USEtox vision 2025-2035

Peter Fantke | 4-Dec-2024

-- BACKGROUND & STATUS --

USEtox is a well-established and operational modelling tool to characterize human toxicity and ecotoxicity impacts in life cycle assessment (LCA). USEtox has been developed based on a series of model comparisons by an international team of experts between 2002 and 2008, under the auspices of the Life Cycle Initiative hosted at the United Nations Environment Programme (UNEP). USEtox is formally endorsed by the Life Cycle Initiative since 2015, has been developed as a scientific consensus model based on a broad model comparison, is applied by a wide range of academic, public and private stakeholders – mostly in the context of using its characterization factors implemented in various life cycle impact assessment (LCIA) methods.

USEtox originally characterizes toxicity and ecotoxicity impacts from chemicals emitted primarily into the outdoor environment along product and service life cycles. Since its major releases in 2008 (version 1) and 2015 (version 2), USEtox has been continuously advanced and expanded, for example in terms of covered pathways, chemicals, and application contexts. From its current beta release version 3, USEtox shows great potential to become a global reference model for assessing human toxicity and ecotoxicity impacts in a wider range of decision-making frameworks beyond LCA.

-- VISION --

USEtox is a widely applied, easy-to-use, life cycle oriented, and reliable, global reference model for quantitative, comparative assessments of human health and biodiversity impacts from releases of and exposure to chemicals and related stressors across decision support tools concerning environmental sustainability.

-- STRATEGY --

To achieve the stated vision 2025-2035 for USEtox, the following strategic elements are defined:

1. ***Application areas:*** Broaden the use of USEtox toward a wider set of relevant decision support contexts and application areas, by:
   - *Decision support contexts:* Identify decision support tools and application areas (including and particularly beyond LCA) potentially relevant for USEtox (e.g. chemical substitution, chemical alternatives assessment, safe and sustainable-by-design (SSbD), exposure and risk screening, risk prioritization based on cumulative assessments, chemical footprinting, absolute environmental sustainability assessment (AESA), ecosystem services modelling, cost-benefit analysis, exposome), and (internally) relate to respectively available tools
   - *Requirements:* Define requirements and elements to make USEtox fit-for-purpose for each context (based on context/application area-specific boundary conditions and workflows)
   - *Regulatory/policy relevance:* Increase the relevance of USEtox for application in regulatory applications (e.g. chemicals regulation, identification of substances of regulatory concern, chemical substitution, reporting of company sustainability metrics according to company reporting obligations under the CSRD, assessment of co-benefits for environmental certificates incl. carbon, biodiversity, and ecosystem services)

2. ***Scientific advancements:*** Define and publish in peer-reviewed ISI journals relevant scientific advancements for USEtox and build synergies with adjacent scientific fields, including:
   - *Damage modelling:* Define relevant metrics and develop damage modelling pathways for human health and especially biodiversity
   - *Ecotoxicity indicators:* Develop indicators for relevant ecosystems, such as terrestrial soil ecosystems, pollinating insects, groundwater ecosystems, sediment-dwelling organisms, marine aquatic ecosystems, and their relevant processes and characteristics
   - *Spatialization:* Expand USEtox toward spatial impact assessment based on reprogramming and aligning Pangea with processes and characteristics implemented in USEtox
   - *Absolute sustainability:* Adapt USEtox for absolute environmental sustainability assessment (AESA), e.g. for boundary setting and impact assessment from local to global scale
   - *In-silico predictions:* Develop machine learning methods to predict substance property data (e.g. environmental degradation half-lives, bioaccumulation factors, ecotoxicity effects)
   - *Uncertainty:* Include quantitative, substance- and parameter-specific uncertainty factors, and make uncertainty transparent, incl. comparison with other approaches (e.g. qualitative)
   - *Substance coverage:* Extend the number of organic chemicals contained in the USEtox chemical input database while applying relevant data curation and quality criteria; globally relevant/acceptable data sources should be prioritised as much as possible over regional priorities in order to maintain global acceptability of USEtox model, results and databases
   - *Other stressors:* Expand the modelling framework to consider stressors other than organic chemicals to which Kow-based partitioning applies and metal ions (e.g. PFAS, inorganic substances, polymers including micro- and nano-plastics, engineered nanomaterials, complex mixtures, bio-pesticides)
3. ***User community:*** Establish a broad user community of practice around USEtox, mainly via:
   - *UNEP interaction:* Strengthen the continuous interaction between the USEtox Team and different UNEP branches ('Life Cycle Initiative' Secretariat, 'Global Framework on Chemicals' (GFC) Secretariat), e.g. by contributing to relevant standardization discussions
   - *Collaboration:* Actively engage in and establish new (e.g. with FAO, OECD) collaborations with national and international institutions, leading academics, authorities and companies to ensure that USEtox continuously integrates relevant scientific expertise, influences the international developments within various relevant decision support contexts, and that the USEtox Team is aware and inspired by the developments among its peers
   - *Education & training capacity:* Foster capacity building by developing regional, national and international education and training elements for USEtox for various decision contexts
4. ***Funding mechanisms:*** Ensure that USEtox is relevant and able to attract funding for scientific advancements, training, as well as wide application and implementation by stakeholders, by:
   - *Visibility:* Strengthen the visibility and relevance of USEtox toward a variety of national and international public and private funding organizations
   - *Network:* Develop and maintain a strong international user network around USEtox
   - *Funding sources:* Systematically identify and exploit national and international funding sources and opportunities to promote, advance and apply USEtox
5. ***Operationalization & application:*** Establish a mechanism to ensure the operationalization of USEtox, including its scientific foundation and advancements, and the broad application of USEtox across various decision contexts and institutions worldwide, by:
   - *Organization of USEtox Team:* Explore the possibility to organize the USEtox Team as a formal legal entity (e.g. non-profit organization) to strengthen interaction with UNEP and foster

collaboration that focuses mainly on training and application of USEtox (e.g. by companies, industry associations or international organizations)

- *Relation to USEtox Int. Centre:* Formalize the relation between the broader 'USEtox Team' and the 'USEtox Int. Centre' hosted at DTU, to clarify mandates for establishing projects, formally allowing to expand the USEtox Team, re-establishing the role of Peter Fantke as 'USEtox Team Director' vs. assigning a formal 'DTU Centre Manager', and clarifying aspects around owning USEtox trademarks, domain names, etc.
- *Web-tool:* Develop a user-friendly, semi-automated USEtox web-tool (USEtox^{WEB}), including a spatialized version of USEtox (USEtox^{GEO}), to broaden its application by a wide range of stakeholders with varying levels of expertise; for example focusing on cloud-computing services (e.g. AWS, Google Cloud, Microsoft Azure) and related data platforms (e.g. Snowflake, Oracle)
- *Update mechanisms:* Formalize a clear, transparent and semi-automated USEtox model and data update mechanism that allows to strike a balance between continuous scientific advancements and maintaining a scientific consensus character of USEtox, including a complete technical model and data documentation (could get a DOI), and different levels of user manuals—all stored e.g. in Zenodo
- *Implementation roadmap:* Define a roadmap for the operationalization and application of USEtox by its stakeholders in relevant decision support contexts, including automated format generation for implementing USEtox results into LCA software, clarification of integrating USEtox into SSbD workflows, and guidance on intersecting USEtox model and data with existing frameworks at companies and authorities (e.g. via the PARC partnership)

-- TIMELINE --

To ensure an effective implementation of the USEtox strategy until 2035, an implementation timeline is established for the strategy elements, differentiating elements that are primarily executed by the USEtox Team (i.e. coordinated by a 'USEtox Director') from elements that are mainly executed by individual USEtox Team members (e.g. multi-partner projects involving a specific USEtox Team member). Continuous strategy elements are not further detailed below.

Strategy elements	Years 2024-2035											
	24	25	26	27	28	29	30	31	32	33	34	35
Define applications & related requirements												
Increase regulatory relevance of USEtox												
Scientific advancements via projects*I**												
Increase interaction with UNEP*												
Strengthen stakeholder collaboration*												
Set up collaboration with FAO/OECD												
Capacity building via training/application*												
Identify new funding sources/options												
Clarify relation to USEtox Int. Centre***												
Develop user-friendly web tool												
Formalize model update mechanism												
Develop implementation roadmap												

Colour key: USEtox Team (mainly via 'USEtox Team Director')
Mainly via individual USEtox Team members

*Continuous strategy elements that appear in the timeline only listed as summary items but are effectively more detailed (i.e. implementing individual scientific advancements via projects, different activities to increase interaction between USEtox and UNEP, setting up various collaborations with individual public and private stakeholders, and establishing different capacity building efforts worldwide, including training application and implementation efforts).

**Scientific advancements via projects refers to different types of project setups with varying timelines, and includes aspects around damage modelling, ecotoxicity indicators, spatialization, absolute sustainability, in-silico predictions, and other stressors than currently considered in USEtox. Definition of USEtox-relevant projects and related timelines depends on USEtox Team members' research interests and funding options. Results of such projects will undergo a formal USEtox Team approval process before taking up aspects into official USEtox consensus model.

***DTU leads the effort on clarifying the formal relationship between the broader USEtox Team and the DTU-affiliated USEtox Int. Centre, incl. assigning a formal Centre Manager.

-- RESOURCES & REQUIREMENTS --

To enable the implementation of the strategic elements in support of achieving the stated vision 2025-2035 for USEtox, specific resources are needed, and certain requirements need to be met.

1. ***Human resources:*** With the current setup of the USEtox Team, different human resource elements are required for a successful implementation of the stated strategy, including:
   - *'USEtox Team Director':* Executing various elements of the USEtox strategy require a formal representative of the USEtox Team (i.e. a 'USEtox Team Director') appointed by the broader USEtox Team, regardless of USEtox Int. Centre setup. Current USEtox Team Director is Peter Fantke.
   - *Research collaboration:* For the various research-based projects, a collaboration among different USEtox Team members might be needed. This can for example refer to industry-funded projects that are easier to implement via collaboration with specific USEtox Team members based on their institutional background (SME vs. university vs. public authority). This may be decided on a project-by-project basis, with strong focus on those projects that produce output that can be directly fed into the official USEtox model.
2. ***Other resources:*** Some of the strategy elements will require additional financial and/or technical resources that should be discussed with stakeholders (e.g. UNEP) for strategically advancing and applying USEtox. This should be discussed and agreed based on each effort or strategy element.
3. ***Requirements:*** To achieve the above-stated vision for USEtox, it is essential to establish a strategic alignment between the USEtox Int. Centre hosted at DTU, and the broader USEtox Team, with a defined role of a 'USEtox Team Director', a 'DTU Centre Manager' and affiliated individuals vs. institutions involved in USEtox.