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Building a model based on scientific consensus for Life Cycle Impact Assessment of Chemicals: the Search for Harmony and Parsimony

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"Perfection is achieved, not when there is nothing more to add, but when there is nothing left to take away"

- Antoine de Saint-Exupéry

Achieving consensus among scientists is often a challenge—particularly in model development. In this article we describe a recent scientific consensus-building process for Life Cycle Impact Assessment (LCIA) models applied to chemical emissions—including the strategy, execution, and results of a process that used model comparison to achieve parsimony. This process has succeeded in establishing a transparent LCIA consensus model. We present the lessons that may be adapted by similar consensus processes in other fields.

LCIA characterizes potential impacts on human health and the environment attributable to chemical emissions over the life cycle of a product. LCIA relies on substance-specific characterization factors (CFs) that combine exposure potential and toxicity to represent the relative contribution of the substance to health and environmental impacts *(1)*. LCIA focuses on comparative assessment, using approaches adapted from risk assessment. In 2003, in response to large variations in available methods, an international model comparison/consensus process was initiated. This process was under the umbrella of the Life Cycle Initiative, a joint effort of the United Nations Environment Program (UNEP) and the Society of Environmental Toxicology and Chemistry (SETAC) *(2)*. The process encompassed an international group of model developers responsible for the most commonly-used worldwide LCIA characterization models and focused on characterization of human and ecosystem health impacts. It also involved disciplinary experts in fate and transport, exposure assessment, health risk assessment, and ecotoxicology.

The comparison/consensus process fostered a common understanding among the participants of which model elements contribute most to the relative magnitude of LCIA characterization factors. It became clear that with a careful focus on the most influential model elements a consensus model could be established. Experience dictated that a more transparent model would be more likely to gain and retain acceptance and wide-spread use. The need for consistent documentation and transparency led the participants to create an entirely new model, building on contributions from the existing models. This required consensus on essential model elements, provided robust results consistent with existing models, and made parsimony a guiding principle. The tangible outcome is "USEtox", named in recognition of the UNEP-SETAC Life Cycle Initiative under which it was developed. The model is supported by all participating model teams as a basis for future global recommendations of LCIA characterization factors.

Historical Context

The Life Cycle Initiative was launched jointly by UNEP and SETAC in April 2002 with its goal to "develop and disseminate practical tools for evaluating the opportunities, risks, and trade-offs associated with products and services over their entire life cycle to achieve sustainable development". One aim of the initiative was to identify recommended practice for conducting life cycle assessment (LCA) within the framework spelled out by the ISO standards *(3,4)*, and to make the data and methodology for performing LCA available and applicable worldwide. For LCIA this required recommendations of specific models and characterization factors for the different categories of environmental impact, based on a global consensus among experts, focusing on the scientific validity of the methods, and their relevance and feasibility in LCIA *(2)*. Such a recommendation from UNEP-SETAC potentially meets the requirement of the ISO standard for LCIA that "…the impact categories, category indicators and characterization models should be internationally accepted, i.e. based on an international agreement or approved by a competent international body" *(4)*. The Task Force on Toxic Impacts (TFTI) was established in 2003 under the LCIA component of the Life Cycle Initiative as one of several task forces addressing the different categories of environmental impacts normally included in an LCA.

Earlier comparative studies revealed that chemical emissions models used in LCIA vary substantially in their scope, modeling principles, and, most importantly, in terms of the characterization factors they produce *(5)*. Available models have produced published characterization factors for between 100 and 900 substances. For the LCA practitioner considering chemical-related impacts, this situation imposes important limitations. First, there may be substances in the life cycle inventory with no characterization factor available from any of the models and second, for some substances, there may be significantly different factors from several models. Faced with this situation, many LCA practitioners elected to exclude the chemical-related impacts from their LCIA, a simplification that de facto reduces the assessment to an energy impact assessment *(1)*. This unsatisfactory situation motivated the TFTI to define its objectives as:

1) Recommend practices for characterization modeling of ecotoxicity, human toxicity and related categories with direct effects on ecosystem and human health
2) Harmonize existing models
3) Recommend a characterization model or models and characterization factors for many substances
4) Provide guidance on the use of characterization factors

The Process and Methods

Prior to the Life Cycle Initiative, SETAC had sponsored harmonization efforts *(6,7,8)* that produced a framework for exposure and toxicity assessment (Figure 1). Our work group began with a survey and pre-selection of existing characterization models that were used within this framework. We then went on to develop criteria for an ideal model, procedures for comparing the pre-selected characterization models, and recommendations of key model elements. Finally, we developed and evaluated the consensus model that forms the basis for recommending characterization factors. A recent Organization for Economic Cooperation and Development (OECD) model comparison exercise that led to the creation of a consensus model for calculating overall persistence (Pov) and long-range transport potential (LRTP) of substances (*11*) was the precedent used for comparison of existing characterization models and defining consensus by creating a new model.

Our task force first recognized that it is not possible to compare models and develop a consensus model without first defining consensus metrics of impact. From a survey of existing characterization models for toxic impacts and a comparative review of available documentation, we elected to (a) combine fate and exposure estimates by using intake fraction *(9)* as our source-to-dose metric for humans, (b) define soil and water concentrations as the metric of ecosystem exposure and (c) use human and aquatic toxicity data to set benchmark doses and damage factors for both ecosystem and human populations. Lessons learned from previous SETAC LCA workgroups, and from the OMNITOX model development effort *(10)* provided the basis for these decisions.

Comparison and harmonization of existing characterization models

Our task force began by comparing fate, exposure and effect parameters and the resulting characterization factors for a variety of substances as calculated by a set of available models. The aim was to identify elements and characteristics of the models that had the strongest influence on the model results and use this knowledge to establish the key elements of an LCIA model. Representatives for ten models from Europe, North America, and Asia were invited to participate in the model comparison. Seven accepted the invitation to participate in the first model comparison workshop on 5-6 May 2006 in Bilthoven, The Netherlands where we compared the participating models to determine how the fate and characterization factors, model structure, and key sensitivities differed. In contrast to greater emphasis on the fate component in previous model comparisons (for example Fenner et al.*(11)*), our first comparison workshop focused on differences in results for exposure, human health impacts and ecotoxicological effects. Because they are capable of providing characterization factors for very large numbers of chemicals and for both human health and ecosystem endpoints and intermediate fate and exposure results, four models remained in the more detailed assessment process carried out over the next six months. Three of the models, CalTOX *(12)*, IMPACT 2002 *(13,14)*, and USES-LCA *(15)*, are integrated multimedia models that use fate modeling to estimate environmental concentrations combined with toxicological effect information. These three differ in spatial resolution and environmental compartments considered. The fourth model, EDIP97 *(16)*, employs fate and effect modeling based on selected key chemical and physical properties. These four models provided the basis for developing the consensus model.

To reduce differences attributable to input variations, all modelers used the same substance database, which covered 76 selected substances. We selected chemicals in this database to be representative of a larger group of chemicals with a similar combination of properties and to capture a range of substance properties for (bio)degradability, hydrophobicity, volatility and toxicity. In the first comparison round, characterization factors differed in some cases by many orders of magnitude. All outliers were thus important, and cases of large differences pointed to the need for further analysis of model differences. Another point of focus was differences in slopes of plots of characterization factors for two models. Parallel slopes typically represent scaling differences that can be removed by calibration of the models, but differences in slopes indicate more fundamental modeling differences.

The Bilthoven workshop led to recommendations for harmonization of the models where feasible by eliminating the sources of difference without fundamentally changing the model structure. The participants made these modifications and ran the models again for the 76 substances. Model results were again analyzed and compared in an iterative process at two subsequent model evaluation workshops--Paris in September 2006 and Montreal in November 2006--with further modifications in-between. These efforts produced harmonization of the characterization models in terms of parameter and algorithm choices with a significant reduction in the variation in characterization factors among the models. A detailed discussion of the technical findings of the model comparison can be found in Rosenbaum et al. *(17)*. The most important factors behind the differences in model performances are listed in Table 1 where we distinguish between factors related to choice of parameter value, which are easily harmonized, and choice of algorithm. Differences in algorithm choices were only removed if the modelers agreed that the change was scientifically defensible and that one algorithm choice could be agreed upon for the purpose of LCIA characterization modeling.

Development of the consensus model

Drawing on experiences from the OECD model comparison, we elected to establish "universally acceptable" modeling practice and then develop a consensus model as a joint effort, rather than merging together all reasonable elements of the participating models. This allowed the group to recognize value in different approaches and develop the consensus model through a systematic and parsimonious reduction in detail, accounting for important elements behind the differences in the models. Based on these general objectives, the group aimed for a consensus model that:

- provides results as strongly correlated to the results of other models their results are to each other;
- produces output that falls within the output range of the existing characterization models;
- is parsimonious in the sense that it contains only those model elements that the comparison of the existing characterization models identified as the most influential;
- provides a repository of knowledge through evaluation against a broad set of existing models;
- is endorsed by the modelers behind all participating models;
- is transparent and well documented.

A prototype of the consensus model was developed after the Bilthoven workshop, and checked against the other models at the two following model comparison workshops in Paris and Montreal. Through an iterative process, the model has been debugged, evaluated, modified, and improved based on the outcome of the model comparisons.

The consensus model is not yet complete and there are chemical classes and impacts yet to be addressed. For example, significant contributors to human health impacts come from toxic air pollutants including benzene and PAHs, pesticides, persistent pollutants, volatile solvents, aldehydes, and numerous other volatile and semi-volatile organic pollutants, as well as from particulate matter, ozone, mercury, carbon monoxide, and nitrogen oxides. We recognized early in the process that we were not in a position to come to consensus about assessing impacts of inorganic pollutants, and therefore we focused first on organics, but we have also developed interim factors for a large number of inorganic pollutants and have efforts underway to address both primary and secondary particulate matter. Similarly, we have not yet addressed the impacts on terrestrial ecosystems because (a) there is a lack of experimental data and dose-response factors linking exposure to terrestrial systems impacts for a majority of substances, and (b) presumably as a result of assumed equilibrium partitioning, there appears to be correlation between terrestrial and aquatic impacts with respect to chemical ranking.

Results: Model Harmonization and Comparison with the Consensus Model

The effort to harmonize existing characterization models by adjusting parameters resulted in remarkable reductions in the differences among the models. Characterization factors for human health impacts varied up to 9 orders of magnitude for some substances at the first workshop in Bilthoven and less than three orders of magnitude for all substances after the final workshop in Montreal. For aquatic ecotoxicity the harmonization lead to similar results. In spite of the remaining differences, the USEtox consensus model characterization factors still meet the goal of producing results within the range of the existing characterization models for human health impacts from air, water and soil emissions and for aquatic ecotoxic impacts from air, water and soil emissions *(17)*. But uncertainty remains and must be addressed.

Confronting rather than ignoring uncertainty is one of the foremost challenges in LCIA. The overall uncertainty in model output depends on the quantity, quality and relevance of input data; the reliability and relevance of algorithms used to fill data gaps or replicate known results; and the assumptions, scenarios, and decision options used in applying the assessment. We recognize that while the consensus model process cannot reduce uncertainty from lack of data and lack of knowledge, it can help define where and how different assumptions, scenarios and decision options give rise to differences in model output. This follows from the findings of a recent report from the US National Research Council on the use of models in decision making *(18)*. This report observes that a scenario assessment approach is particularly appropriate (compared to probabilistic and Bayesian methods) for showing how different models yield differing results and for reducing some key contributors to model uncertainty.

Compared to other impact categories in LCIA (such as global warming or eutrophication), 2-3 orders of magnitude variability among the characterization models for toxic human health and ecosystem impacts still presents a significant uncertainty, because none of the models can be identified as more correct than the others. The uncertainty created by the variation between the models should, however, be seen in the context of a variation of 10-12 orders of magnitude between the substances that were included in the model comparison. This variation is much larger than the uncertainty introduced by the choice of characterization model. Thus, the characterization factors are still able to discern between a majority of the substances and benchmark them according to their toxic impacts to humans or ecosystems.

The consensus model USEtox is currently (Spring 2008) under a scientific review commissioned by the UNEP-SETAC International Life Cycle Panel that will consider recommending its world-wide use in LCIA of chemical emissions. The recommendations will include a database of “recommended” and “interim” characterization factors including fate, exposure and effect parameters for human toxicity (more than 1000 Substances) and for ecotoxicity (more than 2500 substances) calculated using the USEtox model. Interim factors are provided when available data are insufficient to support a recommendation, but still judged to be better than no information, or when the model result is considered too uncertain to support a recommendation. This is currently the case for metals and metal compounds.

Getting Scientists to Agree: Success in Consensus Building

We believe that our experience can offer important insight for others working for consensus among scientists—particularly for model building. Below are some summary observations from the successful LCIA consensus process:

- It is crucial to minimize the obstructing influence of competition between scientists and create an open-minded atmosphere where participants are not territorial about their own work. Here, we found it useful to base the consensus building on a comparison of the models that had been developed by the participants. Thus, the first step was to analyze and learn in common what is important in characterization modeling, recognizing the value in the different approaches.
- The involvement of outside experts specialized in different disciplines was a key factor for reaching a final recommendation and represented a crucial input towards a credible model.
- It is useful to discuss and agree on common criteria for characterization models prior to the comparison and hence detached from the actual performance of the models. The survey of existing models and the development of criteria went on for an extended period prior to the model comparison workshops.
- The goal of creating something new rather than just recommending something already in existence avoids the contentious process of selecting the best among our own models. The quest for parsimony meant that we had the challenge of simplifying rather than discussing which among our own, more complex approaches, were preferable. Instead, we aimed at selecting appropriate model elements.
- The categories of human toxicity and ecotoxicity involve scientific fields that are mature for development of consensus, at least for organic chemicals.
- Rather than starting from scratch we built on the inspiration and experience from earlier projects with similar goals, most notably the OMNIITOX project and the OECD model comparison.

The Future of USEtox and LCIA

USEtox has now been applied using a large database with properties data for thousands of substances to produce recommended or interim human toxicity and ecotoxicity CFs. This database has been compiled from publicly available databases so quality of the CFs cannot exceed the quality of these available data. The origin of the data is clearly referenced, but beyond this no quality assurance has yet been performed. Our first goal for the next phase of the UNEP-SETAC Life Cycle Initiative is to evaluate and update our substance property databases. Other future activities for consensus model include:

- User-friendly programming of the consensus model
- Uncertainty analyses for the USEtox Characterization Factors
- Development of USEtox to better accommodate metals
- Development of USEtox to accommodate indoor emissions
- Full documentation of USEtox
- Inclusion of terrestrial and marine ecotoxicity as endpoints in USEtox
- Industry workshops on comparative assessment of chemicals and training courses in USEtox

Earlier, we identified two major problems confronted by LCIA--there are many substances in the life cycle inventory for which no CF is available, and CFs from different models may vary substantially. The USEtox consensus process has addressed both issues. LCIA practitioners desire characterization factors that are stable in time so that results support consistent decisions. A practical advantage of basing recommendations on a consensus model rather than on individual research models is that the recommendations are stable in the sense that they will not change until an update of the consensus model is undertaken by UNEP-SETAC. However, the research models will continue to develop, and when important new developments have been introduced and peer reviewed, USEtox can be updated based on another application of the model comparison process. This approach provides the desired stability while accommodating new knowledge and information.

Consensus applies to different groups--researchers, policy makers or practitioners who implement the result in their practical work. In our effort we focused on a process for scientific consensus. The next step is to work in consultation with UNEP, government agencies such as the US EPA and the European JRC, stakeholders, professional societies such as SETAC and other NGOs both to get their review and support for our research consensus and to support their needs with respect to consensus building for policy and implementation. This next step is underway.

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Table 1. Factors which were important for the different performance of the characterization models

MODEL COMPONENT	KEY FACTOR	PARAMETER VALUE (P) OR ALGORITHM CHOICE (A)
Fate	Advection as a loss mechanism in some models	**A**
	Inclusion of the intermittent character of rain	**A**
	Residence times of media, particularly marine water, differ greatly	**P**
	Different algorithms used for estimation of partition coefficients	**A**
	Modeling of soil compartment: (i) homogeneous versus vertically layered soil compartment and (ii) generic versus division between agricultural, industrial and natural soils	**A**
Human exposure	Urban air compartment nested within continental air compartment	**A**
	Difference in population density on the urban and rural scale	**P**
	Different algorithms used for estimation of biotransfer and bioconcentration factors (fish, meat, milk, vegetation)	**A**
Human toxic effects	Some models extrapolate between intake routes (inhalation, ingestion, dermal)	**A**
	Models use different effect indicators (TD50, ADI, TD10)	**P**
Ecosystem effects	Models use different effect indicators (PNEC, HC50)	**P**
	Ocean modeled as a sink only (no effects considered)	**A**
	Some models use acute ecotoxicity indicator	**P**

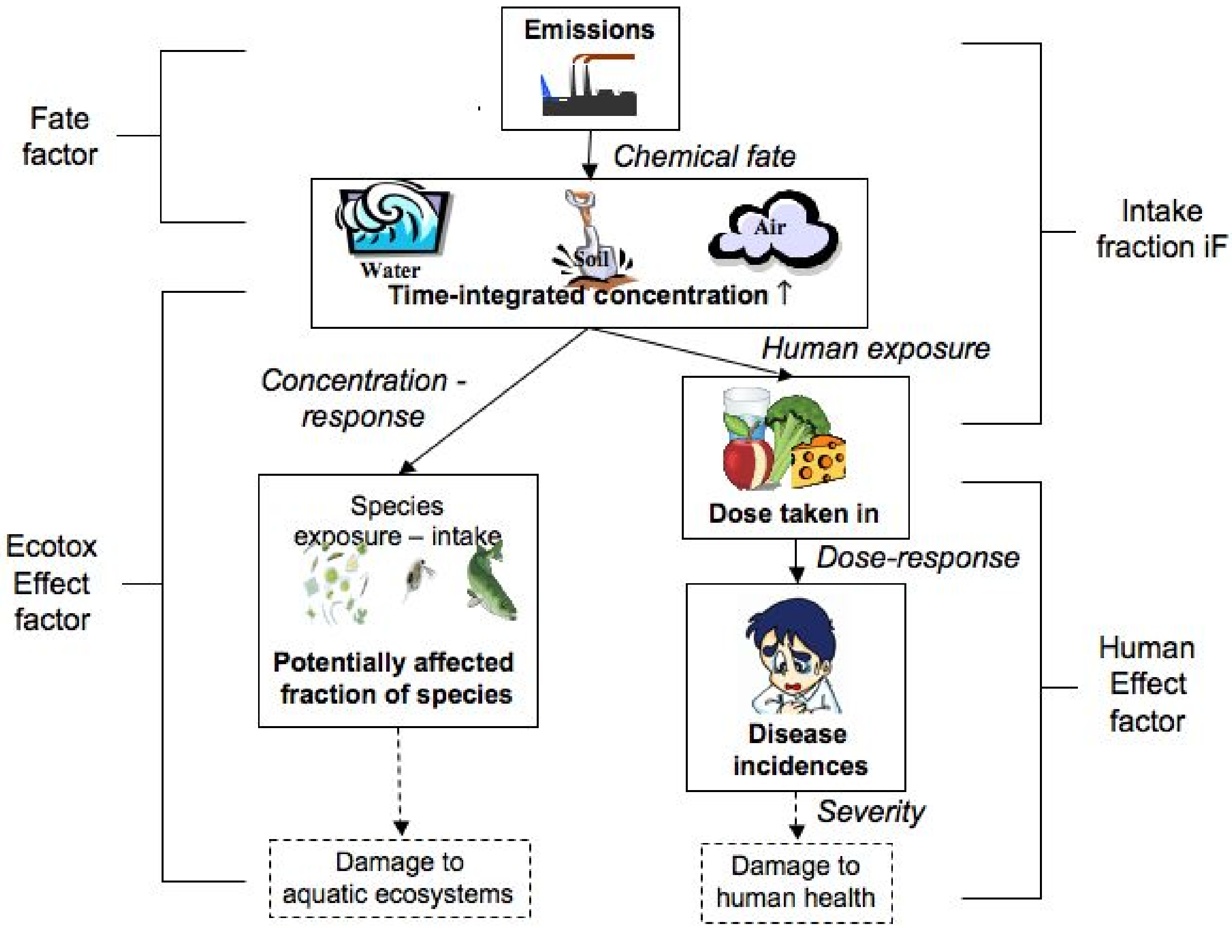

Figure 1. Framework for comparative toxicity assessment.