





# Source to impact framework and uncertainty

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## Overview

- The USEtox model and its structure
- Matrix algebra framework: Combining fate, exposure and effect factors to characterisation factors using matrix algebra
- Walking through a USEtox calculation for TCE
- Uncertainties



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## Principles for USEtox development

- **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

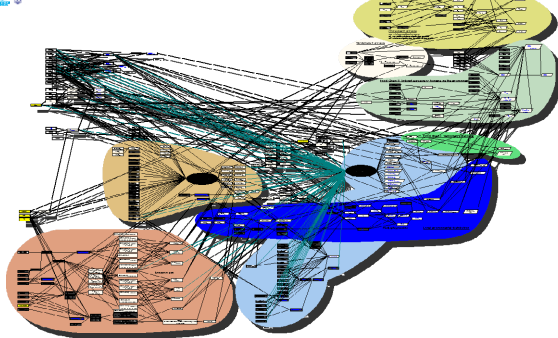





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## Matrix algebra framework: Transparency in multimedia models

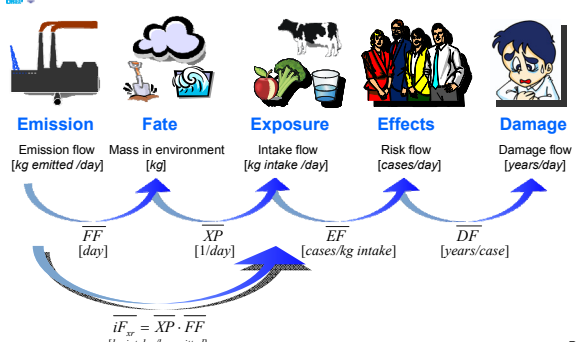







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## Matrix algebra framework: Structure

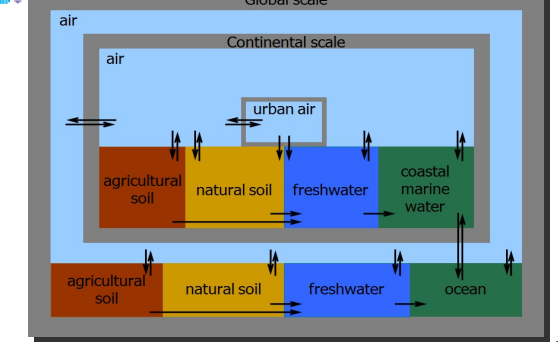







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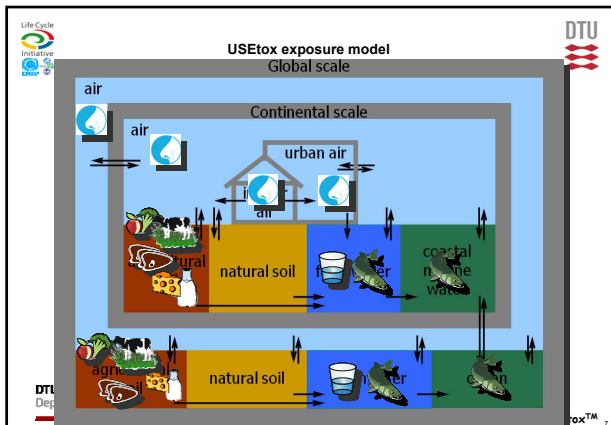



## USEtox fate model compartment structure



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**Matrix algebra framework: USEtox (rate coefficient) k-matrix (TCE)**

receiving compartment urban air emissions continental emissions global emissions

$k [d^{-1}]$

	airU	airC	fr.waterC	seawaterC	nat.soilC	agr.soilC	airG	fr.waterG	oceanG	nat.soilG	agr.soilG
airU	1.87E+01	1.07E-04	0	0	0	0	0	0	0	0	0
airC	1.86E+01	-2.63E-01	1.83E-01	4.59E-03	7.09E-02	7.09E-02	2.37E-03	0	0	0	0
fr.waterC	1.49E-04	6.06E-05	-2.09E-01	0	1.69E-03	1.69E-03	0	0.00E+00	0	0	0
seawaterC	0	2.21E-04	6.97E-03	-2.59E-02	0	0	0	0	4.16E-06	0	0
nat.soilC	0	4.69E-05	0	0	-8.35E-02	0	0	0	0	0	0
agr.soilC	0	4.69E-05	0	0	0	-8.35E-02	0	0	0	0	0
airG	0	1.09E-01	0	0	0	0	-1.97E-01	1.83E-01	2.29E-03	7.09E-02	7.09E-02
fr.waterG	0	0	0	0	0	0	2.06E-05	-2.09E-01	0	1.69E-03	1.69E-03
oceanG	0	0	0	2.76E-03	0	0	1.55E-03	6.97E-03	-2.08E-02	0	0
nat.soilG	0	0	0	0	0	0	1.60E-05	0.00E+00	0	-8.35E-02	0
agr.soilG	0	0	0	0	0	0	1.60E-05	0.00E+00	0	0	-8.35E-02

> Column: emission compartment  
 > Row: receiving compartment  
 > Diagonal elements: total removal rate coefficient per compartment including degradation, advective and intermedia removal [1/day], sum of all off-diagonal elements within the same column + all other removal rates such as degradation or burial  
 > Off-diagonal elements: reflect intermedia or advective transport from source to receiving compartment [1/day]

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**Matrix algebra framework: USEtox fate factor matrix (TCE)**

receiving compartment urban air emissions continental emissions global emissions

$FF [d]$

	airU	airC	fr.waterC	seawaterC	nat.soilC	agr.soilC	airG	fr.waterG	oceanG	nat.soilG	agr.soilG
airU	5.34E-02	2.19E-05	1.94E-05	3.90E-06	1.90E-05	1.90E-05	3.32E-07	2.93E-07	3.74E-08	2.88E-07	2.88E-07
airC	3.80E+00	3.84E+00	3.39E+00	6.82E-01	3.33E+00	3.33E+00	5.81E-02	5.12E-02	6.55E-03	5.04E-02	5.04E-02
fr.waterC	1.18E-03	1.15E-03	7.95E+00	2.04E-04	9.77E-02	9.77E-02	1.74E-05	1.53E-05	1.96E-06	1.51E-05	1.51E-05
seawaterC	3.29E-02	3.32E-02	1.32E+00	3.87E-04	5.48E-02	5.48E-02	5.79E-04	7.69E-04	7.82E-03	5.07E-04	5.07E-04
nat.soilC	2.14E-03	2.15E-03	1.90E-03	3.83E-04	1.02E-01	1.87E-03	3.28E-05	2.88E-05	3.89E-06	2.83E-05	2.83E-05
agr.soilC	2.14E-03	2.15E-03	1.90E-03	3.83E-04	1.02E-01	1.87E-03	3.28E-05	2.88E-05	3.89E-06	2.83E-05	2.83E-05
airG	2.65E+00	2.67E+00	2.96E+00	5.90E-01	3.32E+00	3.32E+00	6.42E+00	5.66E+00	7.06E-01	5.57E+00	5.57E+00
fr.waterG	2.70E-04	2.72E-04	2.40E-04	5.59E-05	2.36E-04	2.36E-04	6.53E-04	4.79E+00	7.21E-05	9.73E-02	9.73E-02
oceanG	2.03E-01	2.04E-01	3.52E-01	5.18E+00	1.81E-01	1.81E-01	4.80E-01	2.03E+00	4.82E+01	4.49E-01	4.49E-01
nat.soilG	3.06E-04	3.06E-04	4.52E-04	1.05E-04	4.42E-04	4.42E-04	1.22E-03	1.08E-03	1.35E-04	1.20E+01	1.08E-03
agr.soilG	3.06E-04	3.06E-04	4.52E-04	1.05E-04	4.42E-04	4.42E-04	1.22E-03	1.08E-03	1.35E-04	1.20E+01	1.20E+01

> Column: emission compartment  
 > Row: receiving compartment  
 > Diagonal elements: residence time in the respective compartment [day]  
 > Off-diagonal element/diagonal element ratio within a row: Fraction of the mass transferred to compartment x from emissions to adjacent compartment y.

The mass transferred from water to air is 88% of the amount emitted to water:  $\frac{3.39}{3.84} = 0.88$

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**Matrix algebra framework: USEtox human exposure factor matrix (TCE)**

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
drinking water	4.51E-04	1.30E-06	0	0	0	0	1.70E-07	0	0	0	0
exposed produce	0	0	2.07E-06	0	0	0	0	7.94E-07	0	0	0
unexposed produce	0	1.09E-09	0	0	0	1.69E-12	1.41E-10	0	0	0	6.44E-13
meat	0	0	0	0	0	1.14E-07	0	0	0	0	4.40E-08
dairy products	0	1.73E-11	5.62E-11	0	0	9.83E-13	2.26E-12	2.16E-11	0	0	3.78E-13
fish	0	2.43E-11	1.76E-10	0	0	2.42E-12	3.18E-12	6.75E-11	0	0	9.28E-13
	0	0	2.98E-07	5.77E-09	0	0	0	1.15E-07	5.37E-11	0	0

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**Matrix algebra framework: USEtox human intake fraction matrix (TCE)**

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
air	2.95E-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	2.64E-09	2.59E-09	6.89E-09	4.66E-10	2.02E-07	2.02E-07	5.54E-10	3.80E-08	6.13E-11	7.73E-08	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	8.48E-10
unexposed produce	2.67E-10	2.69E-10	2.38E-10	4.84E-11	2.33E-10	1.37E-09	5.76E-11	5.08E-11	6.37E-12	5.00E-11	5.26E-07
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	2.01E-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	3.66E-11
fish	9.62E-10	5.76E-09	1.44E-06	2.24E-07	2.95E-08	2.95E-08	1.09E-10	5.49E-07	2.64E-09	1.12E-08	1.12E-08

$iF = XP * FF$

$iF$  (agg)

	airU	airC	fr.waterC	seawaterC	nat.soilC	agr.soilC	airG	fr.waterG	oceanG	nat.soilG	agr.soilG
inhalation	2.95E-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	6.16E-07

[kg intake/kg emissions]

Enables simple identification of the dominate exposure pathways per emission scenario (red circles).

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**Matrix algebra framework: USEtox characterisation factor matrix (TCE)**

$iF$  (agg)

	airU	airC	fr.waterC	seawaterC	nat.soilC	agr.soilC	airG	fr.waterG	oceanG	nat.soilG	agr.soilG
inhalation	2.95E-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	6.16E-07

Human health effect factor matrix  $EF_{hum}$  [cases/kg<sub>intake</sub>]:


	Inhalation	Ingestion
Cancer	0.0017	0.0029
Non-cancer	0.0000	0.0000

$HTP = iF * EF_{hum}$


Midpoint human health characterization factor matrix HTP [cases/kg<sub>emission</sub>]:

	airU	airC	fr.waterC	seawaterC	nat.soilC	agr.soilC	airG	fr.waterG	oceanG	nat.soilG	agr.soilG
cancer	5.06E-08	9.38E-09	4.17E-08	2.35E-09	8.79E-09	1.28E-08	2.00E-09	1.48E-08	2.29E-10	2.00E-09	3.55E-09
non-cancer	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
total	5.06E-08	9.38E-09	4.17E-08	2.35E-09	8.79E-09	1.28E-08	2.00E-09	1.48E-08	2.29E-10	2.00E-09	3.55E-09

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### Matrix algebra framework: Interpretation

**Fate matrix interpretation:**


- Mass increase in row compartment due to an emission in a column compartment
- Diagonal elements: residence time in the respective compartment [day]
- Feedback factor: product of the corresponding diagonal elements of k-matrix and fate matrix, yields the fraction of a chemical being transferred back into the compartment of origin (Margni et al., 2004 ES&T)

**Exposure matrix interpretation:**


- Direct exposure rate: corresponds to fraction of the total mass in a medium, taken in daily by humans & inverse represents the equivalent time required by the population to inhale or ingest the whole mass in the medium
- Indirect exposure rate: can be interpreted as the equivalent intake rate of polluted medium via an exposure substrate



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### Matrix algebra framework: Interpretation

**Intake fraction (iF) matrix interpretation:**

- Intake fraction for individual pathways: each element represents an actual iF
- Pathways contributions: ratio of each element in a column with the sum of all elements of the same exposure route (e.g. inhalation, ingestion, dermal) within this column yields the contribution of this pathway to the corresponding route
- Comparison of exposure routes: dominating exposure route per emission scenario

**Effect matrix interpretation:**


- Human health: increase in cancer or non-cancer disease cases per unit mass ingested or inhaled

**Damage matrix interpretation:**


- Severity of occurring diseases: Years of Life Lost per affected Person (YLLp [year/case]) and Years of Life lived with a Disability per affected Person (YLDp [years/case])

**Human damage matrix interpretation:**


- Increase in affected life time due to cancer and non-cancer diseases



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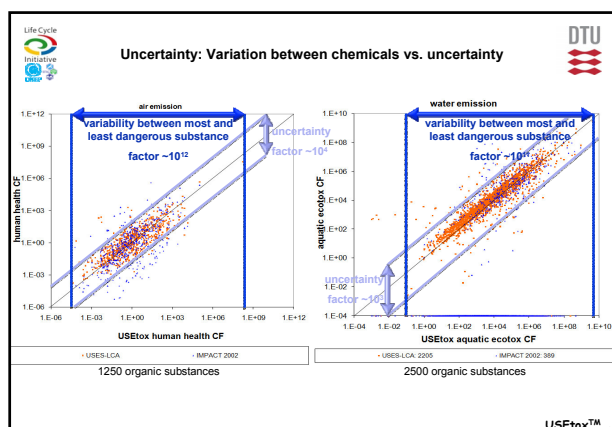
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### Matrix algebra framework: Advantages

- **Flexibility:** adding new compartment, exposure pathway, or effect type -- adding new rows or columns to the respective matrices
- **Interpretability:** e.g. identification of dominating exposure pathways
- **Model comparability and evaluation:**
  - matrices contain all intermediate results
  - low dependency on model and scenario parameters
  - direct matrix comparison of two models yields advantages against comparing single results which often need to be made consistent
- **Computational efficiency** is increased
- **Characterisation of multiple emission scenarios in one calculation run:**
  - current models need to run separately for each emission scenario
  - matrices are stored and can be used for further calculation any time
- **Multidisciplinary work is facilitated:**
  - each of its modules defines a clear interface of intermediate results
  - enables linkage of different models from various disciplines together




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### Uncertainty: Recommendations

- Contributions of 1%, 5% or 90% to the total human toxicity score are essentially equal, but significantly larger than those of a chemical contributing to less than 1 per thousand or less than 1 per million of the total score. Disregarding this fact has been a major cause of complaints about the variability of these factors across LCIA methods, whereas the most important chemicals were often the same within a factor 1000 across methods.
- This means that for LCA practitioners, toxicity factors are useful to identify the 10 or 20 most important toxics pertinent for their applications. The Life Cycle Toxicity scores thus enable the identification of all chemicals contributing more than e.g. 1/1000 to the total score. In most applications, this will allow the practitioner to identify 10 to 30 chemicals to look at in priority, and perhaps more importantly, to disregard hundreds of other substances whose impacts are not significant for the considered application.
- Once these most important substances have been identified, further analysis can be carried out on the life cycle phase, application components responsible for these emissions, and the respective importance of fate, exposure and effect in determining the impacts of this chemical.


Rosenbaum R.K., Bachmann T.K., Gold L.S., Huijbregts M.A.J., Joliet 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. Int. J. Life Cycle Assess. 13, 532-546.



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### USEtox: Future perspectives (next 3 yr)


- Increase of substance coverage and quality assurance of substance data;
- Accommodate metals and indoor emissions;
- Include terrestrial and marine ecotoxicity;
- Include parameter uncertainty;
- Research on how to include chronic data and how to estimate average toxicity (single species or trophic levels);
- Reliability check of freshwater ecotoxicity CFs based on one or two effect data only (including a check for the occurrence of NOEC extrapolation and on the representation of taxa and trophic levels).

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**USEtox: Future perspectives (next 3 yr)**




- Recommendations regarding differentiation between midpoint and endpoint characterisation;
- Industry workshops and practitioner training courses in USEtox (such as this one today);
- User-friendly programming, full documentation and website;
- Consensus building among stakeholders;
- USEtox is considered for further review, evaluation and possible adoption/endorsement by several national, international, and global organisations and bodies.

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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., Jolliet, 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., Jolliet, 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.
- Jolliet, 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.

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