To model or not to model: applying the parsimony principle in fate and effect modelling of chemicals

Level:	Master
Start:	Anytime
Project form:	Data collection and modeling
Supervision:	Rosalie van Zelm

Background and short content of the project

Life cycle assessment (LCA) is a tool to assess the environmental impact of products and services, considering their entire life cycles. One part of this process is the life cycle impact assessment (LCIA), where inventory data are converted into impact indicators for various impact categories, such as human toxicity and ecotoxicity. When it comes to scientific merit, there are major uncertainties about the extent to which outcomes of LCAs reflect (changes in) real-life environmental impacts. Uncertain product or service comparisons, despite their complexity, could be preferable compared to avoiding any quantification. Depiction of uncertainties can be used to evaluate the probabilities and consequences of outcomes by acknowledging that they are uncertain. Knowledge on the magnitude of the uncertainty allows us to assess the robustness of decisions based on LCAs and to focus our resources in reducing uncertainty. In LCIA, simple models with a low number of parameters generally have relatively low parameter uncertainty and larger model structure uncertainty. For more complex models with a large number of parameters, the situation can be reversed. A major challenge lies in comparing and aggregating these two types of uncertainty to recommend the "optimal" model according to the parsimony principle: "as simple as possible, as complex as needed".

Van Zelm and Huijbregts (2013) showed how the trade-off between model structure and parameter uncertainty could be quantified (see Figure 1). For this, the specific case of freshwater ecotoxicity due to pesticide application in The Netherlands was chosen. Parameter uncertainty in pesticide emissions, chemical-specific data, effect and damage data, and fractions of metabolite formation of degradation products was statistically quantified via probabilistic simulation, i.e. Monte Carlo simulation. Model structure uncertainties regarding the concentration−response model to be included, the selection of the damage model, and the inclusion of pesticide transformation products were assessed via discrete choice analysis. To arrive at a minimum level of overall uncertainty the linear concentration−response model was preferable, while the transformation products may be excluded. Selecting the damage model had a relatively low influence on the overall uncertainty. The outcomes on the preferred model can, however, depend to a large extent on the case under study.

To follow-up on this study, more cases need to be viewed, as well as more types of model-structure uncertainty, applying up-to-date data and parameter uncertainty ranges.

The goal of this research is to show the case-specificity of the trade-off between model structure and parameter uncertainty. Model structure uncertainties that can be included are the inclusion of pesticide transformation products (with updated data), applying specific regressions for ionic compounds, and spatial variability. The trade-off between uncertainties will be shown in the case of maize production with a focus on freshwater ecotoxicity due to pesticide application using up-to-date data, and in at least one other case of freshwater ecotoxicity.

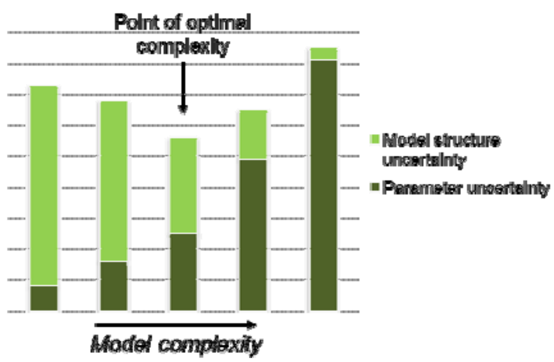

Figure 1: Trade-off between parameter uncertainty and model structure uncertainty to derive at the point of optimal model complexity

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References:

Finkel, A. Toward less misleading comparisons of uncertain risks: The example of aflatoxin and alar. Environ. Health Perspect. 1995, 103 (4), 376−385.

Van Zelm R, Huijbregts MAJ. 2013. Quantifying the trade-off between statistical and model uncertainty in life cycle impact assessment. Environmental Science & Technology, 47 (16),: 9274–9280.