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Stochastic and epistemic uncertainty propagation in LCA

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Abstract

Purpose: When performing uncertainty propagation, most LCA practitioners choose to represent uncertainties by single probability distributions and to propagate them using stochastic methods. However the selection of single probability distributions appears often arbitrary when faced with scarce information or expert judgement (epistemic uncertainty). Possibility theory has been developed over the last decades to address this problem. The objective of this study is to present a methodology that combines probability and possibility theories to represent stochastic and epistemic uncertainties in a consistent manner and apply it to LCA. A case study is used to show the uncertainty propagation performed with the proposed method and compare it to propagation performed using probability and possibility theories alone.

Methods: Basic knowledge on the probability theory is first recalled, followed by a detailed description of epistemic uncertainty representation using fuzzy intervals. The propagation methods used are the Monte Carlo analysis for probability distribution and an optimisation on alpha-cuts for fuzzy intervals. The proposed method (noted IRS) generalizes the process of random sampling to probability distributions as well as fuzzy intervals, thus making the simultaneous use of both representations possible.

Results and discussion: The results highlight the fundamental difference between the probabilistic and possibilistic representations: while the Monte Carlo analysis generates a single probability distribution, the IRS method yields a family of probability distributions bounded by an upper and a lower distribution. The distance between these two bounds is the consequence of the incomplete character of information pertaining to certain parameters. In a real situation, an excessive distance between these two bounds might motivate the decision-maker to increase the information base regarding certain critical parameters, in order to reduce the uncertainty. Such a decision could not ensue from a purely probabilistic calculation based on subjective (postulated) distributions (despite lack of information), because there is no way of distinguishing, in the variability of the calculated result, what comes from true randomness and what comes from incomplete information.

Conclusions: The method presented offers the advantage of putting the focus on the information rather than deciding a priori of how to represent it. If the information is rich, then a purely statistical representation mode is adequate, but if the information is scarce, then it may be better conveyed by possibility distributions.

Keywords: Uncertainty representation, uncertainty propagation, probability, possibility, distribution, fuzzy sets, intervals, confidence index

1. Introduction

Life cycle assessment (LCA) aims at modelling complex systems that usually encompass a number of compartments of the biosphere and the technosphere. Results rely on several choices and large amounts of data are affected by uncertainty. These uncertainties have been described extensively, e.g. by Reap et al. (2008) and Williams et al. (2009). Characterising and assessing uncertainties is important to make decision support models more transparent, robust and reliable. Uncertainty analysis gathers numerous methods with different means and goals from qualitative assessment to sensitivity analysis and uncertainty propagation; see Morgan and Henrion (1990) for an overview on uncertainty analysis and Clavreul et al. (2012) for a tiered approach to uncertainty analysis in LCA applied to waste management.

The focus of the present study is on uncertainty propagation which aims at quantifying the uncertainty of the results of an LCA study. Uncertainty propagation can be performed using different uncertainty representations and propagation methods. With respect to parameter uncertainty, the common practice in LCA consists in representing uncertain parameters by single probability distributions, e.g. a normal distribution characterized by an average and a standard deviation. Databases such as the ecoinvent database (Frischknecht et al. 2005) rely increasingly on probability distributions to represent parameter uncertainty. The most commonly-used method to propagate probability distributions is the Monte Carlo analysis, as shown by Lloyd and Ries (2007) who reviewed 24 LCA studies that included uncertainty analysis. This method is implemented in many calculation tools and consists in randomly sampling values in the probability distributions of input parameters, to obtain the frequency distribution of the calculated results.

However, a fundamental problem of the probabilistic representation lies in the selection of probability distributions when faced with scarce information or expert judgement. The review by Lloyd and Ries (2007) showed that the choice of probability distributions is often poorly justified and relying on estimations. Yet the result of the uncertainty propagation is totally depending on the ‘a priori’ defined probability distributions. Bayesian methods (Lindley 1971) could address this shortcoming by updating these prior distributions based on new data and Bayes’ theorem of conditional probabilities. However this is almost never implemented in LCA due to the impossibility of measuring and validating results. This introduces confusion between the two distinct natures of uncertainty: truly stochastic uncertainty which refers to variability of data e.g. in time, space and technology, and epistemic uncertainty related to our lack of knowledge e.g. due to measurement errors or to an insufficient number of measurements. While

classical probability theory was developed to address stochastic uncertainty (i.e. related to variability and fluctuations), more recent information theories are required to address incomplete/imprecise information (Dubois and Prade 2009).

To address this problem and handle modelling in presence of imprecise information, possibility theory has been developed over the last decades (Dubois and Prade 1988). The simplest example is the representation of parameters as min-max intervals instead of crisp (precise) numbers, as used by Chevalier and Le Téno (1996). The concept can be extended to fuzzy intervals (possibility distributions) which express preferences within intervals. More detailed presentation of fuzzy intervals is provided in the methods section. Fuzzy intervals have been first applied to the field of LCA to save time and costs by avoiding the need for precise quantification of flows e.g. by Weckenmann and Schwan (2001) and Gonzàlez et al. (2002). Fuzzy linguistic descriptors have also been used to calculate life cycle inventories (LCI) and evaluate data quality (Ardente et al. 2004), to normalise and weigh characterised impacts (Guereca et al. 2007) and to support interpretation of results and ranking alternatives using multi-criteria analysis (Benetto et al. 2008). Besides, in an LCA model dedicated to fuel evaluation (namely POLCAGE), Tan et al. (2004) represented parameter uncertainties using possibility distributions and propagated them using fuzzy arithmetics. Tan (2008) formalised the integration of fuzzy intervals into a matrix-based LCI model, supported later by a mathematical proof by Heijungs and Tan (2010) re-examined by Cruze et al. (2013). Finally André and Lopes (2012) proposed to enhance the mathematical and physical understanding of the application of possibility theory to LCA, by providing clear definitions of terms and comparing the possibility and probability representations and propagation results.

The objective of this study is to present a methodology that combines probability and possibility theories to represent stochastic and epistemic uncertainty in a consistent manner, and apply it to LCA. The method is compared to uncertainty propagation performed with probability and possibility theories alone, using a case study where global warming benefits associated with bioenergy from energy crops cultivation are assessed.

2. Methods

This section describes how probability and possibility theories can be used to represent uncertainties and propagate them through a model. A joint-propagation method, proposed by Baudrit et al. (2006), is

presented and applied to a case study. In addition two other propagation methods are also applied for the purpose of comparison.

2.1. Probability theory

A probability is a measure of the likelihood that an event will occur. A probability distribution describes the probabilities of different outcomes of a statistical experience: for a random variable X, a probability distribution gives for each value x the probability P(x) that X takes the value x. Probabilities follow certain rules: they take only values between 0 and 1 and the sum of the probabilities of all possible outcomes is 1. In the case of continuous variables, probability distributions are often represented by their cumulative distribution function (cdf), the probability that X be less than x: $F(X) = P[X \leq x]$. Another representation, the probability density function (noted here pdf), can be obtained by deriving the cdf. It represents the density of probabilities: for some small increment Δx, $f(x).\Delta x$ is the probability that X falls in the interval of length Δx around x (Morgan and Henrion 1990). In theory, selection of a probability distribution should be based on a sufficient amount of data to allow a statistically representative assessment of the parameter's variability. However, in the context of LCA, this is often not technically feasible and the selection of a distribution often relies on partial information (scarce measurements) or on expert judgment.

Uncertainty propagation of probability distributions can be performed by different methods, the most common one being the Monte Carlo analysis, as used by e.g. Huijbregts et al. (2003) or Sonnemann et al. (2003). In this analysis, a value is randomly sampled for each parameter in its distribution and by using the obtained set of values, the model result is calculated. By repeating this operation a sufficient number of times, a cdf is obtained for the result. Other sampling methods are more adapted to large data sets, such as Latin hypercube, as used by Thabrew et al. (2008). Finally, calculations can also be performed analytically using Taylor series expansions to approximate the result's uncertainty, as implemented by Hong et al. (2010) and Imbeault-Tétreault et al. (2013).

2.2. Epistemic uncertainty representation

As shown by several authors (e.g. Ferson and Ginzburg 1996), there is a fundamental difference between true random variability, as depicted by a single probability distribution, and epistemic uncertainty, due to incomplete or imprecise information. Possibility theory (e.g. Dubois and Prade 2008) provides a framework to address this type of information. Possibility theory assigns degrees of likelihood

(possibility) to intervals of values rather than precise values, yielding a fuzzy interval (or fuzzy number or fuzzy set). The simplest fuzzy interval is the well known min-max interval. If the parameters involved in a model are represented by intervals, interval propagation can be performed using either interval calculus in the case of simple models or else an optimisation algorithm in the case of more complex models. In a Bayesian framework, application of the principle of maximum entropy to interval-type information leads to selecting a uniform probability distribution between the limits of a min-max interval (e.g. Shulman and Feder 2004). But this results in selecting only one distribution amongst all the possible probability distributions bounded by the following two cumulative distributions:

$$P_u(X) = 0 \text{ if } X < \min \text{ and } P_u(X) = 1 \text{ otherwise,}$$

$$P_l(X) = 0 \text{ if } X \leq \max \text{ and } P_l(X) = 1 \text{ otherwise.}$$

Where P_u and P_l are the upper and lower limits of the family of probability distributions defined by the min-max interval. Selecting just one representative of the family of probability distributions introduces a bias in the analysis and a confusion between true variability (as depicted by a single distribution) and imprecision (as depicted by an interval).

When richer information is available, the concept of intervals can be extended to fuzzy intervals (also called possibility distributions) where preference is given to certain values (see Dubois and Prade 1988). In a possibility distribution, degrees of likelihood (possibility) between 0 and 1 are assigned to specific parameter intervals. In the example depicted in Figure 1, the most likely interval (the “core” of the possibility distribution), i.e. values between 18 and 20, is assigned a likelihood of unity, while values located outside the “support” of the distribution (i.e. values between 14 and 23) are assigned a possibility of zero. Intervals selected at different levels of possibility, called alpha-cuts, correspond to confidence intervals with confidence 1-alpha. Thus a possibility distribution yields a lower bound ($P_\alpha \geq 1- \alpha$) on the probability that the parameter value should lie within a given alpha-cut. As in the case of the simple min-max interval, a fuzzy interval can be depicted as a family of probability distributions, limited by an upper and a lower cdf, as shown in Figure 1. While the function presented in Figure 1 is a trapezoidal distribution, more complex distributions can be adopted to suit available information (See Dubois and Prade 1988). Fuzzy intervals are particularly well suited for representing subjective judgements, commonly used in most LCA studies, because they adopt the language of experts, when describing the possible values a parameter can take in presence of incomplete information (Dubois 2006). If an expert is able to answer the following two questions: (i) can you provide a range within which you are confident

that the parameter value should lie? and (ii) can you express a preferred value or interval of values within this range? Then the provided information can be formalized as a possibility distribution.

2.3. Propagation methods

The method used to propagate fuzzy intervals in the general case is very analogous to the Monte Carlo method using single probability distributions, except that in the case of parameters represented by fuzzy intervals, intervals are randomly sampled instead of single values, based on α-cuts. As shown above, for a given possibility distribution, an alpha-cut is an interval containing all values with a degree of possibility higher than alpha ($0 \leq \alpha \leq 1$). An example of α-cut is presented in Figure 1: for alpha=0.6 the α-cut is the interval [16.4; 20.9]. If the model is relatively simple and monotonous, propagation of the fuzzy intervals through the model can be performed simply using interval calculus on alpha-cuts. For alpha = 0 to 1 with e.g. step = 0.1, the min and max values of the model are determined for all values of the alpha-cuts. However, if the model is not monotonous, it may not be possible to determine the min and max values of the model based solely on the min and max values of the alpha-cuts. In this case it is necessary to use an optimization algorithm to find the min and max values of the model for all parameter values within the alpha-cuts.

If certain parameters are represented by fuzzy intervals while others are represented as single cdfs, the Monte Carlo method can be used to randomly sample the cdfs, while optimization on the alpha-cuts is performed in a second step (see Guyonnet et al. 2003 and Baudrit et al. 2005). Baudrit et al. (2006) developed a slightly different method (dubbed the IRS; Independent Random Set method), whereby random sampling is performed on both the cdfs and the fuzzy intervals. Couso et al. (2000) showed that the IRS method is a systematically conservative counterpart to the calculation with random quantities under stochastic independence (classical Monte Carlo method on cdfs). The schematic of the IRS method, used herein, is the following.

Given an LCA model with n parameters represented by probability distributions and m parameters represented by fuzzy intervals,

1. Generate n + m random numbers between 0 and 1: $x_1, x_2, ...x_{n+m}$.
2. Sample the n probability distributions to obtain n random variables: $p_1, p_2... p_n$.
3. Sample the m fuzzy intervals to obtain m intervals: $I_1, I_2... I_m$.
4. Calculate the smallest (Inf) and largest (Sup) values of the LCA result obtained for all combinations of values contained in the m intervals I_i.

5. Return to step 1 and repeat ω times.
6. Obtain the probability bounds of the LCA results from the ω Inf and Sup values as shown below.

The IRS method yields a random interval made up of ω intervals. This random interval is then summarized in the form of a pair of upper and lower cdf (see Baudrit et al. 2005) using the Plausibility and Belief functions of the theory of evidence (Shafer 1976). This theory assigns probability weights (noted m) to intervals (called focal sets; A_i) instead of simply point values (the limiting case of a classical probability distribution). Considering the proposal (noted B) "LCA result lies below a specified target level", the probability that this proposal is true is comprised between the degree of Plausibility (an upper bound on probability) and the degree of Belief (a lower bound on probability) defined by Shafer (1976) as:

$$Bel(B) = \sum_{i:A_i \subseteq B} m(A_i) \quad \text{and} \quad Pl(B) = \sum_{i:A_i \cap B \neq 0} m(A_i) \qquad (1)$$

Bel(B) is thus the sum of the weights of all subsets A_i (i = 1 to n where n is the number of subsets) such that A_i is completely included within prescribed set B, while Pl(B) is the sum of the weights of all subsets A_i such that the intersection of A_i and B is non empty. In other words, Bel(B) gathers the imprecise evidence that asserts B, while Pl(B) gathers the imprecise evidence that does not contradict B. The interval [Bel(B), Pl(B)] contains all potential probability values induced by the mass function m. In practice, Pl is obtained by ordering the ω Inf values in increasing order, and assigning a frequency 1/ω to each value. while Bel is obtained likewise from the Sup values. These functions will be depicted graphically in the application section below.

2.4. Interpretation of results in a decision-making framework

If at least one parameter in a model is represented by a fuzzy interval, the uncertainty propagation will result in a family of probability distributions (delimited by the Pl and Bel functions described previously), rather than in a unique probability distribution. As suggested by Dubois and Guyonnet (2011), this may prove impractical in a decision-making framework. These authors therefore propose to compute a single distribution as a weighted average of the upper and lower distributions, with the selected weight reflecting the decision-makers attitude with respect to risk. The resulting distribution, referred to as a "confidence index" by Dubois and Guyonnet (2011), is computed from:

$$f(a_i, b_i) = \alpha\, a_i + (1 - \alpha)\, b_i \qquad (2)$$

where a_i and b_i are the limits of the interval defined at probability level i.

This approach, which is based on earlier work by Hurwicz (1951), thus computes a single indicator as a weighted average of focal element bounds. It achieves a trade-off between upper and lower probability bounds which, following the context, will constitute either optimistic or pessimistic estimates. While it is recognized that the choice of weight α is subjective, it should be underlined that this subjectivity is only introduced at the decision-making step in the form of a single cdf used as a sensible reference displayed along with the pessimistic and optimistic outputs. This approach is very different from displaying a single distribution obtained by propagating single distributions selected arbitrarily at the beginning of the risk analysis step.

3. Case study

3.1. Goal and scope

The objective of this LCA study is to exemplify and apply uncertainty propagation using different hypotheses with respect to input parameter uncertainty, for the purpose of comparison. To this end, a specific LCA case study was selected in order to show the differences between the probability and possibility theories and how they can be combined in order to better represent uncertainties in LCA. The selected case study investigated the environmental sustainability of willow cultivation for bioenergy production through co-firing in large-scale combined heat and power (CHP) plants, based on results from Tonini et al. (2012) (see section 3.2). Emphasis was placed on how the different uncertainties associated with the inventory data can be represented based on available knowledge (e.g. from measurements, literature or expert estimates). The uncertainty associated with the environmental impact of the system was quantified with each individual uncertainty method to identify the major differences between them and recommend a best practice. The focus of this study was on the global warming impact category. The functional unit was the cultivation of 1 hectare of Danish land for bioenergy production (CHP). The geographical scope was Denmark and the temporal scope 20 years. Figure 2 presents the processes included in the LCA system boundary.

3.2. Background – case study

Reduction of fossil fuel consumption in the energy sector through increase of fluctuating renewable energy sources (e.g. wind energy and hydropower) and bioenergy is a fundamental step towards more sustainable energy systems (Tonini and Astrup 2012). However, biomass resources available for

bioenergy are limited as biomass is already used today for a number of purposes (e.g. animal feeding and bedding, improvements of agricultural soil, etc.). Thus cultivation of energy crops for bioenergy production may be needed. One of the most critical impacts associated with energy crops is related to land use changes (LUC) defined as the consequences determined by the conversion of the land from one use to another use (Edwards et al. 2010; Searchinger et al. 2008; Searchinger 2010). LUC are distinguished between direct (dLUC) and indirect (iLUC). The dLUC impacts are associated with the consequences of cultivating the selected energy crops in place of an established food crop. The iLUC impacts are related to the consequences of converting land presently not used for crop cultivation to cropland, as a result of the induced demand for the initially displaced food crop. In order to evaluate the environmental sustainability of bioenergy systems, LCA is often used. For instance, in Tonini et al. (2012), a case study based on cultivation of three perennial crops (ryegrass, willow and *Miscanthus*) in Denmark was presented. The authors compared the environmental performance of anaerobic digestion, gasification, direct combustion and co-firing. With respect to global warming, co-firing of willow appeared to be the most environmentally sound option, though CO_2 savings were generally low as a result of LUC.

3.3. Modelling and data

The modelling of the bioenergy system (primarily CO_2 and N_2O flows) was based on the inventory data provided by recent studies: Hamelin et al. 2012 (cultivation of willow and of the marginal crop displaced, i.e. spring barley) and Tonini et al. 2012 (storage, pre-treatments, energy conversion processes and estimates of iLUC). Spring barley was assumed as the marginal crop, i.e. the food crop which would likely react to changes in demand or supply of energy crops (Dalgaard et al. 2008; Schmidt 2008; Weidema 2003). Coal-fired power plants and natural gas-fired power plants were assumed as the marginal technologies for respectively electricity and heat production (Energistyrelsen 2011; Weidema et al. 1999; Weidema 2003). The overall environmental impact on global warming was thus calculated as the sum of the following processes (see Appendix for further details):

I. Cultivation of willow;
II. dLUC, i.e. the impacts/savings associated with the replacement of the marginal crop;
III. iLUC, estimated after Tonini et al. (2012);
IV. Storage, pre-treatments: emission of carbon dioxide;
V. Co-firing: emissions of carbon dioxide;

VI. Avoided energy production (i.e. avoided emissions of GHGs from fossil fuel combustion).

It was assumed that all carbon degradation during drying, storage and combustion was in the form of carbon dioxide (methane emissions were negligible) and machinery-related processes such as fertilizer spreading and tillage were not included because they contribute to the results only to a minor extend (Tonini et al. 2012). Selected modelling data (referred to below as 'parameters') related to CO_2 and N_2O flows throughout the bioenergy system were associated with uncertainty (after Hamelin et al. 2012 and Tonini et al. 2012). The uncertainty representation modes are shown in Table 1. For the purpose of comparison, trapezoidal distributions were selected for both probability density function and fuzzy interval modes of representations. Their supports and cores are respectively delimited by the values [a, d] and [b, c] presented in Table 1, estimated based on the different sources presented. The choice between probability and fuzzy interval representations was made based on the quantity and quality of data available for each individual parameter. For example, Figure 3 shows the 19 values collected in literature and databases for the lower heating value (LHV) of willow. This significant amount of data enabled to define a trapezoidal distribution and to select a representation with probability distributions in the joint-propagation method. Conversely, very scarce information could be found on iLUC; therefore its uncertainty distribution was defined based on expert judgment and the representation using a possibility distribution was preferred in the joint-propagation method.

Further, it is necessary to fix correlations when they are known, in order to avoid non-physical combinations of parameter values during random sampling process. Correlations between the following parameters were identified and implemented:

- Cultivation yield and net carbon uptake for willow,
- Cultivation yield and net carbon uptake for barley,
- Cultivation yields for willow and barley (as they depend highly on soil and climate properties),
- LHV and carbon content of willow.

These correlations were implemented by direct linear correlation: the carbon content was implemented as a function of LHV while net carbon uptakes for willow and barley and the yield of barley cultivation were all implemented as functions of the yield of willow cultivation. Note that a fuzzy correlation could also be implemented, whereby the selection of one parameter generates an interval for the correlated parameter rather than a precise value (see Guyonnet et al. 2003).

Heat and electricity recovery are assumed to be independent because the power plants are considered as extraction condensing power plants. N_2O emissions (both direct and indirect) were considered as independent for willow and spring barley because they are linked to fertilizer use.

4. Results

Uncertainty propagation was performed using the following three methods: Monte Carlo with cdfs, fuzzy calculation and the IRS method. The algorithm and its implementation in MATLAB 7 are provided as supplemental information. In the 2nd and 3rd uncertainty method, minimum and maximum values were calculated using the global search function of MATLAB 7. The cumulative distribution functions of the calculated results are presented in Figure 4. The x-axis shows the impact of the system on global warming: a positive result means that the cultivation and co-combustion of willow contributed to more greenhouse gases emissions than current practice.

The distribution obtained with Monte-Carlo simulation (in full line) suggests a 65% probability that willow cultivation and combustion was beneficial compared to current practice. According to this simulation, the average benefit was -48 Mg CO_2-eq ha^{-1} for 20 years, with a standard deviation of 124 Mg CO_2-eq ha^{-1}, and a 95% confidence interval between -305 and 194 Mg CO_2-eq ha^{-1}.

When implementing the same distributions as fuzzy intervals instead of probability distributions, two curves were obtained: a plausibility and a belief distribution (Figure 4). They are the respective upper and lower limits of the family of probability distributions obtained with fuzzy intervals. In this case study the proposal evaluated was “The impact of willow cultivation for bioenergy production on global warming is below a specific target”. Thus the plausibility distribution represents here the most “optimistic” probability distribution: it is obtained from the most favourable values of input possibility distributions. On the other hand, the belief distribution represents the most “pessimistic” outcome achievable: the impact on global warming cannot be larger than this distribution, considering the input information. The global warming potentials resulting from the fuzzy calculus were between -603 and 400 Mg CO_2-eq ha^{-1} (95% confidence interval) and most likely between -240 and 100 Mg CO_2-eq ha^{-1}. These very wide ranges result from the fact that the rich information available for some parameters was only modelled as fuzzy information in this calculation.

In the third method, either mode of uncertainty representation was selected, based on available information. Two distributions were again obtained, thus defining a family of distributions which again

encompasses the purely probabilistic result. Note that the distance between the upper and lower probability bounds, which directly reflects the incomplete nature of information regarding certain parameters, is less than in the case of the purely possibilistic calculation, because in this case certain parameters are represented by single cdfs.

Also depicted in Figure 4 is the confidence index calculated by assigning a weight of 1/3 to the "optimistic" IRS result and 2/3 to the "pessimistic" result. Putting all the weight on the pessimistic bound would seem exaggerated, as it would be neglecting all information suggesting a more favourable outcome, while putting all the weight on the optimistic bound would appear as unrealistically biased. The selected weights of 1/3 and 2/3 are proposed as a "reasonably conservative" compromise.

5. Discussion

In this study, it was recognized that the level of information was low for 10 out of the 17 parameters (cf. Table 1). The results highlighted the fundamental difference between the probabilistic and possibilistic representations: while the Monte Carlo analysis produces a crisp (precise) result on the probability of exceeding the baseline emissions (represented by a global warming potential of zero in Figure 4), the IRS method yields a family of distributions. When selecting the most favourable assumption for each of the 10 parameters, the probability of exceeding the baseline emissions fell to less than 5%. But when combining all least favourable assumptions, this probability rose to 82%. Note that both cases are fully realistic as the modeller had no a priori knowledge on the variability of these parameters. The choice of deciding between the optimistic and pessimistic assumptions is left to the decision maker at the interpretation stage.

We see that the Monte Carlo method and the Confidence Index yield very similar results at high levels of probability. This is primarily related to the fact that the same distributions were selected for the pdfs and the fuzzy intervals. However, what we see with the IRS result is the consequence of the incomplete character of information pertaining to certain parameters. This is seen in the distance between the upper and lower probability bounds. In a real situation, an excessive distance between these two bounds might motivate the decision-maker to increase the information base regarding certain critical parameters, in order to reduce the uncertainty. Such a decision could not ensue from a purely probabilistic calculation based on subjective distributions (despite lack of information), because there is no way of distinguishing, in the variability of the calculated result, what comes from true randomness and what

comes from incomplete information. Considering the considerable sources of uncertainty in LCA, it is felt that it would be more faithful to convey, in addition to an indicator for decision-making, an appreciation of the extent of the knowledge gaps and their consequences.

This study used a rather simple case study with only one impact category as the focus was put on the methodology. It should be noted that the exact same methodology can be applied at the characterisation, normalisation and weighting steps, e.g. to propagate uncertainties in characterisation factors. It is however acknowledged that the implementation of such a method in complex systems and in LCA software would require substantial computation power. Indeed the calculations involve an optimisation step over several parameters at each run.

6. Conclusions

This paper underlines the difference between different types of uncertainty in the context of LCA modelling and illustrates a methodology that allows such uncertainties to be propagated through the LCA model. Rather than to arbitrarily select a given mode of uncertainty representation, it is proposed that the investigator first considers the information that is available and then selects the formalism that seems best suited to convey this information. This sets the focus on available information and the importance of gathering information that is both reliable and technically feasible, rather than disguising imprecise information as precise variability. If available information is rich, then a purely statistical representation mode is in order, but if it is scarce, then it may be better conveyed by possibility distributions. The two bounding distributions obtained as a result reflect the incomplete character of the information pertaining to certain parameters: one is the “optimistic” distribution obtained when using all favourable values of input possibility distributions, the other one is the “pessimistic” distribution. Finally, at the interpretation step, a single distribution can be computed by assigning weighs to these two bound distributions, reflecting the decision maker’s aversion to risk.

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Tables

Table 1: Assumed parameter distributions, values rounded to 2 significant digits

Description	Unit	Limits of the trapezoidal distributions				Source of information	Preferred representation
		a	b	c	d		
Net carbon uptake from atmosphere, willow cultivation	Mg C ha^{-1} yr^{-1}	3	6	6	9	Tonini et al. 2012	Fuzzy
Net carbon uptake from atmosphere, barley cultivation	Mg C ha^{-1} yr^{-1}	1	2	2	3	Tonini et al. 2012	Fuzzy
N_2O direct emissions, willow cultivation	kg N ha^{-1} yr^{-1}	0.8	1.69	1.69	2.5	Tonini et al. 2012	Fuzzy
N_2O direct emissions, barley cultivation	kg N ha^{-1} yr^{-1}	0.9	1.9	1.9	2.9	Tonini et al. 2012	Fuzzy
N_2O indirect emissions, willow cultivation	kg N ha^{-1} yr^{-1}	0.1	0.22	0.22	0.33	Tonini et al. 2012	Fuzzy
N_2O indirect emissions, barley cultivation	kg N ha^{-1} yr^{-1}	0.3	0.56	0.56	0.8	Tonini et al. 2012	Fuzzy
Indirect land use change	Mg CO_2-eq ha^{-1}	189	398	398	610	After Tonini et al. 2012 *	Fuzzy
Yield of cultivation of willow	Mg DM ha^{-1}	8.7	12.7	12.7	16.7	Tonini et al. 2012	Probability
Yield of cultivation of barley	Mg DM ha^{-1}	3.35	4.85	4.85	6.35	Tonini et al. 2012	Probability
Carbon content of willow	% DM	0.47	0.48	0.49	0.50	Tonini et al. 2012 **	Probability
Loss of carbon during storage	%	0.035	0.048	0.048	0.061	Tonini et al. 2012	Fuzzy
Lower heating value of dry matter (willow)	GJ Mg^{-1} DM	16.7	17.6	19	19.8	Tonini et al. 2012 **	Probability
Water content of willow after field drying	%	0.15	0.2	0.3	0.35	Tonini et al. 2012	Fuzzy
Electricity recovery from LHV	%	0.35	0.38	0.38	0.41	Danish Energy Agency and energinet.dk (2010)	Probability
Heat recovery from LHV	%	0.44	0.52	0.52	0.6	Danish Energy Agency and energinet.dk (2010)	Probability
GHG emissions from electricity production in DK	Mg CO_2-eq MWh^{-1}	0.66	0.92	0.92	1.05	Personal communication, DONG Energy A/S et al. (2010)	Probability
GHG emissions from heat production in DK	Mg CO_2-eq GJ^{-1}	0.04	0.05	0.06	0.07	Estimations based on the ecoinvent database	Fuzzy

* This includes the conversion of land and the effects of cultivating the reacting crop on newly converted land.

**: 19 values extracted from articles and the Phyllis and Biodat databases referenced in Tonini et al. 2012.

Figure Captions

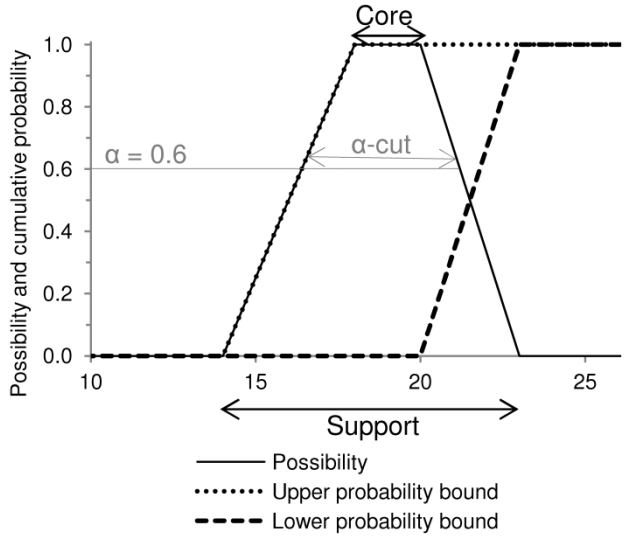

Fig. 1 Example of a possibility distribution

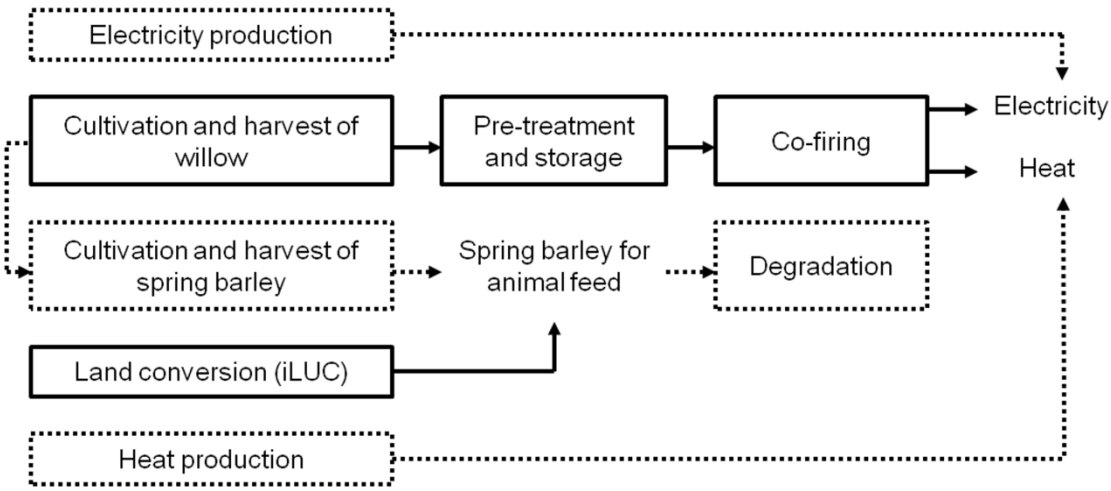

Fig. 2 System boundary of the selected LCA case study (dashed lines: avoided processes)

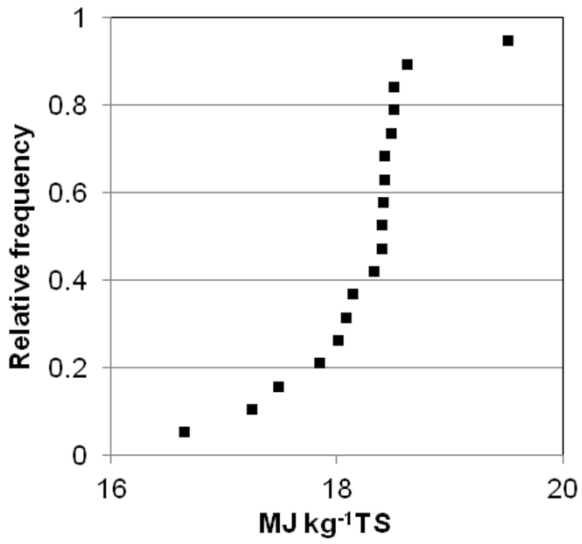

Fig. 3 Data collected in 19 studies for LHV of willow

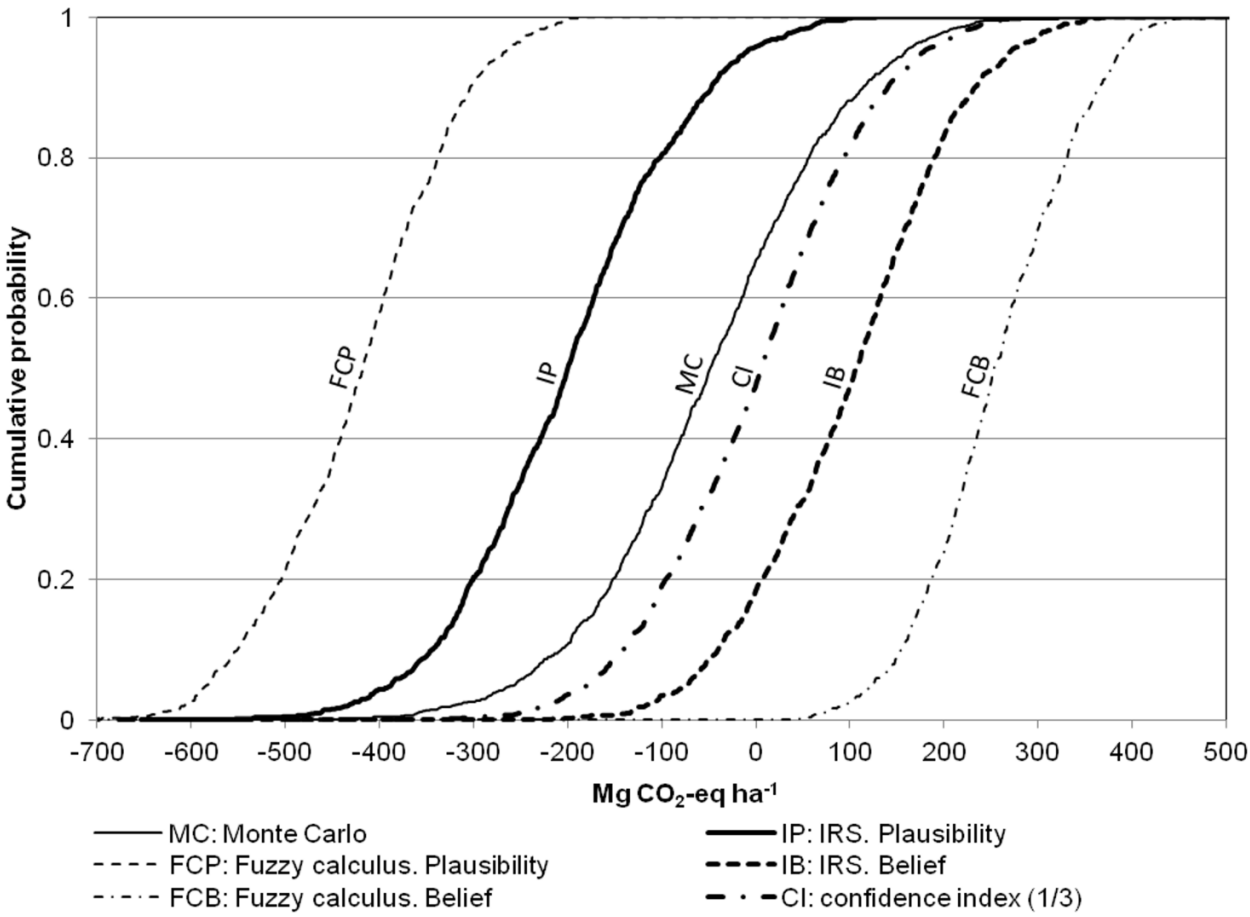

Fig. 4 Cumulative distribution functions of greenhouse gas emissions of cultivation and co-combustion of willow (in Mg CO_2-eq ha^{-1}) obtained with three uncertainty propagation methods: Monte Carlo, fuzzy calculus and IRS method (1000 runs)

Appendix: Calculation of the global warming (GW) impact

Cultivation and harvest of willow (life-cycle of 21 years)

$$CO_{2_in} = (C_{em_y2} - 13 * C_{in_cultivation} - 5 * C_{in_harvest}) / 21 * 44/12 \qquad [1]$$

$$N_2O_{em} = (N_2O_d + N_2O_i) * 44/28 * N_2OCF / 1000 \qquad [2]$$

Where:

CO_{2_in}: yearly (average) CO_2 emissions from cultivation of willow — Mg CO_2 ha^{-1} yr^{-1}

$C_{in_cultivation}$: yearly net uptake of carbon during the 13 cultivation years — Mg C ha^{-1} yr^{-1}

$C_{in_harvest}$: yearly net uptake of carbon during the 5 harvest years (this parameter being strongly correlated to $C_{in_cultivation}$ it is later replaced by $C_{in_cultivation}$ - 0.78) — Mg C ha^{-1} yr^{-1}

C_{em_yr2}: emissions of carbon during year 2 (assumed equal to 5.32) — Mg C ha^{-1} yr^{-1}

N_2O_{em}: yearly emissions of N_2O from cultivation of willow — Mg CO_2-eq ha^{-1} yr^{-1}

N_2O_d: yearly direct emissions of N_2O from cultivation of willow — Mg N ha^{-1} yr^{-1}

N_2O_i: yearly indirect emissions of N_2O from cultivation of willow — Mg N ha^{-1} yr^{-1}

N_2OCF: characterisation factor of N_2O for GW — kg CO_2-eq/kg N_2O

Cultivation and harvest of barley

$$CO_{2_b} = -C_{in_b} * 44/12 + Y_b * C_b * 44/12 \qquad [3]$$

$$N_2O_b = (N_2O_{d_b} + N_2O_{i_b}) * 44/28 * N_2OCF / 1000 \qquad [4]$$

Where:

CO_{2_b}: yearly CO_2 emissions from cultivation and harvest of barley — Mg CO_2 ha^{-1} yr^{-1}

C_{in_b}: yearly net uptake of carbon during cultivation and harvest of barley — Mg C ha^{-1} yr^{-1}

Y_b: yield of cultivation of barley (at the field gate) — Mg DM ha^{-1} yr^{-1}

C_b: carbon content of barley — %DM

N_2O_b: yearly emissions of N_2O from cultivation and harvest of barley — Mg CO_2-eq ha^{-1} yr^{-1}

$N_2O_{d_b}$: yearly direct emissions of N_2O from cultivation and harvest of barley — Mg N ha^{-1} yr^{-1}

$N_2O_{i_b}$: yearly indirect emissions of N_2O from cultivation and harvest of barley — Mg N ha^{-1} yr^{-1}

N_2OCF: characterisation factor of N_2O for GW — kg CO_2-eq/kg N_2O

Co-firing

$$CF = Yield * C_w * 44/12 \quad [5]$$

Where:

CF: yearly CO_2 emissions from co-firing of willow	Mg CO_2 ha^{-1} yr^{-1}
Yield: yield of cultivation of willow (at the field gate)	Mg DM ha^{-1} yr^{-1}
C_w: carbon content of willow	%DM

Avoided energy production

$$EP = Yield * (LHV * (1 - Loss) - watercontent/(1 - watercontent) * H_2Oheating) * (elec_rec/3.6 * GHG_{elec} + heat_rec * GHG_{heat}) \quad [6]$$

Where:

EP: yearly avoided GHG emission from energy production	Mg CO_2–eq ha^{-1} yr^{-1}
Yield: yield of cultivation of willow (at the field gate)	Mg DM ha^{-1} yr^{-1}
LHV: lower heating value of willow as dry matter	GJ Mg^{-1} DM
Loss: loss of carbon during drying and storage of willow	%
watercontent: water content of willow after field drying	%
H_2Oheating: energy needed for water content evaporation	GJ Mg^{-1}
elec_rec: electricity recovery from LHV	%
heat_rec: heat recovery from LHV	%
GHG_{elec}: GHG emissions from electricity production in DK	Mg CO_2-eq MWh^{-1}
GHG_{heat}: GHG emissions from heat production in DK	Mg CO_2-eq GJ^{-1}

Total net impact

$$TNI = iLUC + 20 * (CO_{2_in} + N_2O_{em} - (CO_{2_b} + N_2O_b) + CF - EP) \quad [7]$$

Where:

TNI: total net impact on GW over 20 years	Mg CO_2-eq ha^{-1} yr^{-1}
iLUC: indirect land use change	Mg CO_2-eq ha^{-1} yr^{-1}
CO_{2_in}: yearly CO_2 savings from cultivation and harvest of willow (average)	Mg CO_2 ha^{-1} yr^{-1}
N_2O_{em}: yearly emissions of N_2O for willow cultivation	Mg CO_2-eq ha^{-1} yr^{-1}

CO_{2_b}: yearly CO_2 savings from cultivation and harvest of barley	Mg CO_2 ha^{-1} yr^{-1}
N_2O_b: yearly emissions of N_2O for barley cultivation	Mg CO_2-eq ha^{-1} yr^{-1}
CF: yearly CO_2 emissions from co-firing of willow	Mg CO_2 ha^{-1} yr^{-1}
EP: yearly avoided GHG emission from energy production	Mg CO_2–eq ha^{-1} yr^{-1}

Supplementary information

Stochastic and epistemic uncertainty propagation in LCA

Julie Clavreul, Dominique Guyonnet, Davide Tonini and Thomas H Christensen

This document presents the algorithm used to propagate the uncertainties with the IRS method and obtain the cumulative frequency distributions (CFD).

The general algorithm is presented in Figure S1. To run it, three inputs are required:

- A function f of several parameters,
- An array describing the trapezoidal distributions for all parameters. Each line of the array represents a parameter. In columns 1, 2, 3 and 4 are the numbers a, b, c, d delimitating the support [a, d] and the core [b, c] of each trapezoidal distribution ($a \leq b \leq c \leq d$). In column 5 is stored the information about the preferred representation for the IRS method (probability or possibility),
- The number of iterations w.

An optimisation algorithm is needed to find the minimum of a function f when the vector of parameters x is varying between two vectors of values (x1 and x2). In this study, the algorithm was implemented in MATLAB (v 7.11.0) with the optimisation algorithm called global search provided by MATLAB. The implementation of the algorithm in MATLAB is presented after Figure S1.

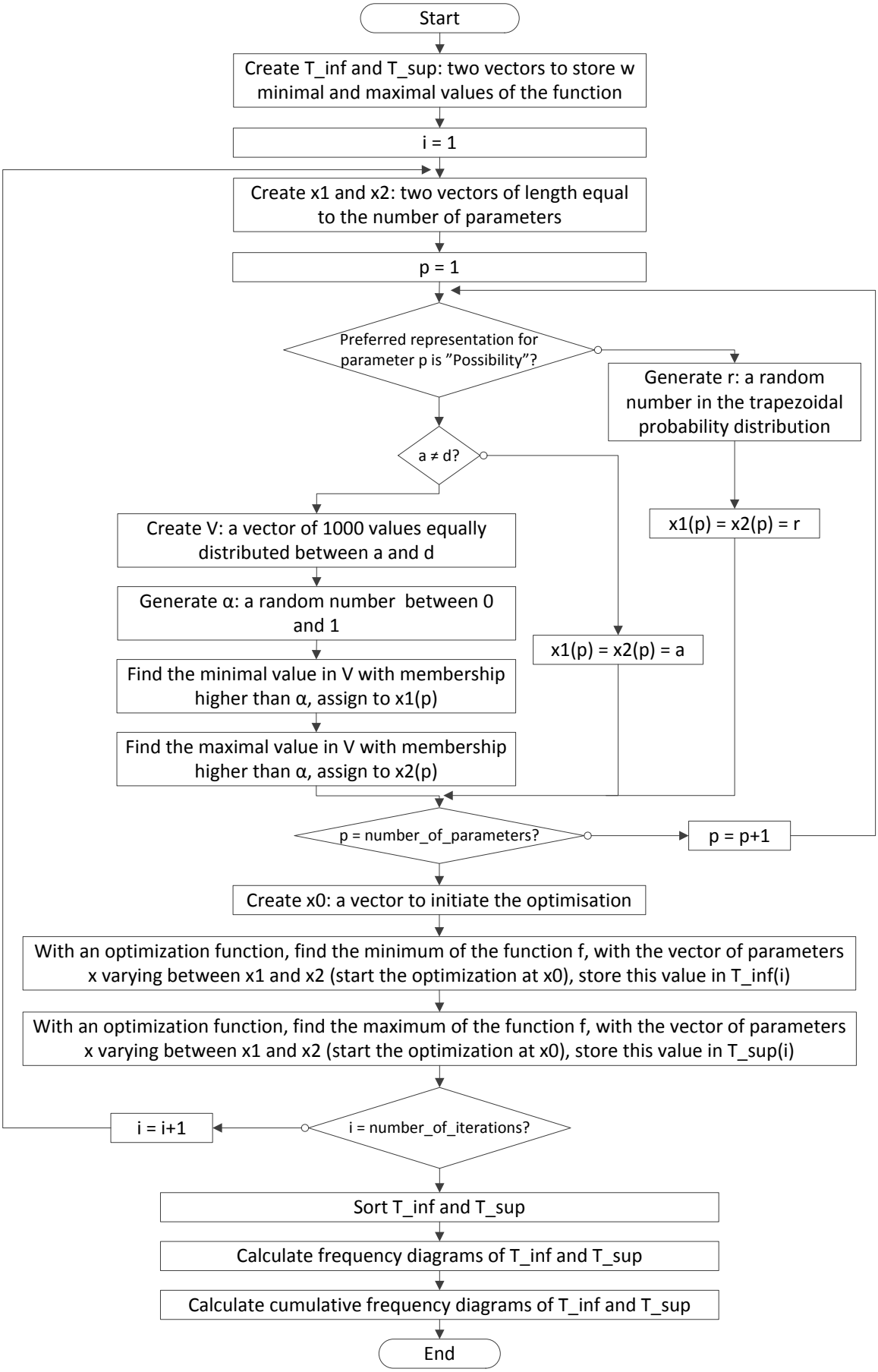

Figure S1: Algorithm of uncertainty propagation using the IRS method

Implementation in MATLAB

Similarly to the previous explanations, the function implemented in MATLAB code has:

- 3 inputs:
  - fhandle is the function that need to be optimised
  - dataArray is the matrix of parameter values: each line is a parameter, columns 1, 2, 3 and 4 contain the limits of the trapezoidal distributions (in ascendant order) and column 5 tells which representation ("probability" or "possibility") should be preferred when propagating with the IRS method
  - w is the number of runs wanted
- 4 outputs:
  - T_inf is a column vector of the w inferior values of fhandle obtained
  - T_sup is a column vector of the w superior values of fhandle obtained
  - IntervalsTable is a column vector of the abscissa of the CFDs
  - CumFreqTable is a matrix of two column vectors which are the two CFD wanted (Pl and Bel)

The algorithm uses different functions provided by MATLAB, such as the trapezoidal-shaped membership function called "trapmf" and the optimisation algorithm "Global search". It uses also a self-made function for random sampling in trapezoidal probability distributions provided after the main function.

```
function [T_inf, T_sup, IntervalsTable, CumFreqTable] = main(fhandle,
dataArray, w )

% Tables to store the minimal and maximal values of the function
T_inf=zeros(w,1);
T_sup=zeros(w,1);

% Declaration of the two functions to minimize
[fn]=fhandle;
minusfn=@(x) -function(x);

gs = GlobalSearch;
opts = optimset('Algorithm','interior-point');

% Vector to initialize the optimisation procedure
x0=dataArray(:,2);

for i=1:w %for each run

    %Random sampling of intervals of values for each parameter
     x=dataArray;
     l=length(x(:,1)); %number of parameters
     x1=zeros(l,1);
     x2=zeros(l,1);

     for p=1:l %for each parameter p

         if (x(p,5)=='Probability') %if the preferred representation is
         probability, the interval is reduced to one value randomly
         sampled in the trapezoidal probability distribution
              x1(p)=tpzrnd(x(p,1),x(p,2),x(p,3),x(p,4));
              x2(p)=x1(p);
```

```
        elseif (x(p,5)=='Possibility') %if the preferred
        representation is possibility, the interval is calculated as a
        random alpha-cut in the trapezoidal membership function
            if (x(p,4)==x(p,1))
                x1(p)=x(p,1);
                x2(p)=x(p,1);

            else
                step=(x(p,4)-x(p,1))/1000;
                grid=[x(p,1):step:x(p,4)];
                alpha=rand();
                y = trapmf(grid,[x(p,1),x(p,2),x(p,3),x(p,4)]);
                ind=find(y>=alpha);
                x1(p)=grid(min(ind));
                x2(p)=grid(max(ind));
            end
        end
    end

    % Search of the minimum of function, by global search function,
for x comprised between x1 and x2
    problemmin = createOptimProblem('fmincon','x0',x0,...
        'objective',fn,'lb',x1,'ub',x2,'options',opts);
    [xming,fming] = run(gs,problemmin);
    T_inf(i)=fming;

    % Search of the minimum of minusfunction i.e. the maximum of
function
    problemmax= createOptimProblem('fmincon','x0',x0,...
        'objective',minusfn,'lb',x1,'ub',x2,'options',opts);
    [xmaxg,fmaxg] = run(gs,problemmax);
    T_sup(i)=-fmaxg;

end

% Sorting of T_inf and T_sup
T_inf=sort(T_inf);
T_sup=sort(T_sup);

% Calculation of the frequency diagram (abscissa: IntervalsTable,
ordinates: FreqTableInf and FreqTableSup)
min_int=round(min(T_inf)-100);
max_int=round(max(T_sup)+100);
IntervalsTable=[min_int:1:max_int];

FreqTableInf=hist(T_inf, IntervalsTable)/w;
FreqTableSup=hist(T_sup, IntervalsTable)/w;

% Calculation of the cumulative frequency diagram (abscissa:
IntervalsTable, ordinates: CumFreqTable (1 and 2))
CumFreqTable=ones(length(IntervalsTable),2);
CumFreqTable(1,1)=FreqTableInf(1);
CumFreqTable(1,2)=FreqTableSup(1);
for i=2:length(IntervalsTable)
      CumFreqTable(i,1)=CumFreqTable(i-1,1)+FreqTableInf(i);
      CumFreqTable(i,2)=CumFreqTable(i-1,2)+FreqTableSup(i);
end

end
```

The function used to generate a random number in a trapezoidal probability distribution defined by support [a, d] and core [b, c] is presented below.

```
function [y] = tpzrnd( a,b,c,d )

x=rand();% Creates a random number between 0 and 1

u=2/(d+c-b-a);
fb=u/2*(b-a);
fc=1-u/2*(d-c);

if x<fb
    y=a+sqrt(2*(b-a)/u*x);
else
    if x<fc
        y=x/u+(a+b)/2;
    else
        y=d-sqrt(2*(d-c)*(1-x)/u);
    end
end

end
```