Two-dimensional Monte Carlo simulations in LCA: an innovative approach to guide the choice for the environmentally preferable option

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Abstract

Purpose: Uncertainty and variability need to be taken into account in Life Cycle Assessment (LCA) studies to make robust decisions. We introduce a novel approach in LCA that allows to decide if either uncertainty or variability is dominating in the results: two-dimensional Monte Carlo simulations (2DMC). We aim to do so in a pedagogical and transparent way, allowing interested readers to fully grasp all technical details for their own potential use in future studies.

Methods: In 2DMC, an approach from quantitative risk assessment, the model parameters are divided into four categories: deterministic, variable, uncertain, and uncertain ánd variable; and appropriate distributions are selected. These distributions are sampled separately, so they can be assessed separately in the output as well. Firstly, the approach was translated to the LCA context with an illustrative *proof of concept model*, freely available on our website. Further, two variants of the post-harvest apple chain in Belgium (bulk versus pre-packed) are worked out as a *real life* comparative LCA case study. This real life case study is also analyzed in a classical, deterministic way and by performing a more often used one-dimensional Monte Carlo simulation (1DMC), allowing a comparison with the 2DMC results and associated interpretations.

Results and discussion: Deterministic results do not reflect the complexity of reality. 1DMC results provide an indication on the robustness and conclusiveness of the result of a comparative LCA, but do not provide a way to guide further decisions. 2DMC results do provide this as results typically belong to one out of three possibilities. Firstly, the 2DMC results may confirm the result of the deterministic results. Secondly, the 2DMC curves may show proof that the two products are equivalent when it comes to environmental impact. One may then decide to analyze the variability causes further or that other reflections, like cost, should be considered as well. Thirdly, the 2DMC curves may indicate that more detailed and accurate information is needed to come to conclusive results.

Conclusions: 1DMC results give a first indication on the need for a 2DMC analysis. If that is the case, 2DMC can be used in a comparative LCA to take uncertainty and variability separately into account. 2DMC results can guide decisions to obtain more conclusive results. We recommend to consider a 2DMC analysis when comparing two products or processes if needed, hereto, our proof of concept model fully documented available online may be a starting point.

Keywords

LCA; uncertainty; variability; two-dimensional Monte Carlo simulation; second-order Monte Carlo simulation; apple

1 Introduction

1.1 The added value of uncertainty and variability

To communicate about reality in a representative way, such as with Life Cycle Assessment (LCA) results, proper data quality reporting is required to fully and correctly understand the study results and their reliability (ISO 2006). For example, uncertainty and variability need to be taken into account. (Epistemic) *uncertainty* refers to the imperfection of our knowledge, such as inaccurate measurements, lack of data, incomplete knowledge, etc. In contrast, v*ariability* represents the inherent heterogeneity of the natural world that will always be observed (Walker et al. 2003; Hauschild et al. 2018). The combination of uncertainty and variability is called *overall uncertainty* (Pouillot et al. 2016).

While the difference in origin of uncertainty and variability is clear, LCA results are still quite often reported as deterministic [e.g., Bosona and Gebresenbet (2018)]. Yet, LCA is a decision-making tool, so the results on which all sectors concerned with environmental impact (e.g., farmers, industry, consultants, research groups, consumers and governmental bodies) base their decisions, should be as reliable as possible to make informed decisions. If those decisions are solely based on some kind of central tendency (e.g., mean or median), comparisons would not be as robust because the possible overlap due to uncertainty and/or variability is being ignored. Even if uncertainty is accounted for, variability is often treated alike or even left unacknowledged (Konstantas et al. 2018; Jiao et al. 2019; Sykes et al. 2019).

Because of this, when products or processes are compared using an LCA study – usually using deterministic input values – researchers are often unable to make an unambiguous conclusion on which is environmentally preferable [e.g., when comparing conventional and organic cultivation systems (Chatzisymeon et al. 2017; Tasca et al. 2017)]. This often leads to the general recommendation of the need for more data. And even when a tentative recommendation is made, questions quickly arise on how robust the LCA results are. Is the chosen option always environmentally preferable? What if we account for variability (e.g., data from a different cultivation period with more severe weather)? What if we *simultaneously* account for uncertainty (e.g. when estimations were used instead of accurate measurements)? Does the decision stay the same? Answering such questions is where the focus of this research paper lies.

In that regard, it is needed to shortly reflect on how products can statistically be compared using LCA results that reflect (overall) uncertainty, which is described in the next section.

1.2 Selecting a preferential product in a comparative LCA

When it comes to comparative LCAs, recent literature has discussed different methods on how the preferential product can be chosen when uncertainty is present (Gregory et al. 2016; Mendoza Beltran et al. 2018; Heijungs 2021). Heijungs (2021) reviews approaches that can be used to single out the superior option of two (or more) products when uncertainty is propagated using (one-dimensional or 1D) Monte Carlo simulations, including: nonoverlap statistics (measures the degree of overlap or the similarity between probability distributions), and comparison indicator/discernability analysis. Heijungs (2021) concludes that two questions need to be answered to select the best product alternative out of two options: (i) "*What is the probability that a randomly selected specimen of product A performs better than a randomly selected specimen of product B?*" and (ii) "*How much will a randomly selected specimen of product A perform better than a randomly selected specimen of product B?*". He proposes the use of a "modified comparison index" to answer these questions, for which a minimum threshold value is used to assess the superiority of option A and of option B.

1.3 The dominance of uncertainty vs. variability: existing approaches

In Michiels and Geeraerd (2020a) we reviewed which methodologies have already been used in LCA that allow to decide whether uncertainty or variability is dominating in the results. This turned out to be very limited, with only 11 studies (of the 562 records identified through database searching) having some kind of visualization showing whether either uncertainty or variability dominates the results when propagating *both* in the LCA calculations.

In 10 of the 11 studies, (one-dimensional) Monte Carlo simulations were conducted to propagate uncertainty and variability, often in combination with some kind of sensitivity analysis. We concluded our review paper (Michiels and Geeraerd 2020a) by recommending – among other things – (one-dimensional) Monte Carlo (1DMC) simulations visualized in either variability and uncertainty ratios to identify which is dominating, which was done by Hauck et al. (2014) and Steinmann et al. (2014). Monte Carlo simulations are a kind of sampling method in which iterations of model calculations are performed using randomly sampled input values from probability distributions, causing the output to be represented as a probability distribution as well (Hauschild et al. 2018; Igos et al. 2019).

In our systematic review (Michiels and Geeraerd 2020a), the most important shortcoming that was identified, was the fact that an input parameter was either categorized as uncertain or variable but could not be separately propagated simultaneously as being both variable and uncertain. It is however possible that a parameter has both characteristics. For example, sorting apples at an auction can be uncertain because the auction does not have an accurate system in place to measure the amounts of apples that are sorted out (due to spoilage or quality requirements), and it can be variable as well, due to the biological nature of apples, causing different percentages of apples to be spoiled in each batch and causing a lack of uniformity for the quality requirements. In the case where a parameter is identified as being both uncertain and variable, it is often categorized under uncertainty [as in Steinmann et al. (2014)], possibly leading to aberrant decisions. An alternative method is needed which allows to classify one parameter as being both uncertain and variable, and which subsequently simultaneously propagates them separately for that parameter.

1.4 Introducing two-dimensional Monte Carlo simulations

A potential solution to these two shortcomings can be found in the field of quantitative risk assessment (Nauta 2000; Vose 2008), where two-dimensional Mont Carlo simulations (2DMC) are used, for example, for simulating:

- the risk of environmental hazards [e.g., for salmonid embryo survival (Wu and Tsang 2004), *Escherichia coli* contamination during the cattle slaughter process (Cummins et al. 2008) and the potential ecotoxicological impacts of shampoo (Douziech et al. 2018)],

- the risk of food hazards [e.g., the possible daily exposure to a carcinogenic substance in breast milk and powder infant formula (Boué et al. 2017) and the risk of acquiring *Listeria monocytogenes* when consuming smoked fish (Vásquez et al. 2014)], and
- health risks [e.g., radiological risk for the public and workers near the vicinity of a field radiological system (Jang et al. 2009) and indoor exposure to semi-volatile organic compounds (Pelletier et al. 2017)].

2DMC allows for a clear and straightforward visualization of uncertainty and variability in the results. However, 2DMC comes with its own difficulties of having to define which parameters are uncertain and/or variable, what probability distributions should be used, and how the results can be interpreted and communicated. We need to conceptualize how 2DMC can be used for LCA, which might differ from its use in other domains.

In this article, we aim to introduce this novel approach, two-dimensional Monte Carlo simulations (2DMC), in LCA that simultaneously propagates uncertainty and variability separately, allowing to decide which is dominating in the results. We aim to clarify in full details the 2DMC procedure using a fully detailed proof of concept (POC) model, of which the technical intricacies are available on our website[1] (Michiels and Geeraerd 2021). In a next step, a real life case-study will be conducted, in which two products are compared (bulk versus pre-packed apples), paying special attention to how data uncertainty and variability is assigned to different input parameters.. Additionally, the 2DMC results will be compared to the deterministic results and the 1DMC results (treating uncertainty and variability alike) for this case study, to assess their different interpretation in the LCA context and their different influence on decision making. For the 1DMC results, the modified comparison index proposed by Heijungs (2021) will be used.

Preliminary results of this research were presented at the 12th International Conference on Life Cycle Assessments of Food (Michiels and Geeraerd 2020b).

2 Methods

The first part of the Methods section describes the steps in a general 2DMC methodology. For the interested reader, a proof of concept (POC) model was constructed for this section, which is available online (Michiels and Geeraerd 2021). The second part of the Methods section introduces the goal, scope and life cycle inventory of the

[1] https://mebios-agri-food.pages.gitlab.kuleuven.be/supplementary/2dmc/

real life case study i.e., the post-harvest chain of apple in Flanders (Belgium). The different inventory results are described for the deterministic, 1DMC and 2DMC analyses.

2.1 Two-dimensional Monte Carlo simulations

Monte Carlo simulations are a sampling method in which iterations of model calculations are performed using randomly sampled input values from probability distributions, causing the output to be represented as a probability distribution as well (Hauschild et al. 2018; Igos et al. 2019). *One-dimensional Monte Carlo simulations (1DMC)* can propagate either uncertainty *or* variability, but not both at the same time. Separate 1DMC simulations can be conducted each time in- or excluding either uncertainty or variability. *Two-dimensional Monte Carlo simulations (2DMC)* do allow to propagate uncertainty and variability simultaneously as well as disentangle their influence on the results. This is possible because in 2DMC, the distributions reflecting uncertainty *and* the distributions reflecting variability are sampled separately, so they can be assessed separately in the output as well (Cohen et al. 1996; Pouillot and Delignette-Muller 2010).

Technically, 2DMC consists of two 1DMC loops, where the outer loop consists of *n* simulations of model parameters to simulate the knowledge uncertainty; and the inner loop consists of *m* iterations of input variables to simulate system variability (Wu and Tsang 2004). First the input parameters need to be divided into four categories: deterministic parameters, variable parameters, uncertain parameters and parameters that reflect both variability and uncertainty (Pouillot et al. 2016). The categorization of these parameters is dependent on the kind of data that can be gathered through measurements, surveys, expert consultation and literature search. The possibility to consider a parameter as being both uncertain and variable is a major benefit of 2DMC, incorporating separate distribution data for the uncertain part and the variable part of the input parameter.

For each model input that is not deterministic, a probability distribution (e.g., Uniform, Binomial, Pert, etc.) is specified based on the distribution of the gathered data (Vose 2008). This is a very important and elaborated step for which a lot of information is needed, as will be detailed in section 3.1. The uncertain parameters are randomly sampled from their respective distributions and considered as fixed while performing 1DMC simulations with random values from the variable parameters (*m* iterations; see Fig. 1). This process is repeated several times (*n* simulations), where each time new random values of the uncertain parameters are fixed before running 1DMC simulations using the variable parameters (Pouillot et al. 2016). This results in a two-dimensional model output of 2DMC curves, where each curve in the 2DMC output represents the variability within the chain for one dimension of uncertainty. The dispersion of the different curves shows the influence of uncertainty, while the steepness is an indication of variability (Vose 2008).

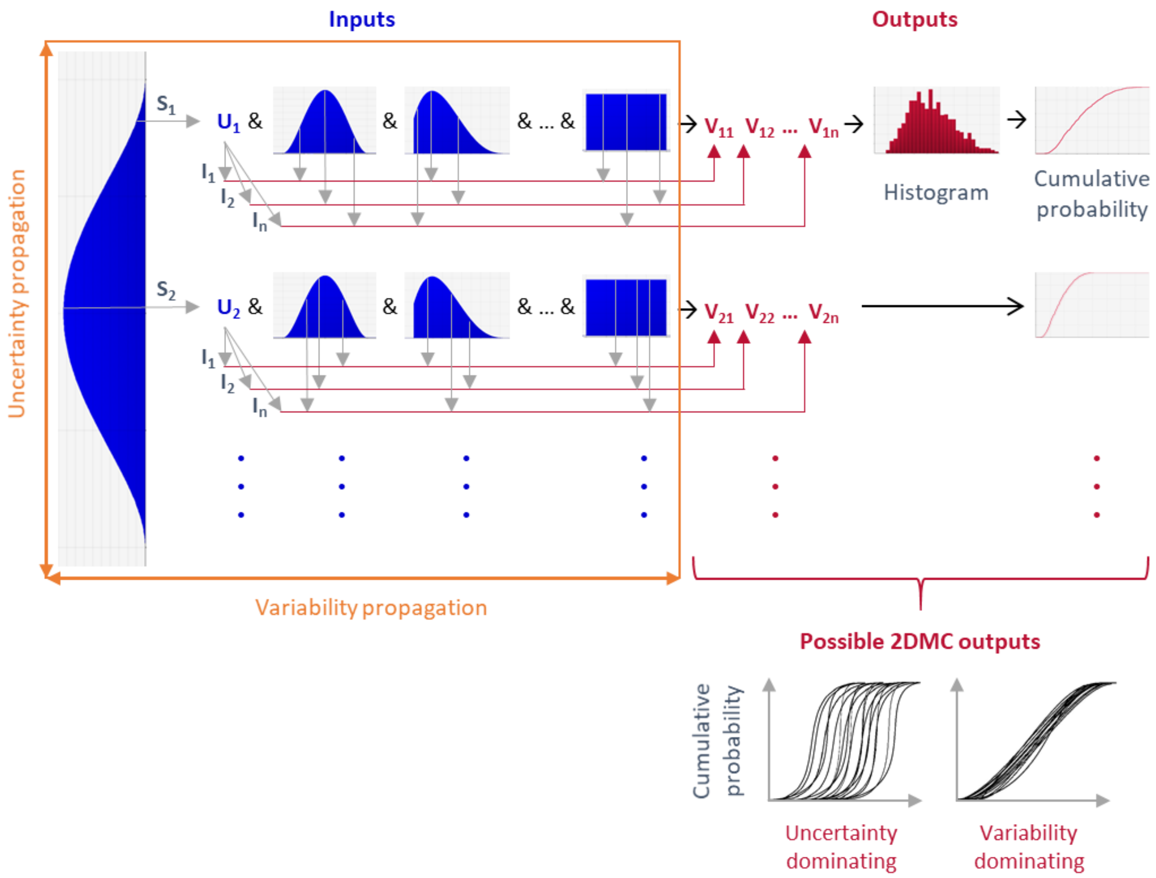


Fig. 1 *Schematic overview of how two-dimensional Monte Carlo simulations are conducted (S = simulation, I = iteration, U = fixed uncertainty parameters, V = possible LCA output), adapted from Cummins (2016).*

In this study, 10 000 iterations and 250 simulations were conducted, leading to 2 500 000 possible LCA outcomes shown in 250 2DMC curves. The number of iterations was chosen because 10 000 iterations are often seen as a rule of thumb in Monte Carlo simulations (Ciroth et al. 2004; Igos et al. 2019). The number of simulations was chosen for compatibility reasons with Microsoft Excel, after making sure that it provided a good sampling of the full range and shape of each input probability distribution. The total number of 2DMC runs provided a good representation of all possible LCA results. The Excel add-in @Risk 7.6 (Palisade, NY, USA) was used to conduct these 2DMC simulations, using the default Latin Hypercube sampling and Mersenne Twister generator. To ensure repeatability of the sampling, a fixed initial seed value was used, which was different for each of the 250 simulations (Michiels and Geeraerd 2021). This fixed initial seed guarantees that the same random values are sampled from each probability distribution for each product and for each impact category. Thus, parameters that are equal for both product systems, have equal influence on their results. This can be seen as “dependent sampling” (Henriksson et al. 2015) or “paired simulation (von Brömssen and Röös 2020).

2DMC results may have a cumbersome look given the large number of cumulative curves. Therefore, they typically are further synthetized using *ratios*, more specifically variability, uncertainty and overall uncertainty ratios [combination of uncertainty and variability (Pouillot et al. 2016)] as described in Pouillot et al. (2016) and proposed by Özkaynaka et al. (2009). These ratios allow to clearly decide if either uncertainty or variability is dominating the overall uncertainty. The ratios can be calculated as followed (Fig. 2):

- Variability Ratio: B / A
- Uncertainty Ratio: C / A
- Overall Uncertainty Ratio: D / A

For which: A is the median of uncertainty for the median of variability; B is the median of uncertainty for the 97.5th percentile of variability; C is the 97.5th percentile of uncertainty for the median percentile of variability and D is the 97.5th percentile of uncertainty for the 97.5th percentile of variability.

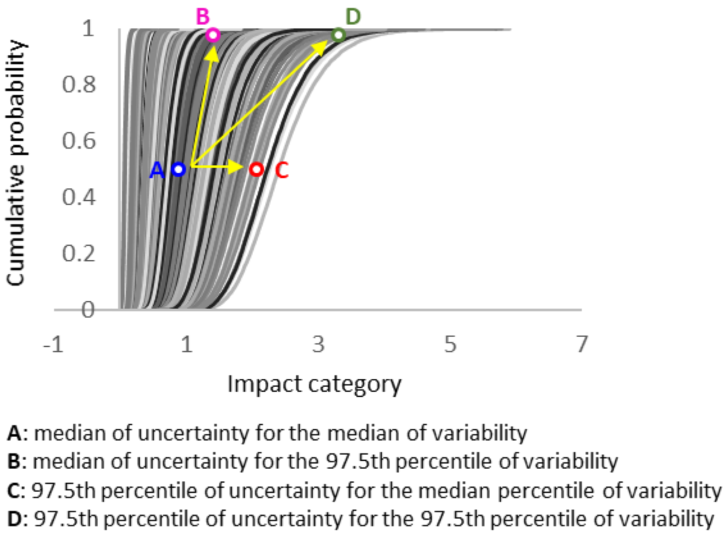


Fig. 2 *Graphical representation of the points A, B, C and D needed to calculate the variability ratio (B/A), the uncertainty ratio (C/A) and the overall uncertainty ratio (D/A) (Özkaynaka et al. 2009; Pouillot et al. 2016)*

An extensive manual explaining the 2DMC procedure for a POC model using @Risk is available on our website (Michiels and Geeraerd 2021). In the POC model, two products are compared using fictious parameters. Each parameter is assigned an uncertainty type and a probability distribution (if needed). These parameters are then combined in LCA input processes and 2DMC simulations are run, leading to LCA outputs reflecting uncertainty and variability. The 2DMC results can be visualized in a cumulative probability graph, using either macros in Excel or an R script (The R Foundation, Vienna, Austria).

2.2 Life Cycle Assessment of the post-harvest apple chain

2.2.1 Goal and scope definition

We implemented 2DMC in an existing attributional LCA of the Belgian (Flanders) apple, developed in our team (Goossens et al. 2019), which describes the apple food chain from farm-gate till consumer disposal of food waste. The post-harvest chain consists of activities at the auction, sorting center, distribution center, supermarket and consumer (Fig. 3). The functional unit is 1 kg of apples purchased by the consumer, either bulk or pre-packed (per 6).

Calculations were performed using SimaPro 9.0.0.49 (Pré Sustainability, the Netherlands) and Microsoft Excel 2016 (Microsoft, WA, USA). The ILCD [2011 Midpoint+; EC-JRC Global, equal weighting] method was used as impact assessment method. Input processes were collected from the database ecoinvent 3.5, using “allocation, at point of substitution”.

2.2.2 Life Cycle Inventory

Goossens et al. (2019) gathered information on the apple post-harvest chain by interacting with three auctions and a retailer through surveys. The chain starts with apples being transported from the farm to the auction. The apples undergo a cooling and storing phase in case they are not sold to the retail immediately, after which they are sorted at the auction, farm or an external facility. Apples fit for sale are packaged in cardboard boxes or plastic crates. Next, the apples are transported to the distribution center of the retailer. Apples, intended to be sold pre-packaged, are packaged per six using a cardboard tray and plastic film. All apples remain shortly in a cold space in the distribution center, before being transported to the supermarket. There, the apples are placed in a cold room where they are bought by consumers. Upon arrival at home, the apples are stored and consumed. Food waste and packaging waste disposal is taken into consideration along the complete post-harvest chain. A more detailed description of the post-harvest chain can be found in Goossens et al. (2019). The *deterministic* case was based on this study, using updated SimaPro processes and calculating the impact of apples bought in March, half a year after the harvest when the highest percentage of apples was bought.

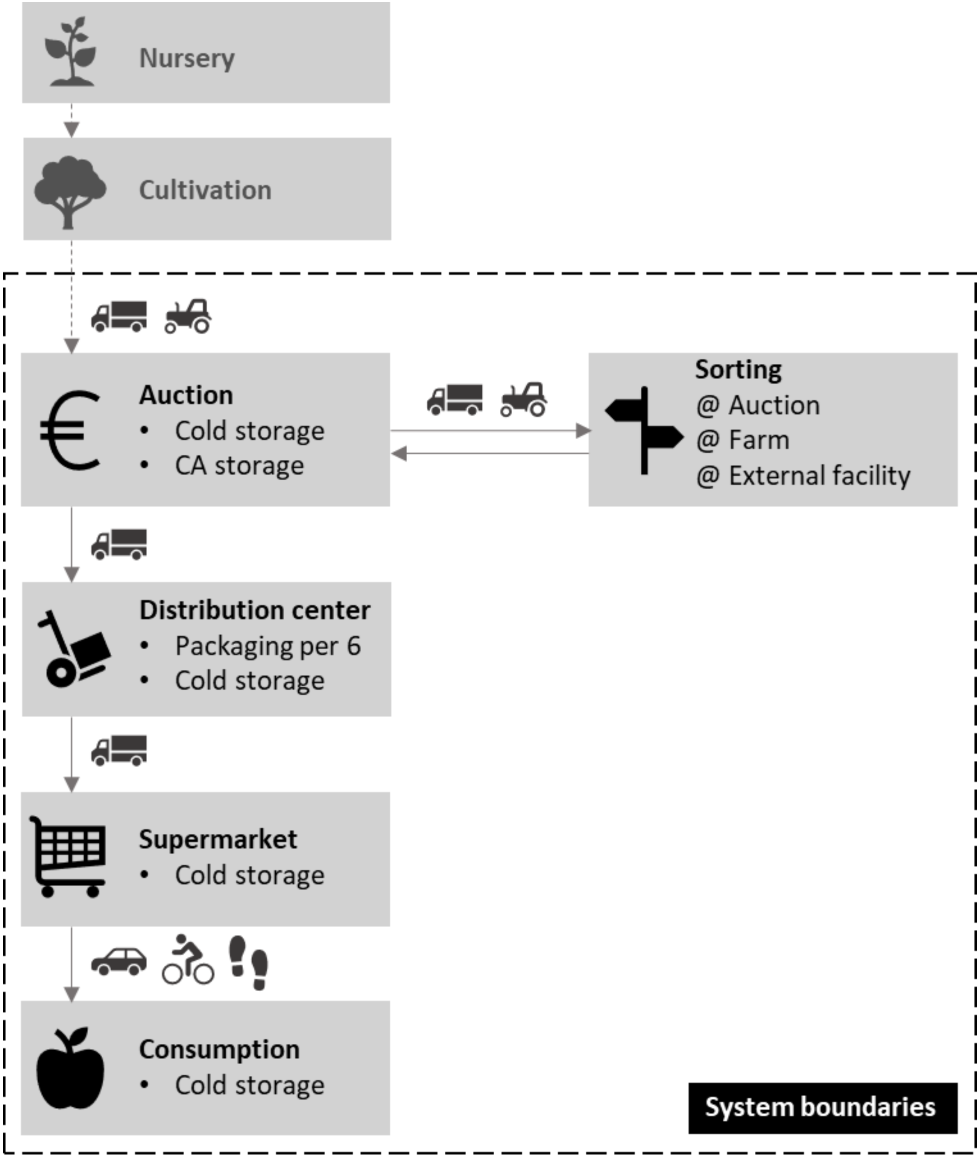


Fig. 3 *System boundaries of the post-harvest apple chain (CA = Controlled Atmosphere)*

2.2.2.1 *Identifying influential parameters*

For the 1DMC and 2DMC analysis, we start with conducting a local sensitivity analysis to identify the most influential parameters for which uncertainty and/or variability data should be gathered. We conducted a simple perturbation analysis with a one-at-a-time approach (Heijungs and Kleijn 2001; Igos et al. 2019; Michiels and Geeraerd 2020a), using the Excel add-in TopRank 7.6 (Palisade, NY, USA). A perturbation analysis shows if a relatively small perturbation, in our case –10% en +10%, of the input parameters propagates as smaller or larger deviations from the deterministic output (Heijungs, Reinout and Suh, Sangwon and Kleijn 2005). The parameters that lead to a change of at least 0.10% (the highest change was 7.21%) of the LCA results were selected as influential parameters, and this for both the bulk as pre-packed apples, and for each impact category.

This resulted in a list of 47 influential parameters for which uncertainty and/or variability information needed to be gathered (as will be detailed below). In addition to this, the variability due to month of purchase and its related loss will also be accounted for in the 1DMC and 2DMC analysis. Table 1 gives a short impression of the parameters that were considered influential and their related data. A full overview of all influential parameters can be found in Table S1 in the Online Resource, where also the complete inventory list and selected SimaPro inputs are available.

2.2.2.2 *Categorizing input data: deterministic, uncertain, variable or uncertain & variable*

The study of Goossens et al. (2019) was based on "most likely" data. However, next to the "most likely" data, they did also inquire about minimum and maximum data for all parameters in their surveys, which can be used to quantify variability. Additionally, they inquired about how certain the companies are of their given data using parameter uncertainty ratings of the Product Environmental Footprint (PEF) quality criteria (European Commission 2012), ranging from no uncertainty, very low uncertainty (≤ 10%), low uncertainty (10-20%), fair uncertainty (20-30%), high uncertainty (30-50%), to very high uncertainty (> 50%), which can be used to quantify uncertainty. This data was used as uncertain and variable data for the influential parameters, supplemented with literature data and own estimations where needed (Table 1). This data allowed us to set up uncertain and variable input probability distributions for the influential parameters which were propagated together in the 1DMC analysis and separately in the 2DMC analysis In the following text, we explain in more detail how the uncertain and variable data is assigned to the parameters for the 2DMC analysis.

Deterministic parameters

As we discussed in the 2DMC methodology (section 2.1), the first step of a 2DMC analysis is done by categorizing the input data into one out of four categories: deterministic, uncertain, variable and, uncertain & variable. All "non-influential" parameters (i.e., cause a lower than 0.10% change in the output) are considered deterministic. A full overview of the influential and non-influential parameters can be found in the Online Resource. Appropriate probability distributions need to be selected for the uncertain, variable and, uncertain & variable categories.

Table 1 Overview of the most influential post-harvest input parameters and their categorization into uncertain, variable and uncertain & variable. For each parameter, the deterministic value or variable data for use in the input probability distribution is shown. If the distribution is PERT, the variable data is "min, most likely, max", if it is uniform, the variable data is "min, max", if it is discrete, the variable data shows the possible values with each one having an equal probability. For other distributions the data is explained in the table itself. Uncertainty is shown using the uncertainty ratings indicated in the surveys or of our own estimation. A complete overview of all parameters can be found in the Online Resource (OR). (DC = distribution center)

Parameter	Unit	Deterministic or variable data	Distribution used for variable data	Uncertainty rating	Category	Source
Share of apples sold throughout the year @ shop	%	See Table S2 in the OR	Discrete	-	Variable	Retailer
Apple loss along the food chain						
Loss of pre-packed apples @ DC	%	0, 3, 5	PERT	Fair	Uncertain & Variable	Retailer
Loss of pre-packed apples @ shop	%	1.42	-	Low	Uncertain	Retailer
Food waste @ consumer	%	6.65, 29	Uniform	-	Variable	(Johnson et al. 2008; DEFRA 2010; Bernaert et al. 2018)
See Table S1 in the Online Resource for the 2 other influential parameters related to apple loss along the food chain.						
Storage and sorting						

Sorting electricity use	kWh/ (ton*week)	CONFIDENTIAL	-	-	Variable	Two auctions
Coldroom electricity use @ shop	kWh/ (ton*year)	CONFIDENTIAL	-	CONFIDENTIAL	Uncertain	Retailer
Share of coldroom used for apples @ shop	%	3, 4, 5	PERT	High	Uncertain & variable	Retailer
Storage time in household fridge @ consumer	days	0, 7, 28	PERT	-	Variable	(European Commission 2018; Voedingscentrum 2021)
See Table S1 in the Online Resource for the 7 other influential parameters related to storage and sorting.						
Packaging						
Weight of 1 EPS M plastic crate	kg	1.6	-	Very low	Uncertain	(Euro Pool System 2017) & own estimation (uncertainty rating)
Weight of apples that fit into 1 plastic crate	kg/plastic crate	8, 9, 15	PERT	-	Variable	Retailer
Rotations of crates	rotations	50, 100	Uniform	-	Variable	(Barthel et al. 2007a)
See Table S1 in the Online Resource for the 16 other influential parameters related to packaging.						
Distribution						
Transport distance farm - auction	km	1, 25, 75	PERT & discrete	-	Variable	Auction

	km	1, 20, 60				Auction
Transport distance DC - shop	km	0.28, 80, 152	PERT		Variable	Retailer
See Table S1 in the Online Resource for the 6 other influential parameters related to distribution.						
Biowaste @ consumer						
Share of Flemish families that compost	%	36, 52	Uniform	-	Variable	(M.A.S. et al. 2012; Goossens et al. 2019)
See Table S1 in the Online Resource for the 3 other influential parameters related to biowaste at the consumer.						

Variable parameters

In general, variability was attributed to those parameters that described management choices, different production sites/companies, biological variation and consumer behavior. Parameters were considered uncertain when the auction and retail indicated being uncertain of the provided data. It is possible that the companies are uncertain about the data of a variable parameter, making it uncertain & variable. If no variable or uncertain data were provided and that information could not be found in literature, an estimation by the authors was made, building on our expertise of the post-harvest apple chain.

For the parameters for which the auctions and retailer provided *variable* data, PERT (based on provided min, most likely and max data) or uniform (in case a most likely value was not provided) distributions were constructed. The PERT (Program Evaluation and Review Technique) distribution is similar to a triangular distribution but is preferred over it because of its curved density, emphasizing most likely values more (Palisade 2016).

Additionally, the data of multiple auctions was taken into account [as opposed to one in the study of Goossens et al. (2019)], by combining their estimates in a discrete distribution, for which we assumed that they were all equally likely to occur. For example, two auctions provided deterministic data on their sorting electricity, causing that parameter to be variable. Another discrete distribution reflecting variability was the percentage of apples sold each month throughout the year, which in turn influenced storage time and the percentage of apples lost at the auction.

Variability was also found in all parameters concerning the consumer phase. Several literature sources (Johnson et al. 2008; DEFRA 2010; Bernaert et al. 2018) were used to construct a plausible uniform distribution that reflects the percentage of food waste by the consumer. This parameter could also be seen as uncertain, since the data is based on estimates from households. However, since there is no data on the certainty and since the parameter is very dependent on consumer behavior and biological variation, it was classified as being variable. Consumer transport was accounted for by combining a probability distribution of how far people usually live from the shop (provided by the retailer) with data from the government on the percentage of car use based on the travel distance (FOD Mobiliteit 2017). Other variable parameters were the storage time in the fridge before consumption, and the percentage of consumer that compost at home or participate in a municipal collection of biowaste.

For packaging, the weight of apples transported by paloxes, cardboard boxes or plastic crates could variate. Additionally, regarding the lifetime of the plastic crates, a conservative reusability scenario of 10 years and a technical scenario of 20 years (Barthel et al. 2007b) was considered using a uniform variability distribution.

Uncertain parameters

When it came to the other influential secondary and primary packaging parameters, no variable or uncertain data was – in general – provided or retrieved. We assume that the production of those has been fine-tuned [e.g., EPS size M and H plastic crate weight (Euro Pool System 2017)] and therefore estimated that the influential packaging parameters (for which no other data was available) had a very low uncertainty.

Thus, *uncertainty* was taken into account by using parameter uncertainty ratings (European Commission 2012). For example, the retailer was not very certain about how much electricity they needed for the coldroom at the shop, and therefore provided an uncertainty rating for that parameter, making it an uncertain parameter. These ratings were used to construct PERT distributions. The most likely value was the given deterministic, while the min and max were based on the provided percentage of uncertainty. For example, the loss of pre-packaged apples at the supermarket for which the retailer provided a deterministic value (x) and very low uncertainty rating (≤ 10%), has distribution [x*PERT(1-10%; 1; 1+10%)]. The parameter is then considered strictly uncertain.

Uncertain & variable parameters

It is also possible that instead of a deterministic value, variable data is provided in combination with an uncertainty rating of that data. In that case, x is replaced by a probability distribution, allowing separate sampling later on. Such is the case for the percentage of apples lost at the distribution center when packaging apples per 6, which is then categorized as being *uncertain & variable*. This means that the apple loss during packaging varies constantly and that there is no system in place in the distribution center to measure this varying loss.

Model and data quality and correlations

Regarding the (potential) *relationship* between different parameters, different methodologies exist for taking those into account (Groen and Heijungs 2017; Gil et al. 2021). We envisioned three ways to include relationships between parameters into the model:

- Building the relationships into the model, based on logic or knowledge (e.g., apples bought in the summer have a long storage time and a higher loss percentage at the auction).
- Letting @Risk calculate a correlation matrix while the distributions for several parameters (for which a correlation is assumed) are being fitted at the same time. This is only possible when multiple data units (e.g., measurements) are available for one parameter, as when using a large database, which is not the case for the post-harvest chain and was therefore not used.

- Specifying correlations directly in the model using correlation coefficients. We assume that correlations were present between several parameters, but we were unable to specify them for the case study due to a lack of data. For example, one of the auctions specified that the transport distance from the farm to the auction varied between 1 and 75 km (25 km most likely), and that in 65% of the cases a tractor is used instead of a truck. It is plausible that for farther distances, a truck is more often used for transportation. Though, we did not have any data on that, so the possible correlation was not incorporated.

The *quality of the data* was assessed using the PEF Data Quality Ratings (European Commission 2012). Data quality refers to the characteristics of data that relate to their ability to satisfy stated requirements (ISO 2006). This includes various aspects such as technological, geographical and time-related representativeness, completeness and precision of the inventory data (European Commission 2012). We want to note here that when the data is rated to be of excellent quality, this does not mean it is deterministic data. It is more an indication of how well the data approximates reality and covers the complete system at hand. Thus, data variability and uncertainty can still be present.

All the necessary parameters, data sources, (non-confidential) data, probability distributions, types of uncertainty and variability, data quality ratings and SimaPro processes can be found in section 1 of the Online Resource. Running the 2DMC simulations for the post-harvest model, generating the 2 500 000 2DMC results in a separate Excel worksheet and producing the cumulative probability graph for 1 impact category for 1 packaging option took around 50 minutes on a PC with Intel® Core ™ i7-7820HG CPU with 4 cores, a RAM of 32 GB DDR4 at 2400 MHz. Generating all 2DMC results for the 16 impact categories for both packaging options thus took a little under 27 hours.

2.2.2.3 *Statistical tests for 1DMC results*

For the 1DMC analysis, all input probability distributions assigned to the influential parameters stayed the same as for the 2DMC analysis (Table 1), but during the simulations, all distributions are sampled from together. Thus, each parameter that was categorized as uncertain, variable and uncertain & variable in 2DMC is categorized as "overall uncertain" in the 1DMC analysis since uncertainty and variability are in such an analysis treated alike. Just as for the 2DMC analysis, 10 000 iterations are run, leading to 10 000 possible LCA results for each impact category.

To see which product is preferred, either bulk or pre-packed apples, the "modified comparison index" was calculated. This index was proposed by Heijungs (2021) and is an adaptation of the discernability analysis. In a *discernability analysis* it is counted how many times one product scores better than another in all Monte Carlo runs (Heijungs and Kleijn 2001; Heijungs 2021). According to Hauschild et al. (2018), there are two frequently used methods for this, either subtracting (A-B) or dividing (A/B), meaning that option A has a lower impact than option B when A-B<0 or A/B<1, respectively. The advantage of this is that if the impacts of two options are subtracted or divided during simulation, the uncertainty of correlated parameters will be the same in both options and will therefore not contribute to the uncertainty of the difference between the two options (Hauschild et al. 2018). For the "*modified comparison index*", two versions of the comparison index (CI) are first defined (Heijungs 2021):

$$CI_{A,i} = \frac{b_i}{a_i} \quad \text{and} \quad CI_{B,i} = \frac{a_i}{b_i}$$

with i representing the number of Monte Carlo runs and a and b the environmental impact of product A and B, respectively. Next, a minimum threshold value is defined $\gamma_0 = 1.2$, the same as in Heijungs (2021). A minimum threshold value of 1.1 was also considered.

The minimum threshold value is used for assessing the superiority (*S*) of product A and of product B (Heijungs 2021):

$$S_{A,i} = \frac{1}{n}\sum_{i=1}^{n} \Theta(CI_{A,i} - \gamma_0) \quad \text{and} \quad S_{B,i} = \frac{1}{n}\sum_{i=1}^{n} \Theta(CI_{B,i} - \gamma_0)$$

with Θ(x) representing the Heaviside step function (which returns 1 if x>0 and otherwise 0). *S* is expressed as the probability of threshold superiority of product A and of product B (in %), respectively.

3 Results

The results section is divided into two parts. In section 3.1, three hypothetical outcomes when using 2DMC for the comparison of two options within an LCA context are illustrated. These possible outcomes are further illustrated using real-life data for the apple post-harvest chain in section 3.2 and the 2DMC results are compared to the deterministic and 1DMC results. The POC model and manual (Michiels and Geeraerd 2021) explain how the 2DMC results can be visualized and synthetized using ratios.

3.1 Possible 2DMC outcomes for LCA

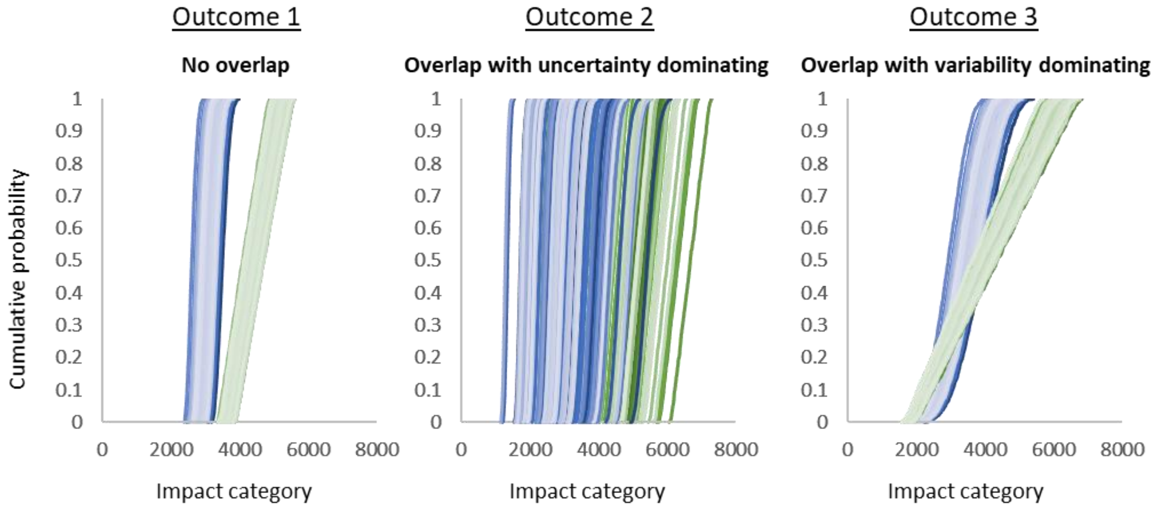
When using 2DMC in quantitative risk assessment, the total range of 2DMC results are often sufficient to allow management decisions to be taken. For example, when estimating the possible daily exposure to a carcinogenic substance in breast milk and powder infant formula (Boué et al. 2017) or the risk associated with the consumption of smoked salmon potentially contaminated with the pathogen *Listeria monocytogenes* (Vásquez et al. 2014), the maximum possible estimation is often of utmost importance. Therefore, obtaining the 2DMC curves of one product is generally sufficient and the focus lies on the probability that the estimation will be above a certain critical value. Two possible 2DMC outputs for this were already illustrated in Fig. 1.

In contrast, the comparison between two products or processes is an important LCA goal. For comparative LCA's, the inventory data are often based on deterministic data from one location during a specific time [e.g., comparing conventional and organic cultivation using data from one cultivation period from one farm each (Chatzisymeon et al. 2017)]. These data are used to choose the environmentally preferable option. However, as already addressed in the introduction, some questions quickly arise in those cases. Is the chosen option always environmentally preferable? What if we account for variability (e.g., data from a different cultivation period with more severe weather)? What if we account for uncertainty (e.g. when estimations are used instead of accurate measurements)? Does the decision stay the same?

Generally, there are three possible 2DMC outcomes in LCA. These are illustrated in Fig. 4 for fictitious data (based on the POC model), showing the cumulative probability of a specific impact category reaching a certain impact.

First, the curves of the 2DMC results could show no overlap between the two products, meaning that one product (the one with its curves at the left of the other) consistently performs better (Outcome 1 in Fig. 4). This allows to base the decision on the central tendency (the median of the median, A in Fig. 2) comparison, or even on the deterministic impact. Secondly, the 2DMC could show overlap either due to high uncertainty (high uncertainty ratio, Outcome 2) or, thirdly, it could show overlap due to high variability (high variability ratio, Outcome 3) in the input data. Outcome 2 and 3 imply that the most environmentally friendly option, still with respect to that specific impact category, cannot yet be decided upon. For uncertain data, this means collecting more accurate information (Vose 2008), for variable data, this means the two products are equivalent when it comes to that specific impact category. One may then decide to analyze the variability causes further or that other reflections, like cost, should be considered as well.

Note that, as illustrated in Fig. 4, we propose to visualize and communicate 2DMC results in two ways: by looking for overlap in the graphs and/or by comparing ratios.



	Product 1	Product 2
UR	1.11	1.07
VR	1.09	1.18
OR	1.21	1.26

	Product 1	Product 2
UR	**1.66**	**1.49**
VR	1.09	1.08
OR	1.81	1.61

	Product 1	Product 2
UR	1.11	1.07
VR	**1.28**	**1.51**
OR	1.42	1.62

Fig. 4 *There are three possible outcomes when comparing two products or processes (P1 and P2) using two-dimensional Monte Carlo simulations in LCA. The two 2DMC curves can be either clearly separated for the two products (outcome 1) or there can be overlap (outcome 2 and 3). In case of overlap, this can be caused by high uncertainty in the data (outcome 2) or high variability (outcome 3), which can be clearly deduced from the ratios (UR = uncertainty ratio, VR = variability ratio and OR = overall uncertainty ratio)*

3.2 Deterministic, 1DMC and 2DMC post-harvest results

Fig. 5 shows the deterministic, 1DMC and 2DMC results for three selected impact categories, which give a good overview of the different outcome trends for the post-harvest apple chain: Water Resource Depletion, Climate Change and Ionizing Radiation (Human Health). The results of the other impact categories can be found in the Online Resource.

For the *deterministic* results, bulk apples are consistently preferred for each impact category over pre-packed apples (Fig 5, shown as rhombi at 0.5 cumulative probability for visibility reasons; the cumulative probability is not a part of the for deterministic results and should be disregarded). This is also the case when looking at the *1DMC* curves (Fig. 5, left), which show no overlap between the two products. The *modified comparison index*, calculated using 1DMC results, gives a more nuanced result. For the pre-packed apples, there is a 0% probability of a threshold superiority for both threshold values (i.e., 1.1 and 1.2). For the bulk apples, however, the probability of a threshold superiority, for a threshold value of 1.2, changes quite a bit depending on the impact category, ranging from 0% for Ozone Depletion, Ionizing Radiation (Fig. 5) and Terrestrial Eutrophication, to 14% for Climate Change (Fig. 5) and up to 100% for Water Resource Depletion (Fig. 5). This means that, for Climate Change, bulk apples have a lower impact than pre-packed apples with a factor of at least 1.2 (i.e., 20%) with a probability of 14%, while reversely, pre-packed apples have a 0% probability. For the 86% other cases, bulk apples might still beat pre-packed apples but with a lower difference. Evidently, when reducing the minimum threshold value to 1.1, the threshold superiority of bulk apples increases significantly. Only Ionizing Radiation (Human Health) still had a probability of threshold superiority of less than 10% (i.e., 6%), followed by Ozone Depletion with 17% (shown in the Online Resource).

Regarding the *2DMC* results, almost all impacts of the bulk and pre-packed apples show clearly divided 2DMC curves (except for a small overlap in the tail ends), with bulk apples being environmentally preferable. This is illustrated in Figure 5 (right) for Water Resource Depletion and Climate Change, clearly showing that the impact category can be categorized as a typical outcome 1 ‘No overlap’ of Fig 4. The impact categories Ozone Depletion, Ionizing Radiation (Environmental in Online Resource and Human Health in Fig. 5c, right) and Freshwater Ecotoxicity, however, show overlapping 2DMC curves between the bulk and pre-packed apples. These results are categorized under outcome 3 ‘Overlap with variability dominating’ of Fig. 4 since variability has a higher ratio than uncertainty. We could have predicted from the modified comparison index (based on the 1DMC results) that those impact categories would show overlap since they had a 0% or very low (i.e., 2%) probability of threshold superiority for both bulk and pre-packed apples for a minimum threshold value of 1.2. Additionally, when reducing the minimal threshold value to 1.1, the probability of threshold superiority for bulk apples for those impact categories showed a limited increase, (with a max of 30%). No impact category from the apple post-harvest chain could be categorized under outcome 2 ‘Overlap with uncertainty dominating’.

When looking at the *ratios* of all impact categories, variability is dominating the overall uncertainty in the complete post-harvest chain. Bulk apples show a higher variability ratio for all categories compared to pre-packed apples. The uncertainty ratio, in contrast, was almost always the same for each packaging method with a maximum ratio of 1.04. This means that the overall uncertainty ratio is dominated by variability.

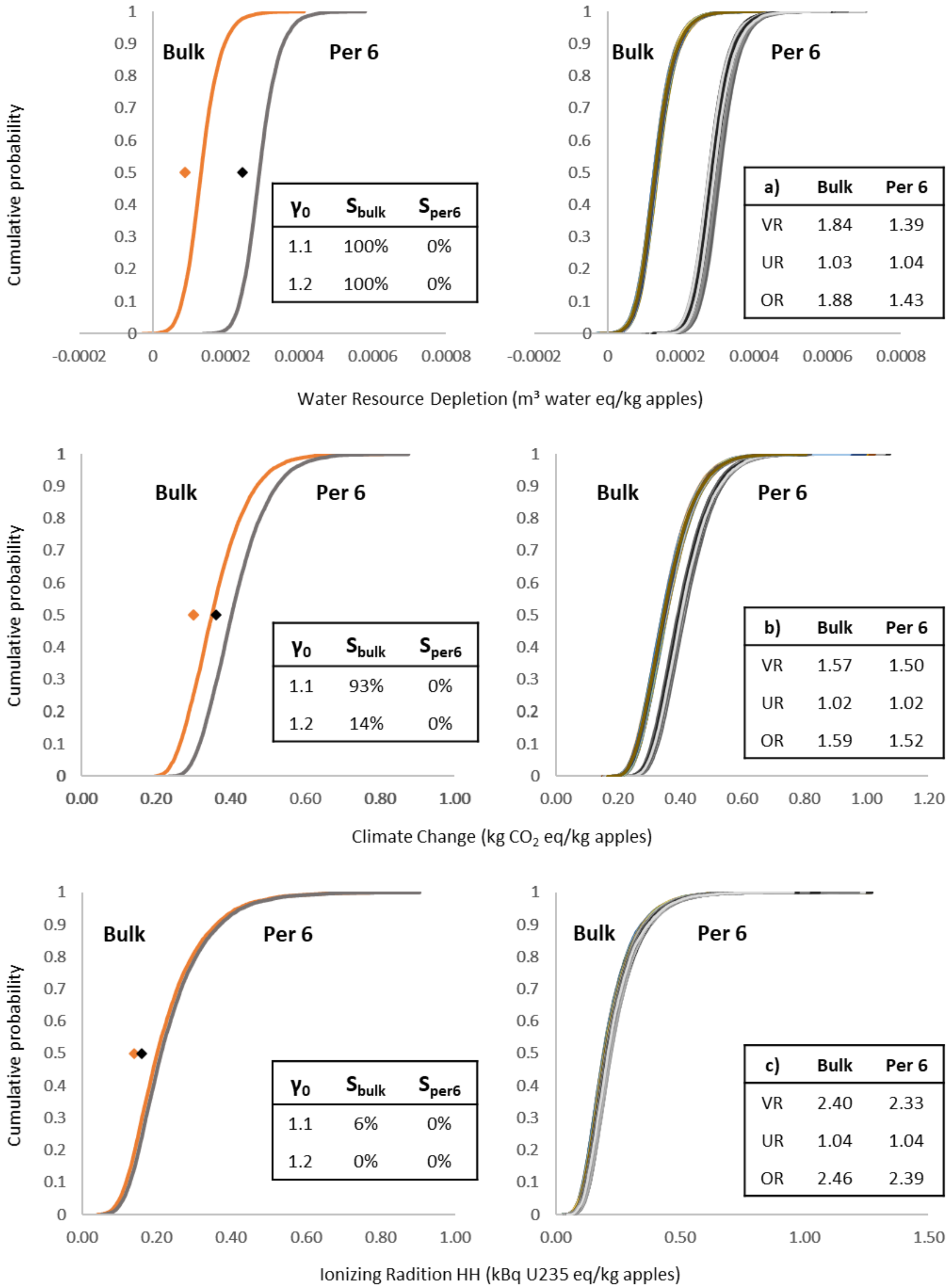


Fig. 5 *Deterministic (left, rhombi, only x-values relevant), 1DMC (left, curves) and 2DMC (right, curves) results for the post-harvest chain (bulk colored and pre-packed in greyscale) with the modified comparison index results (S, expressed as the probability of threshold superiority of either bulk or pre-packed apples, for two threshold values) and the uncertainty ratio (UR), variability ratio (VR) and the overall uncertainty ratio (OR)*

4 Discussion

4.1 Assigning uncertainty and variability

The aim of this study was to *introduce 2DMC as a potential interesting method* for simultaneously propagating uncertainty and variability separately in LCA. To test the method, we used a previously developed case study from our research group (Goossens et al. 2019). A local sensitivity analysis was conducted to identify influential parameters and the associated uncertainty and/or variability was characterized. The remaining, low influential parameters were categorized as deterministic. It is possible that there is still uncertainty or variability connected to those parameters, however, we at least know that these parameters do not really influence the results that much. It is, therefore, justified to not spend extra time on finding additional data for those parameters.

In general, parameters were considered uncertain in this study when the surveyed people (i.e., auction and retail) indicated being uncertain of the provided data. Variability was attributed to those parameters that described biological variation, consumer behavior, management choices and different production sites/companies. For example, the distance between two specific companies is deterministic, but when several different companies deliver the same goods (e.g., different growers bringing their fruit to the auction) the distance is seen as variable.

To be able to actually propagate uncertain and/or variable parameters, data needed to build distributions have to be available/provided. The definition of the *fore- and background system* play a significant role in that. The foreground system is where the LCA practitioner can be in direct contact with the data provider, creating the opportunity for gathering specific data, being potentially uncertain and/or variable.

Data in the background system is generally more uncertain and variable, as it is usually not product, process or location specific. The data quality of the database determines if reliable data is available. Though, one might wonder if the background system is really where the focus should lie when looking for qualitative data. Oftentimes in product/process comparisons, the systems share background processes, and the absolute uncertainty from those can cloud the relevant differences. Rather the relative uncertainty found in the foreground system is of importance to discern between the two options (Henriksson et al. 2015; Bamber et al. 2020) and is more interesting for both LCA practitioners as well as the stakeholders. LCA practitioners can influence the foreground system more, really making sure that the chain they built is representative and realistic. For the stakeholders, they want to use LCA as a decision-making tool, thus for them it is also more relevant that the focus lies on the foreground system since there they have more power to intervene (if necessary).

Even when a sufficient amount of data is available/provided, the distinction between uncertainty and variability is not always a clear-cut decision. Warmink et al. (2010) mention that random variation in the natural world can arguably also be seen as a lack of knowledge, which subsequently can be reduced given enough resources. Yet, it is unrealistic to assume unlimited available resources and variability is therefore seen as random system behavior when a realistic amount of available resources are considered (Warmink et al. 2010). This thought process was followed when distinguishing uncertainty from variability in this case study.

4.2 Basing decisions on deterministic or 1DMC results

While LCA improves the understanding of the environmental impacts associated with each product or process, it is rare that the results identify a clear 'winner' between alternatives (Curran 2014). The deterministic and 1DMC results provide a first indication on which product or process in a comparative LCA is preferable. However, with deterministic results, no ranges in the input data are accounted for, meaning that overlapping output results cannot be observed. The complexity and dynamics of reality are unaccounted for.

1DMC outcomes provide a more nuanced result. First, 1DMC curves can also show overlap, though this was not the case for the post-harvest case study, or can lie very close together, indicating that conclusions may not be robust and a closer inspection is needed. Similarly, the modified comparison index provides a way to tell how much probability there is that a certain product will be superior over another. If those probabilities are low for some impact categories (such as for Ionizing Radiation), this – again – indicates that a closer inspection is needed. The shortcoming, however, is that there is no indication on where the focus should lie for this 'closer inspection'. 2DMC can help in that regard because its ratios show which steps to take when the results of two products show overlap and a clear 'winner' cannot be identified.

4.3 Interpreting 2DMC ratios

While the vast majority of 2DMC results show no overlap between the two products, for Ionizing Radiation (Human Health, Fig. 5c) a lot of overlap can be seen in the results. This means that we cannot conclude which product is environmentally preferable for that impact category. When 2DMC results of two products or processes show overlap, one can look at uncertainty and variability to make informative decisions. The different origin of uncertainty and variability leads to different steps that need to be taken to be able to reduce the overall uncertainty of the model.

Ionizing Radiation (Human Health) showed a high degree of variability (represented by a high variability ratio). This implicates true differences between the two products or processes, which cannot be reduced by further study (Hauschild et al. 2018; Igos et al. 2019). Collecting more accurate information to conduct new calculations would just be a waste of time (Vose 2008). On the one hand, a high variability ratio can indicate that there are ways to have a low environmental impact for a certain product or process, but for some reason, not all companies can achieve that. This may provide the opportunity for companies to learn from each other and to improve their management. In that case, having a closer look at the physical system and examining the differences between different management practices can lead to system optimization, product development or policy (Steinmann et al. 2014).

On the other hand, the high variability can also be due to differences that cannot be reduced, for example, because of the biological nature of the apples, weather variations or differences in soil during cultivation. In such cases, it could be said that the products are equivalent when it comes to their environmental impact. One could then choose to make other reflections when deciding which product is preferable, such as looking at their difference in cost. Or, one might decide to disregard the impact category for which the 2DMC curves show overlap due to a high variability and instead focus on the remaining impact categories. For the post-harvest apple chain, only four of the 16 impact categories show overlap in the results, all due to a high variability. The other 12 impact categories clearly show a preference for bulk apples. The stakeholders could decide that those four impact categories are not of high relevance when looking at the complete picture and may decide to disregard them

In our real life case study, there was no example of a result dominated by uncertainty (represented by a high uncertainty ratio). Yet, if in another study this would be the case then gathering more knowledge through e.g., further measurements, literature research and expert consultations (Huijbregts 1998; Walker et al. 2003; Hauschild et al. 2018; Igos et al. 2019), may be needed before two products or processes can robustly be compared.

Reducing the overall uncertainty by reducing uncertainty and/or variability could lead to more robust conclusions when it comes to recommending one product or process over another. Deterministic or 1DMC results do not allow for a distinction between uncertainty and variability, and therefore cannot guide these types of decisions. When the 2DMC curves of two scenarios overlap, it is always advisable to interpret the ratios and to see how to possibly reduce the spread and range of the curves.

4.4 Towards a communication consensus

We propose to visualize and communicate about 2DMC results in two ways: by looking for overlap in the graphs *and* by comparing ratios.

Regarding the ratios, we used the *50th and 97.5th percentiles* to calculate uncertainty and variability ratios as described in Pouillot et al. (2016) and proposed by Özkaynaka et al. (2009) to communicate about uncertainty and variability in a clear way. However, we could have chosen to use other ratios, such as the ones calculated from the 10th and 90th percentiles, as was done by Douziech et al. (2019) and Huizer et al. (2012). We could even have used the 2.5th and 97.5th percentiles, as to be more in line with the ratios calculated by Hauck et al. (2014) and Steinmann et al. (2014) (section 1.3).

One might also wonder if the variability ratio is truly representative for the steepness of all output probability distributions, since the ratio is calculated using the data from only one curve (i.e., the 50th percentile or median of uncertainty). It might be interesting to see how the variability ratio would differ if another percentile was used, for example the 97.5th percentile of uncertainty (i.e., D/C in Fig. 4-2). In the case of the apple post-harvest chain, this difference is fairly limited with a maximum decrease of 0.02 and maximum increase of 0.01 of the variability ratios across all impact categories. It might be good practice to consistently calculate the variability ratios of a set of percentiles of uncertainty (i.e., a specific set of curves), as to quantify the uncertainty of the steepness of the curves.

Whichever ratios are chosen, the used percentiles should always be equivalent for the uncertainty ratio and the variability ratio, so they can be consistently compared.

5 Conclusions

To the best of our knowledge, this was the first time 2DMC was used in LCA to separately propagate data uncertainty and variability. Conducting a comparative LCA using only deterministic information, can give a first indication of which product/process might be environmentally preferred, but does not reflect the complexity and dynamics of reality. Therefore, it is recommended to always include uncertainty and/or variability information for the most influential parameters. For a quick analysis, these can be treated alike in a 1DMC analysis, using the 1DMC curves and the modified comparison index to see how far the product results are separated from each other. If the results lie too close together to make robust decisions, a 2DMC analysis is needed to identify which steps to take next to (potentially) reduce the overall uncertainty. The ratios indicate if that can be achieved by gathering more knowledge (and thus reducing uncertainty) *or* if the system should be examined more closely and other reflections may be needed (when variability is dominating). Of course, LCA practitioners can also choose to conduct a 2DMC analysis from the start. We propose to visualize and communicate about 2DMC results in two ways: by looking for overlap in the graphs and by comparing ratios, and we look forward to future work on refining the chosen ratio definitions.

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7 Data availability statement

All data generated or analyzed during this study are included in this published article and its supplementary information files.

8 Competing interests

The authors have no competing interests to declare that are relevant to the content of this article.

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10 Online resource caption

Electronic supplementary material containing detailed descriptions regarding the inventory data, assumptions, categorizations into uncertainty and variability and probability distributions. Additional deterministic, 1DMC and 2DMC results can be found in the online resource and the weblink to the manual on 2DMC in LCA using @Risk.