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Abstract: Uncertainty assessment in LCA enables the evaluation of the significance of results, which is important for providing sound decision-support. In this work, an LCA was performed on two plant-growth regulators considering various sources of uncertainty: In the LCI, uncertainties of imprecise measurements of elementary flows, temporal and spatial variation, and different production processes were assessed. In the characterisation phase, the uncertainties of substance properties and the composition of sum-parameters were considered. These uncertainties were expressed as probability distributions and assessed via stochastic modelling (Monte-Carlo Simulation). For most LCI- and LCIA-data, generic uncertainty ranges were used. Uncertainties due to assumptions on the production efficiency were reflected by a best-case and a worst-case scenario. Contributions to variance of all uncertain input parameters were calculated. One plant-growth regulator was defined as significantly better than the other, if the impact score was lower in 90% of the simulations. The results showed that differences in median impact scores of a factor of 1.6 were sufficient in the impact categories global warming, acidification, and eutrophication for a significant distinction of the products. The applied doses and the elementary flows of basic-chemical production and energy supply had the highest contribution to variance in these impact categories. By contrast, dispersions are large concerning the toxicity impact categories and the photooxidant creation potential. This can be mainly attributed to the high contribution to variance of sum-parameters and characterisation factors. The implications of these uncertainties on the decision-making process are discussed. Moreover, tentative rules of thumb for estimating the significance of results are put forward. Finally, a format is proposed how complex results of uncertainty assessments may be presented for decision-support.

***Keywords**:* decision making; Life Cycle Assessment (LCA); pesticides; significance; uncertainty

1 INTRODUCTION

Quantifying uncertainty in LCA is an important step towards reliable and transparent decision support. The theoretical foundation and tools for uncertainty analysis in LCA are published [Huijbregts, 1998a, 1998b, Huijbregts, 2001, Weidema, 1996]. However, there is still a lack of case studies analysing uncertainty in LCA results and implications for decision support.

A prerequisite for an uncertainty analysis is the availability of information quantifying the uncertainty. Unfortunately, specific factors for uncertainty in individual LCI or LCIA parameters are only rarely available today. To handle this lack of specific uncertainty data, the use of generic uncertainty factors has been proposed for groups of parameters (e.g. air emissions, characterisation factors). Concerning the LCI, such generic uncertainty factors were derived by Finnveden and Lindfors [1998] in a comparison of LCI datasets on PVC production from different sources. For characterisation factors of LCIA methods, generic uncertainty factors have been published by method developers (e.g. Huijbregts [2003] concerning the CML-baseline method [Guinée, 2001]).

In this work, we assess the uncertainty of an LCA comparing two plant-protection products using generic uncertainty factors. A simple format for the presentation of uncertain LCA results is proposed. It is discussed to what extent a full uncertainty analysis is necessary to obtain reliable results in routine application of LCA, taking into account implications of uncertainty for decision making. Rules of thumb for simplified significance criteria are suggested.

2 CASE STUDY

A case study on two plant-protection products is used to illustrate consequences of uncertainty in LCA for decision making of pesticide producers. Both products are assessed for their use as plant-growth regulators in winter wheat. The product Moddus contains trinexapac-ethyl as active substance and is relatively new on the market (since 1990). The product Stuntan is established since 1960. Stuntan is a fictive name representing a range of similar products from different suppliers that contain chlorocholine chloride as active substance. The functional unit is the dose applied to 1 ha of crop, as recommended by pesticide registration authorities [BfL, 2002]. Such a product comparison is of interest e.g. for pesticide producers to benchmark new products against established ones.

Published LCIs were used regarding the supply of basic chemicals and energy as well as transport, distribution and tractor operation [Geisler, 2003a]. A specific estimation procedure [Geisler, 2003b] was applied to inventory LCIs of fine chemical production, namely the supply of active substances, formulation ingredients, and their precursors. Uncertainty in this estimation procedure concerning the efficiency of chemical production is depicted by a best and a worst-case scenario (see below). The full LCIs concerning the production of the active substances are published in Geisler [2003a], LCIs for formulation ingredients are documented in Geisler et al. [2003b]. The LCIA was carried out using relevant impact categories of the CML-baseline method [Guinée, 2001].

3 METHODS

The LCA was calculated in Excel using a matrix-inversion algorithm proposed by Cano-Ruiz [2000]. Parameter uncertainty was propagated through this algorithm into impact scores using Monte-Carlo simulation (@Risk [2001], Latin Hypercube sampling, 30'000 iterations). We used correlated sampling for parameters that appear in the life cycles of both plant-protection products. Scenario uncertainty was depicted by calculating one Monte-Carlo simulation for each scenario. The influence of individual parameters on the uncertainty of the impact scores was quantified with the contribution to variance [Fenner, 2001] of each parameter. The contribution to variance measures the influence of a parameter on the results distribution in terms of dispersion and absolute magnitude.

To evaluate the product comparison, we calculated the quotient of impact scores of the two alternatives:

$$Q = I_{Moddus} / I_{Stuntan} \qquad (1)$$

where Q is the quotient of impact scores (dimensionless) and I is an impact score (unit of the impact category). In calculating such a quotient, uncertainty applying to both alternatives cancels out to an extent. Percentile distributions of Q were obtained as output of the Monte-Carlo simulations. Significant differences between the two alternatives were assumed, if 90 % of the values of Q were above or below unity.

We assumed a lognormal distribution for most parameters because it yields only positive values and because its long tail in high values is deemed appropriate for LCA parameters [Huijbregts, 2003]. Lognormal distributions were parameterised using dispersion factors [Huijbregts, 2003, Slob, 1994]:

$$k = X_i(0.975) / \text{median}_i \qquad (2)$$

where k is the dispersion factor, i is the uncertain parameter, and X is the 97.5th percentile of i. The range of uncertainty (uncertainty range, UR, dimensionless) in quotients of impact scores (Equation 1) is expressed as 90 % confidence interval:

$$UR = X_i(0.95)/X_i(0.05) \qquad (3)$$

Sources of uncertainty included in the assessment are shown in Table 1. Concerning LCI flows, uncertainty and different sources of variability are depicted as one single generic dispersion factor per group of flows.

It was of interest here to derive such factors for processes of basic chemical production, because they exhibit a major contribution to the LCI of the production of active substances in the case study [Geisler, 2003b]. Therefore, we derived generic dispersion factors from the differences between elementary flows for the production of benzene and sodium hydroxide. Six and nine LCIs were compared for the production of benzene and sodium hydroxide, respectively [Geisler, 2004]. Calculating dispersion factors for comparable elementary flows in these different LCIs yields information on all sources of uncertainty in the LCI assessed here (Table 1).

A specific model uncertainty in the LCI stems from the use of the estimation procedure for LCIs of chemical production-processes in the supply of the active substances and formulation ingredients [Geisler, 2003b]: Knowledge on the efficiency of production processes is uncertain. Since pesticide producers have an influence on the production efficiency of precursors, we specifically wanted to illustrate the consequences of neglecting environmental objectives in supply chain management. Therefore, production efficiency in the chemical industry was assessed in a best and a worst-case scenario (Table 1) [Geisler, 2003b]. Finally, for those LCI data acquired specifically for this study (e.g., applied doses of the products) probability distributions were fitted.

Table 1: Sources of uncertainty [Huijbregts, 1998] covered in this work.

Source\phase	LCI	LCIA
Parameter uncertainty	Imprecise calculation of flows; Unknown composition of sum parameters	Imprecise knowledge on substance/ environmental properties
Model uncertainty	Assumptions on production efficiency	N/a [a]
Uncertainty due to choices	Different allocation methods, system boundaries, etc.	N/a [a]
Temporal variability	Variation of parameter values between years	N/a [a]
Spatial variability	Variation of parameter values between production sites	N/a [a]
Variability between objects/sources	Different production processes for the same product	Variability in exposure parameters

[a] N/a – not assessed.

To depict uncertainty in characterisation factors of the CML-baseline method [Guinée, 2001], generic dispersion factors were used as published by Huijbregts [2003]. Sources of uncertainty comprised in these factors are parameter uncertainty and variability in exposure assessment parameters (e.g. human characteristics, Table 1). Sum parameters carry a specific uncertainty, because their composition is not known quantitatively. Therefore, uniform distributions were defined for the characterisation factors of sum parameters. The minimum and maximum value of each uniform distribution was defined by the minimum and maximum characterisation factor, respectively, of the range of substances a sum parameter comprises. Additionally to this uncertainty in the composition of sum parameters, the uncertainty of characterisation factors themselves was modelled for sum parameters as for any other characterisation factor.

4 RESULTS

4.1 Case-Study Results

In Table 2, the probability of the quotient of impact scores (Equation 1) to be larger than one and the uncertainty ranges are shown. The spreads in the distributions are caused by uncertainty in LCI flows and in characterisation factors. Uncertainty ranges are considerably higher regarding the toxicity impact-categories than for the other midpoints. Significant differences between the two products occur only in the worst-case scenario, with regard to acidification, photooxidant creation and human toxicity impacts: Moddus shows significantly higher impact scores than Stuntan according to the significance criterion chosen (see Methods).

The applied doses of the two plant-protection products have high contributions to variance in all impact categories (Table 2), because the applied dose is the reference flow of the functional unit. Therefore, uncertainty in this parameter has an effect on all other parameters in the life cycles compared. The doses are uncertain, because in pesticide registration, a dose range is set permitting some flexibility to the farmer. The utilisation of this dose range by farmers is influenced by various factors, e.g. differences in prices between products. Uncertainty in the LCIs of basic chemical and energy supply, expressed as dispersion factors, also contributes considerably to variance. Concerning the toxicity impact categories, the uncertain composition of sum parameters plays a major role for uncertainty. With regard to single substances, the characterisation factor for emissions of chlorocholine chloride to air and water has high contributions to variance in freshwater ecotoxicity impact-scores. This contribution to variance of impacts of chlorocholine chloride explains the large uncertainty range in freshwater ecotoxicity in Table 2, because the generic uncertainty factors for the characterisation factors of chlorocholine chloride are as high as 50 (emission to air) and 100 (emission to water) [Geisler 2003a]. Additionally, air emissions of substrates in chemical production exhibit a considerable contribution to variance in the worst-case scenario, where the emission factor for such substances is relatively high [Geisler, 2003b]. Due to the unavailability of mammalian no-effect data for these substrates, we applied a worst-case no-effect value [Geisler, 2003a] to calculate characterisation factors for the human toxicity potential in USES-LCA [Huijbregts, 1999]. It is common practice in chemical industry in Western Europe to combust off-gases containing such highly toxic substances [Geisler, 2003b]. The high contribution to variance exhibited by these substrate emissions therefore gives a conceptual idea of the consequences of such emissions. Uncertainty in tractor operations largely cancels out in the product comparison due to correlated sampling. Remaining sources of uncertainty have small contributions to variance below 6 %.

4.2 Using Uncertain Results in Decision Making

Considering uncertainty in decision making is important, but may substantially increase the complexity of results. The presentation of uncertain results to decision makers may however be facilitated by a simplified representation, such as presented in Table 3.

The use of highly uncertain LCA results for decision support may not be advisable. For instance, it would not be desirable suppressing the development of the new product Moddus on the grounds that the LCA shows no progress compared to the established product Stuntan concerning freshwater ecotoxicity, as long as method uncertainty is a major cause for this insignificance. Therefore, impact-category results carrying extremely high uncertainty should be marked as such (Table 3).

Table 2: Probability (%) of the quotient of impact scores to be larger than one, with asterisks designating significant differences between the products and contribution to variance (CTV) of groups of parameters.

Impact category	Global warming	Acidifi-cation	Eutrophi-cation	Photoox. creation	Human toxicity	Freshwater ecotoxicity	Terrestrial ecotoxicity
P(Q>1), best case	86	53	33	51	64	29	71
P(Q>1), worst case	88	99*	75	90*	93*	61	84
UR, best case	2.2	2.3	2.5	3.8	5.6	15	40
UR, worst case	2.7	2.8	3.5	3.3	120	45	40
Highest CTV	Applied doses	Applied doses	Basic chemical and energy supply	Applied doses	Sum parameters	Sum parameters	Applied doses
2nd highest CTV	Basic chemical and energy supply	Basic chemical and energy supply	Applied doses	Sum parameters	Applied doses	Chlorocholine chloride to water	Sum parameters, substrates to air

Table 3: Simplified representation of the results of the product comparison under uncertainty (👎 means that the impact score of Moddus is significantly higher than that of Stuntan, -- means that the results are insignificant, and ~ denotes high method uncertainty).

Production efficiency scenario	Implication for supply chain	Likeliness	Global warming	Acidification	Eutrophication	Photo-oxidant creation	Human toxicity	Freshwater ecotoxicity	Terrestrial ecotoxicity
Best case	High environmental standards	High	--	--	--	--	--	~	--
Worst case	Low environmental standards	Low	--	👎	--	👎	👎	--	~

4.3 Significance: Rules of Thumb

It is impossible to fully predict uncertainty in LCA results without conducting a quantitative uncertainty analysis. Since full uncertainty analyses are time-consuming, rules of thumb concerning the significance of LCA results would be helpful in LCA practice.

In deterministic case studies, only expert judgement is available to set significance criteria for results. We found estimated significance criteria in published case studies ranging between 1.1 and 2 (e.g. [Frischknecht, 1996, Ross, 2003]) expressed as quotients of impact scores and only once as high as 10 [Finnveden, 1998], expressed as quotients of elementary flows. In our case study, median quotients (Equation 1) are assumed to approximate deterministic results. Significant differences demanded median quotients larger than 3 concerning toxicity impact-categories, and around 1.6 concerning other impact categories. Compared to our findings, expert judgements common in literature overestimated the significance of LCA results. Our results suggest that a median quotient of impact scores larger than two may be considered on the safe side of being significant, concerning the impact categories global warming, acidification, eutrophication and photooxidant creation. This rule of thumb is supported by inherent characteristics of these impact categories regarding uncertainty, namely few impact pathways and a small number of elementary flows contributing to these categories [Geisler, 2004]. Case-study results exhibiting smaller differences should be evaluated for significance with a full uncertainty analysis. Regarding toxicity impact-categories, no rule of thumb is proposed, because large dispersion factors of individual parameters cause highly varying uncertainty in individual toxicity impact-scores. A detailed uncertainty analysis seems indispensable for reliable decision support concerning toxicity impacts assessed by the CML-baseline method.

The case study used here to establish the rule of thumb compared products with relatively similar life cycles. This was also the case in the work of Huijbregts [2003]. Larger differences between life cycles, e.g. mechanical compared to chemical weed control, often lead to larger differences in impact scores of alternatives. However, strongly differing life cycles also imply weaker correlations among input distributions in these life cycles, leading to larger uncertainty ranges (Equation 3). These two trends counteract each other in their effect on the significance of differences between impact scores of alternatives.

We conclude that in the absence of better data, the rule of thumb may be used in LCA if a full uncertainty analysis is outside the scope of the study. It should however be born in mind, that the rule of thumb proposed here has not been verified yet for products with very different life-cycles.

5 DISCUSSION AND CONCLUSION

The comparison of the plant-growth regulators showed no significant differences in most impact categories. With regard to freshwater ecotoxicity impacts, larger differences between Moddus and Stuntan are superimposed by exceptionally large uncertainty (two orders of magnitude between 5th and 95th percentile of the quotient). High uncertainty also superimposes relatively large differences between impact scores regarding terrestrial ecotoxicity impacts in the worst-case scenario. Measures to reduce uncertainty should be taken before these toxicity impact-scores are used for decision support.

In spite of large uncertainty in some impact categories, the case-study results give the important information that Moddus is not significantly environmentally preferable to Stuntan, regarding the more likely best-case scenario (Table 3). Another useful recommendation from the case study may be the inclusion of environmental objectives in the supply-chain management of pesticide producers, to avoid the worst-case scenario (Table 3).

The ranges of uncertainty of the case-study results can be compared to those published by Huijbregts [2003] for a case-study comparing housing insulation options. Uncertainty ranges in Huijbregts [2003] are considerably smaller than in this work, especially with regard to toxicity impact-scores. One reason for this is that sum parameters play a crucial role for the high uncertainty range (Equation 3) in toxicity impact-scores in our work, while they were of minor importance in the case study of Huijbregts [2003]. Second, higher dispersion factors were assumed in this work compared to Huijbregts [2003] for LCI parameters and characterisation factors. These differences in parameter uncertainty are mainly due to substantial efforts of Huijbregts [Huijbregts, 2003] to acquire specific dispersion factors for parameters in the LCA with high contribution to variance. Such an iterative approach is however not generally practicable in LCA, because it is very labour intensive and necessitates access to substance data and models used in the calculation of characterisation factors.

The rule of thumb for the significance of LCA results (Section 4.3) is useful when a quantitative uncertainty analysis is not feasible (e.g., due to time restrictions). However, routine uncertainty analyses should be aimed at in future LCA practice. To this end, data and guidelines on the definition of uncertainty in LCI and LCIA are needed. To further facilitate an uncertainty assessment, LCI and LCIA data providers should supply quantitative uncertainty information including correlation estimates for individual parameters. Ecoinvent [2003] has already made a first step toward this direction by estimating uncertainty ranges for LCI parameters. In contrast to parameter uncertainty, a large variety of choices and sources of model uncertainty are less accessible to quantitative analysis. It is suggested that choice and model uncertainty of specific interest for goals and scopes of case studies be modelled quantitatively. Choices and model uncertainty generally applying to LCA should be made transparent to decision makers. This enables decision makers to explicitly accept choices and models employed as being an adequate basis for decision support.

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