



Human Exposure Modelling


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using also material from T.E. McKone & M. Margni

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Overview

- What is exposure?
- Exposure concepts and definitions
- Quantifying direct and indirect exposure to contaminants
 - Quantifying exposure: Exposure factors XP, the concentration-to-intake relationship
 - Combining fate and exposure: Intake fraction iF, the emission-to-intake relationship
- The USEtox exposure model

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What is exposure?

EXPOSURE


“Contact between an **agent** (air, water, food, soil etc. containing a potentially harmful substance) and a **target** (human individual or population). Contact takes place at an **exposure surface** (mouth, skin, eyes) over an **exposure period** at an **exposure frequency**”.

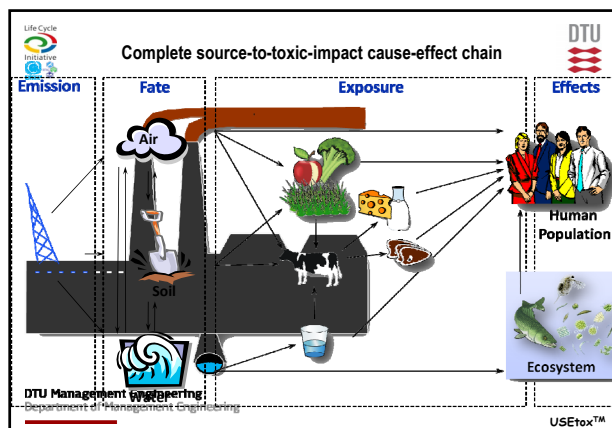



EXPOSURE ASSESSMENT


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.

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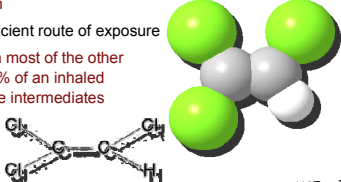








Example Chemical TCE


- Trichloroethylene (TCE) is a chlorinated hydrocarbon solvent, which is still in widespread use as a metal degreaser, and solvent
- Several million kg used world wide
- Ranked as one of the most hazardous compounds (worst 10%) to ecosystems and human health (SCORECARD)
- TCE is absorbed well by the lungs--30 to 50 percent of the inhaled vapor is absorbed into the bloodstream
- Skin contact is also a fairly efficient route of exposure
- TCE is metabolized more than most of the other chlorinated solvents--up to 90% of an inhaled dose is metabolized to reactive intermediates



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Estimating Exposure


- Concentration:
 - You spend **8 hours/day** in a **factory** with a TCE concentration of **1 mg/m³**
 - You spend **16 hours/day** in an **environment** with a TCE concentration of **0.1 mg/m³**
- What is your daily exposure to TCE?




TCE intake

If your average daily breathing rate is 0.8 m³/h:

- What is your daily intake [mg/day]?
- What is your daily dose [mg/kg*day]?
- Do you have confidence in these estimates?



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Estimating Exposure

Consider a lake that contains 1 mg/l of TCE and provides 2 l/d of drinking water to a population of 1 million people whose average weight is 70 kg:

- >What is the TCE intake per person (mg/d)?
- >What is the TCE dose per person (intake per unit body weight) (mg/kg*d)?
- >What fraction of the lake's daily flow is being consumed by this population each day?

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Multi-media

- > Sources are multimedia: the same pollutant can be released to multiple media--air, water, soil, food, ...
- > Pollutants are multimedia (cross-media): they partition among multiple media--air, water, soil, ...
- > Exposures are multimedia: a receptor can have contact with multiple exposure media--air, water, food, soil, ...

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Multi-pathway

- > Exposure to a contaminated medium can lead to human contact through several parallel pathways.
- > Examples:
 - > Pollutants in ambient (outdoor) air can contaminate indoor air, food, water, ...
 - > Pollutants in ground water can contaminate surface water, indoor air, food, ...

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Multi-route

- > Pollutants enter humans through different exposure routes which combine various exposure pathways:
 - > Inhalation (outdoor air, household indoor air, industrial indoor air)
 - > Ingestion (drinking water, agricultural produce, meat, milk, eggs, fish, ...)
 - > Dermal contact (air, water, soil, cosmetics, cleaning agents, ...)
- > Health effects can vary with the route of intake/uptake.

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Quantifying multiple exposure pathways

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Exposure pathways and biokinetics

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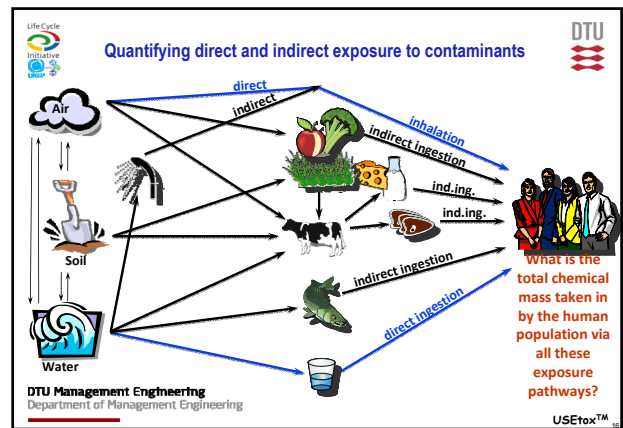
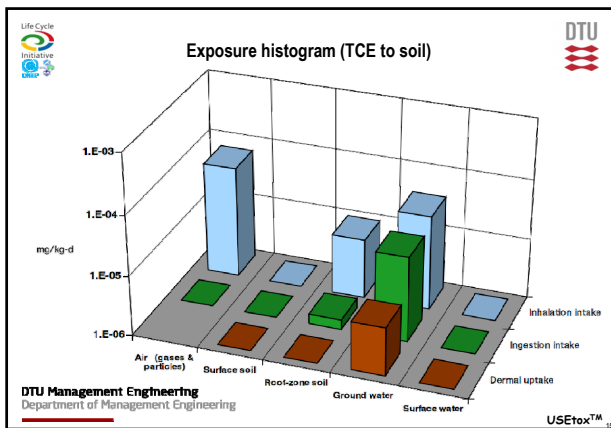
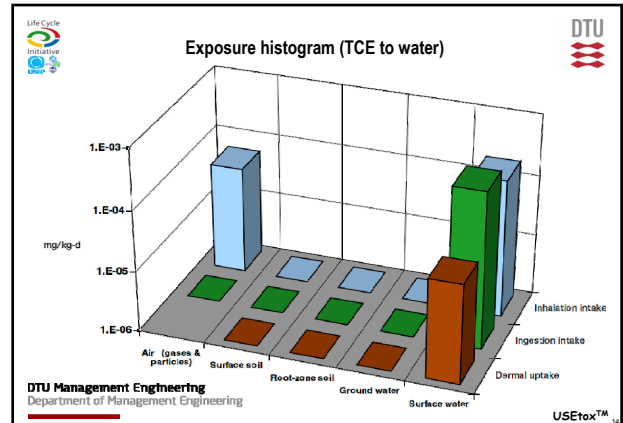
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Quantifying multiple exposure pathways: Exposure matrix

| | ENVIRONMENTAL MEDIA | | |
|---------------|--|--|--|
| | AIR | SOIL | WATER |
| INHALATION | Outdoor air Indoor air | Soil vapors under houses Soil particles transferred to indoor air | Contaminants transferred from tap water |
| INGESTION | Fruits, vegetables, and grains | Human soil ingestion Meat, milk, and eggs (soil ingestion by animals) | Ingestion of tap water |
| | Meat, milk, and eggs (transfer to plants to animals) | Fruits, vegetables, and grains | Irrigated fruits, vegetables, & grains |
| | Meat, milk, and eggs (inhalation by animals) | Meat, milk, and eggs (transfer from soil to plants to animals) | Meat, milk, and eggs (animals consuming contaminated water) |
| | Breast milk | Breast milk | Fish and sea food Breast milk |
| DERMAL UPTAKE | | Dermal contact with soil | Dermal contact in baths and showers Dermal contact while swimming |

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Quantifying exposure: Exposure factors XP , the concentration-to-intake relationship

Conceptually similar to the intermedia transfer rate coefficient calculated in the fate model, the exposure factor $XP_{k,i}$ [1/day] is the transfer rate coefficient for exposure to contaminants in compartment k via exposure pathway i (e.g. inhalation, water ingestion, food ingestion, ...):

$$XP_{k,i} = \frac{ITF_{k,i} \cdot IR_i \cdot \text{population}}{\rho_k \cdot V_k}$$

$ITF_{k,i}$ = C_i/C_k = Intermedia transfer factor from compartment k to medium i [kg_i/kg_k]
 IR_i = Individual human intake rate of i [kg_i/day]
 ρ_k = Density of compartment k [kg_i/m_k^3] (irrelevant if IR_i in [m^3/day])
 V_k = Volume of compartment k [m_k^3]

The total exposure factor $XP_{k,\text{tot}}$ for compartment k is then given as the sum of alldirect and indirect exposure factors:

$$XP_{k,\text{tot}} = \sum_{i=\text{direct}} XP_{k,i} + \sum_{i=\text{indirect}} XP_{k,i}$$

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Rosenbaum, R.K., Margni, M., Joliet, O., (2007). A flexible matrix algebra framework for the multimedia multipathway modeling of emission to impacts. Environment International 33, 624-634. USEtox™

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Direct exposure: Exposure factor $XP_{k,\text{direct}}$

The exposure factor $XP_{k,\text{direct}}$ [1/day] is the rate coefficient for direct exposure to contaminants in compartment k , through consumption of drinking water or inhalation of air. Here $ITF_{k,i} = C_i/C_k = 1$ since $i = k$, meaning that the compartment is directly ingested.

$XP_{\text{air,direct}} [1/\text{day}] = \frac{IR_{\text{air}} [\text{m}^3/\text{day}] \cdot \text{population}}{V_{\text{air}} [\text{m}^3]}$

$XP_{\text{water,direct}} [1/\text{day}] = \frac{IR_{\text{water}} [\text{m}^3/\text{day}] \cdot \text{population}}{V_{\text{water}} [\text{m}^3]}$

The inverse of $XP_{k,\text{direct}}$ is a 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).

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Indirect exposure: Exposure factor $XP_{k,indirect}$

$XP_{k,indirect}$ [1/day] is the rate coefficient of indirect exposure to a contaminant in compartment k through consumption of an exposure medium i that was contaminated from compartment k .

$$XP_{k,i-indirect} = \frac{ITF_{k,i-indirect} \cdot IR_i \cdot population}{\rho_k \cdot V_k}$$

$ITF_{k,i} = C_i/C_k$ = Intermedia transfer factor from compartment k to medium i [kg_i/kg_k]
 IR_i = Individual human intake rate of i [kg/day]
 ρ_k = Density of compartment k [kg/m^3] (irrelevant if IR_i in [m^3/day])
 V_k = Volume of compartment k [m^3]

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Indirect exposure: Intermedia transfer factors $ITF_{k,i}$

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

- Bioconcentration factor ($BCF_{k,i}$) at steady-state:

$$BCF_{k,i} = \frac{C_i(\text{chemical conc. in exp. medium } i)}{C_k(\text{chemical conc. in compartment } k)}$$
- Biotransfer factor (BTF_i) – measure of bioaccumulation at steady-state:

$$BTF_i = \frac{C_i(\text{chemical conc. in exp. medium } i)}{I_{chem.}(\text{animal chemical intake})}$$

Rosenbaum, R.K., McKone, T.E., Jolliet, O., (2009). CKow: A Dynamic Model for Chemical Transfer to Meat and Milk. *Environmental Science and Technology* 43, 8191-8198. **USEtox™**

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Indirect exposure: Production-based vs. subsistence scenarios

Pennington, D.W., Margni, M., Ammann, C., Jolliet, O., 2005. Multimedia fate and human intake modeling: Spatial versus nonspatial insights for chemical emissions in Western Europe. *Environmental Science and Technology* 39, 1119-1128. **USEtox™**

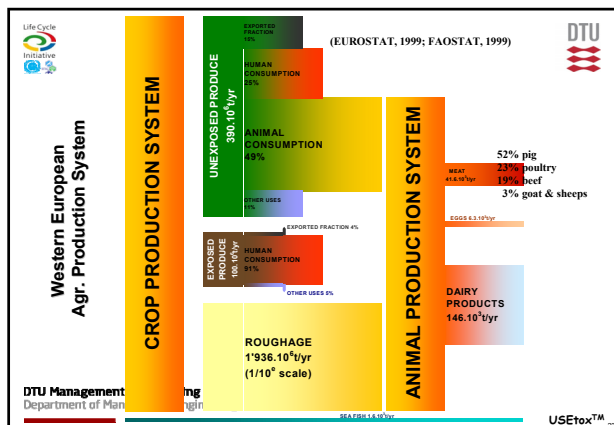
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Indirect exposure: Production-based scenario

Usual exposure models used for environmental risk assessment: individual or cohort risk + conservative assumptions

- « Subsistence scenario »
 - receptor perspective,
 - consumed food produced in the same region
- « Production scenario »
 - Chemical transfer to food = f(production area)
 - Tracks long-range chemical transport via food

Pennington, D.W., Margni, M., Ammann, C., Jolliet, O., 2005. Multimedia fate and human intake modeling: Spatial versus nonspatial insights for chemical emissions in Western Europe. *Environmental Science and Technology* 39, 1119-1128. **USEtox™**



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Total intake of the human population via all exposure pathways I_k

Contaminant mass in compartment k : M_k [kg]

Total exposure factor XP_k [1/day]:

$$XP_k = \frac{Intake_k}{V_k} = XP_{k,direct} + XP_{k,indirect}$$

Total chemical mass intake from compartment k by the human population: I_k [kg/day]

$$I_k = M_k \cdot XP_k$$

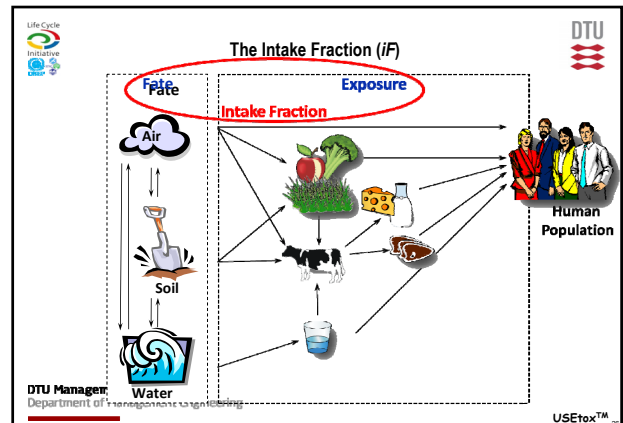
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Rosenbaum, R.K., Margni, M., Jolliet, O., (2007). A flexible matrix algebra framework for the multimedia multipathway modeling of emission to impacts. *Environment International* 33, 624-634. **USEtox™**

Combining fate and exposure: Intake fraction iF , the emission-to-intake/uptake relationship

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Intake fraction (iF) for outdoor exposure

$$iF = \frac{\sum_k M_k \cdot XP_k}{S} = \frac{\text{Population Intake}}{\text{Total Emissions}} = \frac{\int_{T_1}^{\infty} \left[\sum_{k=1}^P \{C_k(t) \cdot In_k(t)\} dt \right]}{\int_{T_1}^{\infty} S(t) dt}$$

M_k = Mass in compartment k [g]
 XP_k = Exposure factor via compartment k [1/day]
 S = Emission rate to a compartment [g/day]
 C_k = Concentration in compartment k [g/m³]
 In_k = Intake rate [m³/person*day], e.g. breathing rate
 P = Population [persons]

Bennett, D. H., Margni, M., McKone, T. E., & Joliet, O. (2002). Intake Fraction for Multimedia Pollutants: A Tool for Life Cycle Analysis and Comparative Risk Assessment. *Risk Analysis*, 22(5), 903-916.
 Bennett, D. H., McKone, T. E., Evans, J. S., Nazaroff, W. W., Margni, M. D., Joliet, O., et al. (2002). Defining Intake Fraction. *Environmental Science and Technology*, 36(9), 207A-211A.

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Intake fraction (iF) for indoor exposure

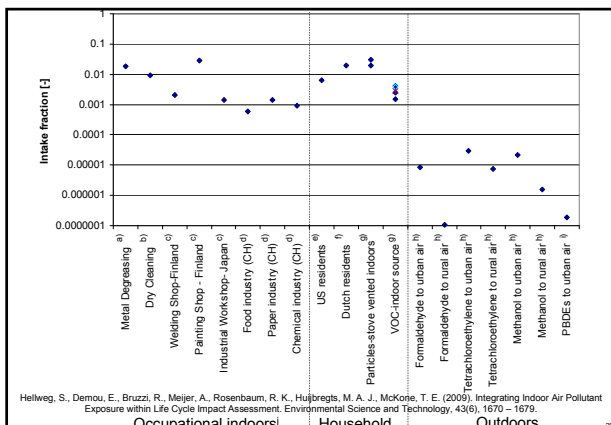
$$iF = \frac{IR}{V \cdot m \cdot k_{ex}} \cdot N$$

iF = population intake fraction of a chemical [-]
 IR = daily inhalation rate of air of an individual [m³/day]
 N = number of people exposed [-]
 V = volume of the exposure area [m³]
 k_{ex} = air exchange rate of the volume in the exposure area [-]
 m = mixing factor [-]

Hellweg, S., Demou, E., Bruzzi, R., Meijer, A., Rosenbaum, R. K., Huijbregts, M. A. J., McKone, T. E. (2009). Integrating Indoor Air Pollutant Exposure within Life Cycle Impact Assessment. *Environmental Science and Technology*, 43(6), 1670 – 1679.

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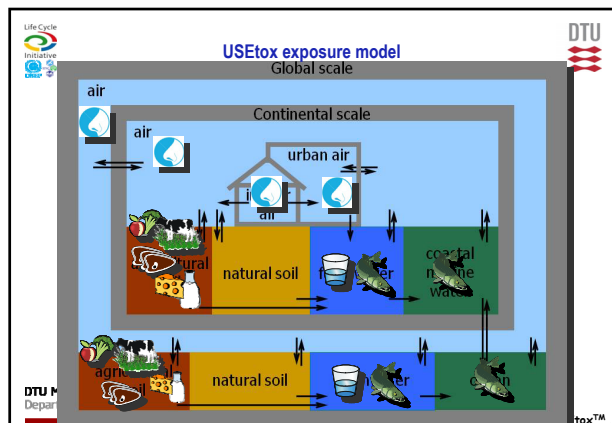
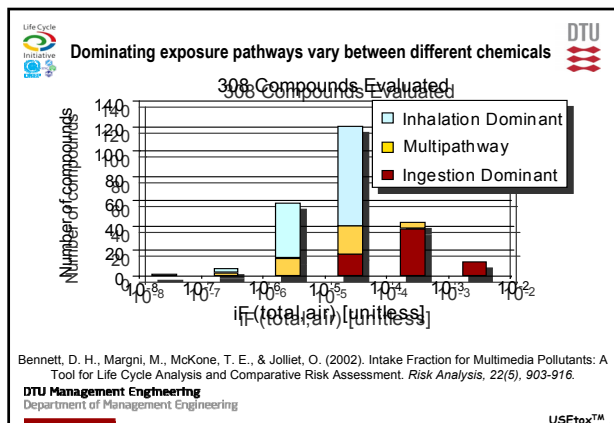
Intake fraction for a simple case (TCE)


Consider a lake that contains 1 mg/l of TCE and provides 2 l/d of drinking water to a population of 1 million people whose average weight is 70 kg:

- >How many kg of TCE per day does this population of 1 million consume from the lake?
- >What is the characteristic time of intake (CTI) for this lake (how many days does it take for a million people to consume the volume of the lake)?
- >What is the intake fraction?
- >Use the ratio of TCE residence time to CTI to determine iF .

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Institute

exposure medium

urban air

continental compartments

global compartments

XP (d⁻¹)

| airU | airC | fr.waterC | seawaterC | nat.soilC | agr.soilC | airG | fr.waterG | oceanG | nat.soilG | agr.soilG |
|-------------------|----------|-----------|-----------|-----------|-----------|----------|-----------|----------|-----------|-----------|
| 4.51E-04 | 1.30E-06 | 0 | 0 | 0 | 0 | 1.70E-07 | 0 | 0 | 0 | 0 |
| drinking water | 0 | 0 | 2.07E-08 | 0 | 0 | 0 | 0 | 7.94E-07 | 0 | 0 |
| exposed produce | 0 | 1.09E-09 | 0 | 0 | 0 | 1.68E-12 | 1.41E-10 | 0 | 0 | 6.44E-13 |
| unexposed produce | 0 | 0 | 0 | 0 | 0 | 1.14E-07 | 0 | 0 | 0 | 4.40E-08 |
| meat | 0 | 1.73E-11 | 5.62E-11 | 0 | 0 | 9.83E-13 | 2.28E-12 | 2.16E-11 | 0 | 3.78E-13 |
| dairy products | 0 | 2.43E-11 | 1.76E-10 | 0 | 0 | 2.42E-12 | 3.18E-12 | 6.75E-11 | 0 | 9.28E-13 |
| fish | 0 | 0 | 2.98E-07 | 5.77E-09 | 0 | 0 | 0 | 1.15E-07 | 5.37E-11 | 0 |

exposure medium

urban air

continental emissions

global emissions

iF

| airU | airC | fr.waterC | seawaterC | nat.soilC | agr.soilC | airG | fr.waterG | oceanG | nat.soilG | agr.soilG |
|-------------------|----------|-----------|-----------|-----------|-----------|----------|-----------|----------|-----------|-----------|
| 2.99E-05 | 5.44E-06 | 4.81E-06 | 9.80E-07 | 4.72E-06 | 4.72E-06 | 1.16E-06 | 1.03E-06 | 1.29E-07 | 1.01E-06 | 1.01E-06 |
| drinking water | 2.84E-09 | 2.59E-09 | 9.89E-08 | 4.66E-10 | 2.02E-07 | 2.02E-07 | 5.54E-10 | 3.80E-06 | 6.13E-11 | 7.73E-08 |
| exposed produce | 4.48E-09 | 4.52E-09 | 4.00E-09 | 8.14E-10 | 3.92E-09 | 3.94E-09 | 9.69E-10 | 8.54E-10 | 1.07E-10 | 8.40E-10 |
| unexposed produce | 2.67E-10 | 2.69E-10 | 2.38E-10 | 4.84E-11 | 2.33E-10 | 1.37E-06 | 5.76E-11 | 5.08E-11 | 6.37E-12 | 5.00E-11 |
| meat | 7.18E-11 | 7.24E-11 | 3.33E-10 | 1.30E-11 | 6.82E-11 | 8.00E-11 | 1.55E-11 | 1.17E-10 | 1.72E-12 | 1.55E-11 |
| dairy products | 1.01E-10 | 1.02E-10 | 9.31E-10 | 1.84E-11 | 1.05E-10 | 1.34E-10 | 2.19E-11 | 3.42E-10 | 2.42E-12 | 2.55E-11 |
| fish | 5.82E-10 | 5.76E-10 | 1.44E-06 | 2.24E-07 | 2.95E-08 | 2.95E-08 | 1.09E-10 | 5.49E-07 | 2.64E-09 | 1.12E-08 |

iF (agro)

| airU | airC | fr.waterC | seawaterC | nat.soilC | agr.soilC | airG | fr.waterG | oceanG | nat.soilG | agr.soilG |
|-----------|----------|-----------|-----------|-----------|-----------|----------|-----------|----------|-----------|-----------|
| 2.99E-05 | 5.44E-06 | 4.81E-06 | 9.80E-07 | 4.72E-06 | 4.72E-06 | 1.16E-06 | 1.03E-06 | 1.29E-07 | 1.01E-06 | 1.01E-06 |
| ingestion | 8.15E-09 | 8.13E-09 | 1.13E-05 | 2.25E-07 | 2.36E-07 | 1.61E-06 | 1.73E-09 | 4.35E-06 | 2.82E-09 | 8.94E-08 |

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USEtox exposure model input data

Substance specific data (see worksheet "Substance data"):

- > Bioaccumulation factor in root crops BAF_{root}
- > Bioaccumulation factor in leaf BAF_{leaf}
- > Biotransfer factor in meat BTF_{meat}
- > Biotransfer factor in milk (dairy products) BTF_{milk}
- > Bioaccumulation factor in fish BAF_{fish}

Exposure model parameters for continental and global scale respectively (see worksheet "Landscape data"):

- > Human population
- > Human breathing rate
- > Water ingestion
- > Production-based food ingestion for exposed produce, unexposed produce, meat, dairy products, freshwater fish, marine fish

Exposure model parameters for urban and indoor air (household/industrial) exposure:

- > Human population/average room occupation
- > Human breathing rate

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Concluding Points

- > While the fate model provides the contaminant mass in each compartment,
- > the exposure model estimates the contaminant intake of the human population due to the chemical mass in the environment.
- > Combining fate and exposure, the intake fraction estimates the fraction of an emission which is ultimately taken in by the population. It is obtained from the multiplication of exposure factors (XP) and fate factors (FF) or the respective matrices containing these factors.
- > Exposure happens via many direct and indirect pathways in parallel and varies depending on the exposure magnitude, duration, and frequency.

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Further reading (USEtox)

- > Rosenbaum, R.K., Bachmann, T.K., Gold, L.S., Huijbregts, M.A.J., Jolliet, O., Juraske, R., Koehler, A., Larsen, H.F., MacLeod, M., Margni, M., McKone, T.E., Payet, J., Schuhmacher, M., Van de Meent, D., Hauschild, M.Z., (2008). USEtox - The UNEP/SETAC-consensus model: recommended characterisation factors for human toxicity and freshwater ecotoxicity in Life Cycle Impact Assessment. *International Journal of Life Cycle Assessment* 13, 532-546.
- > Hauschild, M.Z., Huijbregts, M.A.J., Jolliet, O., MacLeod, M., Margni, M., Van de Meent, D., Rosenbaum, R.K., McKone, T.E., (2008). Building a model based on scientific consensus for Life Cycle Impact Assessment of Chemicals: the Search for Harmony and Parsimony. *Environmental Science and Technology* 42, 7032-7037.
- > Rosenbaum, R.K., Margni, M., Jolliet, O., (2007). A flexible matrix algebra framework for the multimedia multipathway modeling of emission to impacts. *Environment International* 33, 624-634.
- > Hellweg, S., Demou, E., Bruzzi, R., Meijer, A., Rosenbaum, R.K., Huijbregts, M.A.J., McKone, T.E., (2009). Integrating Indoor Air Pollutant Exposure within Life Cycle Impact Assessment. *Environmental Science and Technology* 43, 1670 - 1679.

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Further reading (UNEP-SETAC LCA-toxicity expert workshops)



- Diamond, M.L., Gandhi, N., Adams, W.J., Atherton, J., Bhavsar, S.P., Bulle, C., Campbell, P.G.C., Dubreuil, A., Fairbrother, A., Farley, K., Green, A., Guinee, J., Hauschild, M.Z., Huijbregts, M.A.J., Humbert, S., Jensen, K.S., Joliet, O., Margni, M., McGeer, J.C., Peijnenburg, W.J.G.M., Rosenbaum, R.K., van de Meent, D., Vijver, M.G., (2010). The clearwater consensus: the estimation of metal hazard in fresh water. *International Journal of Life Cycle Assessment* 15, 143-147.
- McKone, T.E., Kyle, A.D., Joliet, O., Olsen, S.I., Hauschild, M., (2006). Dose-Response Modeling for Life Cycle Impact Assessment - Findings of the Portland Review Workshop. *International Journal of Life Cycle Assessment* 11, 137-140.
- Joliet, O., Rosenbaum, R.K., Chapmann, P., McKone, T., Margni, M., Scheringer, M., van Straalen, N., Wania, F., (2006). Establishing a framework for Life Cycle Toxicity Assessment: Findings of the Lausanne review workshop. *International Journal of Life Cycle Assessment* 11, 209-212.