Overall modelling with USEtox "Exercise"

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USEtox exercise: Objectives

- See what can be found on the www.USEtox.org website.
- Get your hands on the USEtox model and find your way through it.
- Learn how to use the USEtox model with its most important functions and where to find the most important information.
  - Single substance data input and substance database import function;
  - Performing single-substance and multi-substance calculations and where to find the results;
- Learn how to interpret and use the main intermediate and final results of the model.

USEtox exercise: What you can find on www.usetox.org

1. Download (via acceptance of the licence terms) of the latest versions of:
   1. USEtox model + user manual:
   2. Organics database + user manual;
   3. Inorganics database + user manual;
   4. Readily calculated results for organics and inorganics;
2. Contact to the USEtox helpdesk via email support@usetox.org
3. Some background information and links to the directly related publications;
4. Some short information on the USEtox team;
5. In the future:
   1. This course as stream/download;
   2. The course material from this course;
   3. Dates for future iterations of this course;
   4. Complete scientific documentation of the model and data (still to be funded).
   5. **Any further ideas what you would like to find here?**

USEtox exercise: Usage – User-relevant worksheets

- Unless you want to change a model parameter (not a substance parameter), you only need to know your way around the worksheets "**Substance data**", "**Run**", and "**Results**" to use the model:
  - The chemical dependent input data (those describing the physico-chemical and (eco)toxicological properties of the substances) are stored in the worksheet "**Substance data**". The substances properties are entered in the corresponding columns per substance in each line.
  - The main calculations are performed in the worksheet "**Run**", where you will find all the fate, exposure, and effects matrices on the left side, and some interpretations of these on the right side.
  - The results of a multiple-substance (batch) calculation can be found in the worksheet "**Results**".
- The worksheets "Version", "Agreements", and "Instructions" only have informative/reference character. The rest contains model parameters and calculates the inputs to the matrices in "Run". You should not change those if you want to obtain consistent results, compatible to other USEtox factors.

USEtox exercise: Usage – Preparation

1. Open USEtox and the chemical database Organics. Make sure that your security settings allow macros to run.
2. Import the database into USEtox using the button "Import Database Organics" in the worksheet "Substance data".
3. Using the Find function in the worksheet "Run", look for the substance "trichloroethylene".
4. Set the model to a single-substance calculation for TCE. Note that the Find function only serves to find a search term in the database and does not automatically set the model to run the chemical found. One has to manually enter the corresponding row number into the "Single Substance or First Row" field (C5).
5. Answer the following questions using the information provided in the worksheet "Run".

USEtox exercise: Usage – Characterisation factors

1. Where can the characterisation factors for human toxicity and aquatic ecotoxicity for emissions to air, water and soil be found?
2. What is the characterisation factor for total human health effects for an emission to continental air?
3. What is the freshwater ecotoxicity characterisation factor for an emission to continental freshwater?
4. Why do we need fate, exposure, and effect factors to calculate human health characterisation factors?

USEtox exercise: Usage – Effect factors

1. What is the ecotoxicity effect factor for freshwater ecosystems?
2. Why does the effect factor matrix for aquatic ecotoxicity contain so many zeros?
3. What is the human health effect factor for cancer via inhalation?
4. Why is there no effect factor for total human health effects?

USEtox exercise: Usage – Exposure factors

1. What is the inhalation intake fraction respectively for 1 and 10 kg TCE emitted to urban air per day?
2. Who is taking this intake fraction in?
3. Why are these iFs higher for urban air than for continental or global air?
4. What does the first row (air) in the iF matrix distinguish from the other rows?
5. Why are there so many zeros in the Human exposure factors (XP) matrix?

USEtox exercise: Usage – Fate factors

1. What is the Fate factor for TCE in water for an emission to air?
2. What is the overall residence time of TCE in air?
3. Why does the k-matrix contain so many zero values?

USEtox exercise: Usage/Interpretation – Multiple-substance calculation

1. Run USEtox for TCE and the ten following chemicals in the database. The results can be found in the worksheet “Results” in the same rows where the chemicals are located in the “Substance data” worksheet.
2. Rank those chemicals in terms of their characterisation factor for total human health effects for an emission to air and to water respectively.
   1. Why is the ranking somewhat different for both scenarios?
   2. Why are there so many ”n/a” values in the columns with either the cancer or non-cancer characterisation factors?
   3. Name five factors that will determine where a chemical ends up in such a ranking/comparison and categorise each whether it represents a fate, exposure or toxicity related process.

USEtox exercise: Interpretation – Exposure factors

1. Intake fraction matrix:
   - How do you interpret the factors within the same column? What information do they provide?
   - Does it make sense to sum up within the same row? What would the result mean?
2. Exposure matrix:
   - How do you interpret the exposure factors within the same column?
   - Interpret the physical meaning of the exposure factor for drinking water – fresh water and meat – air.
   - Can you sum over all exposure factors within the same row of the exposure matrix? How would you interpret it?

USEtox exercise: Interpretation – Fate factors

1. What is the meaning of non-diagonal and non-zero elements in the k-matrix?
2. Pick three non-diagonal elements of the fate matrix and explain the processes they represent. Does any non-diagonal element represent a realistic process? How can you tell?
3. What are the dominant removal pathways of TCE in air?
4. What fraction is removed by degradation?
5. How to interpret the $FF_{w,a}$
   - in term of residence time Θ_w and transfer fraction $F_{a,w}$?
   - Which is the dominant pathway (air-water vs. air-soil-water)?