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Uncertainty Analysis in Life Cycle Assessment (LCA): Case Study on Plant-Protection Products and Implications for Decision Making

Georg Geisler, Stefanie Hellweg* and Konrad Hungerbühler

Institute for Chemical- and Bioengineering, Swiss Federal Institute of Technology, ETH-Hönggerberg, 8093 Zürich, Switzerland

* Corresponding author (<u>Stefanie.hellweg@chem.ethz.ch</u>)

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Abstract

Goal, Scope, and Background. Uncertainty analysis in LCA is important for sound decision support. Nevertheless, the actual influence of uncertainty on decision making in specific LCA case-studies has only been little studied so far. Therefore, we assessed the uncertainty in an LCA comparing two plant-protection products.

Methods. Uncertainty and variability in LCI flows and characterization factors (CML-baseline method) were expressed as generic uncertainty factors and subsequently propagated into impact scores using Monte-Carlo simulation. Uncertainty in assumptions on production efficiency for chemicals, which is of specific interest for the case study, was depicted by scenarios.

Results and Discussion. Impact scores concerning acidification, eutrophication, and global warming display relatively small dispersions. Differences in median impact scores of a factor of 1.6 were sufficient in the case study for a significant distinction of the products. Results of toxicity impact-categories show large dispersions due to uncertainty in characterization factors and in the composition of sum parameters. Therefore, none of the two products was found to be significantly environmentally preferable to the other. Considering the case study results and inherent characteristics of the impact categories, a tentative rule of thumb is put forward that quantifies differences in impact scores necessary to obtain significant results in product comparisons.

Conclusion. Published LCA case-studies may have overestimated the significance of results. It is therefore advisable to routinely carry out quantitative uncertainty analyses in LCA. If this is not feasible, for example due to time restrictions, the rule of thumb proposed here may be helpful to evaluate the significance of results for the impact categories of global warming, acidification, eutrophication, and photooxidant creation.

Keywords: Acidification; decision making; eutrophication; global warming; impact categories; Monte-Carlo simulation; pesticides; plant protection products; photooxidant creation; significance of data sources; uncertainties

Introduction

Life Cycle Assessment (LCA) is a method to analyze the environmental performance of products, for instance via product comparisons [1, 2]. Decision support by LCA, however, may be misleading due to uncertainty in LCA results. Quantifying such uncertainty is therefore an important step towards reliable and transparent decision support. Further, it allows the identification of improvement potentials in LCA models and

data. The theoretical foundation and tools for uncertainty analysis in LCA are published [3–6]. However, there is still a lack of case studies analyzing consequences of uncertainty in LCA results and implications for decision support.

Of the manifold sources of uncertainty in LCA, Huijbregts [4] distinguishes between

- Parameter uncertainty due to imprecise knowledge of LCI and LCIA parameters (e.g. mass flows and substance properties, respectively);
- Temporal and spatial variability in LCI and LCIA parameters;
- Variability between sources in the LCI (e.g. different processes supplying the same output) and between objects of the assessment in the LCIA (e.g. humans);
- Uncertainty in the models used (e.g. the strongly simplified description of the environment by multimedia fate models); and
- Uncertainty due to choices in LCA (e.g. which allocation method to apply).

Uncertainty and variability in parameters is conveniently propagated into LCA results using Monte-Carlo simulation, while model and choice uncertainty is accessible by calculating LCA results for different scenarios [3–5]. The term uncertainty generally refers to random errors, for instance imprecision in measurements, whereas variability accounts for stochastic variation in data, e.g. seasonal and spatial variation of precipitation.

Typically, large amounts of published data are used in LCA case-studies to set up the LCI and to carry out the LCIA. A prerequisite for an uncertainty analysis is the availability of information quantifying the uncertainty mentioned above in such published data. No specific factors for uncertainty in individual LCI or LCIA parameters are available today, with the exception of ecoinvent 2000 [7] that recently published uncertainty estimates for LCI parameters. 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, characterization factors). Concerning the LCI, such generic uncertainty factors were derived by Finnveden and Lindfors [8] in a comparison of LCI datasets on PVC production from different sources. For characterization factors of LCIA methods, generic uncertainty factors have been published by method developers (e.g. Huijbregts et al. [9] concerning the CML-baseline method [2]).

In this work, we assess the uncertainty of an LCA comparing two plant-protection products. Generic uncertainty factors for parameters in LCIs of chemical production are derived and compared to factors published. 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 the routine application of LCA, taking into account implications of uncertainty for decision making.

1 Case Study and Methods

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. Application of growth regulators leads to reduced stem height and increased stem thickness in wheat, which avoids yield losses due to bending or breaking of stems in storms [10]. The product Moddus contains trinexapac-ethyl as an active substance and is relatively new on the market (since 1990). The product Stuntan has been established since 1960. Stuntan is a fictive name representing a range of similar products from different suppliers that contain chlorocholine chloride as an active substance. The functional unit is the dose applied to 1 ha of crop, as recommended by pesticide registration authorities [11]. Such a product comparison is of interest, e.g. for pesticide producers to benchmark new products against established ones. A schematic representation of processes considered in the LCIs of each product is given in Fig. 1.

Published LCIs were used regarding the supply of basic chemicals and energy as well as transport, distribution and tractor operation. Detailed information on the data sources is given in [12]. A specific estimation procedure [13] was applied to inventory LCIs of fine chemical production, namely the supply of active substances, formulation ingredients, and their precursors. 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 (see below). The full LCIs concerning the production of the active substances are published in [12], LCIs for formulation ingredients are docu-



Fig. 1: Life cycle of a plant protection product, with processes (boxes) and process outputs (plain text). Data sources are indicated by bold text and processes covered by these data sources by dashed lines

mented in [13]. The LCIA was carried out using relevant impact categories of the CML-baseline method [2]. The case study was evaluated on the level of characterization.

Uncertainty Analysis. The LCA was calculated in Excel using a matrix-inversion algorithm proposed by Cano-Ruiz [14]. Parameter uncertainty was propagated through this algorithm into impact scores using Monte-Carlo simulation (@Risk [15], Latin Hypercube sampling, 30,000 iterations). Correlated sampling was used concerning parameters that appear in both life cycles of the plant-protection products compared, with rank order correlation coefficients set to unity. 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 assessed by calculating the contribution to variance (CTV, see **Supporting Information**, online only at <<u>http:// dx.doi.org/10.1065/lca2004.09.178.1</u>>) for each parameter.

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

$$Q = I_{Moddus} / I_{Stuntan}$$
(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 these distributions of Q were above or below unity. The choice of this rather strict confidence interval was adequate here, as considerable investments are involved in decisions concerning the development of pesticides. In other cases, lower significance intervals might be sufficient, for instance, if products are compared that perform equally with respect to other criteria, such as price. It needs to be born in mind, however, that a lower confidence interval bears a higher risk of erroneously classifying a difference between two alternatives as significant.

The specific form of probability distributions for individual parameters is generally not known in LCA, because parameter values are mostly based on few measurements or on estimates. Choosing the same probability distribution for all parameters is therefore reasonable to avoid bias among parameters. 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 [9]. The available inventory data for these parameters was then assumed to represent the mean value of the lognormal distribution. The spread of the lognormal distributions was parameterized using dispersion factors [9,16]:

$$k = X_i(0.975) / \text{median}_i$$
(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 (Eq. 1) is expressed as 90% confidence interval:

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

Source \ phase	LCI	LCIA
Parameter uncertainty	Imprecise calculation of flows; Unknown composition of sum parameters	Imprecise knowledge on properties of substances and the environment
Model uncertainty	Assumptions on production efficiency in estimation of LCIs [13]	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 assessment parameters
^a N/a – not assessed		

 Table 1: Sources of uncertainty [4] related to phases of LCA, and uncertainty covered in this work. Font styles indicate the method of analysis used (bold – scenario analysis; italic – stochastic modelling)

Uncertainty Sources. Sources of uncertainty included in the assessment are shown in Table 1. Concerning LCI flows, uncertainty and different sources of variability are all depicted in one single generic dispersion factor per group of flows. Such factors are published for LCIs on PVC production [8].

It was of interest here to derive such factors for processes of basic chemical production, which exhibit a major contribution to the LCI of the production of active substances in the case study [13]. 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 (see Supporting Information, online only at http://dx.doi.org/10.1065/lca2004.09.178.1). Many data sources are interdependent, e.g. versions from different years or data adapted to specific needs of secondary data providers. Hence, only two to three primary data sources underlie the LCIs compared. Still, temporal variability in processes and uncertainty due to choices of data suppliers (e.g. allocation methods or system boundaries) are recorded even by an analysis of such interdependent datasets. Calculating dispersion factors for comparable elementary flows in these different LCIs therefore 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 [13]: Knowledge on the efficiency of production processes is uncertain. This model uncertainty was assessed in a best and a worst-case scenario of production efficiency in the chemical industry ([13]; Table 1). Finally, probability distributions of LCI data acquired specifically for this study (e.g. applied doses of the products) are documented in the Supporting Information (online only at <<u>http://dx.doi.org/10.1065/lca2004.09.178.1</u>>).

To depict uncertainty in characterization factors of the CMLbaseline method [2], generic dispersion factors were used as published by Huijbregts et al. [9] (values see **Supporting Information**, online only at <<u>http://dx.doi.org/10.1065/</u> <u>lca2004.09.178.1</u>>). Sources of uncertainty comprised in these factors are parameter uncertainty and variability in exposure assessment parameters (e.g. human characteristics, Table 1). Sum emissions such as AOX, PAH, metals, etc. carry an additional uncertainty, because their composition is not known quantitatively. We chose a 2-step procedure for such sum emissions. In Fig. 2A we illustrate this procedure using the example of PAH (polycyclic aromatic hydrocarbons) with regard to freshwater ecotoxicity. First, we selected all emissions that belonged to such a sum parameter and for which the CML-baseline method [2] provided characterization factors. The minimum and the maximum of these characterization factors represent a best- and worstcase scenario, respectively, to be seen in Table S3 (see Supporting Information, online only at <http://dx.doi.org/ 10.1065/lca2004.09.178.1>). Since no quantitative information about the *composition* of sum parameters was available, we assumed that the total impact of the sum emissions would follow a uniform distribution between this minimum and maximum characterization factor. Second, in addition to this uncertainty in the composition of sum parameters, the uncertainty of *characterization factors* themselves was modeled for sum parameters with lognormal distributions as for any other characterization factor. Instead of this approach, we also could have taken all single substances of a sum parameter and assumed that their share to the sum emission be a uniform distribution between 0 and 1. As the sum of all emissions must equal 100%, we need to divide the share of each substance by the sum of all substances (Fig. 2B). In a second step, the amounts of all these substances could be multiplied to the respective log-normally distributed characterization factors and summed up. It should be noted that the share of each substance in the sum emission is not a uniform distribution because of the normalization. For instance, A can only be equal to 100% if at the same time all other substances are simulated to have a content of 0%; otherwise, the content of A gets reduced. Therefore, the distribution for each substance is not a uniform distribution but rather a distribution that has a peak value towards the left center (the more substances, the more to the left is this peak). The overall uncertainty therefore tends to be smaller than according to the first approach. For reasons of simplicity and in order not to underestimate possible uncertainties, we did not choose the latter approach (see Fig. 2B) but the former (see Fig. 2A).



Fig. 2: Two procedures for modelling the uncertainties of sum emissions (example: PAH emissions, freshwater ecotoxicity). Above (A): Procedure followed in this work. Below (B): Alternative procedure

2 Results

Generic Uncertainty Factors for LCIs. Dispersion factors for elementary flows were derived from the comparison of LCIs on the production of sodium hydroxide and benzene. Most elementary flows display dispersion factors between 1.1 and 5.0 (Table 2). Considerably higher spreads of up to 1100 appear in a few cases. Such extreme dispersions are often due to large differences at rather low absolute levels of flows (e.g. in the benzene datasets, inputs of oil for energy generation are low as well as emissions of ammonia and benzene to air). Energy flows have median dispersion factors of 2 in both products compared. Oil used as feedstock in the cumulated LCIs of benzene production has a similar dispersion factor as the total energy demand. The air emission mass-flows show median dispersion factors of three for both products. There is no relevant difference between dispersion factors for sum parameters and specified emission massflows. Water emissions comprise mainly sum parameters and specific metals. Median dispersion factors for water emissions are similar to those for air emissions.

The dispersion factors from Table 2 are compared to dispersion factors from Peereboom et al. [17], Finnveden and Lindfors [8], with additional modifications by Huijbregts et al. [9] in Table 3. In general, dispersion factors from literature correspond fairly well with the factors found here. However, median dispersion factors smaller than 2 are not supported by the results of this work (Table 2). Minimum factors of 3 are generally used here in order not to underestimate uncertainty. Further, no relevant difference between median dispersion factors for air and water emissions were

 Table 2: Dispersion factors (k; Eq. 2) for selected elementary flows derived from the comparison of LCIs of sodium hydroxide and benzene production (Table S1 Supporting Information, online only at <<u>http://dx.doi.org/10.1065/lca2004.09.178</u>>). Median dispersion factors were calculated from all elementary flows per group

	Energy der		Air emis	sions	3		Water emissions							
	NaOH k	n ^a	Benzene k	nª		NaOH k	nª	Benzene k	nª		NaOH k	nª	Benzene k	nª
Coal	1.7	8	1.3	5	Chlorine	11	5	7.2	2	Mercury	13	7	49	3
Oil	1.3	9	190	2	Mercury	10	7	6.0	3	Metallic ions	3.5	7	7.9	5
Natural gas	1.9	8	1.3	5	Benzene	1.1	6	68	2	TOC	2.1	6	31	2
Hydropower	1.5	9	8.8	5	CO ₂	1.4	9	2.6	6	BOD	4.3	9	1.4	5
Nuclear energy	1.6	9	1.8	5	N ₂ O	3.3	7	30	4	COD	2.3	9	1.4	6
Total energy	1.4	9	4.0	6	Ammonia	2.6	6	1100	4	AOX	1.4	6	-	1
					Metals	-	1	2.8	3	Nitrate	2.1	7	6.4	5
Oil (feedstock)	None		2.2	6	Heavy metals	3.1	6	1.4	2	NH_4^+	9.2	2	1.4	5
					VOC	5.0	9	2.8	6	N-tot	1.5	7	1.5	4
					SOx	3.4	9	1.5	6	Phosphate	1.1	6	13	2
					NO _x	2.8	9	1.3	6	P ₂ O ₅	_	1	1.9	2
Median	2		2			3		3			2		3	
^a Total number of	of datasets d	ocumer	ting the elem	ienta	ary flow.	•				-	•			

Table 3: Generic dispersion factors (Eq. 2) for groups of LCI flows: Values published by Peereboom et al. [17], Finnveden and Lindfors [8] and interpreted as dispersion factors by Huijbregts et al. [9], factors derived here by comparing LCI datasets for the production of benzene and sodium hydroxide, and factors used in the case-study

Flow group	Flow name	Flows included	Generic dispersion factors								
			[17] ^a	[8] and [9]	This study (Table 2)	Factors used in the case study					
		Technos	phere flows								
	Energy	Energy flows	1.1–1.3	2	-	3					
	Materials	Energy inputs to energy supply processes are counted as materials		1.05	_	2					
	Wastes	Any solid waste output		100	-	100					
		Elemer	ntary flows								
Resources	Central	Nuclear and fossil fuel energy and mass flows	1.2–2	2	Median 2	3					
	Non-central	Any other resource input	1.6–32	10	1.5–8.8	10					
Air emissions	CO ₂		1.4	1.05	Median 3	3					
	SO _x , NO _x		2.0–2.2	2	Median 3	3					
	Any other		1.6–220 median 11	10	1.1–1100	10					
Water emissions	Any		1–940 median 7.6	100	1.1–49	10					

^a Peereboom et al. [17] provide minimum and maximum values of inventory flows. We assumed that these values would enclose 95% of all values of a lognormal distribution. Median values were calculated as the square root of the product of the minimum and maximum value (calculation derived from Slob [16]). Dispersion factors were then calculated according to Equation 2.

found here. Therefore, a considerably lower dispersion factor for water emissions was used compared to the other sources. We assigned a dispersion factor of ten to most air and water emissions, which is somewhat higher than the median factors found for the corresponding groups in Table 2. Such a conservative choice is reasonable, because median uncertainty may be underestimated in the dispersion factors derived here due to interdependencies among datasets (see above). No dispersion factors for technosphere flows were calculated, because most datasets analyzed were cumulated. Dispersions of energy flows were assumed to be similar to those of air emissions from fossil fuel consumption, such as CO_2 and SO_x . Material flows were assumed to show the highest precision of all flow groups [8,9].

Case-Study Results. Impact scores of the two plant-growth regulators are compared in Fig. 3, displaying distributions of quotients of impact scores (see Eq. 1). Results are juxtaposed in the best and worst-case scenario of production efficiency [13] for active substances, formulation ingredients and their precursors. The results are less favorable for



Fig. 3: Percentiles of the quotient of impact scores (Eq. 1) comparing the two plant-growth regulators. Above: Distributions obtained for scenarios of production efficiency for chemicals [13] are juxtaposed: Best-case scenario on the left, worst case on the right of each pair of distributions. Below: Probability (%) of the quotient of impact scores to be larger than one, with asterisks designating significant differences between the products, and uncertainty range (UR, dimensionless, Eq. 3)

Group	Subgroup	Gle war pote	obal ming ential	Acidi pot	fication ential	Eutrop pote	hication ential	Photo crea pote	Photooxidant creation potential		Human toxicity potential		Freshwater ecotoxicity potential		estrial oxicity ential
		Best case	Worst case	Best case	Worst case	Best case	Worst case	Best case	Worst case	Best case	Worst case	Best case	Worst case	Best case	Worst case
Elementary	Applied doses	79	90	62	69	41	38	18	64	17	11	2	8	31	24
or techno- sphere flows	Basic chemical and energy supply	13	8	32	19	41	48	16	19	9	1	2	4	16	6
	Tractor operations	4	< 0.5	< 0.5	6	4	3	< 0.5	1	1	1	< 0.5	< 0.5	1	< 0.5
	Transport and packaging	1	< 0.5	3	< 0.5	2	< 0.5	1	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	1	< 0.5
	Waste treatment	1	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
Characteri- sation	Sum parameters	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	62	13	69	31	66	56	15	21
factors	Chlorocholine chloride to air	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	7	6	N/a ^b	N/a ^b
	Chlorocholine chloride to water	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	20	19	N/a ^b	N/a ^b
	Mercury to air	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	21	1
	Substrates to air	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	N/a ^b	< 0.5	55	< 0.5	3	< 0.5	33
	Other single elementary flows	< 0.5	< 0.5	1	4.4	10	9	1	2	2	< 0.5	1	2	13	13

Table 4: Contribution to variance (in %) in the quotient of impact scores (Eq. 1) for groups of parameters. Both scenarios of production efficiency for fine chemicals [13] are depicted. 99% of the total variance in the quotient is included a

Rounding in the Excel-software may lead to deviations of +/- 1 % in the table

^b Parameter does not contribute to this impact category

Moddus in the worst-case scenario compared to the bestcase scenario, because Moddus is penalized more strongly by the worst-case assumptions, as the production of Moddus involves more process steps than the production of Stuntan (Fig. 3). The spreads in the distributions are caused by uncertainty in LCI flows (see Table 3) and in characterization factors (Table 1 and Supporting Information, online only at <<u>http://dx.doi.org/10.1065/lca2004.09.178.1</u>>). Spreads 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 (Methods).

The sources of uncertainty in the quotient of impact scores are assessed by their contribution to variance (Supporting Information, online only at <<u>http://dx.doi.org/10.1065/</u> lca2004.09.178.1>), which is shown for groups of parameters relevant to the case study (Table 4).

The applied doses of the two plant-protection products have high contributions to variance in all impact categories (up to 90%). This strong influence occurs because the applied dose is the reference flow of the functional unit, and 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 utilization of

this dose range by farmers is influenced by various factors, e.g. differences in prices between products or different attitudes of farmers against the risk of lodging when using low doses or the risk of crop damage when using high doses. While uncertainties in functional units are, in general, common in LCA, it is rather exceptional that such uncertainties can be modeled as distribution functions. In most cases, they will be accessible only as scenarios.

Uncertainty in the LCIs of basic chemical and energy supply, expressed as dispersion factors (Table 3), shows considerable contributions to variance of up to 48%. The latter uncertainty sources are of lower relevance concerning the toxicity impact-categories in both scenarios, because here characterization factors show high contributions to variance. Specifically, the uncertain composition of sum parameters plays a major role for uncertainty in these impact categories (contribution to variance 15 to 69%). Concerning single substances, the characterization 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 emissions explains the large uncertainty range in freshwater ecotoxicity in Table 1, because the generic uncertainty factors for the characterization factors of chlorocholine chloride are as high as 50 (emission to air) and 100 (emission to water, Supporting Information, online only at <<u>http://dx.doi.org/10.1065/lca2004.09.178.1</u>>). Additionally, air emissions of substrates in chemical pro-

Production efficiency scenario	Implication for supply chain	Likeliness	Global warming	Acidifica- tion	Acidifica- tion	Eutrophi- cation	Photo- oxidant creation	Human toxicity	Freshwater ecotoxicity	Terrestrial ecotoxicity
Best case	High environmental standards	High	_	-	1	-	1	-	~	_
Worst case	Low environmental standards	Low	_	Ţ	P	_	P	Ţ	-	~

Table 5: 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)

duction exhibit a considerable contribution to variance in the worst-case scenario, where the emission factor for such substances is relatively high [13]. Due to the unavailability of mammalian no-effect data for these substrates, we applied a worst-case no-effect value [12] to calculate characterization factors for the human toxicity potential in USES-LCA [18]. It is common practice in chemical industry in Western Europe to combust off-gases containing such highly toxic substances [13]. 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 show small contributions to variance below 6%.

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, however, may be facilitated by a simplified representation, such as the list of symbols in Table 5. Qualitative information on the scenarios is helpful for decision making. In the case study used here, scenarios encode uncertainty in production efficiency of the supply chain for active substances and formulation ingredients. The worst-case scenario was found to be less likely than the best case, regarding chemical industry in Western European countries [13]. Further, using highly uncertain results of LCA 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 (see Table 5).

3 Discussion

Case Study. The comparison of the plant-growth regulators showed no significant differences regarding most results (see Fig. 3). In these cases, either the uncertainty of the quotient of impact scores (see Eq. 1) may be too large or the difference in impact scores may be too small to allow a significant distinction of the alternative products. The latter possibility applies in the best-case scenario, where the median quotient takes values equal to or below 1.3 relating to impacts of all categories (see Fig. 3). An exception occurs with regard to freshwater ecotoxicity impacts, where larger differences between Moddus and Stuntan (median quotient of 0.56, see Fig. 3) 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 (see Table 5). Other objectives (such as economic ones) therefore would need to be weighted against environmental objectives to decide between the two products. Another useful result of the product comparison may be the inclusion of environmental objectives in the supply-chain management of pesticide producers, to avoid the worst-case scenario (see Table 5).

The ranges of uncertainty of the case-study results (see Fig. 3) are compared with those published by Huijbregts et al. [9] for a case-study comparing housing insulation options. This comparison is meaningful, because comparable methods were used for uncertainty analysis and LCIA in both case studies. Uncertainty ranges (see Eq. 3) in [9] take values between 2.2 and 3 concerning toxicity impact-categories and between 1.1 and 1.6 for other impact categories. Hence, uncertainty ranges in [9] are considerably smaller than in this work (see Fig. 3), especially with regard to toxicity impact-scores. These can be explained by three factors. First, sum parameters are more relevant in the current work (e.g. emissions of hydrocarbons to air) than in [9]. Second, higher dispersion factors were assumed here compared to [9] for LCI parameters and characterization factors. These differences in parameter uncertainty are mainly due to substantial efforts of Huijbregts et al. [9] to acquire specific dispersion factors for parameters in the LCA with a high contribution to variance. Such an iterative approach, however, is not generally practicable in LCA, because it is very labor intensive and necessitates access to substance data and models used in the calculation of characterization factors. Third, the large uncertainty of the functional unit influences all other parameters as well, and leads to large uncertainty ranges. As discussed above, it is rather unique to this work that uncertainty in the functional unit can be modeled as a simple distribution function. However, this result indicates that uncertainty in the functional unit may play an important role in LCA.

Significance Criterion and a Rule of Thumb. It is impossible to fully predict uncertainty in LCA results without conducting a quantitative uncertainty analysis. However, it would be of interest to derive rules of thumb concerning the sig-

Impact category	Variety of impact pathways (fate, exposure, effect)	Number of elementary flows [19]	Generic uncertainty factor ^a	Sum parameters relevant?							
Global warming potential	Low	43	1.4	No							
Acidification potential	Low	16	2.2	No							
Eutrophication potential	Low	53	1.8	No							
Photooxidant creation potential	Medium	127	1.2–2.1	Yes							
Human toxicity potential	High	178	50	Yes							
Freshwater ecotoxicity potential	High	178	50 to 100 ^a	Yes							
Terrestrial ecotoxicity potential	High	178	500 to 1000 ^a	Yes							
^a Supporting Information (online	^a Supporting Information (online only at < <u>http://dx.doi.org/10.1065/lca2004.09.178.1</u> >)										

Table 6: Inherent characteristics influencing uncertainty in impact-category results of the CML-baseline method [2]

nificance of LCA results. To this end, it is useful to consider inherent characteristics of impact categories influencing uncertainty in impact scores (**Table 6**).

The global warming, acidification, and eutrophication potentials exhibit similar characteristics with regard to uncertainty: They depict impact pathways of relatively little variety. Consequently, generic uncertainty factors are relatively low. Few elementary flows contribute to these impact categories, and thus highly uncertain sum parameters (see Table 6) are not necessary to simplify inventorying. Hence, relatively low uncertainty is expected concerning impact scores of these three impact categories. Relatively small differences between product alternatives will lead to significant distinctions (see 99% significance of the case-study result in the acidification potential, regarding the worst-case scenario, see Fig. 3). Toxicity impact-categories, by contrast, comprise a relatively high variety of impact pathways and a large number of elementary flows (see Table 6). High generic uncertainty factors apply and sum parameters are frequently used. It is therefore expected that uncertainty in toxicity impact-scores will be relatively high. This was observed in the case study by uncertainty ranges (see Eq. 3) spanning one to two orders of magnitude (see Fig. 3). Hence, large differences between product alternatives are necessary to achieve significant results concerning toxicity impactscores (e.g. a median quotient larger than 3 concerning the human-toxicity result (see Fig. 3), which is realized only because highly toxic substances are modeled in the worst-case scenario to be emitted in the life cycle of Moddus). The photooxidant creation potential takes an intermediate position between toxicity impact-categories and categories similar to the global warming potential, with regard to inherent characteristics influencing uncertainty (see Table 6). Thus, a relatively small median quotient in the case study leads to 90% significance concerning photooxidant creation impact-scores (see Fig. 3).

In deterministic case studies, only expert judgment 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. [20, 21]) expressed as quotients of impact scores and only once as high as 10 [8], expressed as quotients of elementary flows. In our case study, median quotients (see Eq. 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 (see Fig. 3). Compared to our findings, expert judgments 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 the similar inherent characteristics of these impact categories regarding uncertainty (see Table 6). Casestudy 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 (Table 6) cause highly varying uncertainty in individual toxicity impact-scores (see Fig. 3). 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 et al. [9]. Larger differences between life cycles 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 (see Eq. 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 out of the scope of the study. We think that our rule of thumb is a more qualified value than common expert judgment, as it is based on a thorough uncertainty analysis. It should be born in mind, however, that the rule of thumb proposed here has not been verified for products with very different life-cycles yet (e.g. mechanical compared to chemical weed control). Moreover, for toxicity categories we are not able to propose a rule of thumb. We suspect that few case studies will actually have significant results in these categories due to the high uncertainties of characterization factors and sum parameters. In order to enable a meaningful application of toxicity impact categories in LCA, these uncertainties need to be reduced in future research.

Method. Several sources of uncertainty are not comprised in this analysis, namely (a) model uncertainty in LCIA models, (b) uncertainty due to choices in LCIA (e.g. the choice of time horizons for the integration of impacts), and (c) uncertainty in the definition of probability distributions and generic dispersion factors. Concerning points (a) and (b), Huijbregts et al. [9] found that such uncertainty sources were of lower relevance than parameter uncertainty in their case study. To reduce uncertainty of type (c), a best practice should be developed concerning the definition of appropriate types of probability distributions as well as uncertainty ranges. One possible step towards this goal is the use of the generic dispersion factors for LCI parameters derived here (see Table 3).

It is infeasible to comprehensively model all uncertainty sources in the complex systems analyzed by LCA. However, it may be sufficient to consider only the most important uncertainty sources. At the current state of research, these appear to be the various sources of parameter uncertainty depicted in this and other studies [9,22], as well as specific sources of model or choice uncertainty that are exceptionally relevant to the study, such as the production efficiency scenarios modeled here [13]. International consensus on best LCIA methods to be used (e.g. [22]) can help to clarify which choice uncertainty needs to be considered depending on the goals of specific case studies. In routine applications of LCA, choices and models should reflect the preferences of decision makers, in order not to bias results with the preferences of LCA analysts.

Finally, the significance of results depends on the choice of the significance criterion (Methods), which itself depends on the goal and scope of a study. For assessments that may trigger high financial investments, a confidence interval of 90% is appropriate. By contrast, in cases where the investigated alternatives perform relatively equally with respect to all other criteria, lower levels of confidence may be sufficient.

4 Conclusions and Outlook

The case study demonstrated a need for consideration of uncertainty in LCA to evaluate the significance of results. High uncertainty in LCI and LCIA may impede obtaining significant LCA results regarding toxicity impact-scores. High uncertainties in toxicity categories are not specific to our case study, but they are method inherent (see Table 6). The reduction of uncertainties in toxicity characterization factors and a better definition of sum-emissions are therefore a clear future research need.

Concerning the impact categories of global warming, acidification, eutrophication and photooxidant creation, a tentative rule of thumb for the significance of LCA results was derived (factor of two between impact scores). Lower significance criteria have been suggested in the past by experts. Thus, the results of many LCA may have been overestimated in the past. The rule of thumb is useful to evaluate case studies where quantitative uncertainty analysis is practically infeasible. 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. Parameter uncertainty is relatively easily accessible to modeling via generic uncertainty factors and stochastic uncertainty propagation. To further facilitate an uncertainty assessment, LCI and LCIA data providers should supply quantitative uncertainty information including correlation estimates for individual parameters. By contrast, a large variety of choices and sources of model uncertainty are less accessible to quantitative analysis. It is suggested that only choice and model uncertainty of specific interest for goals and scopes of case studies be modeled quantitatively. Choices and model uncertainty generally applying to LCA should be made transparent to decision makers in a more simple manner. This enables decision makers to explicitly accept choices and models employed as being an adequate basis for decision support. Notwithstanding, an analysis of choice and model uncertainty is important to guide LCA research and model development.

The relatively high uncertainty in LCA may also have consequences for its general application: The discriminatory power of LCA may be much larger in analyses of relatively strongly differing scenarios than to assess differences of specific, rather similar products in detail. This would imply a larger usefulness of LCA to support strategic compared to operational decisions. However, there is still a need to analyze the influence of reduced correlations on the magnitude of uncertainty, concerning such fundamentally different scenarios.

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