



USEtox updates – Quality assurance, transparency, and peer review process

The USEtox team intends to regularly publish updated versions of the software as well as updates to model inputs and output as often as necessary, attempting at the same time to minimize changes. In practice, updates that do not affect existing and published characterization factors (CFs) can be done anytime. Updates affecting existing/published CFs are planned every three to five years, but in case of important (error/modeling) corrections, this interval might occasionally be shorter. To address these issues, the USEtox team has adopted an updating procedure that aims to provide an optimal mix of transparency, stability and scientific quality of the model and the characterization factors calculated. This document identifies and illustrates the process for assuring the quality, transparency, and credibility of the USEtox model, its input data, and its results.

Update procedure:

The USEtox team distinguishes three kinds of model updates, each with its own updating protocol

1. Corrective updates (of models and data)

Corrections affecting existing characterization factors that are found to be potentially erroneous, e.g. corrections to algorithms, or substance parameters with errors. We expect these types of corrections will be made once per year. Suggestions for corrections may arise via use of the software in specific research activities and may find their ways to the USEtox team directly (person-to-person), via the USEtox help desk or via other channels to be opened in the future. Generally, proposals for correction will be discussed, decided on, carried out and published by the USEtox team without consultation of external experts.

2. Updates based on data, scientific and technical progress

a. substance specific data (affecting one or very few CFs)

i) Updates affecting existing characterization factors, e.g. alternative (improved) data, especially updates promoting existing “interim” CFs to “recommended”. Such progress-based updates affecting existing/published CFs will be made at the maximum once a year.

ii) Updates adding new characterization factors while not affecting existing ones, e.g. extension of substance coverage, adding or changing uncertainty information. Progress-based updates NOT affecting existing/published CFs can be made anytime.

b. model structure, parameters and algorithms (affecting many CFs)

i) Updates affecting existing characterization factors, e.g. alternative (improved) algorithms; additional mechanisms; changing of landscape or exposure parameters of previously published scenarios, and updates promoting existing “interim” CFs to “recommended”. Progress-based updates affecting existing/published CFs will be made at the maximum once a year.

ii) Updates adding new characterization factors while not affecting existing ones, e.g. extension of substance coverage, adding new impact pathways (e.g. indoor, dermal), adding or changing uncertainty information, adding spatial differentiation/variability or regionalized parameterization for previously unpublished scenarios. Progress-based updates NOT affecting existing/published CFs can be made anytime.

Documented suggestions for progress-based updating, made by any party, will be considered by the USEtox team. When judged worthwhile, the USEtox team will ask the review chair of the UNEP/SETAC life cycle initiative to invite at least two external experts to review the proposal and advise on possible implementation. The USEtox team can suggest potential reviewers. The external experts should be knowledgeable of the specific elements to be updated (substance classes, modeling, regions, etc.) and at least one should be familiar with the USEtox model, its purpose, and its underlying principles or with toxicity assessment in LCA. The external experts will carry out a peer review of the submitted/proposed updates with respect to the following criteria (defined by the USEtox team and based on the USEtox development criteria in Rosenbaum et al., 2008):

- Scientific quality/viability (Is the method/data published in peer-reviewed literature?)
- Level of parsimony (What is the added complexity and is it justified?)
- Level of evaluation
- Level of transparency (documentation)
- Level of scientific acceptance/consensus in the community (Is the method/data already used in published methods?)
- Level of consistency with the data selection hierarchy (for previously published CFs and databases) as published in the official USEtox papers in IJLCA.
- Feasibility/influence in application (Is this possible to consider in practice?)
- Meaningfulness/added value (Is this meaningful to consider in practice? What is the improvement from a practical point of view? Does it entail an additional effort and is it worth it?)

An external review panel can also take on the form of a workshop, organized by the USEtox team.

The USEtox team will consider the recommendations made by the review panel and decide whether and how to implement the proposed changes. If the USEtox team decides not to implement a proposal that was recommended for implementation by the review panel, the reasoning shall be published (e.g. on the USEtox website).

In all cases, the USEtox team shall document the entire updating process, from update suggestions, acceptance/rejection decisions, review reports, decisions on implementation, implementation actions, to eventual updated model and input/output, making all documents publicly accessible through the USEtox website.

Annex: Background and motivation

Model performance testing and evaluation

Models such as USEtox accrue credibility through ongoing model performance testing and evaluation. There is testing of both model algorithms and overall model performance.

Our approach to model performance testing and evaluation includes both model specific evaluations that test the overall soundness of USEtox as well as scenario specific evaluations that need to be performed on a case-by-case basis to explore the relevance or usefulness of the model for chemical class or decision questions.

Model algorithm auditing

All USEtox model algorithms are tested first using hand calculations and simple spreadsheet calculations to ensure that the mathematical model works as intended. We next conduct and audit the model by having at least one other group/individual independently test the same algorithm on another computer system. The two tests are compared against each other and all differences are resolved before the algorithm is determined to be acceptable for USEtox.

To further assure the reliability of the algorithms, the documentation for the algorithm and the spreadsheet are submitted for publication in peer-reviewed journals. This adds a second layer of audit and quality assurance.

Model performance evaluation

Model performance evaluation is an ongoing, iterative process that is expected to continue for the life of USEtox. Among the key elements of this process are publications on the basic model evaluation framework and on specific details related to identifying and reducing various types of uncertainty. Another key element is continued participation in model evaluation workshops as well as inter-agency and multinational model evaluation exercises.

A first approach for model performance evaluation is benchmark testing with similar models developed independently by other investigators. The USEtox model was developed as a result of a multi-year exercise to build a consensus model from a range of existing and well-vetted life-cycle impact models. Its performance has been tested against and among all of these models.

Sensitivity and uncertainty analysis are fully integrated into the model development, performance testing, and evaluation process. We anticipate that this framework will lead to a reduced but informative set of model relationships. Sensitivity and uncertainty analyses are powerful tools for assessing the performance and reliability of models.

As the USEtox model evolves and addresses a broader range of chemical substances, this type of rigorous model performance evaluation will continue.

Peer review

The USEtox peer-review process began early in the model development process. The peer review process involves SETAC, UNEP, the academic community, scientists from private sector for-profit entities, and scientists from non-government non-profit research organizations. The peer review is based on information exchanges with and contributions from professional societies, government entities, industry groups, and NGOs.

Peer review of the conceptual model

Conceptual model evaluation was initiated in the early stages of model development. During the process of framing the problem and designing the conceptual model, the appropriate level of modeling complexity (e.g., what to include and what to exclude), the availability and quality of information needed to run the model (i.e., input data), and the theoretical basis for the model were evaluated. A literature review was used to identify and evaluate the state-of-the-science for processes to be included in the model, as well as to compile and document the initial set of values that will be used as model inputs.

Peer review of model performance

Confidence is further enhanced if the user can easily inspect or verify the operation of the algorithms and data transformations and determine whether the model is internally consistent and contains no logical flaws or technical errors, such as incorrect code implementation. Easy access to the raw data used as inputs, transformed data and the steps of data transformations used in the calculation, and the computer coded algorithms underlying these data transformations will thus enhance user confidence in the model. The availability of clear documentation for model structure, and the possibility of performing calibration against an external standard (test data sets) or an internal standard (parallel algorithms to perform the same calculation) all increase user confidence in a model.

Peer review of model outcomes

The USEtox team maintains an ongoing effort to evaluate model outcomes using both internal evaluation exercises and peer review publication.

Quality assurance and vetting of model inputs

USEtox does not have its own process for data development. All data used for this effort are obtained from existing databases and the peer review literature.

The USEtox team reviews all data for consistency and reliability before entering these data as USEtox inputs. Inputs to USEtox include basic chemical properties data, landscape/climate data, exposure factors, human toxicity, and ecotoxicity data. The data used for these inputs have been reviewed and assessed in the peer review literature, reviewed and assessed by credible entity such as the US EPA, or reviewed for use by the USEtox team with adequate vetting or publication.

Availability of training for model users

The USEtox model is documented with a guide that outlines the theory, shows the mathematical algorithms, identifies data inputs and calibration/validation data used, and includes a sensitivity and uncertainty analysis.

The USEtox team has developed USEtox training courses and makes these available one or more times a year at major international conferences. Team members are also available to respond to specific invitations from governments, professional societies, and industrial organizations.