A statistical approach to deal with uncertainty due to the choice of allocation methods in LCA

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Unresolved debates on the application of allocation methods constitute a major source of uncertainty in Life Cycle Assessment (LCA) results. Some ways to deal with this issue are standardization, sensitivity analysis and scenario modeling. Standardization reduces uncertainty, while the latter two methods serve to analyze the system using one allocation at a time in order to show a range of possible outcomes. However, the full range of outcomes given all possible choices has never been shown. This can be misleading when evaluating the environmental impacts of a production system, particularly when comparing two systems. We investigate the use of Monte-Carlo simulations as a statistical approach for analyzing uncertainty propagation to the LCA outcomes, depending on the choice of allocation method. In this approach, a probability of occurrence is assigned to each allocation method, for each multi-functional process in the system. The allocation methods are sampled according to the probability of occurrence using Monte-Carlo simulations. The range and frequency of LCI outcomes was analyzed with and without this approach, including data uncertainty in both cases. The LCI results show the influence of many possible allocation choices and combinations in a system besides the influence of data uncertainty. Further implementation for more complex systems and broader LCI and LCIA outcomes is required.

Keywords: uncertainty in LCA, allocation, data, Monte-Carlo

1. Introduction

Methodological choices in all phases of Life Cycle Assessment (LCA) are unavoidable and are a potential source of uncertainty. A typical example of such choices is the choice between different methods to solve multi-functionality of unit processes. Generally, practitioners choose ambiguously between the following three types of methods to solve this issue: substitution (avoided burden), system expansion or partitioning, and within partitioning between different principles, e.g., mass, energy, or economic value[1]. This ambiguous choice could be a major source of uncertainty in LCA results since, as mentioned by Guinée et al. (2004): *"... it is impossible to have an ultimate best solution accepted by everybody for a problem that is an artefact of wishing to isolate one function out of many"*. In fact, several studies have shown the influence of the choice of allocation method in the dispersion of LCA results and e.g. policy implications (van der Voet et al. 2010; Wardenaar et al. 2012), and this is one of the reasons why ways to deal with uncertainty due to the choice of allocation method have been a key topic of discussion and development in the LCA arena in recent years.

Until today, the main approaches for accounting for uncertainty introduced to LCA results by the choice of allocation method include: standardization, critical reviews (peer review), sensitivity analysis, and scenario modelling (Björklund 2002). Standardization refers to consensus seeking on which allocation methods to use, and which procedures to follow if multi-functionality is encountered in LCA. Uncertainty due to allocation choices is reduced with standardization, but it does not explicitly lead to LCA results that account for uncertainty due to the choice made. In 1998, ISO (International Standardization Organization) provided guidelines to solve multi-functionality[2] (ISO 2006), which have become more widely applied by practitioners nowadays.

Another method to account for uncertainty due to the choice of allocation methods is sensitivity analysis. This method studies the influence that input parameters (independent) have on output parameters (dependent) (Björklund 2002). A sensitivity analysis that shows the influence of the choice of allocation method (independent parameter) on the LCA outcomes e.g. as Life Cycle Inventory (LCI) or as Life Cycle Impact Assessment (LCIA), is usually implemented by means of scenarios using different allocation methods. This type of sensitivity analysis approach is applied by most LCA practitioners and is referred to as scenario analysis (Björklund

[1] From this point on substitution, system expansion and partitioning (including different principles) are referred to as allocation methods

[2] ISO guidelines for allocation procedure are as follows: first, allocation should be avoided by substitution or system expansion where possible; second, where avoiding allocation is not possible physical partitioning should be applied and where this is not possible economic allocation should be applied. ISO also requires a sensitivity analysis where more than one allocation method seems applicable.

2002). Scenario analysis is still ambiguously defined in LCA because the scenarios design, i.e. which allocation methods to choose and for which multi-functional processes, remains vague and leaves room for debate.

Beside uncertainty introduced by methodological choices, other sources of uncertainty exist in LCA and perhaps the most recognized and addressed one is data uncertainty (Björklund 2002). Data uncertainty at the unit process level has three sources of uncertainty according to Henriksson et al. (2013): representativeness, inherent uncertainty and spread due to averaging of data. The authors developed a practical protocol quantifying the total dispersion of unit process data due to these three uncertainty sources. The explicit description of the input parameters, using distributions, mean values and standard deviations, is systematically facilitated by the protocol of Henriksson et al. (2013), which goes beyond the post-normal pedigree matrix based treatment of data uncertainty in LCA (Weidema & Wesnæs 1996; Funtowicz & Ravetz 1990).

Subsequently, a method has to be selected to propagate these data uncertainties into output uncertainties through the LCA model. For this, several methods exist and have been used in LCA (Heijungs & Lenzen 2014). Among the most popular ones are statistical methods, which include sampling methods such as Monte Carlo (MC) simulations. MC is becoming more and more commonly used in LCA, as it relies on computing capacity, which has increased in time (Heijungs & Huijbregts 2004). Other methods have also been studied, such as analytical uncertainty propagation using e.g. Taylor series expansions. Taylor expansions and analytical methods have been found to lead to similar results as MC simulations, while providing the contribution to uncertainty from each parameter and strongly reducing calculation time (Hong et al. (2010), Heijungs et al. (2005)). Nonetheless, more recently (Heijungs & Lenzen 2014) showed that both analytical and sampling methods are equally important and required for a good analysis, particularly sampling methods when uncertainties are large.

Analytical propagation of uncertainty for allocation factors was developed by Jung et al. (2013). The authors developed a method integrating allocation factors in matrix based LCA calculations and propagating the uncertainty in allocation factors to the LCA outcomes. In other words, the choice for an allocation method is made, but the factors themselves are described as uncertain input parameters leading to uncertainty in the LCA outputs. This method described by Jung et al. (2013) to address uncertainty in allocation factors and in data together is the most recent attempt in literature to deal with both sources of uncertainty together and uses an analytical method for propagation of uncertainty to LCI and LCIA results, i.e. a first-order approximation.

Despite these efforts to deal with data related and allocation related uncertainties, no statistical sampling method exists yet, to our knowledge, to simultaneously propagate through LCA, uncertainties due to data and to the choice of allocation methods. The aim of this study was to develop such a method, so that it can be used in LCA calculations and software. This study uses the CMLCA software as a testing software and implements an illustrative simple case study. Finally, we will simultaneously explore spread of LCI results when propagating uncertainty due to the choice of allocation method and due to unit process data uncertainties using MC simulations.

2. Methods

2.1. Uncertainty sources and propagation methods

Focusing on unit process and allocation uncertainties, we can distinguish the following sources of uncertainty: i. uncertainty in data at the unit process level (covering representativeness, inherent uncertainty and spread); ii. uncertain allocation factors per se (e.g. fluctuating prices lead to uncertain allocation factors for economic value allocation) and iii. choice of allocation methods (substitution, system expansion or partitioning). The main methods for propagating these uncertainty sources into LCA outcomes are: a) scenario analysis, b) analytical methods and c) sampling methods.

Table 1 shows the field of options that results from combining the previously described uncertainty sources and propagation methods. The table also shows some of the studies that have addressed particular sources with particular methods and combinations of both. Table 1 indicates that there are many studies that deal with allocation choices by applying scenario analysis, and that there are no studies that propagate uncertainty due to the choice of allocation method in an analytical way (perhaps because of its impossibility) and finally, that this study is the first one propagating uncertainties due to data and to the choice of allocation method in a simultaneous way.

Table 1. Field of options and examples of literature studies combining different propagation or analysis methods for addressing selected sources of uncertainty in LCA

Propagation / analysis method / **Uncertainty source**	**a) Sensitivity Analysis / scenario Analysis**	**b) Analytical Methods**	**c) Sampling Methods**
i. Unit process data	e.g. Middelaar et al. (2012) van der Harst & Potting (2014)	e.g. Heijungs et al. (2005) Hong et al. (2010) Imbeault-Tétreault et al. (2013) Jung et al. (2013)	e.g. Guo & Murphy, (2012) Gregory et al. (2013) Imbeault-Tétreault et al., (2013) Sonnemann et al. (2003) ***This Study (Option 2 and 3)***
ii. Allocation factors	e.g. Ardente & Cellura (2012) Huppes (1993)	e.g. Jung et al., (2013)	-
iii. Choice of allocation method + principles	e.g. Ardente & Cellura (2012) Ayer, N.W. et al. (2007) González-García et al. (2012) Jeroen B Guinée & Heijungs (2007) Heijungs & Jeroen B Guinée (2007) van der Harst & Potting (2014) Luo et al. (2009) Svanes et al. (2011) Wardenaar et al. (2012) ***This study (Option 1 and 2)***	-	***This study (Option 3)***

The options we analyze in this study are the following:

Option 1: Scenario analysis for different allocation methods without statistical propagation for data uncertainty

This option consists of the classic scenario analysis to evaluate the influence of the allocation method on the LCA results. In this case, no data uncertainty is considered and only different allocation methods are applied to some multi-functional processes in the system, resulting in scenarios with punctual values for LCI outcomes given different allocation methods chosen for the calculations. For a large system with several multi-functional processes, it is unrealistic to analyze all the possible scenarios. The total number of scenarios is equal to a^n, where *n* is the number of multi-functional processes in the system and *a* is the number of allocation methods possible per process. Usually, LCA practitioners undertake a contribution analysis to help them decide which processes to analyze further and then they only create scenarios for the most important multifunctional processes, thereby significantly reducing the amount of scenarios. However, this approach can be misleading as the multi-functional process itself may have no direct emissions, but still have a big influence on the LCA results via upstream inputs.

Option 2: Scenario analysis for fixed allocation settings with statistical propagation for data uncertainty

Data at the process level is uncertain. In this option, we will apply the protocol of Henriksson et al. (2013) to quantify unit process data dispersions due to inherent uncertainty, unrepresentativeness and spread, and derive data distributions to be used as input parameters for the LCA model. Furthermore, we use MC simulations as a propagating method of the unit process data uncertainties and calculate LCI results based on the MC simulations outputs. For the choice of allocation method, fixed choices are specified, as is done in the scenario analysis.

Option 3: Statistical propagation for choice of allocation method and data uncertainty

This option propagates both data and choice of allocation uncertainties simultaneously, using MC simulations based on data distributions as in option 2 and probabilities of occurrence for the choice of allocation method as will be described in section 2.2. This option represents the novel contribution of this study. We will illustrate the possible advantages of this new method by showing the outcomes of the options described above for a simplified agricultural system i.e. rapeseed oil production in Northern Europe.

2.2. Implementation of a statistical propagation method for uncertainty due to the choice of allocation method in this study

For a multi-functional unit process, several *allocation methods* can be applied in order to solve multi-functionality. For partitioning-type of allocation methods, *allocation factors* are defined as the fraction that divides the non-functional economic and environmental flows to the functional flows (i.e. the co-products) of a multi-functional process (Guinée et al. 2004). For each *multi-functional unit process* in the system, allocation factors are defined to be able to solve the matrix algebra (Heijungs & Suh, 2002) behind LCA modeling. Typically, the sum of all allocation factors for each allocation method is equal to 1. This is, in very general terms, the normal parameter definition for partitioning type of methods using different principles such as mass, energy content and economic allocation. For substitution type of allocation, equivalent flows are found for the co-product to be substituted by another product(s), as well as the ratio of substitution.

In this study we introduce a parameter named the *probability of occurrence* (*p*) (as a percentage) for each allocation method which ranges from 0 to 100% and which sum for all *p*-values equals 100%. This means that for each multi-functional process, possible allocation methods are: method 1, 2, 3, 4 etc., which have an associated p_1, p_2, p_3, p_4 etc. percentage of occurrence between 0 and 100% and all together add up to 100%. Together they describe *ranges of occurrence* for each method i.e. from 0 to p_1 for method 1, from p_1 to $p_1 + p_2$ for method 2, from $p_1 + p_2$ to $p_1 + p_2 + p_3$ for method 3, until from $p_1 + p_2 + p_3 + p_a$ to 1 for method a.

In principle, to propagate the uncertainty due to the choice of allocation method through the LCA model into the LCA outcomes, a random real number R is taken from a continuous uniform distribution U (0,100), each time a multi-functional unit process is encountered in the calculation of the system, for every Monte Carlo simulation. This value (R) is evaluated for the ranges of occurrence, and this is how the allocation method and factors are defined for each individual simulation. If for example four allocation methods are defined for a specific multi-functional process*:*

$$
\begin{array}{rcl}
 & R \sim U(0{,}100) & \\
0 \le R \le p_1 & \Rightarrow & \text{use allocation method 1} \\
p_1 < R \le p_1 + p_2 & \Rightarrow & \text{use allocation method 2} \\
p_1 + p_2 < R \le p_1 + p_2 + p_3 & \Rightarrow & \text{use allocation method 3} \\
p_1 + p_2 + p_3 < R \le 100 & \Rightarrow & \text{use allocation method 4}
\end{array}
$$

By repeating the evaluation of R for a large number of runs, for example using MC simulations, several choices for an allocation method for each multi-functional process are taken into account, leading to the propagation of uncertainty due to the choice of allocation method to the LCA results. In each single MC simulation the allocation method for each unit process is selected using the ranges of occurrence for each method, and the results are calculated using such choice. The higher the sample the more combinations of allocation choices are taken into account in the results.

When analyzing a system with a relative large number of multi-functional processes the previously described propagation method becomes very powerful, as a large amount of scenarios can be reproduced minimizing the amount of inputs. For example, if the number of multi-functional processes is 10 and two allocation methods are possible for each process, then 1024 combinations exist if all allocation methods are combined for all multi-functional processes. A complete scenario analysis should show the outcomes for all the combinations. However, that is rarely the case in LCAs as it is a very time consuming process. With the proposed method 1024 combinations can be covered while defining the ranges of occurrence for each method per unit process only one time.

An example of the input parameters necessary for the method to propagate uncertainty due to the choice of allocation method as was described are shown in Table 2. For one multi-functional process four allocation methods are displayed in Table 2. These are the methods currently implemented in CMLCA. For each method the corresponding allocation factors for each co-product are shown. The sum of these factors for one method is equal to 1. For example, partitioning-2, has allocation factors 0.7 and 0.3 for co-product one and two of this example multi-functional unit process. Furthermore, the percentage of occurrence for each method is also defined. For the example, substitution occurs 2.5%, surplus 2.5%, partitioning-1 25% and partitioning-2 70%. Together the percentage of occurrence for the four allocation methods adds up to 100% as well. Thus, the ranges of occurrence for each allocation method in the example of Table 2 are: from 0 to 2.5% substitution, from 2.5% to 5% surplus, from 5% to 30% partitioning-1 and from 30% to 100% partitioning-2.

Table 2. Parameters for different allocation methods for a multi-functional unit process. This table displays the allocation methods implemented in the CMLCA software only

	One Multi-functional Unit Process			
Allocation Method	**Co-product**	**Allocation Example**	**% of occurrence (*p*)**	**Example**
1.Substitution	Co-product 1	1 kg rapeseed cake replaced by 1.5 kg peas	P_1	2.5%
	Co-product 2	-		
2.Surplus	Co-product 1	0	P_2	2.5%
	Co-product 2	1		
3.Partitioning-1	Co-product 1	0.55	P_3	25%
	Co-product 2	0.45		
4.Partitioning-2	Co-product 1	0.7	P_4	70%
	Co-product 2	0.3		
a. Allocation method	Co-product 1	C_1	P_a	P_a %
	Co-product 2	C_2		
	Co-product Y	$1-C_1-C_2$		

2.3. Illustrative case study

We have implemented in CMLCA version beta 5.2 a simple system: Rapeseed Oil production in Northern Europe, similar to Wardenaar et al., (2012). We focus on three key processes (1) cultivation, (2) transport to mill and (3) rapeseed oil extractions by cold pressing of rapeseed. Process one produces straw and rapeseed and process three rapeseed oil and rapeseed cake. Thus both processes are multi-functional and require allocation between the co-products. The system is described in Figure 1. The functional unit is 1 kg of rapeseed oil at mill and the system includes the production, storage and transport of the main inputs to these three key processes. For the description of the background processes, ecoinvent data from version 2.2 is used (http://www.ecoinvent.org/database/). Also, background processes are assumed to be allocated as done by the ecoinvent database and this assumption remain constant for all the options analyzed in this study.

For the two multi-functional processes, we assume two allocation methods are applicable i.e. surplus and mass for rapeseed cultivation and energy content and economic values for oil extraction. The allocation parameters defined for the case study are shown in Table 3. For *option 1* we use the four combinations possible using two multi-functional processes with two allocation methods each. This leads to four fixed allocation scenarios (Table 3) and the LCI results of this option are presented as point values given that no data uncertainty is assumed. For *option 2* we use the same fixed allocation scenarios as option 1, but in this case data uncertainties are propagated to LCI outcomes with MC simulations. We used a sample size of 700 simulations for the four fixed allocation scenarios. Table 3 shows that the percentage of occurrence assigned to each method is equal to 100, simply because choosing for one method corresponds to 100% probability of occurrence of that method, according to the method described in section 2.2. This holds for both options 1 and 2. Finally, for *option 3* we use 50% probability of occurrence of the allocation methods in both multi-functional processes, because this allows an equal chance of occurrence for all the methods. We ran option 3 for 2000 MC simulations which is different than the number of simulations in option 2 a choice made for practical reasons.

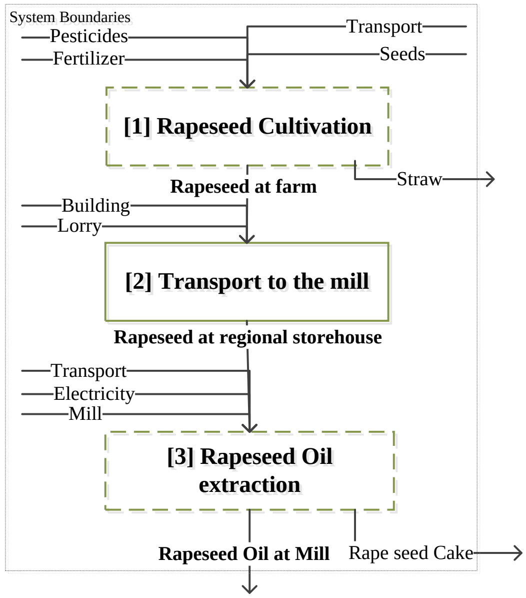

Figure 1. System for rapeseed oil production in Northern Europe. Boxes represent processes, dashed boxes are multi-functional.

Table 3. Allocation factors and probability of occurrence of each allocation methods for the two multi-functional processes in the rapeseed oil production system

	Multi-functional Process		Probability of occurrence p (%) for the different options				
	[1] Rapeseed cultivation		Option 1(no data uncertainty) and 2 (with data uncertainty, 700 MC)				Option 3 (data + choice of allocation method uncertainty)
Allocation Method	**Co-product**	**Allocation factor**	**Fixed Allocation1**	**Fixed Allocation2**	**Fixed Allocation3**	**Fixed Allocation4**	**2000 MC**
Surplus	Straw	0	100	0	0	100	50
	Rapeseed	1					
Mass	Straw	0.43	0	100	100	0	50
	Rapeseed	0.57					
	[3] Rapeseed oil extraction						
Energy Content	Rapeseed Oil	0.55	100	100	0	0	50
	Rapeseed Cake	0.45					
Economic value	Rapeseed Oil	0.7	0	0	100	100	50
	Rapeseed Cake	0.3					

3. Results

Results for option 1 are given in Table 4 and for option 2 and 3 in Figure 2. Option 1 shows the LCA results for a scenario analysis for different allocation methods without statistical propagation for data uncertainty. The results presented in Table 4 only show carbon dioxide emissions to air per kg of rapeseed oil at mill for the four fixed allocation scenarios. Emissions range from 0.7 to 1.19 kg CO_2 / kg of rapeseed oil depending on the allocation settings chosen for the two multi-functional processes under study. As expected, for those allocation scenarios in which rapeseed and rapeseed oil get a higher allocation factor (fixed allocation 1 and 4), the emissions per kg of rapeseed oil are higher.

Table 4. Carbon dioxide emissions to air per kg of rapeseed oil for fixed allocation (Table 3) and no data uncertainty propagation (Option 1)

Allocation Settings	CO_2 (kg CO_2 / kg of rapeseed)
FixedAllocation1	0,94
FixedAllocation2	0,70
FixedAllocation3	0,89
FixedAllocation4	1,19

Figure 2 shows a series of histograms that corresponds to the results for carbon dioxide emissions to air for option 2 and 3. The outcomes for option 2 correspond to the histograms for the four possible fixed allocation combinations with statistical propagation for data uncertainty (i.e. dashed lines in Figure 2). The outcomes for option 3 correspond to the histogram including statistical propagation of the choice of allocation method together with statistical propagation of data uncertainty (i.e. continuous line in Figure 2).

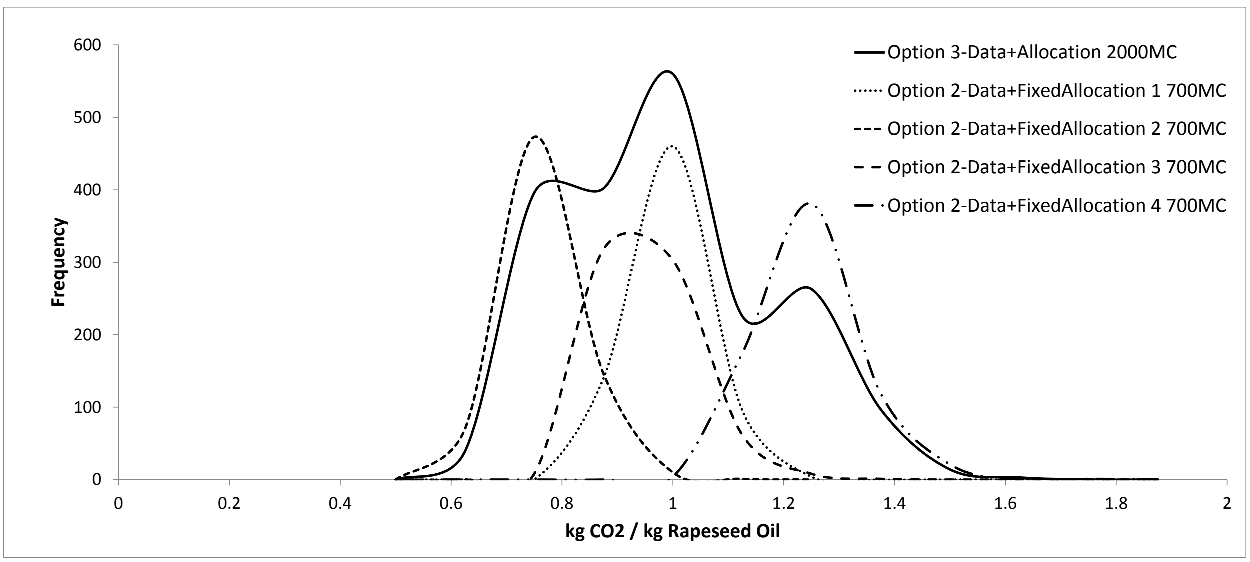

Figure 2. LCI results for carbon dioxide emissions to air per kg of rapeseed oil under four fixed allocation settings (Table 3) and for random allocation choice using MC simulations to propagate uncertainty

4. Discussion

The method presented here to simultaneously propagate uncertainties in data and due to the choice of allocation methods through an LCA, is based on the introduction of the probability of occurrence of each allocation method for a multi-functional process. This parameter can be used by assigning equal probability of occurrence to all allocation methods for a multi-functional process, as shown in the illustrative case of this study. Assuming this, helps to propagate, with equal chances, the uncertainty around the fact that one can choose for different allocation methods in different multi-functional processes. Therefore, assigning equal probability of occurrence to the allocation method per process, is expected to have an influence on the size of the peaks of the histograms i.e. the frequencies with which an outcome is observed, but not on the ranges of the outcomes. The shape of the histograms also depends on the sample size of the MC simulations which at the end determines the distributions of the LCI results.

Also, the use of this parameter allows a full statistical propagation of uncertainty with a large sample size to make sure all methods are sampled more or less equally. It can be argued, nevertheless, that this method could be intensive in terms of computing capacity requirements as it uses MC simulations as a propagating method. Analytical methods do not yet exist - despite recent efforts in the field -, which could be a less computing intensive alternative to MC simulations as proposed in this study, for propagation of the choice of allocation methods if possible at all.

The results showed how scenario analysis for allocating different multi-functional processes in order to explore the dispersion of the LCI outcomes i.e. option 2, leads to a similar range of outcomes for carbon dioxide emissions to air than option 3 which takes into account data uncertainty and allocation choice simultaneously in MC simulations. This is an indication of the strength of the method presented here that allows capturing in LCI results the influence of all possible allocation choices in a system next to the influence of data uncertainty without actually making an explicit choice for one or another method per process. Also, showing the likelihood for which an outcome can be expected given many possible combinations of input parameters and allocation methods for a specific system is another strength of the proposed method. Besides, both option 2 and 3, lead to a broader range of CO_2 emissions than when no data uncertainty is taken into account in the LCA, showing the importance of accounting for data uncertainty as emphatically pointed out by many other studies.

Further research is required to evaluate the method shown here for systems with a large number of multi-functional processes and broader LCI outcomes too. Finally, in the future, the method could be expanded to deal with uncertainties due to other sources not yet addressed in this study.

5. Conclusion

Unresolved debates on the application of allocation methods constitute a major source of uncertainty in LCA results. The full range of outcomes given all possible choices for allocation methods and combinations in a system with several multi-functional unit processes is hardly shown.

We propose the use of Monte-Carlo simulations as a statistical approach to simultaneously propagate uncertainties due to data and to the choice of allocation methods to LCA outcomes. For this purpose the probability of occurrence was introduced and assigned to each allocation method, for each multi-functional process in a system.

The distribution of LCI outcomes was analyzed with and without the previous approach and in both cases including data uncertainty and we conclude that the proposed method enables, in a relatively simple way i.e. with few additional parameters definition and modest computational calculation capacity, to propagate uncertainties due to the choice in allocation method and data uncertainty to the LCA results while not requiring an actual choice for one or another allocation method. Further implementation for more complex systems is required.

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