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EDITORIAL: LCIA OF IMPACTS ON HUMAN HEALTH AND ECOSYSTEMS (USEtox)

A bright future for addressing chemical emissions in life cycle assessment

Michael Z. Hauschild · Olivier Jolliet · Mark A. J. Huijbregts

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1 USEtox—the UNEP–SETAC toxicity model

What you have in your hands or on your screen is a special issue of the *International Journal of Life Cycle Assessment* dedicated to the impact assessment of chemical emissions occurring along the life cycle of products and services. It counts in total 13 papers on human toxicity and ecotoxicity impacts in life cycle assessment (LCA) and, in particular, on the recently developed international consensus model USEtox. The model was officially launched in May 2010 and has since then been downloaded and applied by users in multiple settings. Since its release, USEtox has been disseminated through the official web page (www.usetox.org), training courses (also accessible as video-streaming—see home page) and incorporation into the major LCA software tools. Its use is encouraged by the United Nations Environment Programme–Society for Environmental Toxicology and Chemistry (UNEP–SETAC) Life Cycle Initiative, and it is under consideration for recommendation as part of the European Commission's ILCD system. A full issue of the journal is dedicated to the further documentation of the model and discussions of experience with its use. Here, we summarize the challenges of assessing chemical impacts in LCA, as identified by the papers in this special issue.

Depending on the properties of a chemical, its toxic impacts on human beings and natural organisms and ecosystems can occur through many different mechanisms, e.g. carcinogenicity, neurotoxicity, or endocrine disruption. An emission inventory for a product system easily contains hundreds of substances, and many of these will have the potential to cause toxic impacts depending on the fate and exposure that can follow very diverse routes. Overall, the number of chemicals that are applied in products totals well above 10,000. In principle, all of these may occur as an emission in a life cycle inventory, and they should therefore be covered in the life cycle impact assessment. The coverage with human or ecotoxicity characterization factors of the emission flows in the inventory thus represents a grand challenge. The challenge is further increased by the absence of measurements of key substance properties like toxicity and biodegradability for the majority of all these chemicals.

A number of different models for characterization of toxic impacts from chemical emissions have been developed over the last 15 years with differences in scope, modelling principles, and in the characterization factors they provide. The number of substances for which the models provide characterization factors is typically 100–500 substances. This unsatisfactory situation was the background on which a Task Force on Toxic Impacts under the UNEP–SETAC Life Cycle Initiative launched a comparison and harmonization of existing characterization models. The comparison formed the basis of a scientific consensus process that eventually led to the development of

M. Z. Hauschild
DTU Management Engineering,
Technical University of Denmark,
Produktionstorvet, Building 424,
2800 Lyngby, Denmark

O. Jolliet
Department of Environmental Health Sciences,
School of Public Health, University of Michigan,
Ann Arbor, MI, USA

M. A. J. Huijbregts (✉)
Department of Environmental Science, Institute for Water
and Wetland Research, Radboud University Nijmegen,
P.O. Box 9010, 6500 GL Nijmegen, The Netherlands
e-mail: m.huijbregts@science.ru.nl

the USEtox model. The USEtox model is an environmental model for characterisation of human and ecotoxicological impacts in Life Cycle Impact Assessment (LCIA). It has been developed by a team of researchers from the Task Force on Toxic Impacts under the UNEP–SETAC Life Cycle Initiative. USEtox is designed to describe the fate, exposure and effects of chemicals. The USEtox model and the process behind its development were previously described by Rosenbaum et al. (2008) and Hauschild et al. (2008). Following a year of testing, it was released spring 2010 together with characterisation factors covering several thousand substances. In this issue, Henderson et al. (2011) indicated that for an emission directly to water, the effect factor strongly controls freshwater ecotoxicity, with a range of up to ten orders of magnitude for the chemicals in the dataset of USEtox. However, for an emission to air or soil, differences in chemical properties may influence characterisation factors for freshwater ecotoxicity by up to ten orders of magnitude, as a result of intermedia transfer and degradation. Rosenbaum et al. (2011) showed for human exposure that for most chemicals in the dataset of USEtox, inhalation and intake of above-ground agricultural produce and fish are the important exposure pathways. The analysis of carcinogenic potency (TD50) when volatile chemicals are administrated by both inhalation and an oral route suggested that results by one route can reasonably be used to represent another route. This paper also proposed extrapolation factors for acute-to-chronic toxic effects to further expand the number of chemicals covered by USEtox. One possible step to further increase the chemical coverage in USEtox was suggested by Birkved and Heijungs (2011) in this issue via Partial Least Squares Regression. The applied statistical approach illustrates that it is possible to derive meta-models from full fate and exposure models with limited data demand.

The USEtox characterisation factors are classified as recommended or interim according to how appropriate the model is and/or how reliable the data are for the substance in question. As an example, dissociating substances have their characterisation factors classified as interim because the dissociation is not appropriately represented in the current version of USEtox. Even though interim factors have this preliminary status, they are still seen as better than not applying any characterisation factor (equivalent to assuming that the factor is zero). Therefore, their use is encouraged, but caution should be taken in the interpretation if very large contributions to human toxicity or ecotoxicity come from emissions for which the characterisation factors are interim. In this context, Askham (2011) found that the toxicity comparison between two competing powder coating solutions with USEtox was indeed highly sensitive to the inclusion of interim characterisation factors.

2 Chemical ranking

LCA is often used for comparisons; it is therefore important to avoid biases and ensure that the impact assessment gets the relative impacts and ranking between substances right. Mattila et al. (2011) compared three recent LCIA models (IMPACT 2002+, ReCiPe and USEtox) in prioritizing substances and products from national emission inventories. The aim was to test model output against expert judgement on chemical risk assessment. It was found that the studied models differed from expert assessment mostly for substances that are bioaccumulative. Saouter et al. (2011) compared USEtox impact scores with critical dilution volume (CDV) scores from the European Ecolabel. Chemicals listed in both the USEtox database and the EU Ecolabel detergent ingredient database (DID list) were used for the comparison. Overall, fair agreement was found between the two models; both highlighted the same five high-concern chemicals. The reasons of the presence of outliers lay in the selection of the physical–chemical, fate and ecotoxicity data within the two models. Van Hoof et al. (2011) also presented the results of a comparison of USEtox and CDV approaches, focusing on laundry products. The two methods showed a lack of agreement in the laundry product comparison, which is somewhat in contrast to the findings of Saouter et al. (2011). Although the CDV method covers most laundry ingredients, a potential drawback is that it lacks a comprehensive environmental fate component in the modelling procedure. Berthoud et al. (2011) conducted an LCA on winter wheat, including ecotoxicity. The USEtox model helped identify the most relevant active ingredients in terms of ecotoxicity and showed that the average impact could be decreased 50% by substituting only three active ingredients. Laurent et al. (2011) developed normalisation factors for Europe and North America to be applied together with the USEtox characterisation factors in support of the integration of USEtox into LCIA methods that cover a broader range of environmental impact categories. Only a limited number of metals and pesticide emissions ($n<10$) were shown to have high contribution to the overall normalization references.

3 Spatial differentiation

With its life cycle focus, LCA is not naturally geared for spatially differentiated assessments, and historically, LCIA has been site generic. Over the last decade, it has become clear that for some impacts, differences in geographical conditions and spatial emission characteristics can be quite influential, and this is now an important field of new research in LCIA. Sala et al. (2011) developed guidelines to help decide the appropriate spatial resolution to address the environmental fate of chemicals and compared the results of a highly spatially differentiated model with USEtox for air removal rates. The study demonstrates the potential relevance of considering spatial variability in chemical fate and supports further development of spatial scenarios and archetypes. Querini et al. (2011) tested USEtox on three energy pathways: gasoline, diesel fuel and hard coal electricity. The emissions studied are mainly volatile organic compounds and heavy metals. For human health impacts from organic chemicals, they observed a clear difference between urban and rural emissions. The distinction in USEtox between rural and urban emissions supports a more relevant assessment of internal combustion engine cars compared with electric and hybrid cars, which is especially useful for the automotive industry.

4 Difficult chemicals

Characterisation models for human and ecotoxic impacts are typically developed for non-ionising organic chemicals of a certain hydrophobicity, but in life cycle inventories, there are many emissions of both inorganic and organic compounds that do not belong to this group. Notably, the metals have been challenging in the characterisation modelling of chemical emissions. Since the Apeldoorn workshop in 2004, there has been agreement that the metal compounds are not well modelled by any of the existing models, and work is going on to develop the characterisation models so they are able to represent the most influential fate, exposure and effect characteristics of metals in the environment. An expert workshop on characterisation modelling of metal freshwater ecotoxicity in 2009 resulted in the Clearwater Declaration with recommendations to this work (Diamond et al. 2010). Results that make these recommendations operational are presented in the papers by Gandhi et al. (2011) and Christiansen et al. (2011) in this special issue, focusing on the speciation behaviour of selected metals and its consideration in the modelling of freshwater ecotoxicity. Gandhi et al. (2011) compared and assessed the consequences of using a new life cycle impact assessment method for metals that includes the influence of ambient chemistry on metal speciation versus currently available LCIA models for calculating freshwater ecotoxicity. The production of a copper pipe and a zinc gutter system was used for the comparison. They compared the LCIA outcomes for freshwater ecotoxicity of these case studies using four models: USES-LCA 1.0, USES-LCA 2.0, USEtox and the new method incorporated in USEtox. Significant differences in characterisation factors, overall freshwater ecotoxicity score and the ranking of metals were traced back to differences in modelling methods, the choice of metal partition coefficients and the calculation of effect factors. Christiansen et al. (2011) also emphasized that speciation should be taken into account in the modelling of the effect factor for copper in the aquatic environment and demonstrated how large differences in reported toxicity values for copper can be traced back to different speciation patterns due to variation in test media composition. Similar work is needed for other metals and for metal ecotoxicity in other compartments, and also for the characterisation modelling of human toxicity of metals. The focus on the speciation behaviour of metals has also highlighted the need for better specification in the life cycle inventory of the form in which metals are emitted from the product system. Without an appropriate link to the inventory, the impact assessment is bound to do a poor job. Organic substances do not speciate in the same way as metals, but dissociating organics do appear in more than one form, and this behaviour is also here potentially influential for the fate and exposure behaviour and needs to be taken into account in the characterisation modelling. The next version of USEtox is foreseen to address both metal compounds and dissociating organic compounds in accordance with the Clearwater Declaration and recent developments in the modelling of the environmental fate of dissociating organic chemicals.

5 An operational method with a bright future

One of the strengths of characterisation modelling is the focus on getting the relative importance between substances right. In combination with the life cycle perspective applied in LCA, this has led to the development of carbon footprint (life cycle climate change impact of a product) that is, for instance, communicated for ecolabelling purposes. In order not to forget the chemical impacts that a product may have, a "chemical footprint" or "toxicity footprint" has been discussed. In the development of such a metric, it seems obvious to build it on a consensus-driven model, such as USEtox, and base the calculation of the toxicity footprints on the USEtox characterisation factors. With the focus on "mainstreaming" of LCA in the third phase of the UNEP–SETAC Life Cycle Initiative and in the work of The Sustainability Consortium on dissemination of LCA in product chains from multiple fields of consumption, it is important that the toxic impact assessment is included and LCA is not reduced to being primarily an energy and resource analysis. We consider that USEtox represents an important step forward for the inclusion of impacts from chemical emissions in LCA, being a consensus model built on a good understanding of the central elements of the characterisation modelling and providing a substance coverage that is much broader than what has been offered earlier. In the last two decades, the process of comparative toxicity assessment has advanced very significantly. USEtox is also tested and applied outside the LCA field for chemical screening and has now acquired a sufficient maturity to be systematically used in LCA when properly interpreted. We, however, also acknowledge that there is still a way to go in further understanding and reducing sources of uncertainty and error. The number of ongoing activities in the field of toxic impact assessment in LCA is high, and ongoing efforts aim to include other product relevant impact pathways in USEtox, such as indoor emissions and direct consumer exposure. A number of the activities that involve the USEtox model are documented in this special issue. Their quality and variety give us good hope for the future development of USEtox and more broadly for the assessment of chemical impacts in LCA within the coming decade.

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