-field environmental fate assessment

Impact Pathway: Environmental Fate







Emission

Emission flow
[$kg_{emitted}$ /d]

Fate

Mass in environment
[$kg_{in\ compartment}$]

Exposure

Dissolved mass fraction
[$kg_{bioavailable}$]

Effects

Potential effects
[PAF x m³]

Fate factor, FF

[$kg_{in\ compartment}$ per $kg_{emitted}$/d]

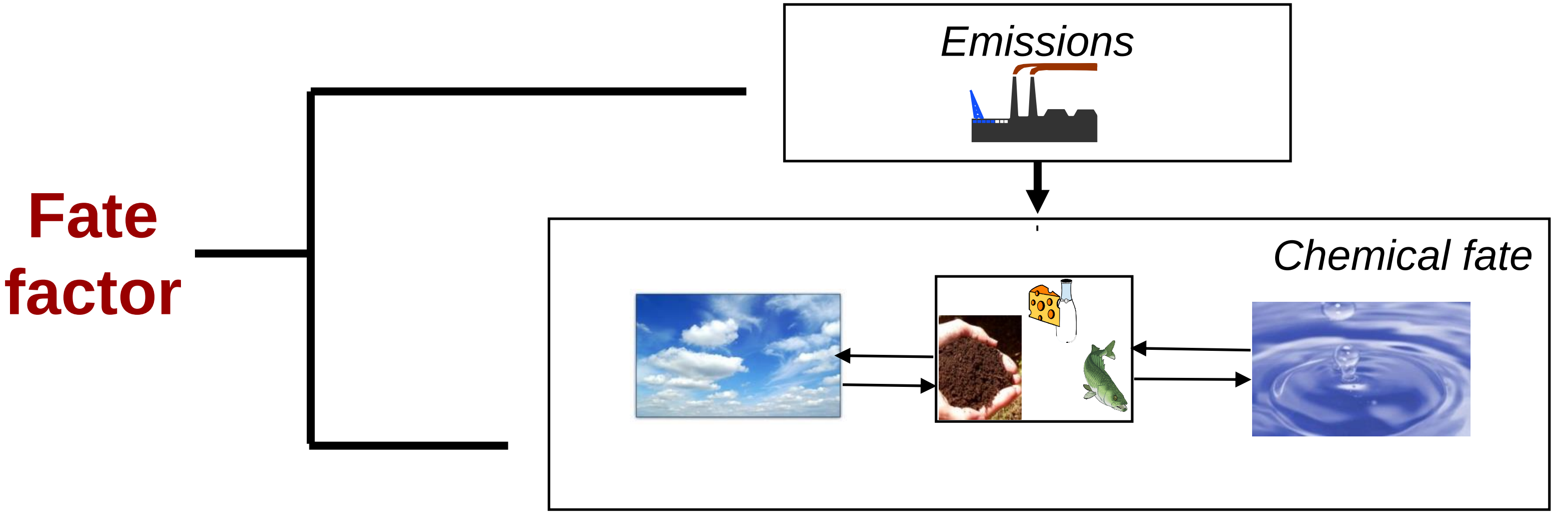
Environmental Fate Definitions

Defining the «Fate Factor»

→ Links the chemical mass in a given compartment to the quantity released into any compartment

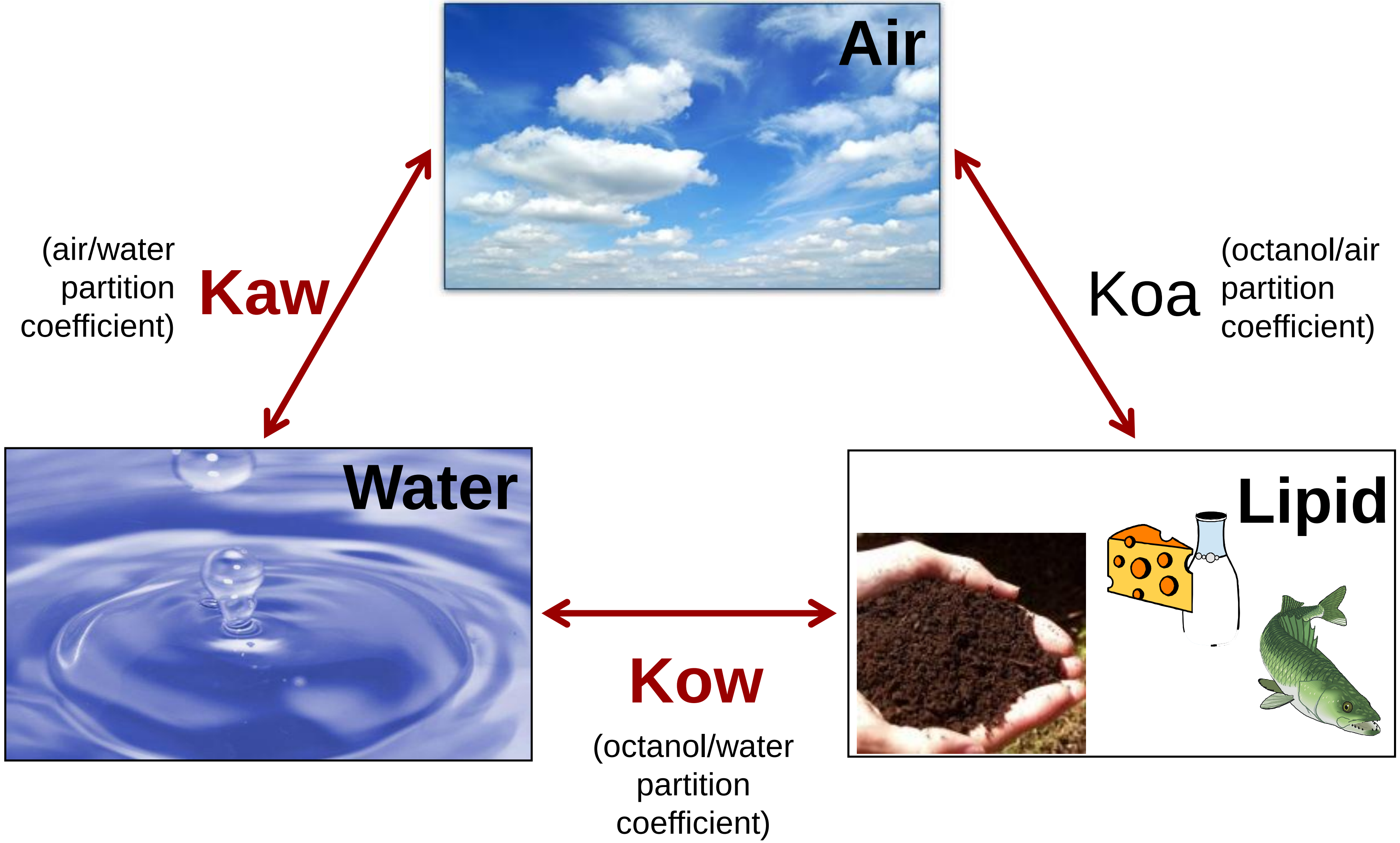
→ Accounts for multimedia & spatial transport between environmental media (e.g. air, water, soil, etc.)

→ Can be interpreted as the «increase of chemical mass in compartment *i* [kg] due to an emission into compartment *j* [kg/day]».

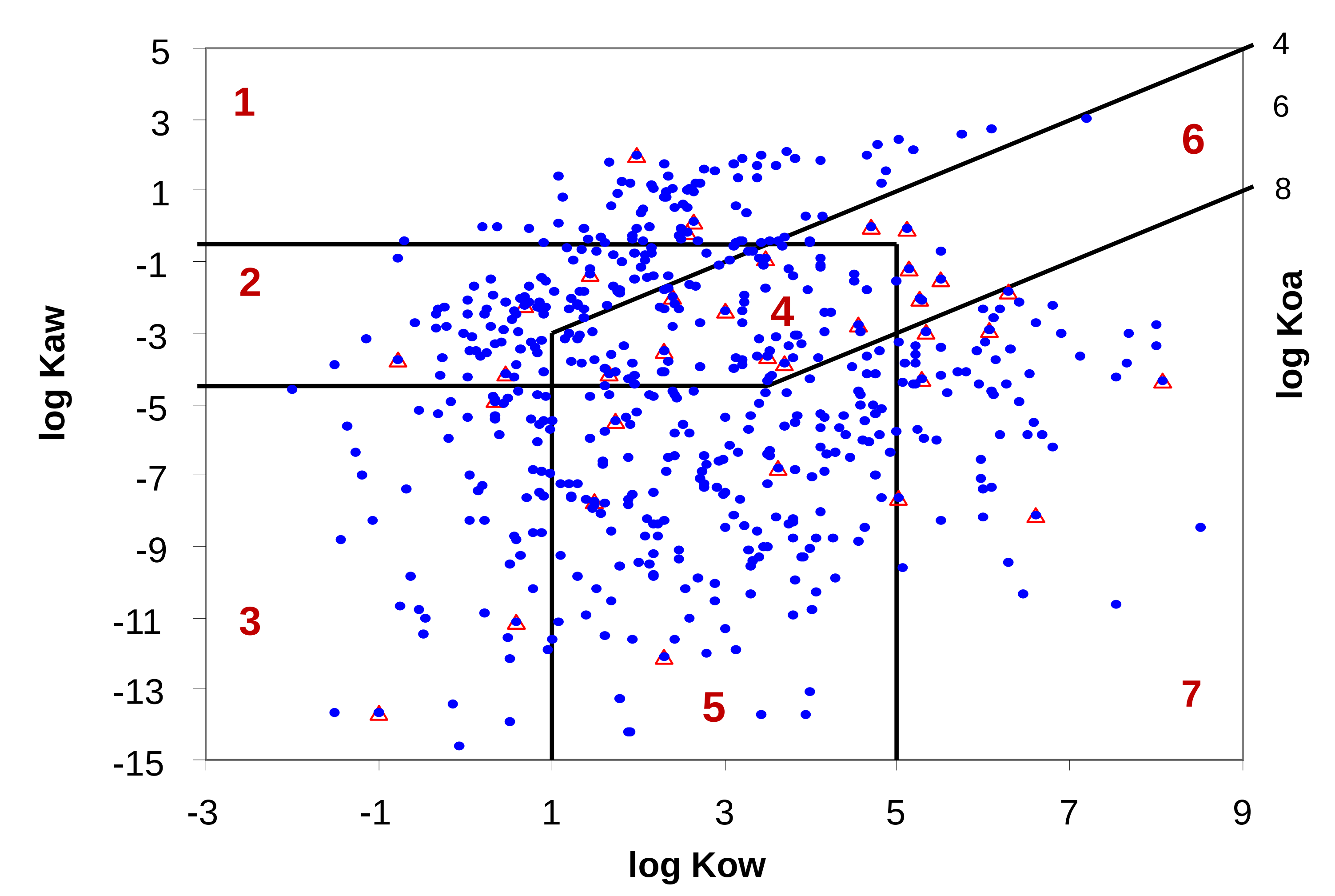


Time-integrated concentration

Chemical Partitioning: Main Phases

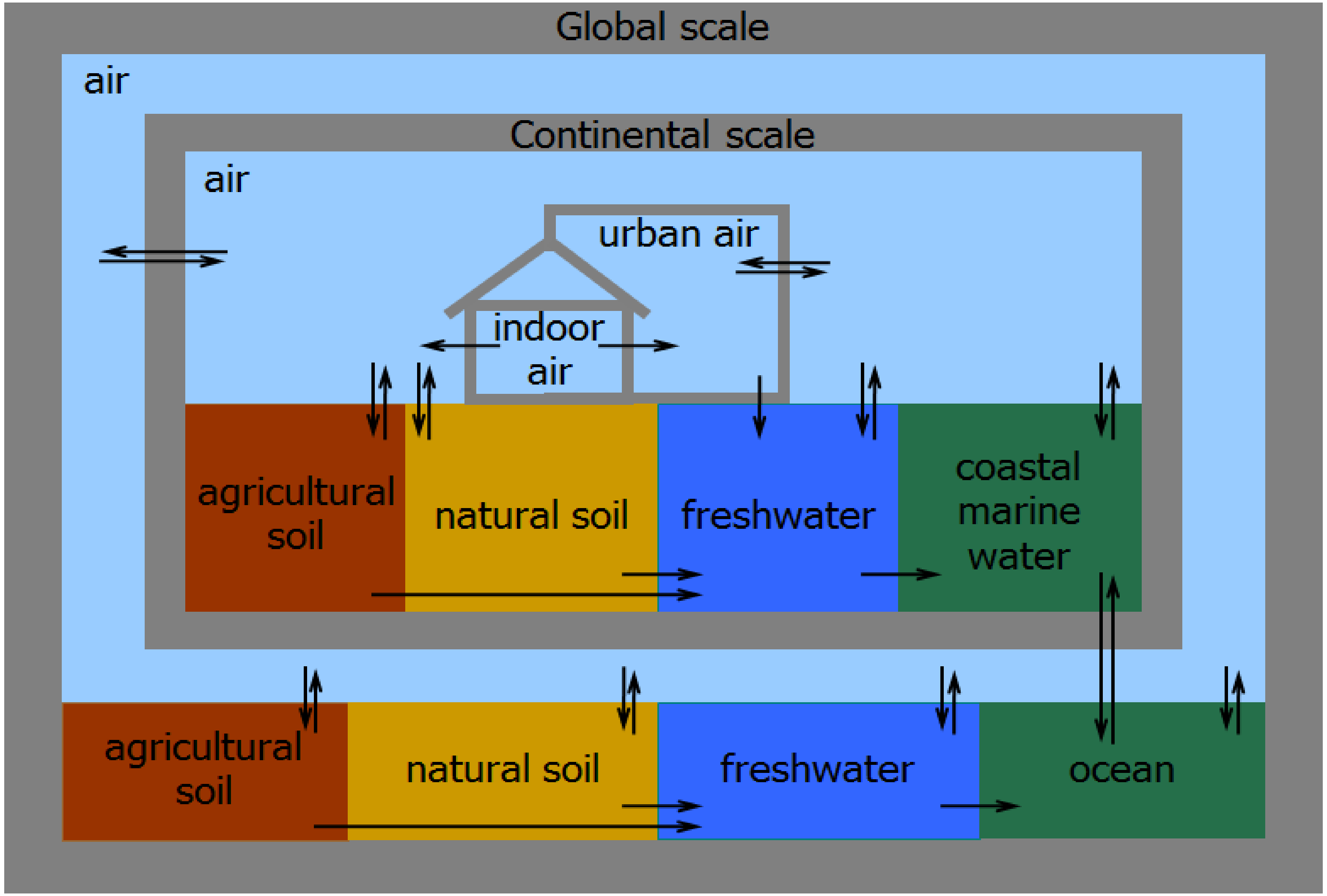


Chemical Partitioning: Why Multimedia?



Multimedia partitioning:
Bennett et al. 2002

USEtox: Environmental Fate System



USEtox: UNEP-SETAC scientific consensus model for characterizing human toxicity and ecotoxicity in LCA and comparative risk screening

Boxes = compartments

Arrows = processes

USEtox documentation

Main Environmental Fate Processes

Degradation processes

→Chemical decomposition (photochemical decomposition, photolysis, hydrolysis)

→Biodegradation/bio-transformation (metabolism)

Transport removal processes

→ Sorption

→ Sedimentation

Transport to other media (diffusion and advection)

→ Deposition

→ Evaporation

→ Air flow

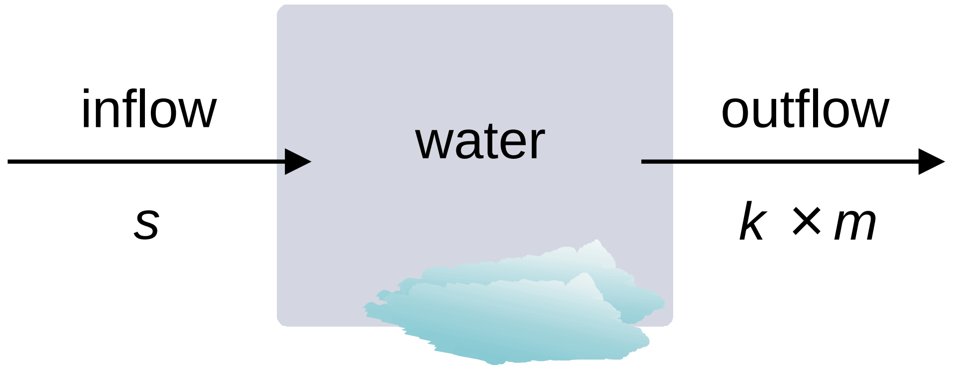
→ Volatilization

→ Re-suspension

Rate constants: $k_{w,tot} = k_{deg} + k_{sed} + k_{w\text{->}a} + \ldots$

Mass Balance Modeling: Residence Time (Fate Factor)

Steady state: inflow = outflow → dm/dt = 0



Emission source rate: s [kg/d] $$s = k \times m$$

Mass in compartment: m [kg] $$m = s/k$$

Removal rate coefficient: k [1/d] $$k = \ln(2)/t_{1/2}$$

(mass eliminated per day; $t_{1/2}$: half-life [d])

Residence time: τ [d] $$\tau \triangleq m/(k \times m) = 1/k$$

K matrix of rate constants [1/day]

Expresses how many times per day is the chemical removed from the media and /or direrectly transferred to another media or to humans

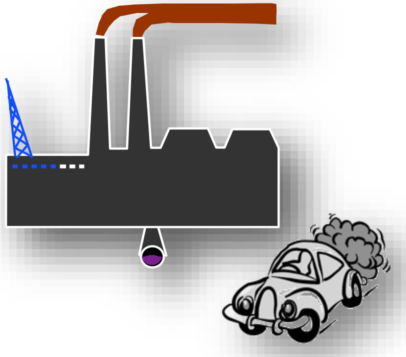
The diagonal is equal to minus the total removal rate:

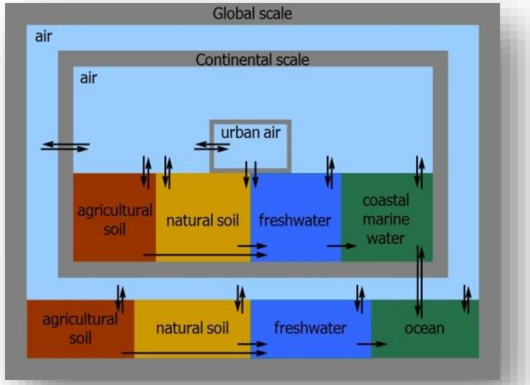
$k_{ia,tot} = k_{ia,deg} + k_{ia,sorption} + k_{oa\leftarrow ia} + k_{inh\leftarrow ia} + k_{derm\leftarrow ia}$

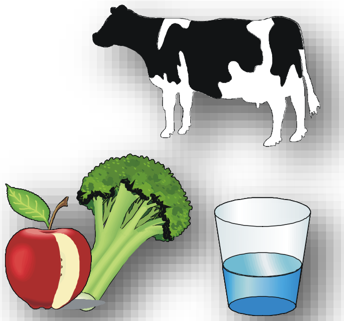
To: \ From:	indoor air	outdoor air	freshwater	respirat. tract	GI tract+skin
indoor air	$-k_{ia,tot}$	$k_{ia\leftarrow oa}$	0	$k_{ia\leftarrow inh}$	0
outdoor air	$k_{oa\leftarrow ia}$	$-k_{oa,tot}$	$k_{oa\leftarrow w}$	$k_{oa\leftarrow inh}$	0
freshwater	0	$k_{w\leftarrow oa}$	$-k_{w,tot}$	0	$k_{w\leftarrow ing\&derm}$
respirat. tract	$k_{inh\leftarrow ia}$	$k_{inh\leftarrow oa}$	0	$-k_{inh,tot}$	0
GI tract+skin	$k_{derm\leftarrow ia}$	$k_{derm\leftarrow oa}$	$k_{ing\leftarrow w}$	0	$-k_{ing\&derm,tot}$

USEtox far-field human exposure and intake

Impact Pathway: Human Exposure







Emission

Emission flow
[$kg_{emitted}$ /d]

Fate

Mass in environment
[$kg_{in\ compartment}$]

Exposure

Human intake
[kg_{intake}/d]

Effects

Potential effects
[disease cases/d]

Exposure factor, XF

[kg_{intake}/d per $kg_{in\ compartment}$]

Exposure

Defining Exposure:

«Contact between stressors and receptors, and the associated sources, pathways and processes.» (Fantke et al. 2020)

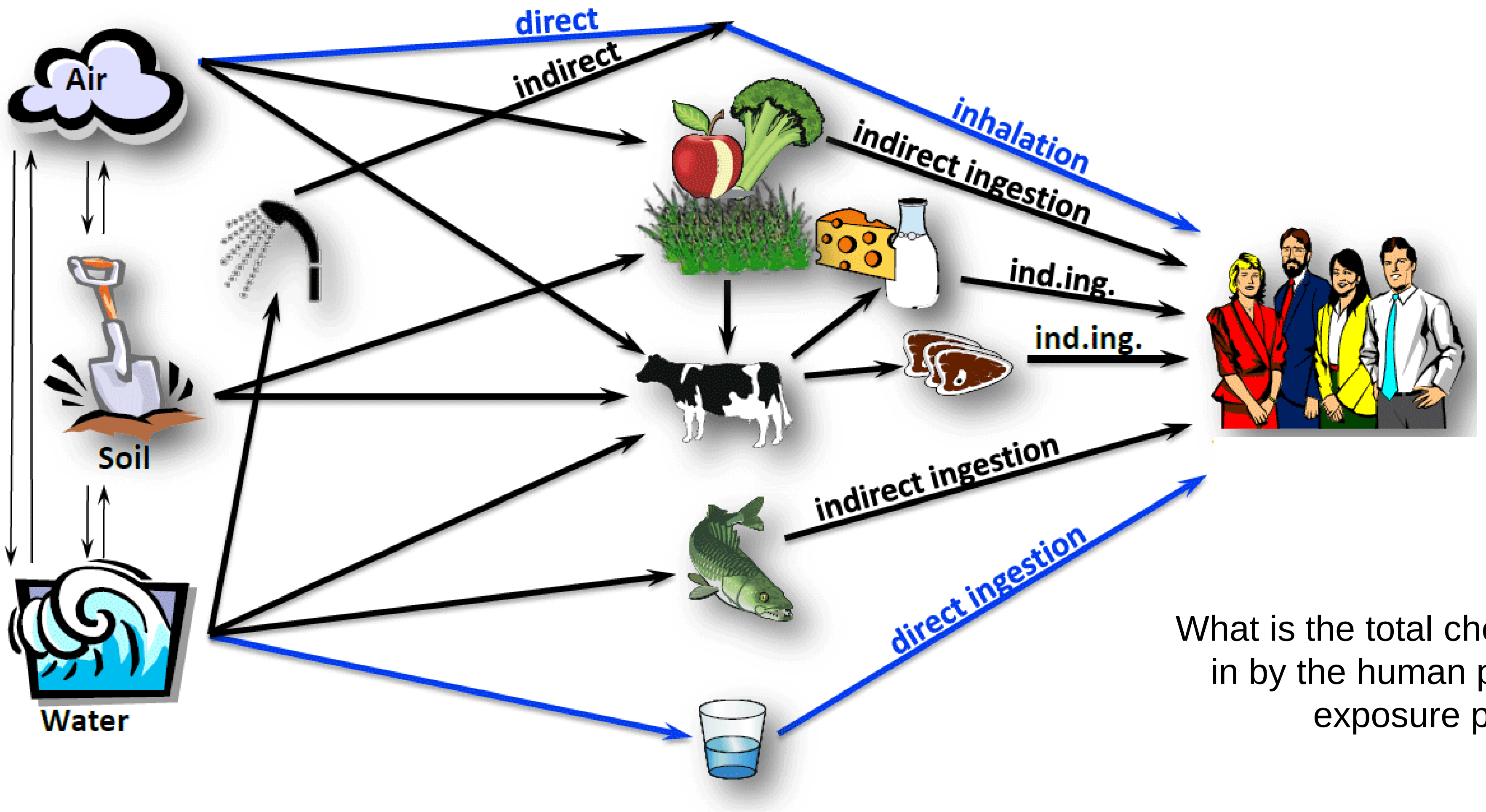
Contact takes place at an exposure surface (mouth, skin, eyes) over an exposure period.

→ Contact with air, water, soil, food, or consumer products containing potentially harmful substances

Exposure Assessment

The process of estimating or measuring the magnitude, frequency and duration of exposure to an agent, along with the number and characteristics of the population exposed. Ideally, it describes the sources, pathways, routes, and the uncertainties in the assessment.

Human Exposure Pathways



What is the total chemical mass taken in by the human population via all exposure pathways?

Human Exposure Factors (XF)

Direct exposure: $\boldsymbol{XF_{k,i}^{\mathrm{direct}}}$

The exposure factor for direct exposure is the rate coefficient for transfer of contaminants in compartment *k*, through consumption of drinking water or inhalation of air to humans. Here, $TF_{k,i} = C_i/C_k = 1$, since *i* = *k*, meaning that we interpret the compartment *k* is directly taken in:

$$XF_{\mathrm{air,inhalation}}^{\mathrm{direct}} = \frac{IR_{\mathrm{inhalation}}\ [\mathrm{m^3/d}] \times n_{\mathrm{persons}}}{V_{\mathrm{air}}\ [\mathrm{m^3}]}$$

$$XF_{\mathrm{water,ingestion}}^{\mathrm{direct}} = \frac{IR_{\mathrm{water\ ingestion}}\ [\mathrm{m^3/d}] \times n_{\mathrm{persons}}}{V_{\mathrm{water}}\ [\mathrm{m^3}]}$$

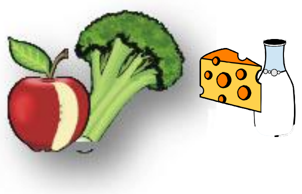
Residence time

The inverse of the direct exposure factor is the **residence time**, reflecting the average time required for the population in compartment *k* to take in the volume of the respective compartment (inhale the volume of air or drink the volume of water.

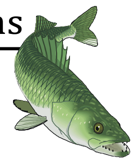
Human Exposure Factors (XF)

Indirect exposure: $\boldsymbol{XF_{k,i}^{\text{indirect}}}$

The exposure factor for direct exposure is the rate coefficient for transfer of contaminants in compartment *k*, through consumption of an exposure medium *j* that was contaminated from compartment *k* – additional fraction of V_k taken in every day:

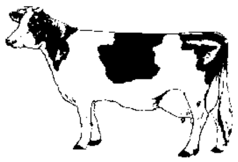


$$XF_{k,j}^{\text{indirect}} = \frac{TF_{k,j}[\text{kg/kg}] \times IR_j[\text{kg/d}] \times n_{\text{persons}}}{\rho_k[\text{kg/m}^3] \times V_k\ [\text{m}^3]}$$



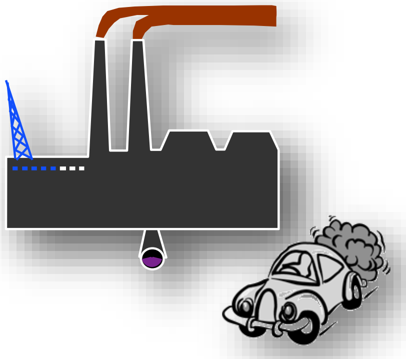
$TF_{k,j}$ quantifies the **transfer efficiency** for a contaminant from an environmental compartment *k* to an exposure medium *j*. Various definitions and measures are used to model it, which can be found in literature. Examples:

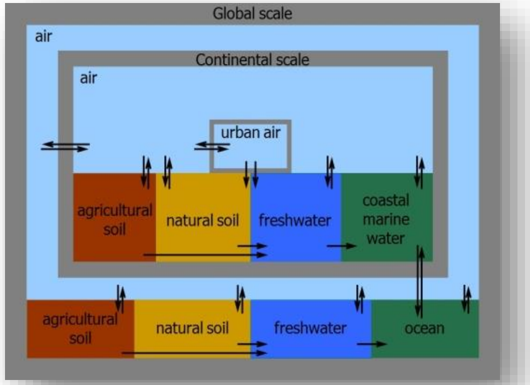
Bioconcentration factor at steady-state, $BCF_{k,j} = \dfrac{C_j\ (\text{conc. in exposure medium } j)}{C_k\ (\text{conc. in compartment } k)}$

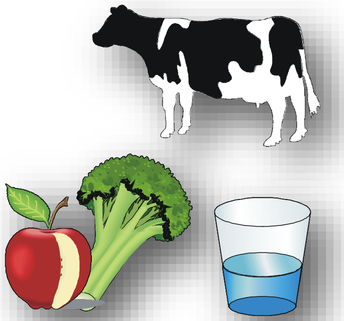


Bioaccumulation factor at steady-state, $BAF_{k,j} = BCF_{k,j} \times f_{\text{uptake from diet}}$

Impact Pathway: Human Intake Fraction







Emission

Emission flow
$[kg_{emitted} /d]$

Fate

Mass in environment
$[kg_{in\ compartment}]$

Exposure

Human intake
$[kg_{intake}/d]$

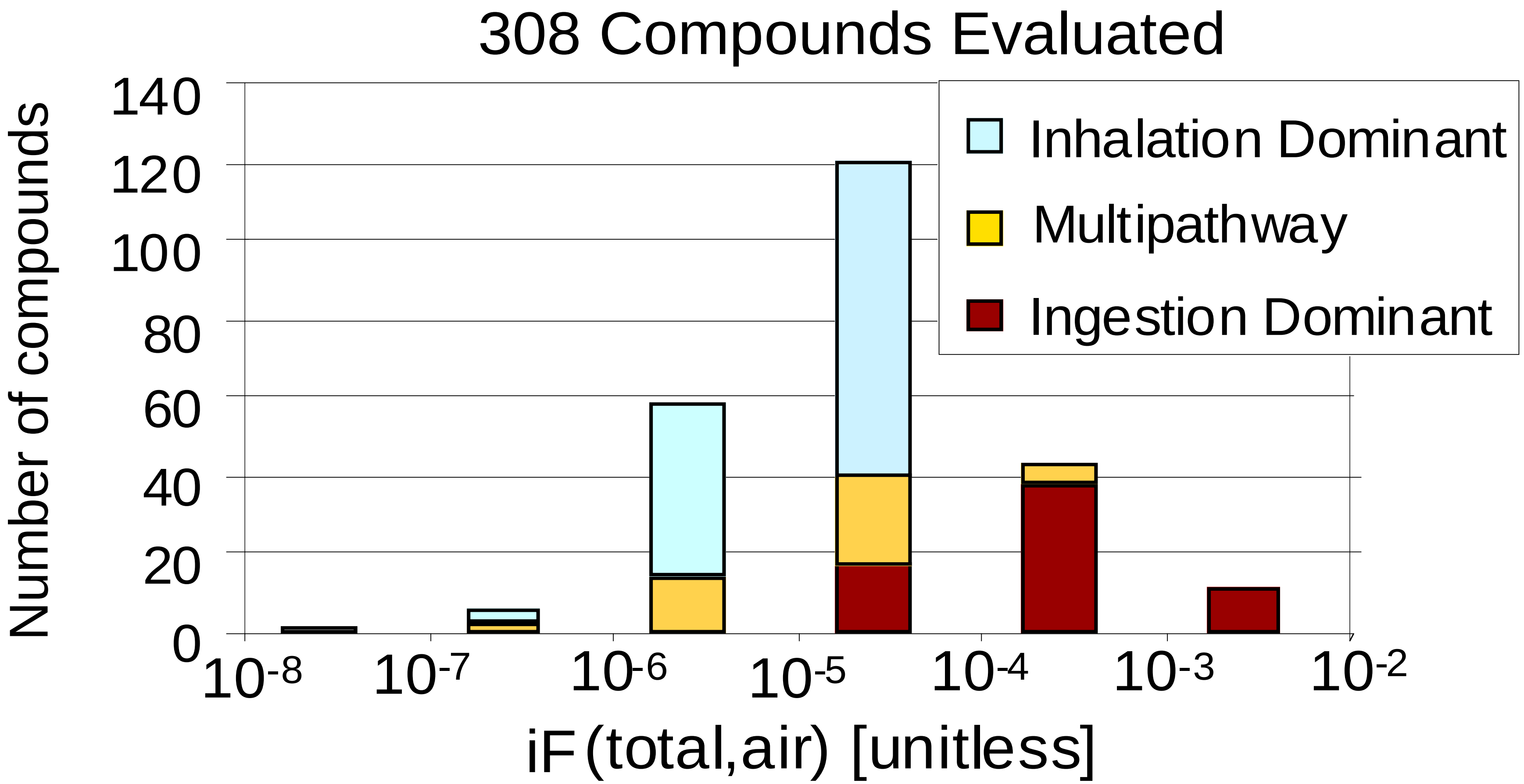
Effects

Potential effects
[disease cases/d]

Fate factor **Exposure factor**

Intake fraction, iF

Human Intake Fraction (iF)



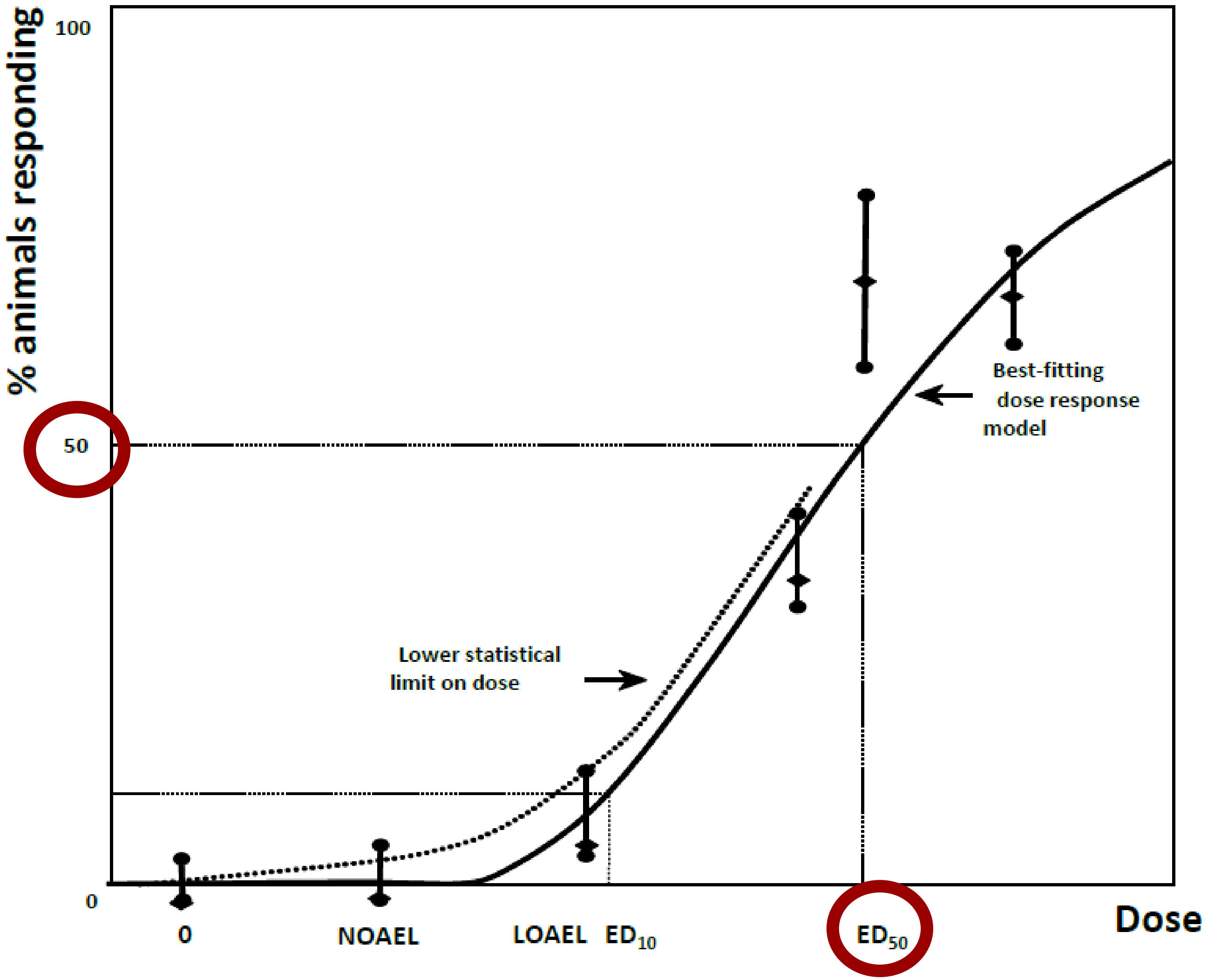
USEtox human toxicity and ecotoxicity effects

Dose Response Models

Effect dose: ED_x
(lifetime) dose generating an **additional risk of x%** over background

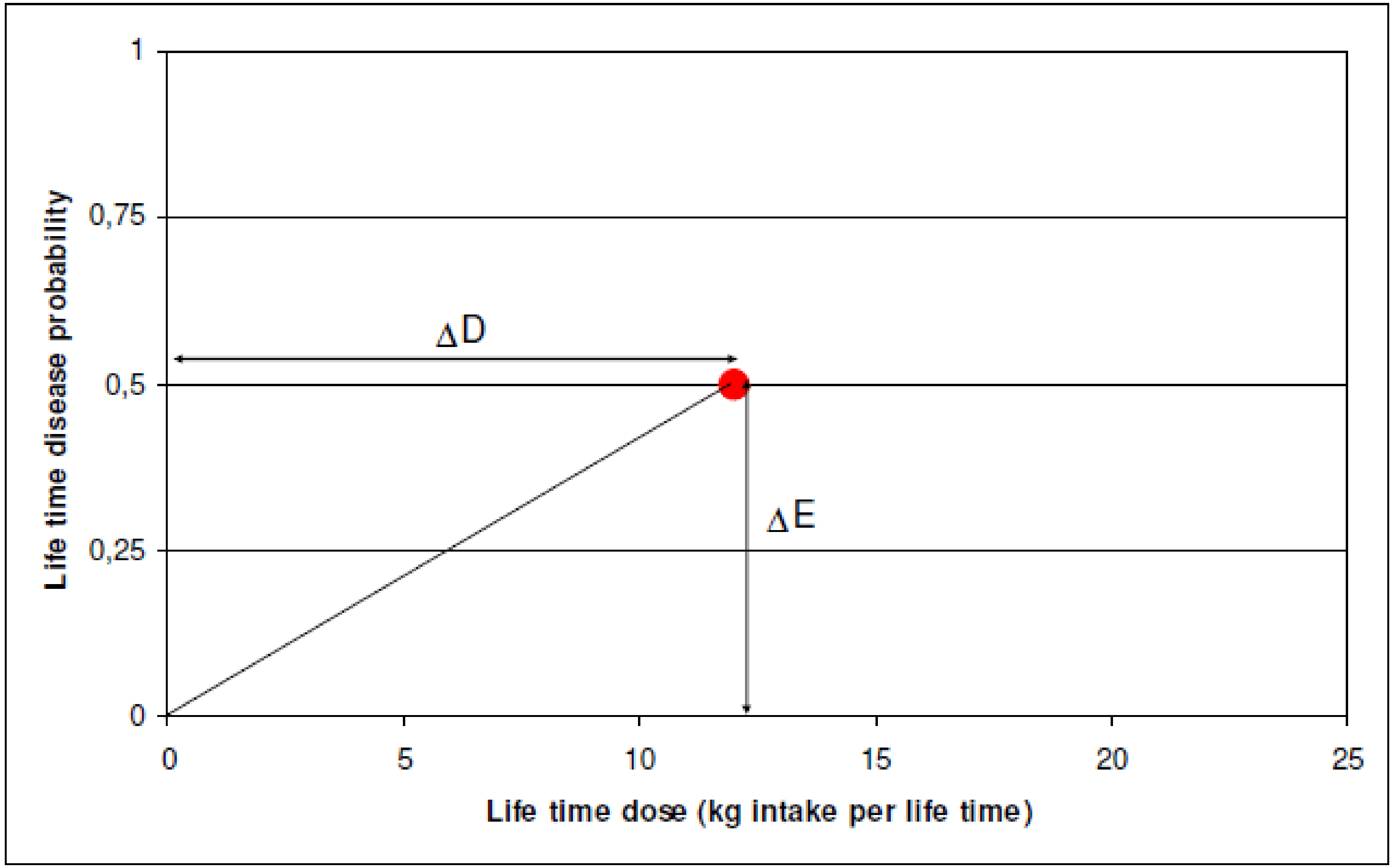
e.g 50% over background for ED_{50}

Dose-response Assessment:
Defines the quantitative relationship between the **dose** of a chemical **received** and the **incidence** of adverse health **effects** in the exposed population.



Dose Response in LCIA: Curve

Cancer / non-cancer effects



Via inhalation / ingestion exposure

Human Toxicity Effect Factor (EF)

$$\text{Incremental risk} = \text{Intake dose} \times \frac{0.5}{\text{Life time dose generating 50\% of additional risk}}$$

$$\text{EF} = \frac{0.5}{\text{ED50}_{\text{human}} \times 365\,\frac{\text{d}}{\text{yr}} \times 70\ \text{kg}_{\text{bodyweight}} \times 70\ \text{yr}_{\text{lifetime}} \times 10^{-6}\,\frac{\text{kg}}{\text{mg}}}$$

$$= \frac{0.5}{\text{ED50}_{\text{human}}^{\text{lifetime}}}\left[\frac{\text{cases}}{\text{kg}_{\text{intake}}}\right]$$

EF : Substance-specific human toxicity effect factor [incidence risk / kg intake]

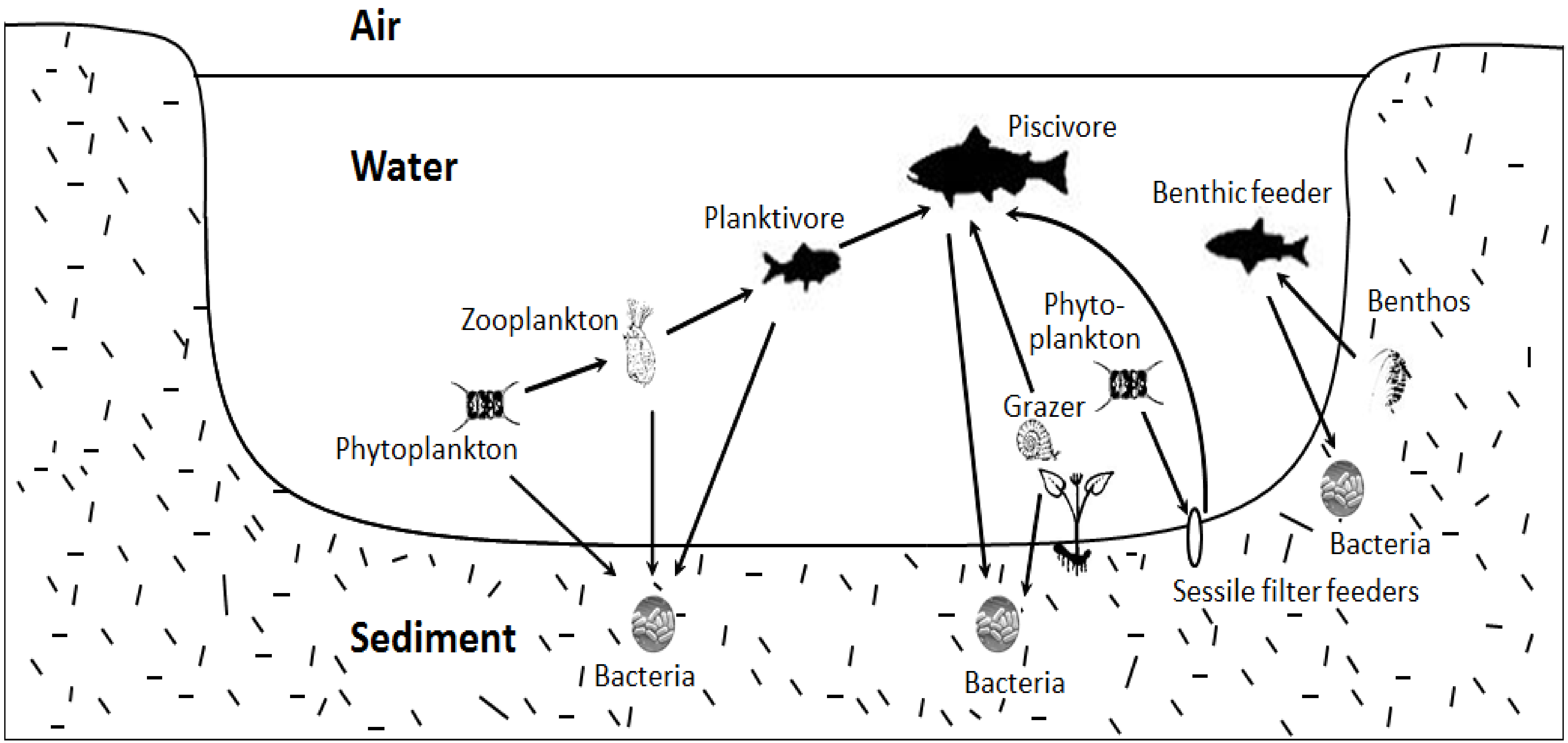
$\text{ED50}_{\text{human}}$: Effect dose inducing a response over background of 50% for humans [mg/kg/d]

$\text{ED50}_{\text{human}}^{\text{lifetime}}$: Effect dose inducing a response over background of 50% in humans over lifetime [kg intake over lifetime]

0.5 : Response level corresponding to the ED50 [lifetime incidence risk]

Aquatic Ecosystem Species Network

Who is exposed e.g. in an aquatic ecosystem? Species with different sensitivities!



Aquatic Ecosystem Exposure Assessment

Exposure factors for aquatic ecotoxicity represent the fractions of a chemical dissolved in contaminated aquatic compartment, calculated by:

$$XF_{\text{aquatic}} = \frac{m_{\text{dissolved}}}{m_{\text{total}}} = \frac{1}{1 + (K_P \times \text{SUSP} + K_{\text{doc}} \times \text{DOC} + BCF_{\text{fish}} \times \text{BIO})}$$

where

K_P : partition coefficient between water and suspended solids [l/kg]

SUSP : suspended matter concentration in freshwater [kg/l]

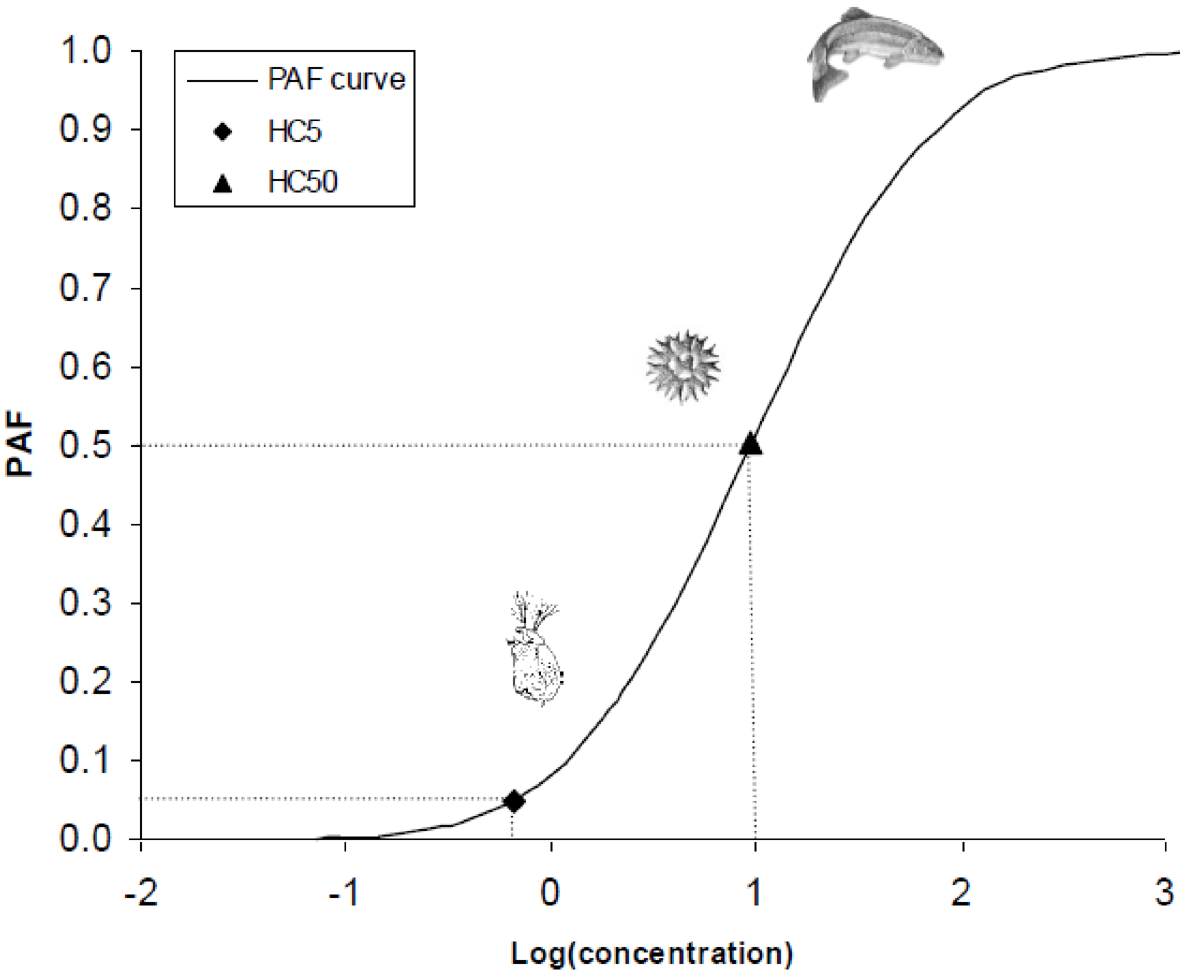
K_{doc} : partitioning coefficient between dissolved organic carbon and water [l/kg]

DOC : dissolved organic carbon concentration in freshwater [kg/l]

BCF_{fish} : bioconcentration factor in fish [l/kg]

BIO : concentration of biota in water [kg/l]

Potentially Affected Fraction (PAF) of Species



$$\mathrm{PAF} = \frac{1}{1 + \mathrm{e}^{\frac{-\log C - \alpha}{\beta}}}$$

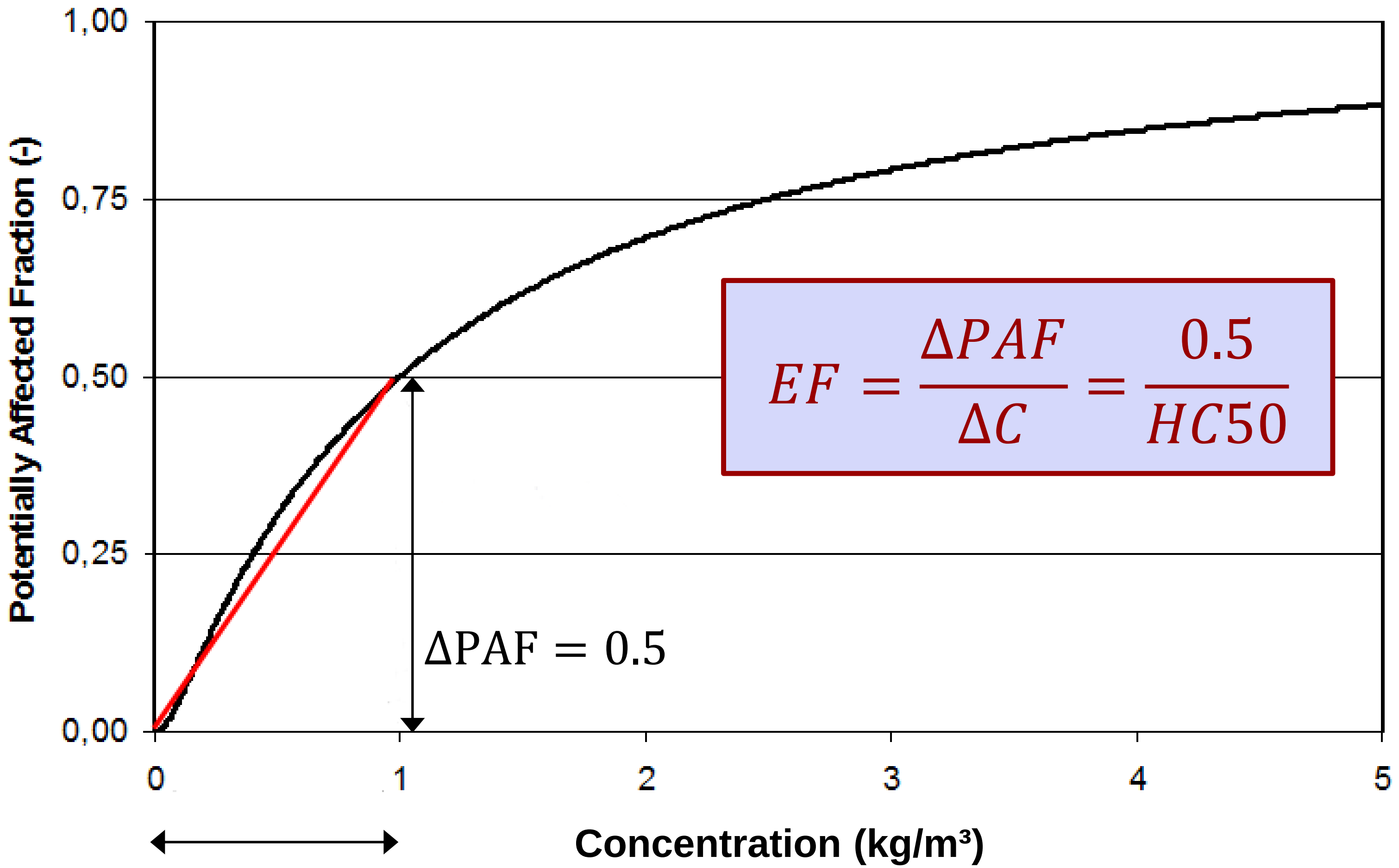
with

$$\alpha = \log \mathrm{HC50}$$

$$= \frac{1}{n_{\mathrm{species}}} \times \sum_{i=1}^{n} \log \mathrm{EC50}_{\mathrm{species}}$$

$$\beta = \frac{\sqrt{3}}{\pi} \times \sigma_{\log \mathrm{EC50}}$$

Ecotoxicity Effect Factor (EF)



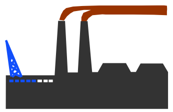
$$EF = \frac{\Delta PAF}{\Delta C} = \frac{0.5}{HC50}$$

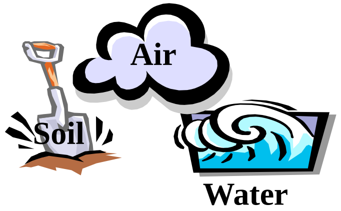
$$\Delta C = \mathrm{HC50} = 1\ \mathrm{kg/m^3}$$

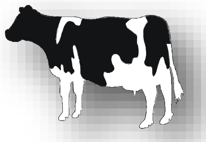
HC: Hazard concentration = concentration at which the indicated % of species is affected above their individual EC

Integration of USEtox far-field and near-field environments

Integration of far-field and near-field in USEtox







Emission flow
$[kg_{emitted}/d]$
Emission mass
$[kg_{emitted}]$

Mass in environment
$[kg_{in\ compartment}]$
Time-integrated mass
$[kg_{in\ compartment}\ d]$

Exposure level
$[kg_{intake}/d]$ $[kg_{dissolved}]$

Toxicity impacts
[cases/d] [PAF m³]

Health damage
[DALY/d] [PDF m³]

Fate factor
$FF = -K^{-1}$

Exposure factor
XF

Effect factor
EF

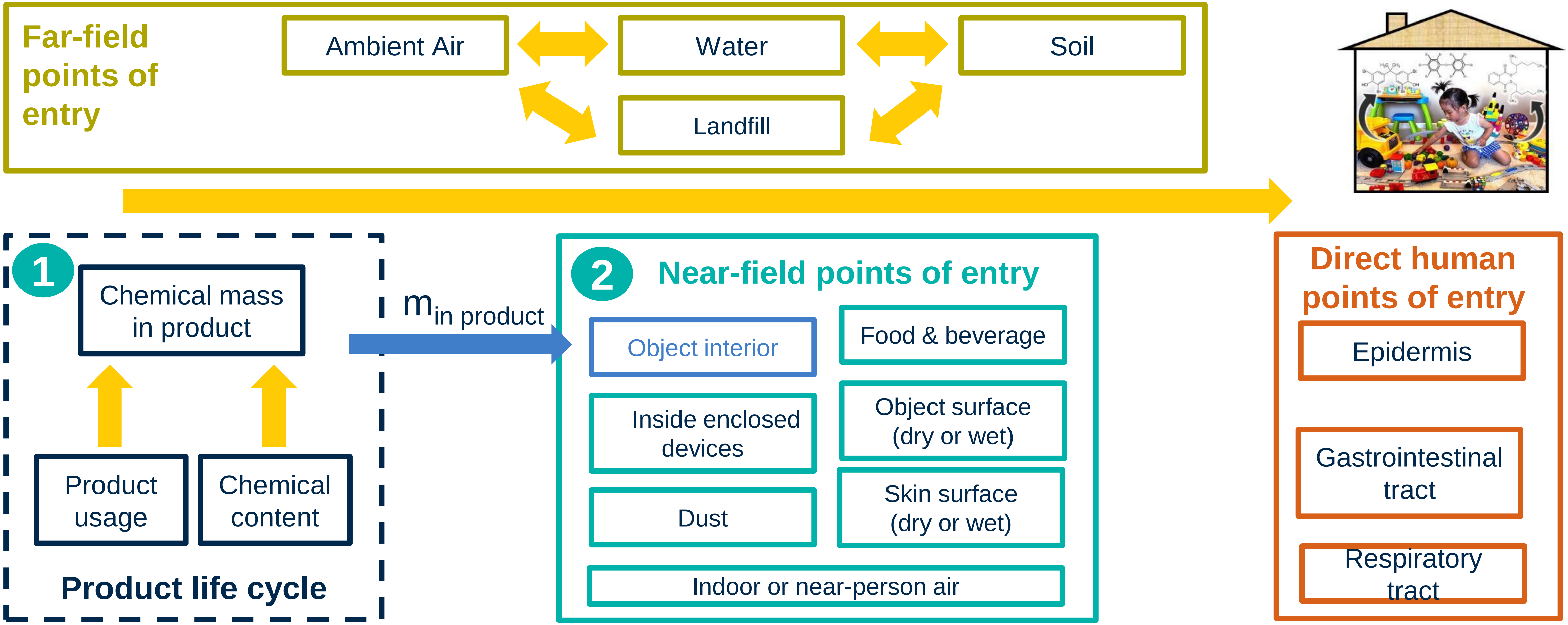
Severity factor
SF

Transfer fractions
$TF = (k_x/k_{\sum x})^{-1}$ ⟵ $XF = k_{x=exposure}$

Midpoint characterization factor , $CF_{midpoint}$ $[impacts/kg_{emitted}]$

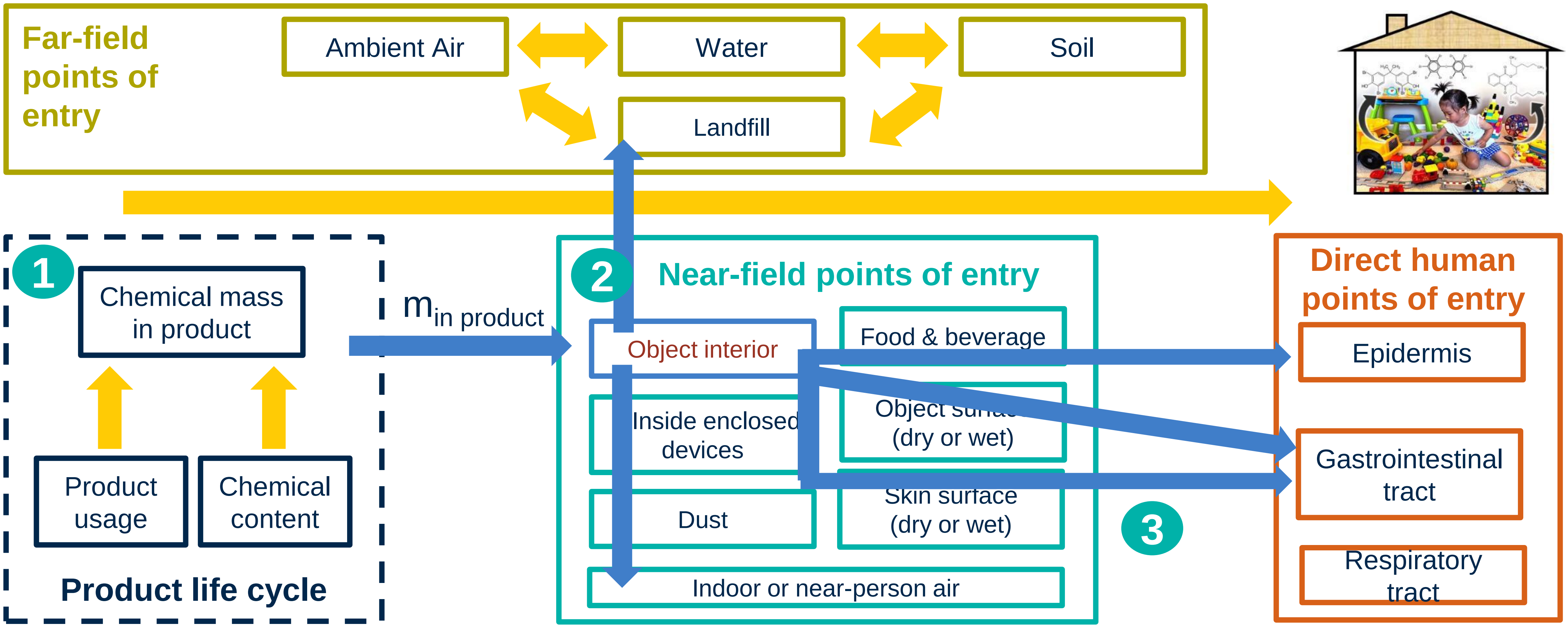
Damage characterization factor , $CF_{damage} = XF \times FF \times ERF \times SF$ $[damage/kg_{emitted}]$

Near-Field Consumer Exposure to Chemicals in Toys



Fantke et al. 2018. Environ Health Perspect 126: 125001

Near-Field Consumer Exposure to Chemicals in Toys



Fantke et al. 2018. Environ Health Perspect 126: 125001

K matrix of rate constants [1/day]

Expresses how many times per day is the chemical removed from the media and /or direrectly transferred to another media or to humans

The diagonal is equal to minus the total removal rate:

$$k_{ia,tot} = k_{ia,deg} + k_{ia,sorption} + k_{oa\leftarrow ia} + k_{inh\leftarrow ia} + k_{derm\leftarrow ia}$$

To: \ From:	indoor air	outdoor air	freshwater	respirat. tract	GI tract+skin
indoor air	$-k_{ia,tot}$	$k_{ia\leftarrow oa}$	0	$k_{ia\leftarrow inh}$	0
outdoor air	$k_{oa\leftarrow ia}$	$-k_{oa,tot}$	$k_{oa\leftarrow w}$	$k_{oa\leftarrow inh}$	0
freshwater	0	$k_{w\leftarrow oa}$	$-k_{w,tot}$	0	$k_{w\leftarrow ing\&derm}$
respirat. tract	$k_{inh\leftarrow ia}$	$k_{inh\leftarrow oa}$	0	$-k_{inh,tot}$	0
GI tract+skin	$k_{derm\leftarrow ia}$	$k_{derm\leftarrow oa}$	$k_{ing\leftarrow w}$	0	$-k_{ing\&derm,tot}$

How can we determine the chemical fraction transferred from e.g. indoor to outdoor air?

Direct Transfer Fractions matrix T [–]

Diagonals: 100% entry in compartments , non-diagonals: transfers to other compartments

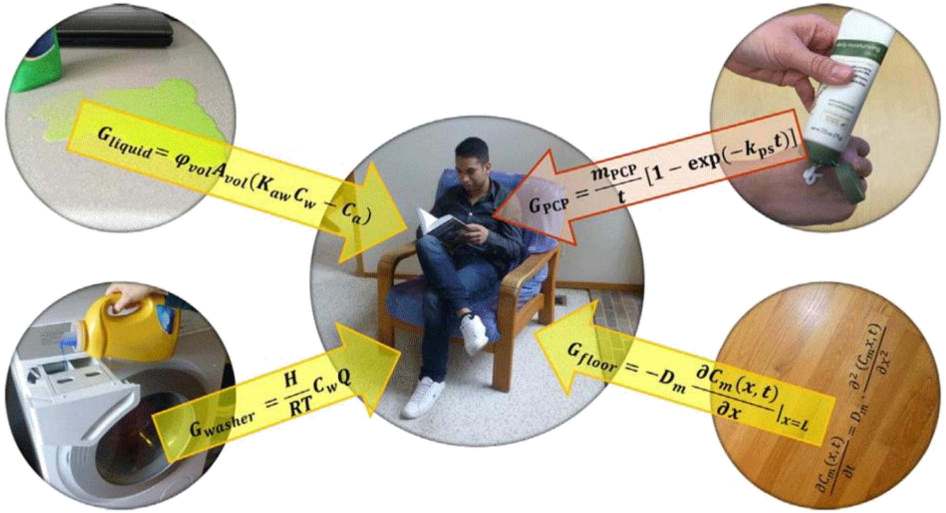
$$t_{oa\leftarrow ia} = k_{oa\leftarrow ia} / -k_{ia,tot}$$

From: indoor air, outdoor air, freshwater, respirat. tract, GI tract+skin

To: indoor air, outdoor air, freshwater, respirat. tract, GI tract+skin

$$\begin{pmatrix} 1 & -\frac{k_{ia\leftarrow oa}}{k_{oa,tot}} & 0 & -\frac{k_{ia\leftarrow inh}}{k_{inh,tot}} & 0 \\ -\frac{k_{oa\leftarrow ia}}{k_{ia,tot}} & 1 & -\frac{k_{oa\leftarrow w}}{k_{w,tot}} & -\frac{k_{oa\leftarrow inh}}{k_{inh,tot}} & 0 \\ 0 & -\frac{k_{w\leftarrow oa}}{k_{oa,tot}} & 1 & 0 & -\frac{k_{w\leftarrow ing\&derm}}{k_{ing\&derm,tot}} \\ -\frac{k_{inh\leftarrow ia}}{k_{ia,tot}} & -\frac{k_{inh\leftarrow oa}}{k_{oa,tot}} & 0 & 1 & 0 \\ -\frac{k_{derm\leftarrow ia}}{k_{ia,tot}} & -\frac{k_{derm\leftarrow oa}}{k_{oa,tot}} & -\frac{k_{ing\leftarrow w}}{k_{w,tot}} & 0 & 1 \end{pmatrix}$$

Near-field sub-models in USEtox



USEtox base model + 6 sub-models for 10000 chemicals in ~500 products

→ customized to particular applications + developed necessary QSARS for high throughput determination

Direct environmental emission

Food contact materials

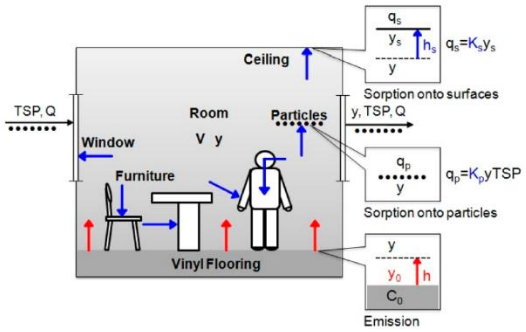
Skin surface

Object surface

Article interior
(with indoor sorption)

Pesticide residue

Article Interior Sub-Model (emission from solid products)



Transfer from product to air:

Diffusion-limited:

$$TF^{\text{diffusion-limited}}_{\text{product}\rightarrow\text{air}} = \alpha \times \left(1 - e^{-\beta_1^2 \times D_m \times t}\right) + (1-\alpha) \times \left(1 - e^{-\beta_2^2 \times D_m \times t}\right)$$

Partition-limited:

$$TF^{\text{partition-limited}}_{\text{product}\rightarrow\text{air}} = 1 - \left(v_1 \times e^{\lambda_1 \times t} + v_2 \times e^{\lambda_2 \times t}\right)$$

Criteria for applying these two models: $\begin{cases} D - limited\text{: } K_{ma} < 0.4 \cdot {D_m}^{-0.61} \\ K - limited\text{: } K_{ma} > 0.4 \cdot {D_m}^{-0.61} \end{cases}$

Key parameters: solid-phase diffusion coefficient D_m (m^2/s), solid material-air partition coefficient K_{ma}

Transfer via dermal contact: $TF^{\text{direct dermal}}_{\text{product}\rightarrow\text{skin}} = \frac{1}{m_0} \times N_{\text{persons}} \times FQ_{\text{contact}} \times f_{\text{home}} \times A_{\text{contact}} \times \frac{K_{\text{p-aq}}}{K_{ma} \times K_{\text{aw}}} \times \int_{t_1}^{t_2} C_m(d_m, t)\, dt$

(Assumes equilibrium between skin surface and material surface)

Transfer via dust ingestion: $TF^{\text{dust ingestion}}_{\text{product}\rightarrow\text{GI tract}} = \frac{1}{m_0} \times f_{\text{home}} \times f_{\text{dust,ingested}} \times \frac{IR_{\text{ing}}}{K_{md} \times \rho_{\text{dust}}} \times \int_{t_1}^{t_2} C_m(d_m, t)\, dt$

(Assumes dust ingested is related to hand contact frequency)

http://doi.org/10.1016/j.jhazmat.2021.127574

USEtox overall framework and interpretation

USEtox Impact Pathway Framework: Ecotoxicity

FF

Fate factors - FF [d]

Receiving compartment	Emission compartment: home.airI	occ.airI	airU	airC	fr.waterC	sea.waterC	nat.soilC	agr.soilC
home.airI	5.27E-02	0	0	0	0	0	0	0
occ.airI	0	3.47E-03	0	0	0	0	0	0
airU	2.58E-02	4.13E-02	5.16E-02	1.43E-05	1.26E-05	2.54E-06	1.24E-05	1.24E-05
airC	2.55E+00	2.52E+00	2.51E+00	2.58E+00	2.28E+00	4.60E-01	2.24E+00	2.24E+00
fr.waterC	3.30E-02	5.22E-02	6.51E-02	8.08E-04	4.79E+00	1.44E-04	9.84E-02	9.84E-02
sea.waterC	3.12E-02	3.62E-02	3.96E-02	2.29E-02	1.31E+00	3.87E+01	4.61E-02	4.61E-02
nat.soilC	1.46E-03	1.45E-03	1.44E-03	1.48E-03	1.31E-03	2.64E-04	1.21E+01	1.28E-03
agr.soilC	1.49E-03	1.49E-03	1.49E-03	1.48E-03	5.10E-03	2.64E-04	1.36E-03	1.21E+01
airG	3.86E+00	3.83E+00	3.80E+00	3.91E+00	3.46E+00	7.70E-01	3.39E+00	3.39E+00
fr.waterG	3.76E-04	3.72E-04	3.70E-04	3.81E-04	3.37E-04	7.50E-05	3.30E-04	3.30E-04
oceanG	3.08E-01	3.06E-01	3.04E-01	3.11E-01	4.46E-01	5.20E+00	2.73E-01	2.73E-01
nat.soilG	7.05E-04	6.99E-04	6.95E-04	7.15E-04	6.32E-04	1.41E-04	6.19E-04	6.19E-04
agr.soilG	7.07E-04	7.01E-04	6.96E-04	7.17E-04	6.34E-04	1.41E-04	6.20E-04	6.20E-04

XF_{eco}

Available Fraction - XF_{eco} [-] *(expand using the "+" button at the beginning of the line to see the matrix)*

Fraction in dissolved/ gaseous phase	Emission compartment: home.airI	occ.airI	airU	airC	fr.waterC	sea.waterC	nat.soilC	agr.soilC
home.airI	1.00E+00	0	0	0	0	0	0	0
occ.airI	0	1.00E+00	0	0	0	0	0	0
airU	0	0	0.00E+00	0	0	0	0	0
airC	0	0	0	1.00E+00	0	0	0	0
fr.waterC	0	0	0	0	1.00E+00	0	0	0
sea.waterC	0	0	0	0	0	1.00E+00	0	0
nat.soilC	0	0	0	0	0	0	7.04E-02	0
agr.soilC	0	0	0	0	0	0	0	7.04E-02
airG	0	0	0	0	0	0	0	0
fr.waterG	0	0	0	0	0	0	0	0
oceanG	0	0	0	0	0	0	0	0
nat.soilG	0	0	0	0	0	0	0	0
agr.soilG	0	0	0	0	0	0	0	0

EF_{eco}

Ecotoxicological effect factor matrix EF_{eco} [PAF m3/kg]:

Ecotoxicity Effect Factors - EF_{eco} [$PAF.m^3.kg^{-1}$]

	Emission compartment: home.airI	occ.airI	airU	airC	fr.waterC	sea.waterC	nat.soilC	agr.soilC
freshwater ecosystems	0	0	0	0	1.74E+01	0	0	0

CF_{eco}

Midpoint ecotox characterization factor matrix CF_{eco} [PAF m3 d /$kg_{emitted}$]:

Midpoint Ecotoxicity Potentials expressed in Comparative Toxic Units [CTU_e = $PAF.m^3.day.kg_{emitted}$]

	Emission compartment: home.airI	occ.airI	airU	airC	fr.waterC	sea.waterC	nat.soilC	agr.soilC
freshwater ecosystems	5.78E-01	9.13E-01	1.14E+00	2.06E-02	8.31E+01	3.79E-03	1.71E+00	1.71E+00

Endpoint ecotox characterization factor matrix CF_{eco} [PDF m3 d /$kg_{emitted}$]:

Endpoint Ecotoxicity Potentials expressed in Comparative Damage Units [CDU_e = $PDF.m^3.day.kg_{emitted}$]

	Emission compartment: home.airI	occ.airI	airU	airC	fr.waterC	sea.waterC	nat.soilC	agr.soilC
freshwater ecosystems	2.89E-01	4.56E-01	5.68E-01	1.03E-02	4.15E+01	1.90E-03	8.56E-01	8.56E-01

Uncertainty, variation, and discerning power

- Uncertainties are important for interpretation and typically capture only precision when quantified, not accuracy
- Comparing uncertainties of CFs from different impact categories? Consider how much of the impact pathway they capture
- Toxicity impacts can be caused by 1000’s of substances
- Overall variation of CFs from most to least toxic substances ranges 11-20 orders of magnitude with uncertainties in the range of 2 to 4 orders of magnitude
- Discerning power of toxicity CFs still meaningful and comparable to other impact categories

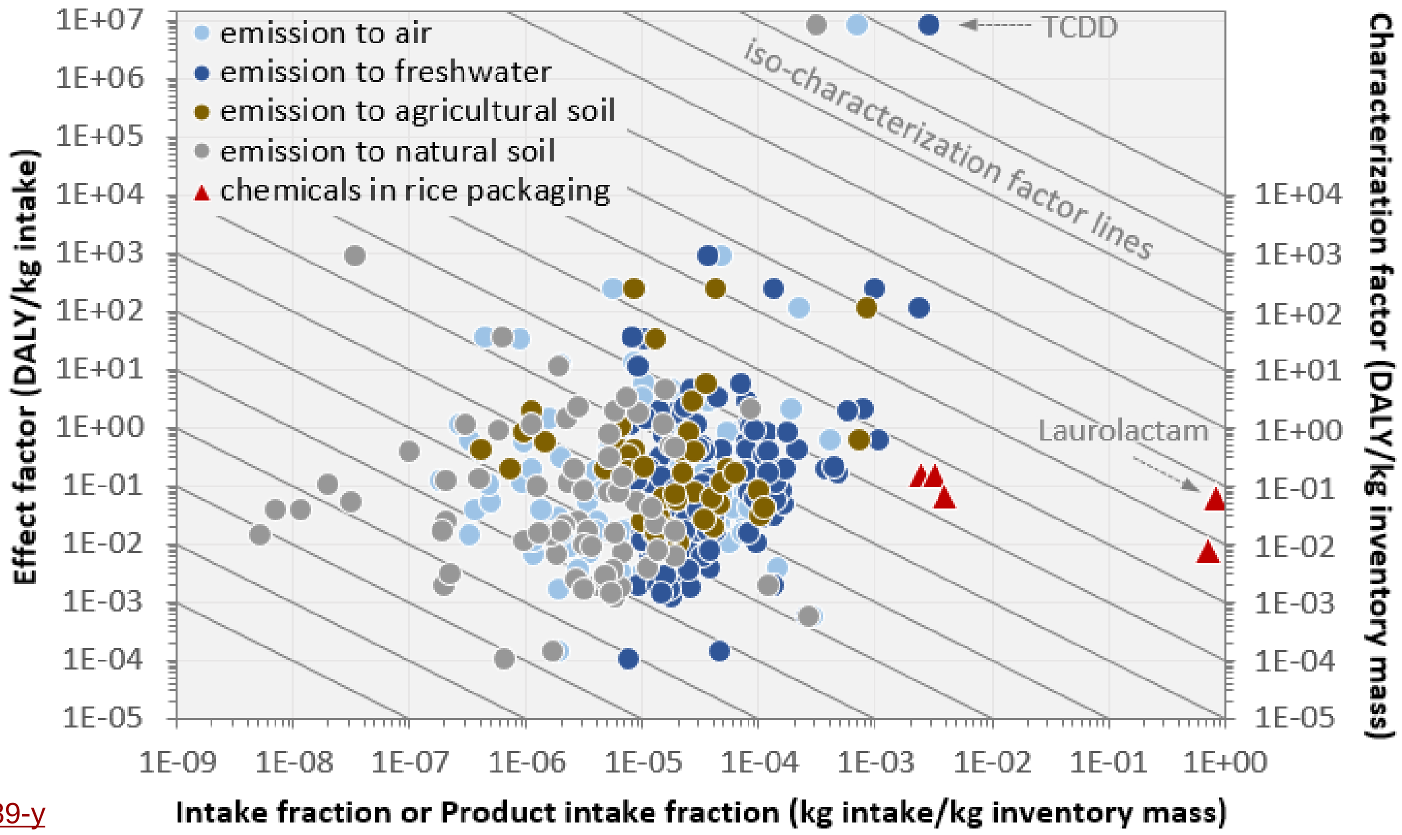
Key Information of USEtox

- Initial model differences were considerably reduced by **harmonisation**, as their sources were identified
- Relative **accuracy** of the new CFs is within a factor of
  - 100-1’000 for human health
  - 10-100 for freshwater ecotoxicity
  - compared to 12 orders of magnitude variation between CFs

- USEtox falls **within range of the other models**, emulating their results, but avoiding their complexity and their pitfalls
- **Characterisation factors** are available for:
  - Human toxicity: ~1’000 recommended + ~100 indicative CFs (= ~1’100 substances covered)
  - Ecotoxicity: 1’184 recommended + 1’335 indicative CFs (= 2’519 substances covered)

How to interpret and apply USEtox CFs in LCA

- Always show and compare toxicity scores in **log-scale**
- Always include **ALL** available characterization factors including “indicative” – consider higher uncertainty
- Identify **10-20** most contributing substances
- Ignore the ranking among them
- Identify most contributing processes
- Check sensitivity of conclusions to choice of LCIA model



http://doi.org/10.1007/s11367-021-01889-y

USEtox Deliverables and publications: Further Reading

- Rosenbaum et al. (2008) → general model
- Hauschild et al. (2008) → consensus process
- Henderson et al. (2011) → ecotoxicity
- Rosenbaum et al. (2011) → human toxicity
- Special issue ‘LCIA of impacts on human health and ecosystems’
- Rosenbaum et al. (2015) → indoor settings
- Westh et al. (2015) → user requirements survey
- Fantke et al. (2021) → near-field/far-field model

- USEtox is **used by U.S. EPA** for screening of chemicals
- USEtox is **recommended by the EC** for PEF and by **ILCD**
- USEtox is **endorsed by the UNEP/SETAC Life Cycle Initiative**

USEtox future development: UNEP GLAM

- 1992-1999 SETAC LCIA working groups (Society for environmental toxicology and chemistry): Assessment framework → LCIA ISO recommendations
- 1999: contacted UNEP → 2 weeks in Paris
  2002 Launch of the UNEP-SETAC Life cycle Initiative!
- 2002 – 2012 LCIA programme of the Life Cycle Initiative:
  LCIA Midpoint-Damage Framework, **USEtox**, WULCA
- 2012-2019 GLAM Phase 1 & 2: Consensus finding for environmental assessment indicators and methods in multiple impact categories → Pellston workshop™ 1 (January 2016) & 2 (June 2018, Valencia)
- **2019-2023 Phase 3: Dissemination and stewardship**
  Creation of a Global LCIA method
  https://www.lifecycleinitiative.org/applying-lca/lcia-cf/