QUANTIFYING THE SUSTAINABILITY OF OUR FOODS IN AN UNCERTAIN AND VARIABLE WORLD:

LIFE CYCLE ASSESSMENT OF THE APPLE CHAIN FROM ORCHARD TO CONSUMER

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Uncertainty is an uncomfortable position.
But certainty is an absurd one.

Voltaire

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Abstract

The need for sustainable production and consumption is strongly present in today's society. To achieve this goal, a realistic quantification of environmental sustainability is needed. Calculating the environmental impact of products and processes can be done by conducting Life Cycle Assessments (LCA). The life cycle perspective ensures that all necessary inputs, processes and outputs are considered, and that environmental impacts are addressed at the point in the life cycle where they will most effectively reduce the overall impact. LCA results can guide the way for making decisions without the risk of burden shifting, but only if those results are robust and unambiguous. However, a few methodological shortcomings obstruct this, especially in the agri-food sector, such as only using central tendencies to calculate impacts thereby ignoring the possible range of input values; and the lack of consensus between the multiple possibilities that exist for allocating impacts between different products generated by the same system. In this PhD thesis, the focus lies on those two shortcomings using the apple agri-food chain as case study.

Making conclusive decisions on what product or process is environmentally preferable is not possible when only using deterministic data. Yet, LCA results based on this kind of data is still being widely disseminated, meaning that uncertainty and variability are being ignored. Uncertainty and variability have a different origin and thus also a different implication, the combination is called "overall uncertainty". While uncertainty shows lack of knowledge, which can be reduced, variability reflects the natural heterogeneity in the world, which will always be observed.

Published LCA studied were assessed through a systematic review, to identify to which extent uncertainty and variability have been separately accounted for. This turned out to be very limited, with only eleven studies having some kind of visualization showing which dominates the results. All methods had drawbacks attached to them. Two-dimensional Monte Carlo simulations (2DMC) was identified as a possible approach that allows solve these drawbacks.

2DMC was introduced in the Belgian apple chain, comparing Jonagold and Kanzi apples in the cultivation chain and comparing bulk and pre-packed apples in the post-harvest chain. 2DMC allows to separately portray uncertainty and variability in LCA studies in a clear and representative way. This can help decision makers in judging the robustness of differences in product comparisons, while also indicating how the overall uncertainty can be reduced. Either the decision maker can already robustly conclude that one product could be preferred over the other, or it might be that the uncertainty and/or variability does not yet allow this. In the case that uncertainty is dominating, more knowledge should be gathered before making any decisions. In contrast, if variability is dominating, the only way to possibly reduce the overall uncertainty would be by examining the production system and making physical changes in the system itself. However, the latter is not always possible or even wanted.

The second necessity for making accurate comparisons using LCA, is the equivalence of the system boundaries of the two options. However, equivalent system boundaries are currently lacking when organic crop production systems are compared to more conventional ones. Generally, when residual products from livestock systems get a second life as organic fertilizers, the impact of producing those residual products are ascribed to the livestock system, thus the system where it originates from. Meaning that no production impacts of those organic fertilizers are allocated to organic cultivation, the system where it is used and very much needed. This is in contrast with mineral fertilizers, used in conventional crop production systems, for which the production impact is allocated to the system where it is used. This inconsistency between organic and conventional crop production can lead to skewed LCA results. Multiple procedures exist to still allocate production impacts of organic fertilizers to organic cultivation, however, these can lead to very different results.

Those different allocation procedures were therefore applied in an LCA of organic apple cultivation, to see where the difficulties for each procedure lies and to assess how much the results can be influenced by the chosen procedure. In the end, mass allocation was selected as the best way to approximate reality if a representative mass allocation factor is chosen that reflects the function of the organic fertilizers. The influence of factors from outside the system is limited for this procedure.

In conclusion, the results show that with the discussed methodological improvements, comparing products and processes to assess their relative environmental impacts will be much more robust and conclusive. Clear decisions are much needed on industry, consumer and policy level to guide the way to sustainable production and consumption.

Samenvatting

De duurzaamheid van ons voedsel kwantificeren in een onzekere en variabele wereld

Levenscyclusanalyse van de appelketen van boomgaard tot consument

De nood aan duurzame productie en consumptie is sterk aanwezig in onze huidige samenleving. Om dit doel te bereiken, is een realistische kwantificering van de ecologische duurzaamheid nodig. Het berekenen van de milieu-impact van producten en processen kan door middel van een levenscyclusanalyse (LCA). Het levenscyclusperspectief zorgt ervoor dat alle noodzakelijke inputs, processen en outputs in rekening worden genomen en dat milieueffecten worden aangepakt op het punt in de levenscyclus waar ze de algehele impact het meest effectief zullen verminderen. De LCA-resultaten kunnen dus richtinggevend zijn bij het nemen van beslissingen zonder daarbij het risico te lopen dat de milieulasten worden verschoven, maar alleen als die resultaten robuust en eenduidig zijn. Er zijn echter methodologische tekortkomingen die dat in de weg staan, en dat vooral in de agrovoedingssector, zoals wanneer enkel centrummaten gebruikt worden om de milieueffecten te bereken waardoor de mogelijke range van inputwaarden genegeerd worden; en het gebrek aan consensus dat er is tussen de vele mogelijkheden die er zijn om effecten toe te wijzen aan verschillende producten die eenzelfde systeem produceert. In dit proefschrift ligt de focus op die twee tekortkomingen waarbij de appel agrovoedingsketen gebruikt wordt als casestudie.

Overtuigende beslissingen nemen over welk product of proces de voorkeur verdient vanuit milieuoogpunt is niet mogelijk wanneer alleen deterministische gegevens worden gebruikt. Toch worden LCA-resultaten op basis van dit soort gegevens nog steeds op grote schaal verspreid, waarbij dus onzekerheid en variabiliteit worden genegeerd. Onzekerheid en variabiliteit hebben een verschillende oorsprong en dus ook een verschillende implicatie; de combinatie wordt "totale onzekerheid" genoemd. Terwijl onzekerheid wijst op een gebrek aan kennis, die kan worden verminderd, weerspiegelt variabiliteit de natuurlijke heterogeniteit in de wereld, die altijd zal worden waargenomen.

Gepubliceerde LCA-studies werden beoordeeld door middel van een systematische review, om na te gaan in hoeverre al met onzekerheid en variabiliteit afzonderlijk rekening is gehouden. Dit bleek zeer beperkt te zijn: slechts elf studies hadden een of andere vorm van visualisering waaruit bleek welke van de twee in de resultaten overheerst. Aan alle gebruikte methoden waren bovendien nadelen verbonden. Tweedimensionale Monte Carlo simulaties (2DMC) werd geopteerd als een mogelijke manier om die nadelen op te lossen.

2DMC werd geïntroduceerd in de Belgische appelketen, waarbij Jonagold en Kanzi appels in de cultivatieketen, en bulk en voorverpakte appels in de naoogstketen vergeleken werden. 2DMC laat toe om onzekerheid en variabiliteit in LCA-studies op een duidelijke en representatieve manier apart weer te geven. Dit kan besluitvormers helpen bij het beoordelen van hoe robuust de verschillen zijn in productvergelijkingen, terwijl het ook aangeeft hoe de totale onzekerheid kan worden verminderd. Ofwel kan de besluitvormer al op robuuste wijze concluderen dat het ene product de voorkeur verdient boven het andere, ofwel kan het zijn dat de onzekerheid en/of variabiliteit dit nog niet toelaat. In het geval dat onzekerheid overheerst, moet eerst meer kennis worden vergaard voordat een beslissing kan worden genomen. Indien de variabiliteit overheerst, zou men enkel de totale onzekerheid eventueel kunnen verminderen door het productiesysteem te bestuderen en fysieke veranderingen in het systeem zelf aan te brengen. Dit laatste is echter niet altijd mogelijk of zelfs gewenst.

De tweede vereiste voor het maken van accurate vergelijkingen met behulp van LCA, is de overeenkomstigheid tussen de systeemgrenzen van de twee opties. Momenteel ontbreekt het echter aan zulke overeenkomstige systeemgrenzen wanneer biologische cultivatiesystemen worden vergeleken met meer conventionele systemen. Wanneer restproducten van veeteeltsystemen een tweede leven krijgen als biologische meststoffen, worden de effecten van de productie van die restproducten doorgaans toegeschreven aan het veeteeltsysteem, dus aan het systeem waaruit ze afkomstig zijn. Dit betekent dat er geen milieu-impact van de productie van die organische meststoffen worden toegerekend aan de biologische teelt, het systeem waar ze worden gebruikt en hard nodig zijn. Dit in tegenstelling tot minerale meststoffen die worden gebruikt in conventionele teeltsystemen, waarvoor de productie-impact wel wordt toegerekend aan het systeem waar ze worden gebruikt. Deze inconsistentie tussen biologische en conventionele plantaardige productie kan leiden tot scheve LCA-resultaten. Er bestaan verscheidene procedures om de productie-impact van biologische meststoffen toch toe te rekenen aan de biologische teelt, maar deze kunnen tot zeer uiteenlopende resultaten leiden.

Die verschillende procedures werden daarom toegepast in een LCA van biologische appelteelt, om te zien waar de moeilijkheden voor elke procedure liggen en om te beoordelen in hoeverre de gekozen procedure de resultaten beïnvloedt. Uiteindelijk werd een impacttoewijzing op basis van massa geselecteerd als de beste manier om de werkelijkheid te benaderen, maar enkel als een representatieve massatoewijzingsfactor wordt gekozen die de functie van de biologische meststoffen weerspiegelt. De invloed van factoren die buiten het systeem liggen, is bij deze procedure beperkt.

Concluderend is er aangetoond dat met de besproken methodologische verbeteringen het vergelijken van producten en processen om hun relatieve milieueffecten te beoordelen, veel robuuster en overtuigender zal zijn. Er is grote behoefte aan duidelijke beslissingen op industrie-, consumenten- en beleidsniveau in onze weg naar duurzame productie en consumptie.

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Abbreviations and symbols

1DMC	(one-dimensional) Monte Carlo simulations
2DMC	Two-dimensional (or second-order) Monte Carlo simulations
AIC	Akaike Information Criterion
B2B	Business to Business
B2C	Business to Consumer
C	Carbon
CO_2	Carbon dioxide
DE	Germany
Distr.	Chosen input probability distribution
E	Environment
ES	Spain
EPS	EuroPoolSystem
eq	Equivalent
EU	European Union
FAO	Food and Agricultural Organization
FADN	Farm Accountancy Data Network
FR	France
GHG	Greenhouse gas
HH	Human Health
IC	Impact Category
ILCD	International Reference Life Cycle Data System
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
K	Potassium
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LPG	Liquefied Petroleum Gas
LUC	Land use change
N	Nitrogen
N_2O	Nitrous oxide
N.A.	Not applicable

NC	North Carolina
NH_3	Ammonia
NL	The Netherlands
NTP	Novatein Thermoplastic Protein
NZ	New Zealand
P	Phosphorus
P_2O_5	Phosphorus pentoxide
PEF	Product Environmental Footprint
PEFCRs	Product Environmental Footprint Category Rules
PERT	Program Evaluation and Review Technique
POC	Proof of concept
PT	Portugal
UK	United Kingdom
UN	United Nations
US	United States of America
WA	Washington state

PART I

Laying the foundations

Chapter 1

General introduction

Since the global population keeps increasing and is expecting to reach an all-time high of 9.73 billion by 2050 (FAO, 2017; medium scenario), governmental bodies are focusing more and more on making sure that everyone has access to sufficient, nutritious and sustainable food (European Commission, 2020). In 2015, the United Nations agreed on new global Sustainable Development Goals for 2030. The second goal specifies the need to “end hunger, achieve food security and improved nutrition and promote sustainable agriculture”, while the twelfth wants to “ensure sustainable consumption and production patterns” (UN General Assembly, 2015). To achieve these goals, the European Commission recently launched – among other things – the European Green Deal (European Commission, 2020). With their Farm to Fork Strategy, the aim is to ensure that the food chain has a “neutral and positive environmental impact”.

Meanwhile, there is also growing concern among consumers about the sustainability of their food consumption. However, they currently lack a uniform and consistent way of being informed on the sustainability aspects of their food choices. For example, Goossens et al. (2017b) discussed 16 eco-labels for fresh produce that are currently being used in Flanders (Belgium), none of which gave the consumer an adequate indication of the produce’s environmental friendliness.

This illustrates the growing need for sustainable food production and consumption. But how can we know how sustainable something is? How can we identify which products or processes should be preferred over another and, how can we correctly communicate the consequences of their food choices to consumers or – alternatively – to decision makers? For this, the sustainability of the current food production and consumption needs to be quantified. Sustainability entails social, economic and environmental aspects, but for the purpose of this thesis, the focus will lie on environmental sustainability.

1.1 Quantifying sustainable production and consumption

To quantify the sustainability of actual food production systems, accurate calculation methods are indispensable**.** The European Commission (2016) declared *Life Cycle Assessment (LCA)* as "the best framework for assessing the potential environmental impacts of products currently available". LCA addresses the environmental aspects and potential environmental impacts (e.g., environmental consequences of emissions) throughout a product's life cycle, from raw material acquisition, production, use, to final disposal (ISO, 2006a).

Hauschild et al. (2018) described four main characteristics of an LCA. First, the life cycle perspective (e.g., cradle-to-grave) ensures that all processes required to deliver the studied function or product are considered. Second, the calculated environmental impacts are not limited to for instance climate change (such as for the carbon footprint) or water depletion (such as for the water footprint). LCA ensures a comprehensive coverage of environmental issues. Third, the quantitative nature of LCA makes it possible to compare the environmental impacts of different products or processes. As a last characteristic, Hauschild et al. (2018) emphasize that LCA is science based. It uses measurements and models that are based on proven or empirically observed causalities.

ISO 14040/44 (2006a, 2006b) developed an LCA framework consisting of four iterative phases (Fig.1-1). In phase one, the *Goal & Scope Definition*, the reasons for carrying out the study, the intended audience, the product system to be studied, the functional unit[1] (e.g., 1 ton apples leaving the farm; see section 1.4.1), the system boundary[2], allocation[3] procedures (see section 1.4.2), impact calculation methods, etc. are defined. The potential environmental impacts generated by LCAs are relative expressions since they are related to the functional unit of a product system.

[1] "Quantified performance of a product system for use as a reference unit" (ISO, 2006a, 2006b)
[2] "Set of criteria specifying which unit processes that are part of a product system" (ISO, 2006a, 2006b)
[3] "Partitioning the input or output flows of a process or a product system between the product system under study and one or more other product systems" (ISO, 2006a, 2006b)

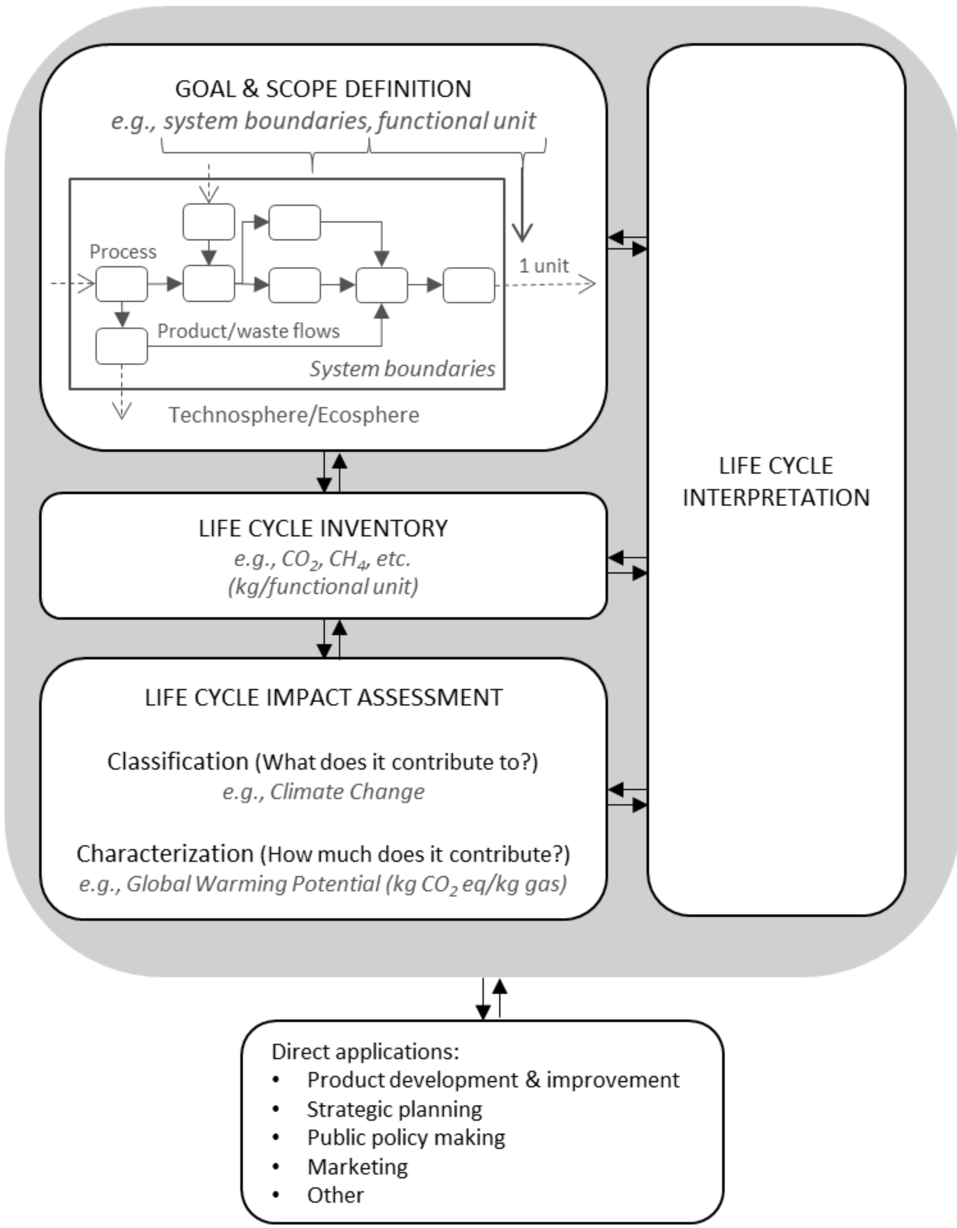


Figure 1-1 Phases of an LCA, adapted from ISO 14044 (2006a) and Hauschild et al. (2018).

During the second phase of the LCA, a *Life Cycle Inventory (LCI)* is built (ISO, 2006a, 2006b). This entails collecting all the input (e.g., energy inputs, raw material inputs, etc.) and output data (e.g., output products, waste, releases to air, etc.) within the system boundaries of the system being studied.

This inventory is then used in the third phase, the *Life Cycle Impact Assessment (LCIA),* to evaluate the potential environmental impacts associated with each inventory in- and output (ISO, 2006a, 2006b). These are classified into specific environmental issues called impact categories[4] [e.g., Climate Change (kg CO_2 eq), Freshwater Eutrophication (kg P eq), Water Resource Depletion (m^2 water eq), etc.] and multiplied with their characterization factor[5] (e.g., Global Warming Potential, P equivalents, water consumption equivalent, etc., respectively). This results in category indicator[6] results (i.e., impact per functional unit).

The chosen impact calculation method, or LCIA method, determines which impact categories will be included during the classification and which environmental mechanisms will be used as a basis for the characterization factors. For example, the ILCD method (which stands for "International Reference Life Cycle Data System") was developed by the Joint Research Centre of the European Union and considers 16 impact categories (Wolf et al., 2012), while the ReCiPe method was developed in the Netherlands and considers 18 impact categories (Huijbregts et al., 2017). This is – among other things – because the impact category "Ionizing Radiation" is split between its effect on human health and its effect on the environment in the ILCD method, which is not the case for the ReCiPe method. Furthermore, ReCiPe considers Terrestrial, Freshwater and Marine Ecotoxicity separately, while ILCD only acknowledges Freshwater Ecotoxicity. ILCD expresses Freshwater Ecotoxicity using CTUe as a unit, while ReCiPe uses kg 1,4-DCB. Next to ILCD and ReCiPe, Hauschild et al. (2018) list six other LCIA methods, all with their individual characteristics.

[4] "Class representing environmental issues of concern to which life cycle inventory analysis results may be assigned" (ISO, 2006a, 2006b)

[5] "Factor derived from a characterization model which is applied to convert an assigned life cycle inventory analysis result to the common unit of the category indicator" (ISO, 2006a, 2006b)

[6] "Quantifiable representation of an impact category" (ISO, 2006a, 2006b)

Finally, during the *Life Cycle Interpretation*, the LCI and LCIA results are summarized and discussed as a basis for conclusions, recommendations and decision-making; all in line with the goal and scope definition.

LCA outcomes should ensure that impacts are addressed at the point in the life cycle where they will most effectively reduce overall environmental impact and resource use (European Commission, 2003). This will also reduce the chance of possibly inducing burden shifting, where a potential environmental burden is shifted between life cycle stages, individual processes or environmental issues (Hauschild et al., 2018; ISO, 2006a). For example, a single-use aluminum container has a large impact on e.g., depletion of elements, ozone layer depletion and human toxicity. Single-use polypropylene containers might be proposed as a better alternative, however, they perform worse when it comes to e.g. climate change, acidification and eutrophication (United Nations Environment Programme, 2021).

A distinction is made between attributional and consequential LCAs. These two types of approaches answer very different questions, which were originally defined during the 2001 workshop on life cycle inventory data for electricity production (Curran et al., 2005). While the *attributional* approach seeks to answer the question "how are things (pollutants, resources and exchanges among processes) flowing within the chosen temporal window?", the *consequential* approach attempts to answer, "how will flows change in response to decisions?". To answer these questions, different types of data are needed i.e., average or marginal data, respectively. Average data represent the average environmental burdens connected to a product or process of the studied system. In contrast, marginal data reflect the effects of a small change in the outputs from a system on the environmental burdens of that system (Finnveden et al., 2009).

The two different approaches can be illustrated with the research of Kua and Maghimai (2017) who studied the environmental performance of steel versus reinforced concrete using both an attributional and consequential life cycle perspective. Depending on the design of a building, 1 kg of structural steel can be replaced by either 1 or 4.25 kg of concrete. Kua and Maghimai (2017) used an attributional LCA on the one hand, to assess the environmental impact of using these two different amounts of reinforced concrete. On the other hand, they used a consequential LCA to consider the environmental impact of the possible short-term and long-term change caused by the reduced consumption of steel and increased consumption of concrete. For the long-term, this could lead to a new market equilibrium, causing an increased import of concrete's constituents and a reduced import of steel. By considering these two types of perspectives, Kua and Maghimai (2017) could propose integrated technology policies to improve the sustainability of those building materials. In this PhD thesis, as in most studies, I will use attributional LCAs: I aim to compare potential impacts of current agriculture and food choices without introducing any changes.

LCA can contribute to the analysis of the environmental performance of production and consumption patterns at various levels (European Commission, 2016). Many business associations and companies [such as BASF (2021), Colruyt Group (2021) and Unilever (2021)] already use the life cycle approach to help reduce the overall environmental burdens of their goods and services, to improve the competitiveness of their products, in B2B and B2C communication, and in communication with governmental bodies. LCA is used in benchmarking and decision making as a tool to improve product system and design [e.g., Tool to Optimize the Total Environmental impact of Materials (totem, 2018)] and in criteria setting [e.g., Environmental Product Declarations (EPD International, 2021)]. The public sector equally makes use of life cycle thinking in stakeholder consultations and policy implementation [e.g. LCA4Regions (Interreg Europe, 2021)], ensuring that the big picture is considered.

1.2 The need for more transparency in LCAs

LCA is a comprehensive assessment, which minimizes – at least in theory – the chance of ignoring or devaluing important environmental issues. It highlights potential environmental trade-offs and challenges conventional wisdom (Curran, 2014). Though, this comprehensiveness comes with a cost, since it requires simplification and generalizations in the modeling of the considered system. LCA follows the "best estimate" principle, causing models to be based on the average performance of the product system and disregarding rare or very problematic events such marine oil spills or nuclear disasters (Hauschild et al., 2018). On top of that, there is often a lack of the lack of reliable, available inventory data (Curran, 2014). This prevents the calculation of *actual* environmental impacts, rather it is more accurate to say that impact *potentials* are calculated (Hauschild et al., 2018). However, some environmental, ethical and societal impacts (e.g., animal welfare)

are not easily measurable and thus cannot yet be ranked in terms of environmental impact (Notarnicola et al., 2015).

Furthermore, it is rare that LCA results identify a clear ‘winner’ between alternatives (Curran, 2014), especially since much of the interpretation is left to the person conducting the assessment, which can even result in producing different results for seemingly the same product (Notarnicola et al., 2015). LCAs can indicate which product or process is better for the environment, but it does not tell you if the better option is in fact “good enough” (Hauschild et al., 2018).

The above-mentioned inadequacies and limitations underline the *need for more transparency*. ISO 14040/44 (2006a, 2006b) specifically states that “the results, data, methods, assumptions and limitations shall be transparent and presented in sufficient detail to allow the reader to comprehend the complexities and trade-offs inherent in the LCA”. However, the majority of LCA reports and publications lack such degree of transparency when it comes to the applied methodology and underlying data, making it difficult for other researchers to build upon the data and/or the results. Unambiguous descriptions of the methods and decisions in, e.g., appendices or online available material [such as in Goossens et al. (2019)], need to be urgently included, respecting confidentiality issues where applicable. The European Commission (2016) has stressed the need for more development and consensus of LCA methodologies by providing a platform to facilitate communication, and data and model exchange.

The lack of an appropriate LCA implementation and transparency is especially the case for LCAs related with the agri-food chain. Its application is not as mature as LCAs for, e.g., solid waste and energy, which were the primary adoption drivers (McManus and Taylor, 2015), and thus not as comprehensive yet. Agri-food LCAs are especially challenging since plant and animal life in the agricultural stage comes with an inherent biological, and time and region dependent variability (Notarnicola et al., 2015).

1.3 The ignorance towards uncertainty and variability

When two products or processes are compared using LCA, this is sometimes based on one production cycle (which is further discussed in section 1.4.2 for perennial production systems). In such cases, the input values and the LCA results are often seen as definite, while reality is much more dynamic and complex. For example, when comparing two crop production system, organic and conventional cultivation, it might be so that the results point to the conventional cultivation as having the lower environmental impact. However, it is quite possible that the reverse is true in the next year, just because the weather is different.

This illustrates a major shortcoming in LCA where results are still being reported as deterministic, while in reality the used data is uncertain and variable (Table 1-1). *(Epistemic) uncertainty* is related to the assessor's incomplete state of knowledge about the parameters that characterize the physical system that is being modelled and can therefore be reduced through further research efforts. *Variability* (or aleatory uncertainty) is an observable variation related to the inherent randomness of the natural world (Hauschild et al., 2018; Vose, 2008; Walker et al., 2003). Given enough resources, this variability could be mapped by measuring and quantifying the total population, but the observed variation cannot be reduced – if that is even wanted – by gaining more knowledge (Hauschild et al., 2018), only by making physical changes to the system (Vose, 2008). The combination of uncertainty and variability is called *overall uncertainty* (Pouillot et al., 2016).

Table 1-1 Examples and reducibility of uncertainty and variability.
This table is based on information from various sources (Hauschild et al., 2018; Vose, 2008; Walker et al., 2003).

Type	Example sources	Possibly reducible through
Uncertainty	Systematic/random measurement errors, low measurement accuracy, ignorance, outdated information, subjective judgement, lack of data, lack of knowledge, etc.	more literature research, more expert consultation, more precise emission factors, increasing measurement resolution, further measurements, refining models, etc.
Variability	Varying climate regions, time aspects, soil textures, management strategies, unpredictability of natural processes, human behavior/preferences, etc.	making physical changes within the system

While the theoretical difference between uncertainty and variability might be clear, the distinction might not be so straightforward in practice. For example, the Intergovernmental Panel on Climate Change (IPCC) defines an uncertainty range around the emission factors of N_2O from fertilizer application. However, this range might also include variation caused by variability due to differences in climate conditions or soil types (Groen, 2016).

If the range of LCA results is dominated by uncertainty then more knowledge may be needed before one can robustly conclude that a product's impact is significantly different from another. Omitting uncertainty from a study can thus lead to over-interpretation and biased decisions (Verones et al., 2017). In contrast, results with a high degree of variability show true differences among alternative production processes, supply chains, etc. This information can further guide system optimization, product development or policy (Steinmann et al., 2014).

Thus, separating uncertainty and variability can help decision makers in judging the significance of the differences in product comparisons, in identifying options for product improvement and in assigning ecolabels (Huijbregts, 1998). Considering the rising importance and ambiguity of ecolabels (Goossens et al., 2017b), it is important to know how representative the results are when they are later expressed with one value. While the benefits of including uncertainty and variability are clear, they are still quite often unacknowledged in LCAs. Limited data availability and time constraints can cause a great hindrance in including them. Even when uncertainty is included, uncertainty and variability are almost always treated alike, even though their origin and implication clearly differ (Notarnicola et al., 2015).

In recent LCA studies, attempts are being made at quantifying uncertainty and/or variability – still treated alike – using methods such as sensitivity analysis (Konstantas et al., 2018; Longo et al., 2017), uncertainty analysis (Bautista et al., 2018; Romero-Gámez et al., 2017); or a combination of both (Jiao et al., 2019; Sykes et al., 2019). In an *uncertainty analysis*, the range of possible LCA results is quantified based on the uncertainty and/or variability range of the input parameters. In *sensitivity analysis*, the focus lies more on figuring out which input parameters have an important influence on the results, rather than the possible spread in the results (Hauschild et al., 2018; Igos et al., 2019).

It is important to truly grasp this distinction. An input parameter may be very uncertain or variable, but if the LCA result is insensitive towards it (i.e., a change in the input value does not change the output), it would be a waste of time to improve the certainty of the parameter. On the other hand, if the model output is very sensitive towards a specific input parameters, but this input parameter is very certain or even deterministic, better data would also not increase the robustness of the result (Fig. 1-2) (Hauschild et al., 2018).

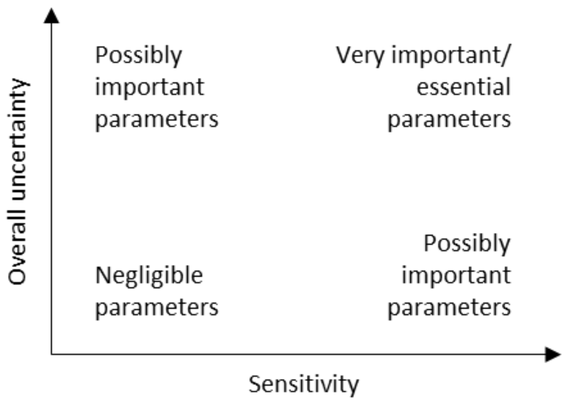


Figure 1-2 Identifying the very important or essential parameters by combining sensitivity and uncertainty/variability, based on Hauschild et al. (2018).

LCA studies that propagate the data uncertainty and/or variability, often do so using (one-dimensional) Monte Carlo simulations (1DMC) (Groen et al., 2014). In the 1DMC approach (Fig. 1-3), an iterative calculation process is performed using computer power. For each uncertain/variable input parameter, a probability distribution is specified containing all probable input values that the parameter can have (Vose, 2008). Ideally, interaction effects and correlation between input parameters are incorporated. Ignoring correlation during uncertainty propagation can lead to an under- or overestimation in the output variance. However, the knowledge about correlation coefficients is often not available (Groen and Heijungs, 2017), yet, a correlation matrix can be calculated when the distribution of several parameters are fitted at once [for example when using the Excel add-in @Risk (Palisade, NY, USA), see Chapter 5].

Once the input probability distributions (and correlations) are specified, a random sample is taken from the probability distribution for each input parameter. The complete set of samples is then analyzed in a deterministic model and the result is stored. This procedure is repeated several times, each time taking other random samples from the input probability distributions. After repeating the procedure for e.g., 10000 times, the 10000 different possible results form a probability distribution for the output (Vose, 2008). The output probability can then guide decision making, after all, knowing the probability of making the wrong decision can alter the final decision you make (Heijungs, 2021).

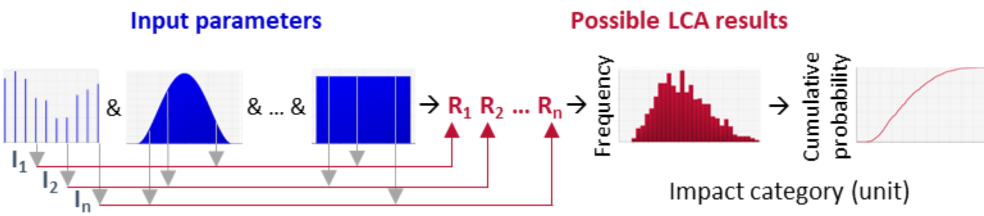


Figure 1-3 Schematic overview of one-dimensional Monte Carlo simulations. I_1 to I_n represent the n number of iterations and R_1 to R_n the resulting possible LCA results. The output can be graphically shown for each separate impact category using a histogram or cumulative probability curve.

1DMC can only propagate variability or uncertainty, but not both separately at the same time when a parameter is both uncertain and variable. A notable attempt at a methodology for separating them in LCA was made by Steinmann et al. (2014), for the LCA of coal-fueled power generation. They used 1DMC to calculate a variability and an uncertainty ratio, separately. Further attempts that have been made in LCAs to account for uncertainty and variability separately will be identified through a systematic review and their methods thoroughly discussed in Chapter 3.

It has been shown in quantitative risk assessment (Boué et al., 2017; Wu and Tsang, 2004) that separating uncertainty and variability could potentially be done effectively by conducting two-dimensional (or second-order or two-stage) Monte Carlo simulations (2DMC). 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). 2DMC has been applied in studies related to LCA, such as for the ecotoxicological impact assessment of down-the-drain products (Douziech et al., 2019) which can be used to calculate the ecotoxicological results of an LCA. However, I found no indication of its application in a typical LCA as it is described in ISO 14040/44 (ISO, 2006b, 2006a).

1.4 Arbitrariness in the goal and scope of agri-food LCAs

Turning now to food chain sustainability, the ‘Environmental Impacts of Products’ project of the EU Joint Research Center (Tukker et al., 2006) found that of all areas of consumption, ‘food and drink’ has the greatest impact throughout its life cycle (alongside private transport and housing), causing 20-30% of the environmental impact of private consumption. Moreover, several cradle-to-grave agri-food LCA studies show the agricultural stage as one of the most burdening (Svanes and Johnsen, 2019; Vinyes et al., 2017; Winkler et al., 2015).

It is evident that the sustainability of the agri-food chain needs to increase. However, there are some challenges connected to this research field when it comes to LCA. Conducting an LCA of the agri-food chain is not as straightforward as when studying a typical non-biological industrial products or processes, due to their inherently different production systems (Notarnicola et al., 2015). For this reason, I will focus on the methodological improvement of agri-food LCAs in this PhD thesis. As a case study, I will built further on the apple agri-food chain of Flanders (Belgium) which was previously developed in our research group (Goossens et al., 2019, 2017a)

As I already pointed out in the sections 1.2 and 1.3, the lack of full transparency and not acknowledging variability together with uncertainty is especially a shortcoming when it comes to agri-food LCAs. I will now further focus on some additional challenges that arise when defining the goal and scope of agri-food LCAs, paying special attention to perennial fruit production systems.

Ideally, the goal and scope should be aligned for all products to make comparisons possible. Comparing LCA results where the LCA practitioner defined different functional units, system boundaries, allocation procedures, LCIA methods, etc., is – quite honestly – meaningless. Complete uniformity is a prerequisite for fair comparisons. Guidelines in the form of Product Environmental Footprint Category Rules (PEFCRs) are slowly being provided to achieve the needed level of reproducibility and consistency for each product category. However, to this day, there has not been one provided for fruit products (European Commission, 2021).

1.4.1 Choosing a representative functional unit

In LCA, the functional unit is used as a reference to fairly and quantitatively compare different products or processes that provide the same function, typically answering questions such as "what?", "how much?", "for how long?", "how well?", etc. (Hauschild et al., 2018). An LCA is in fact the environmental assessment of needs fulfillment, meaning that first a function from the perspective of the user should be identified (Hauschild et al., 2018). However, when it comes to agriculture, three functions could be envisioned: food production, land management and providing an income for the farmer (Nemecek et al., 2011).

Cerutti et al. (2014) identified those three possible categories of functional units in LCAs of the fruit sector. The first category is *mass based*, which is the most commonly used in agri-food LCAs. Here the environmental impact is related to a specific amount of product that was produced. For fruit products, this is typically "1 ton of fruit at the farm gate" or "1 kg of fruit packed and delivered to the customer", depending on the goal and scope of the study.

The second type of functional unit is *land based*, where the impacts are related to the management of a specific amount of land (e.g., 1 hectare of orchard). An example of a land based functional unit from the study of Ferrari et al. (2018) is "the productivity per hectare of wine grapes in the thirty years of an espalier vineyard […]".

Mass and land based functional units are complementary in fruit production because they give different results and interpretations (Cerutti et al., 2014). While mass based units may lead to a preference for high input-high output systems, which can cause concentrated pollution problems on a regional scale; land based units will rank low input-low output systems better, decreasing impacts at a regional level but possibly creating the need for additional land use elsewhere (van der Werf et al., 2007). This can for instance lead to results that show a favorable environmental performance for organic cultivation when they are expressed per unit area, while conventional cultivation outperforms organic when results are expressed per product unit (Foteinis and Chatzisymeon, 2016; Meier et al., 2015). Mass based unit can thus indicate which production system is the most environmentally efficient and the land based unit could be useful when investigating the environmental impact in sensitive areas where a reduction in emissions is required (Cerutti et al., 2013).

The last category identified by Cerutti et al. (2014) is the *economic value-based* functional unit, where the environmental impact is related to a particular amount of grower income from wholesale fruit sales. This type of functional unit has a strong social dimension, seeing as the potential of the system (i.e., the farm) to generate money is assessed rather than its ability to grow food (Cerutti et al., 2013). While the results are very dependent on the local economic context, it does provide opportunities to account for product (i.e., fruit) quality, which is less straightforward in the other categories (Cerutti et al., 2011). In this context, Ponsioen and van der Werf (2017) recommend reporting environmental footprints per economic value (expressed in currency units). They state that this will reflect "the way a consumer values the different functionalities of the food or beverage and takes the possible rebound effects of spending saved money on other environmentally damaging activities into account".

Another possible category to assess food production are functional units related to the food's *nutritional function*. However, this kind of functional unit is very complicated since food products supply a wide variety of micro and macro nutrients (Ponsioen and van der Werf, 2017). This kind of functional unit seems to be primarily researched for protein rich food products or to assess whole diets, it is not often seen when assessing individual fruit products. Functional units that have been proposed and that did include individual fruit products (sometimes as part of a food basket) in the assessment were e.g., 100 g protein (Heller et al., 2013), 100 kcal (Drewnowski et al., 2015; Masset et al., 2015), a dietary dependent nutrient quality index (Sonesson et al., 2019), the amount of fruit containing the daily reference energy intake for one person, the amount of fruit containing the reference daily intake for vitamin C for one person, and the amount of fruit containing the reference daily intake for dietary fiber for one person (Svanes and Johnsen, 2019).

It is clear that when it comes to the functional unit of food products, no consensus has been reached and research is still actively going on. Depending on the perspective of the user (e.g., the farmer vs. the consumer), different functional units seem appropriate. While mass, land and economic value-based functional units might be more meaningful for the farmer, a nutritional functional unit would be more representative from a consumer-perspective (Notarnicola et al., 2015). Different food products can otherwise not be fairly compared when they constitute different nutritional roles in the diet (Heller et al., 2013; Ponsioen and van der Werf, 2017). Yet, these nutritional functional units also do not grasp the entirety of the functions of food, which also include pleasure, cultural values, social interaction, satiety, etc. (Heller et al., 2013; Sonesson et al., 2017). Since mass based functional units are the most commonly used in agri-food LCAs (Djekic et al., 2018) and are recommended by Cerutti et al. (2014) for profiling the environmental burdens of a fruit product, I will use "1 ton of fruit at the farm gate" and "1 kg of fruit purchased by the customer", in this PhD thesis.

1.4.2 Defining the orchard life cycle in perennial food production

First and foremost, it is important that the system boundaries of a studied product reflect the goal of the LCA study. For fruit products, this can mean different stages of the fruit's productive and logistic chain, but consumption and end-of-life can be included too (Fig. 1-4) (Notarnicola et al., 2015). The foreground processes [those processes that are specific to the studied product system and are largely modelled using data collected first hand by the LCA practitioner (Hauschild et al., 2018)] of the productive stage (i.e., the agricultural core) are those directly occurring on the cultivated land, such as fertilization, crop protection, irrigation, etc. (Bamber et al., 2020). In contrast, the background processes [those processes that are linked to the foreground system but also take part in many other product systems and are typically modelled using more generic data from LCI databases such as ecoinvent and agri-footprint (Hauschild et al., 2018)] include processes related to society's electricity supply, the production of fertilizer products, etc. (Bamber et al., 2020).

A lot of studies [e.g. Bamber et al. (2020), Ferrari et al. (2018), Goossens et al. (2017a) and, Romero-Gámes and Suárez-Rey (2020)] choose to focus on the productive part of the fruit chain, namely the perennial food production system. Unlike food crops (for which the life cycle is completed in under a year), perennial food production systems (such as apple orchards) involve plants with a variable life span, depending on crop and management practices (Cerutti et al., 2014). When looking at LCAs of perennial food production systems, different system boundaries [or "time boundaries" (Notarnicola et al., 2015)] for the orchard life span are being used, often depending on data accessibility. Cerutti et al. (2014) considered six stages that define fruit production (Fig. 1-5):

1. a nursery stage,
2. establishment of the orchard (i.e., field preparation and planting),
3. a low productive stage due to the orchard's immaturity,
4. a mature, full productive stage,
5. a low productive stage due to plant senescence, and
6. orchard destruction and disposal.

Though, for economic reasons, the orchard is often already replaced at the end of stage 4.

The productive life span of an orchard thus comprises three stages: the young, low productive stage, followed by full production and subsequently followed by an old, low productive stage (Cerutti et al., 2014; Goossens et al., 2017a). However, most commonly, the inventory used for conducting an LCA of a perennial food production system is limited to the production data of *one year* while the orchard is in full production (Fig.1-5a) (Ingwersen, 2012; Longo et al., 2017). To attenuate production fluctuations and external factors (e.g., varying weather conditions, pest occurrences, etc.), researchers also conduct LCAs on a dataset covering *three or more years* (Fig.1-5b) (Bartzas et al., 2017; Mouron et al., 2006). Cerutti et al. (2014) further suggests to collect field data in even numbers of years (at least four), to take into account the possible alternation of production (biennial bearing) of perennial crops. Bessou et al. (2016) tested how this partial modelling of a perennial crop cycle affected the LCA results. They deduced that the one-year model leads to very uncertain results and that a 3-year average model can still possibly be misleading as it is not sufficient at capturing the environmental impacts of the full perennial cycle.

Thus, LCA practitioners generally only consider the mature trees, because data-recovery for the nursery, establishment, low-yield and destruction stages is difficult (Notarnicola et al., 2015). Though, researchers are getting more and more aware of the increased representativeness of their results when they do not limit a perennial food production LCA to the full productive stage. Fruit production LCAs have been conducted that included e.g., the establishment, young and full productive stages (Vinyes et al., 2017, 2015); all three productive stages (Fig. 1-5c) (Goossens et al., 2017a); and the full orchard life cycle (Alaphilippe et al., 2015; Cerutti et al., 2013; Ferrari et al., 2018).

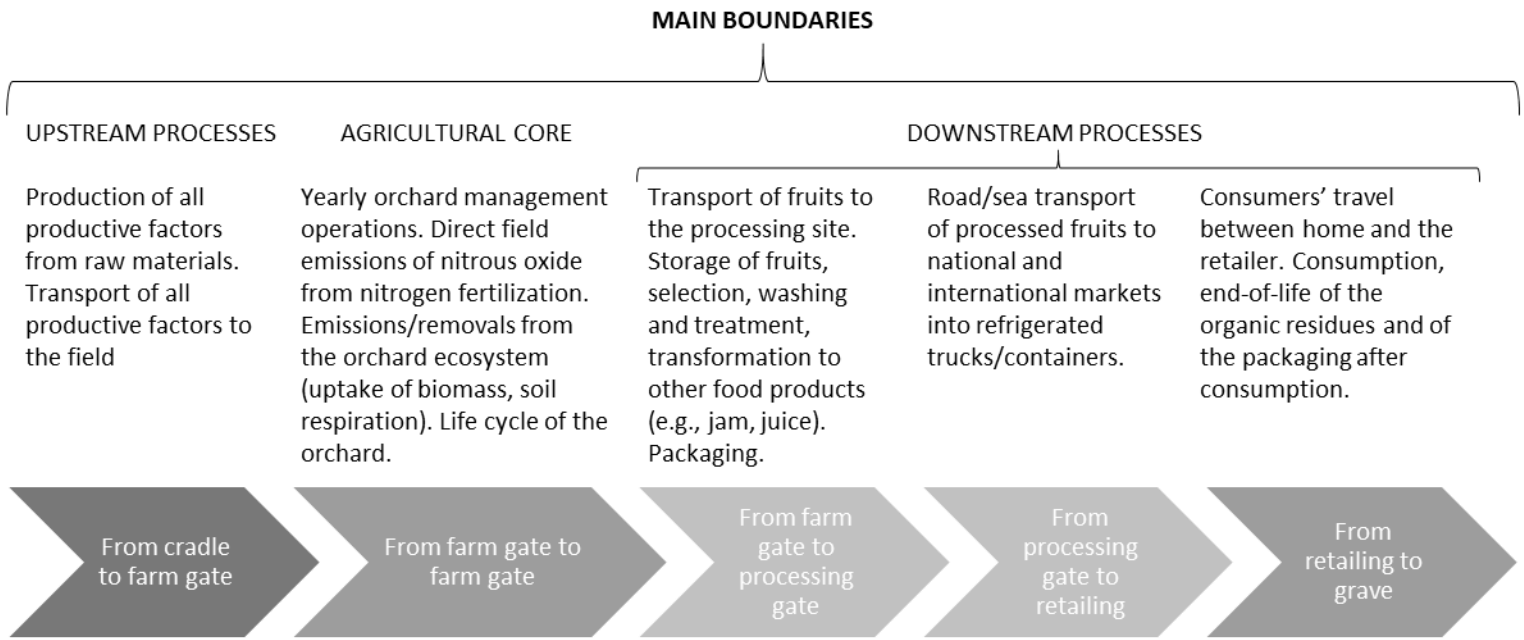


Figure 1-4 Main system boundaries for an LCA on fruit production and post-harvest processes (cradle-to-grave), based on Notarnicola et al. (2015)

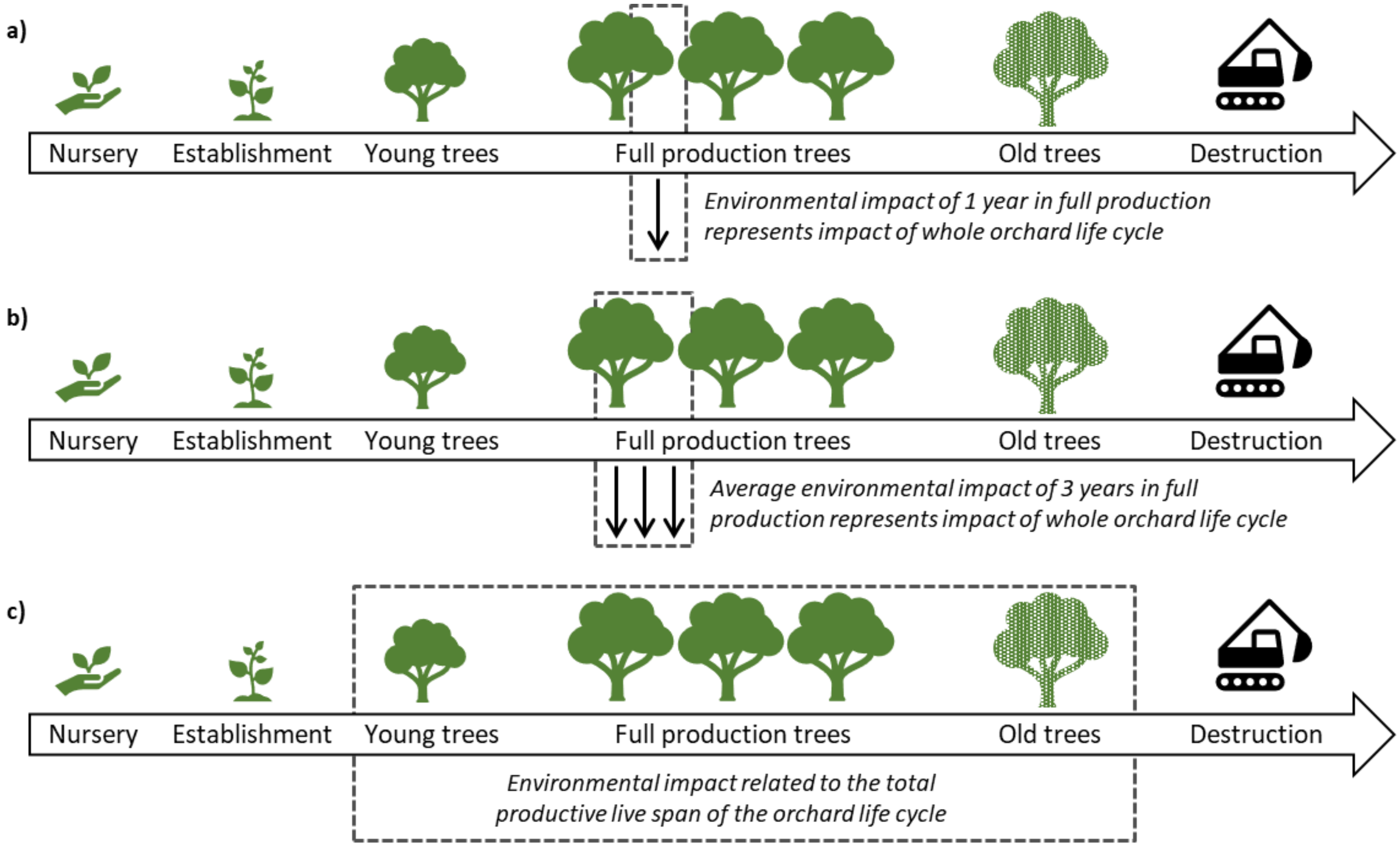


Figure 1-5 Possible definitions of system boundaries for the LCA of a perennial food production system.

Alaphilippe et al. (2015) found that the unproductive stages of apple orchards entailed 9% to 28% of the environmental burdens, depending on the impact category. The contribution of the unproductive stages were generally lower for a semi-extensive orchard than for an intensive one, except for energy demand. The authors stated that the higher contribution for the intensive orchard could be explained by the longer duration of the establishment stage and by the shorter orchard lifespan.

Similarly, Goossens et al. (2017a) discovered in our research group that including all three productive stages of the orchard life cycle in an agri-food LCA could lead to counterintuitive results. Our group found that a mere focus on high productive apple trees in comparison with the complete productive phase, leads, on average, to an *underestimation* of the environmental impact for conventional and integrated farming, yet to an *overestimation* for organic farming. The underestimation was mainly caused by young trees which are often associated with low yields in perennial production systems. To ensure good plant health and to transform young trees into highly productive trees for later years, a lot of agricultural inputs are needed. As such, the resulting impacts per ton of apple produced by young trees tend to be a lot higher than those of full productive trees, leading to an underestimation of the impact when they are not accounted for. The overestimation in organic cultivation was due to – among other things – a difference in orchard lifespans. Organic cultivation has a generally lower impact in the old, low productive phase which lasts longer (six years) than in the conventional and integrated orchards (two years).

It should be noted here that the *carbon storage* of a fruit orchard is generally not accounted for, though it has been included more in case studies in recent years (Aguilera et al., 2015; Bamber et al., 2020; Pirlo and Lolli, 2019) and methods are actively being developed (Albers et al., 2020; Boone et al., 2018) and tested (Bessou et al., 2020; Goglio et al., 2015; Sevenster et al., 2020). Carbon storage in fruit orchards can be divided into two types (Notarnicola et al., 2015):

- temporary storage in the above- and below ground tree biomass for the life cycle of the orchard, and
- medium to long-term soil carbon stock change, which relates to a balance between inputs of organic matter in the soil in the form of senescent leaves, thinned fruits, pruning material, grass cover, dead roots, compost and manure; and output in the form of CO_2 due to the degradation of organic matter.

The carbon stock variations of the trees and soil can be attributed to either land use change (LUC) or land management change (Notarnicola et al., 2015), but is limited in time until a new equilibrium is reached (Aguilera et al., 2015).

In that regard, it is often not clear what happens to the trees when orchards are destructed. Notarnicola et al. (2015) describe in their general review of LCAs in the fruit sector, that “the trees are removed and usually burned for production of domestic heat or in open air” in the destruction stage. This is often not elaborated on in published case studies, again emphasizing the need for more transparency. Alaphilippe et al. (2015) only mention that their destruction stage encompassed the removal of trees and infrastructure, while Cerutti et al. (2013) limit the stage to needing “machinery and fuel”. Ferrari et al. (2018) just state that they include the “disposal” and leave it at that. When it comes to carbon storage accounting, it would be relevant to clearly know the end-of-life-treatment of the trees.

Lastly, when including orchards in an LCA, Cerutti et al. (2014) recommend to always investigate at least three orchards per set of agronomic parameters (i.e., all aspects that make the plantation specific, such as production system, cultivar, etc.). This both for profiling the environmental burdens of a product, supply chain or production area, as well as when comparing different products or farming practices.

1.4.3 Dealing with multifunctionality issues related to organic fertilizers

To keep an LCA clear and feasible, system boundaries are established during the goal and scope definition phase to define the life cycle. Ideally, these system boundaries should include all unit processes that are required to deliver the reference flow defined by the functional unit (Hauschild et al., 2018). This can be difficult when dealing with processes that deliver more than one product or function. Typical examples are livestock systems that deliver both meat and milk or, energy production systems that deliver both electricity and heat These multifunctional processes cause a methodological challenge, because LCA is based on the idea of analyzing the environmental impact of the total system based on the primary function it provides (European Commission et al., 2010; Hauschild et al., 2018). Appropriate methods are needed to partition the environmental impacts among the different functions of the system.

ISO 14044 (2006a) provides a hierarchy of methods to deal with this multifunctionality problem. First, allocation should always be tried to be avoided, preferably by *subdividing* the unit process into multiple sub-processes, collecting separate inventory data for each sub-process. This requires there to be a physical separation between the different processes within the system, which is not always the case (Hauschild et al., 2018). Alternatively, ISO (2006a) proposes to *expand* the product system to include the additional functions related to the co-products. In the case where two systems are compared, one of them being multifunctional, this can be achieved by adding the most likely alternative way of providing the additional function to the other system, thereby expanding its system boundaries (Hauschild et al., 2018). For example, when comparing two power plants, one of which co-generates heat and electricity while the other only generates electricity, an alternative way of generating heat is added to the second system.

Sometimes a different approach is followed in this context where the first power plant is *credited* for the impacts that are avoided by providing the secondary function of producing heat, by subtracting the impacts of the alternative way of generating heat from the power plants' impacts. Both approaches are mathematically equivalent (Hauschild et al., 2018). While system expansion is preferred over allocation, it is not commonly used in agri-food LCAs because of its complexity and high demand in data collection (Notarnicola et al., 2017).

When those procedures are not possible, only then should *allocation* be considered according to ISO 14044 (2006a). The in- and outputs of the multifunctional process are then partitioned among the different products or functions based on an underlying *physical relationship*. Meaning that it should reflect the way in which the inputs and outputs are affected by quantitative changes in the products or functions that are delivered by the system. This physical relationship is preferably a causal relationship, and if not, a representative common physical parameter should be used (Hauschild et al., 2018). The physical property can be for example mass-, quantity-, volume-, length- or energy-based (European Commission et al., 2010). Ponsioen and van der Werf (2017) emphasize here that a common relationship is not the same as a common property. It is not because two products have a mass, that they are therefore related. It is their common origin that determines the relationship between two co-products. They argue that the physical or biological mechanism reflecting the common origin should thus be used as the basis for their relationship.

Finally, when a physical relationship cannot be identified, ISO (2006a) suggests using other representative relationships such as the *economic value* of the products. The impacts are then partitioned based on the prices of each co-product, which strongly depend on the actual market situation, governmental policies and the producer-buyer relationship (Ponsioen and van der Werf, 2017). As it turns out, the last tier option of economic allocation is one of the most frequently used methods to solve multifunctionality problems in LCA (European Commission et al., 2010; Pelletier et al., 2015; Wilfart et al., 2021). Ponsioen and van der Werf (2017) even recommend the method for environmental footprints of food and beverages, though (i) representative public statistics should be used, and when those are unavailable, that stakeholders should agree on the price statistics; and (ii) multiple year averages should be used.

FAO (2016) developed a decision tree (Fig. 1-6), based on ISO's allocation hierarchy, in their guidelines for the assessment of the environmental performance of large ruminant supply chains. The right part of the figure ("3. Split single production units into single products") shows how different methods are chosen based on if the studied product is considered as waste, residual or co-product. This often depends on if the studied product has an (economic) value when leaving the system (FAO, 2016; Ponsioen and van der Werf, 2017). These three options will be further discussed in Chapter 6.

Whichever method is chosen in the end, it is obvious that the different procedures can lead to very different results (Notarnicola et al., 2017). Therefore, ISO (2006a) requires a sensitivity analysis to be conducted whenever several alternative allocation procedures seem applicable. Several studies have applied this recommendation. For example, in their study on the impact of using blood meal as a raw material in the production of a thermoplastic (NTP), Bier et al (2012) had LCA results ranging from 0.21 kg CO_2 eq/kg NTP (substitution with urea) to 14.52 kg CO_2 eq/kg NTP (mass allocation for raw blood), depending on which of the five considered allocation procedure was selected.

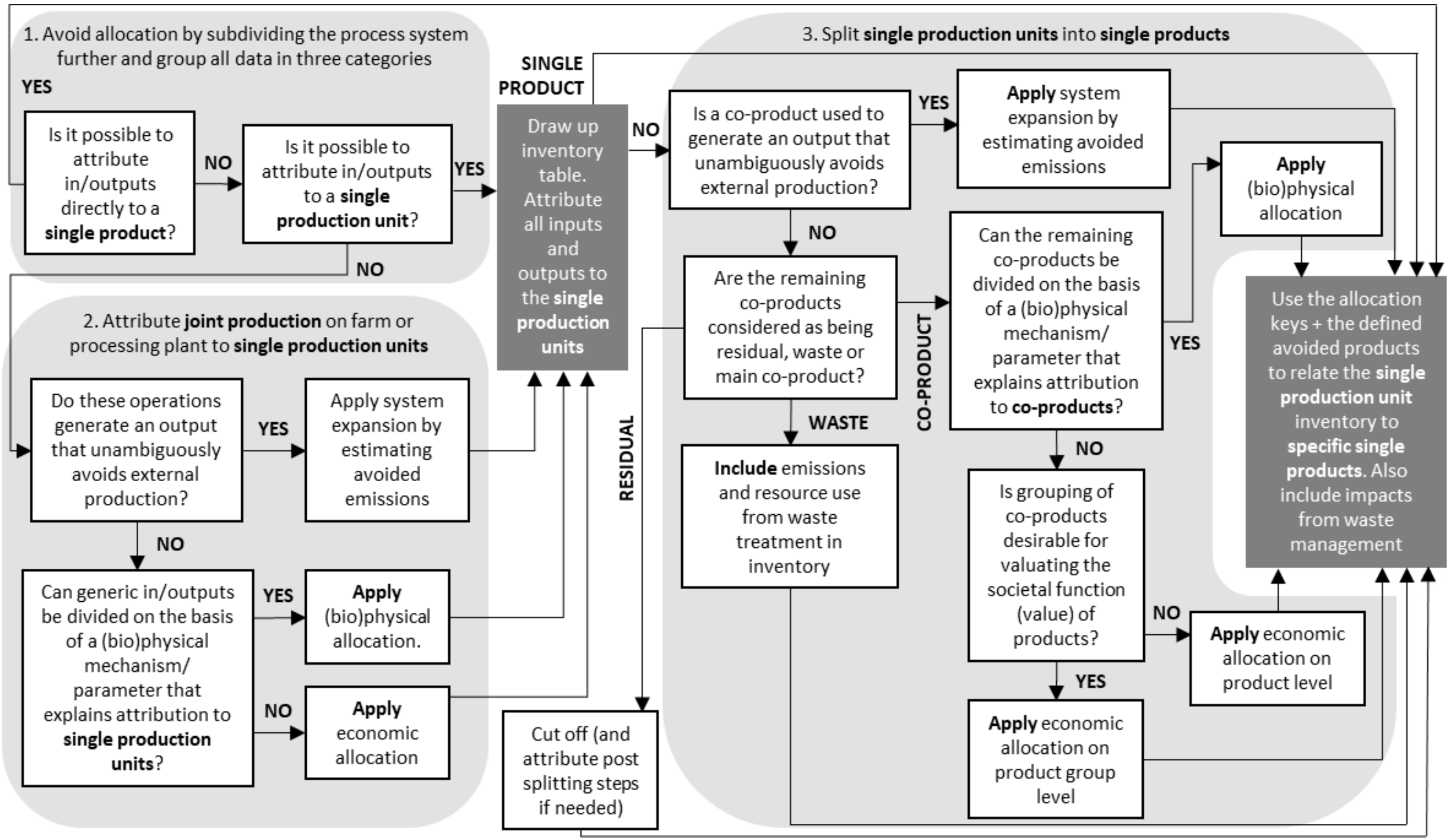


Figure 1-6 Decision tree for choosing the method for handling multifunctional outputs, based on FAO (2016)

Similarly, Hermansson et al. (2020) compared twelve possible allocation methods for ascribing impacts to lignin. Their results ranged from -23 kg CO_2 eq/kg lignin (credited for substituting cotton) to 4 kg CO_2 eq/kg lignin (lignin is selected as main product to bear all burden). Houssard et al. (2020) found that their conclusions were sensitive to the use of mass versus economic allocation, causing whey to be allocated 29% to 47% for mass allocation on dry matter depending on the life cycle stage of the Greek yoghurt product being studied, and 0% or 17.5% for economic allocation depending on its potential value on the market. As a final example, the five allocation factors that Chen et al. (2017) used to partition livestock co-products at the slaughterhouse to human food ranged between 38% (using dry matter content) and 95% (using economic values).

The previously mentioned studies illustrate how multifunctionality can cause problems in agri-food LCAs. For the case of fruit production, multifunctionality can for example cause problems when using organic fertilizers such as manure or compost since those are typically seen as residual products of which the future use is considered as having no impact on the production of it (Durlinger et al., 2017a; Notarnicola et al., 2015). This means that their realized environmental impacts are completely ascribed to the primary products of the systems of origin. Thus, the impacts of producing organic fertilizers are usually not accounted for within the agri-food LCAs where these products are used during cultivation [e.g., Goossens et al. (2017a) and Spångberg et al. (2011)].

This raises questions on how realistic comparisons are between conventional crop production systems that use mineral fertilizers and organic systems that use organic fertilizers. The flows of resources and associated impacts are not represented equivalently in both systems since, unlike for organic cultivation, the production impact of the (mineral) fertilizers they use, are typically included within the system boundaries of conventional crop production systems. It seems relevant to conduct extensive sensitivity analyses to see how the total impact of cultivation systems would change depending on the chosen allocation procedure. This way, the knowledge on how the different allocation procedures can influence results, can be advanced with the goal of finding a solution for the current skewed comparisons of organic and conventional crop systems.

Chapter 2

Aim and objectives

The overall aim of this PhD thesis is to lift LCA approaches to a higher scientific level, specifically for the agri-food sector and potentially for other sectors as well. I will do this by introducing more appropriate methods to calculate environmental sustainability and obtain more accurate potential environmental impacts. That way, conclusions and recommendations to decision makers will be more reliable, leading to more informed and effective decisions. Choosing the environmentally friendliest option will be more conclusive.

I will use agri-food chains to present my methodological improvements, so I can focus on furthering an area of LCA that needs further development and improvement when it comes to obtaining accurate results. In Chapter 1, I described several improvement opportunities related to agri-food LCAs. In this thesis, I will mainly focus on furthering the research regarding uncertainty and variability, and regarding allocation of organic fertilizers.

By using data from the Farm Accountancy Data Network (FADN), I can ascertain that no distinction is made between low and full productive systems. Thereby helping to eliminate the practice of excluding burdens in the low productive parts of the perennial production chain. Because of its significance for Flanders, I use fruit production, more specifically the apple agri-food chain, as a case study to test my research objectives. The apple is one of the most consumed fruit in Flanders, with 9.8 kg/capita in 2015 (Platteau et al., 2016), and apple orchards cover approximately 32% of the Flemish fruit area (Danckaert et al., 2018). Throughout the research, the apple agri-food chain that was previously developed in our group (Goossens et al., 2019, 2017a), is used as my starting point (Fig. 2-1).

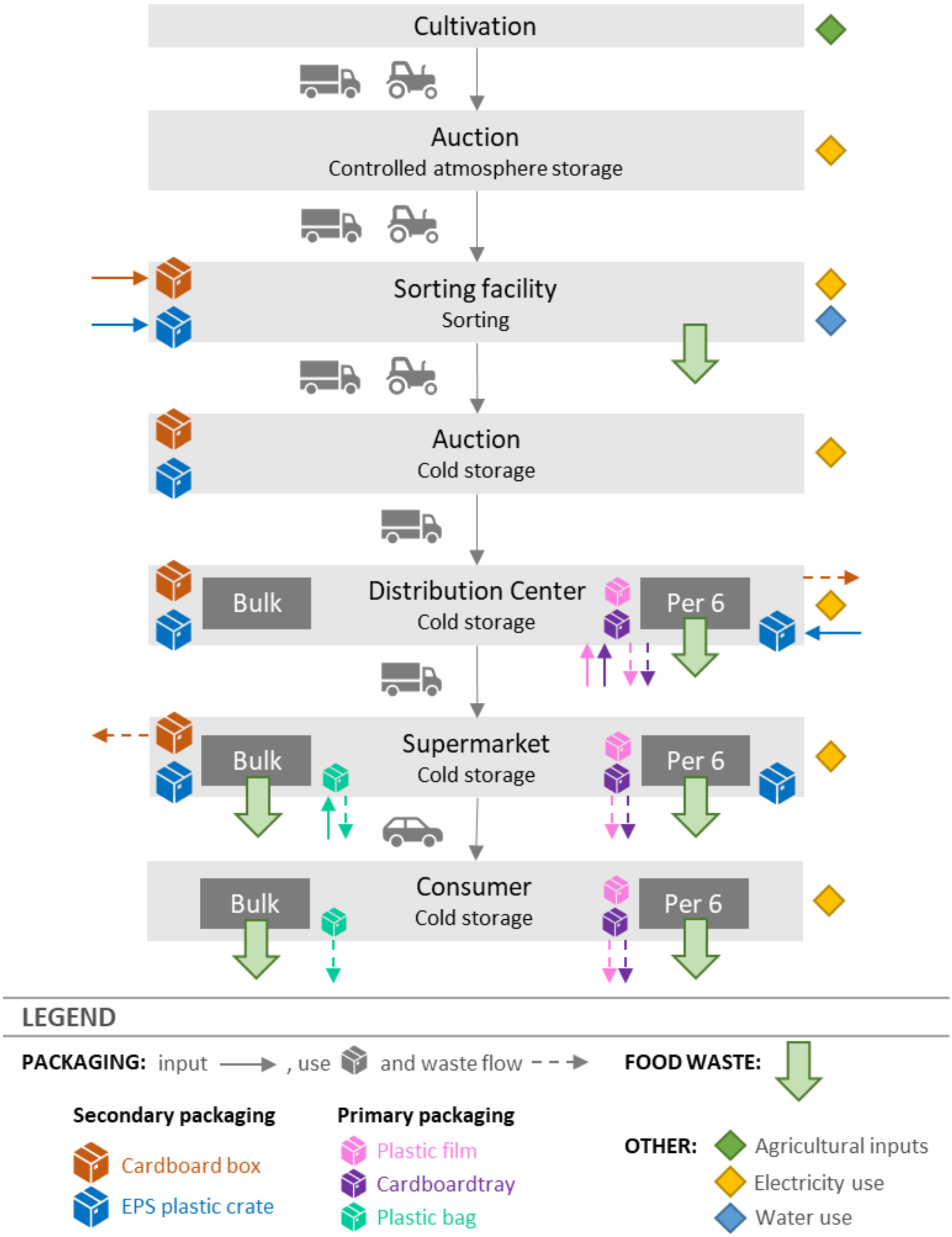


Figure 2-1 Flow chart of the Belgian apple chain for bulk and pre-packed (per 6) apples, based on Goossens et al. (2019).

Objective 1 – Review all the attempts that have been made in LCA to separately account for uncertainty and variability

LCA results are typically reported as deterministic, while reality is uncertain and variable. Through a systematic review, all the methodologies that have already been used to assess both uncertainty and variability, as separate concepts, in the same LCA study will be identified and analyzed. An LCA study will only be included in the review if a clear distinction between uncertainty and variability is made within the life cycle inventory phase *and* the study results show some indication of either uncertainty or variability being dominant.

Thus, the research question that I aim to answer with this systematic review is: *"How can we methodologically assess how important both uncertainty and variability are in LCA results?"* From the included methodologies, I will select the most appropriate one(s) that allow to decide whether uncertainty or variability is dominating in the results. Special attention will be given to how this is visualized. The systematic review can be found in Chapter 3 and will introduce Part II of this PhD thesis, where the focus lies on improving the LCA methodology by complementing uncertainty with variability in the assessments.

Objective 2 – Increase the robustness of results by conducting two-dimensional Monte Carlo simulations for the first time in LCA

The field of quantitative risk assessment has shown that 2DMC can be successful method when it comes to incorporating both data uncertainty and variability in an assessment. Therefore, the 2DMC method is introduced in LCA in Chapter 4, using the apple post-harvest chain as a case study, comparing bulk and pre-packed apples. Afterwards, the apple chain is completed in Chapter 5 with the cultivation part of the chain, comparing Jonagold and Kanzi cultivation. The research question that I wish to answer here is: *"Can 2DMC be used to analyze and visualize uncertainty and variability in LCA results, and how does this differ to 2DMC used in risk assessments?"*

I believe Monte Carlo simulations will be a good fit for LCA. Firstly, because it is widely recognized in widely disparate fields [e.g., finance, project management, energy, manufacturing, engineering, research and development, insurance, oil & gas, transportation and the environment (Palisade, 2021)] and within the LCA community as a valid technique, so its results are more likely to be accepted. Since 1DMC is already being predominantly used – over other approaches such as Taylor series or fuzzy sets – in LCA (Igos et al., 2019; Lloyd and Ries, 2007), introducing 2DMC is feasible. Secondly, software is commercially available to automate the tasks involved in the simulation, and correlations and other interdependencies can be modelled. Lastly, changes to the model can be made very quickly and the results compared with previous ones.

Successfully separating and propagating data variability and uncertainty (using 2DMC) will play an important role in the LCA interpretation phase, as this approach will clearly indicate whether the results demonstrate natural differences or if more data is needed. Additionally, when two products or processes are being compared, basing decisions on clearly separated model outputs is much more meaningful. Overlapping model outputs due to uncertainty and/or variability should be taken into consideration before making definite decisions. If the model outputs only depict a central tendency (e.g., mean or median), comparisons will not be as robust because the possible overlap is being ignored. 2DMC outputs will thus lead to more robust conclusions, accurate decisions, effective Life Cycle Management approaches, and so on.

Objective 3 – Analyze the influence of the allocation choice in organic production systems

One of the first prerequisites when comparing two systems is that the system boundaries should be equivalent. This prerequisite is often not fulfilled in agri-food LCAs when organic crop production systems are compared to more conventional ones. The impact of the production of residual products that are given a second life as organic fertilizers, are typically ascribed to the system of which they originate. This means that organic growers do not carry any share of the burdens of producing such organic fertilizers, even though they do definitely need them for cultivation. For more conventional crop production systems, the production of their fertilizers are included within their system boundaries, leading to skewed comparisons of the two systems. This mismatch of system boundaries is a serious shortcoming in the comparative LCAs of crop production systems, leading to the research question: *"What is a representative allocation procedure for accounting for the production of organic fertilizers within cultivation LCAs?"*

I therefore review the different allocation methods that could be used to include the production impact of organic fertilizers in the organic production system, thereby making sure that the system boundaries match. This will be the challenge of part III of the PhD thesis. In Chapter 6, sensitivity analyses for different possible allocation procedures are conducted and the most preferable one for further use in organic cultivation LCAs is subsequently selected. I again use the apple chain as a case study, however, this time the focus will specifically lie on the organic cultivation of apple. In Chapter 7, I will further reflect on how applicable the findings for the agri-food sector for industrial processes in the secondary sector.

A schematic overview of the three research objectives and their related chapters in this thesis can be found in Figure 2-2. Finally, in part V of this PhD thesis, the general conclusions and reflections are presented, together with opportunities for future improvements (Chapter 7). Extensive and structured appendices are provided alongside my results, respecting confidentiality issues where applicable. Other LCA researchers will be able to easily build upon my research and to use my proposed methods and approaches, hopefully inspiring them to go for the same level of transparency.

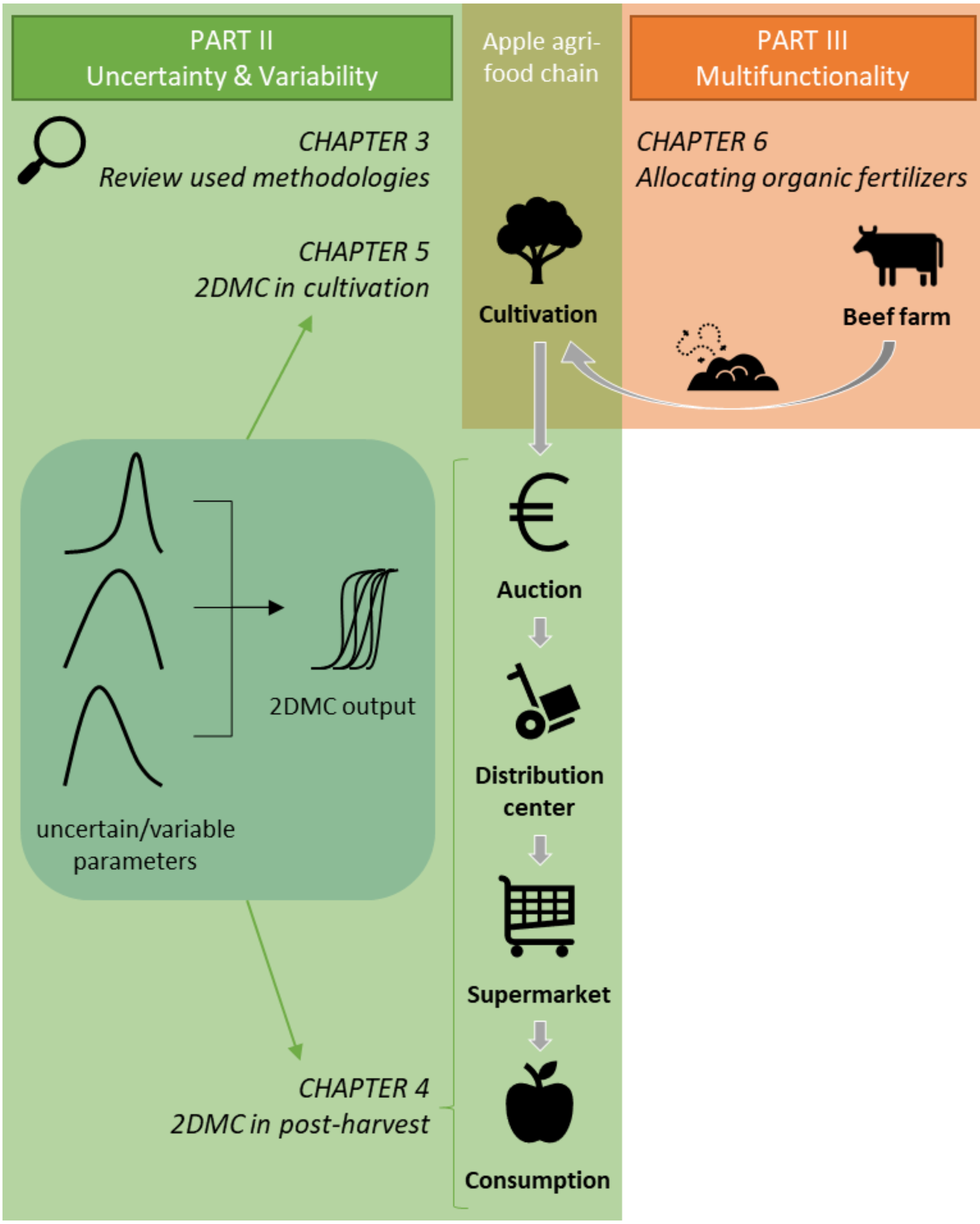


Figure 2-2 Schematic overview of the research objectives and their related chapters.

PART II

Complementing uncertainty with variability

Chapter 3

How to decide and visualize whether uncertainty or variability is dominating in Life Cycle Assessment results: a systematic review

This chapter is based on: Michiels, F., Geeraerd, A., 2020. How to decide and visualize whether uncertainty or variability is dominating in life cycle assessment results: A systematic review. Environmental Modelling and Software, 133, 104841. https://doi.org/10.1016/j.envsoft.2020.104841

Author's contributions: Michiels F. performed the analysis and drafted the manuscript

3.1 Introduction

Proper uncertainty reporting is becoming more and more important in different research fields. Finding a straightforward and transferable methodology for that purpose can be challenging, especially since there are different viewpoints regarding the sources and classification of uncertainty. Additionally, variability is often not accounted for or even acknowledged, causing valuable information for stakeholders and decisions makers to be lost.

Walker et al. (2003) distinguished between three dimensions of uncertainty. The first one, location of uncertainty, deals with where the uncertainty is located within the whole model complex (e.g., context, model and inputs). The second dimension was defined as the level of uncertainty, which expresses the degree of which something is known (from deterministic to total ignorance). The third dimension is the *nature of uncertainty* – and is the main focus of this systematic review – which focuses on how uncertainty relates with reality and more importantly, which strategy we can use to deal with it.

By looking at the nature of uncertainty, a distinction can be made between epistemic uncertainty and variability (Walker et al., 2003). *Epistemic uncertainty* reflects the imperfection of our knowledge (Walker et al., 2003), i.e. "everything we do not know" (Hauschild et al., 2018). This includes systematic or random measurement errors, lack of data, outdated information, subjective judgement, etc. (Hauschild et al., 2018; Walker et al., 2003). Therefore, epistemic uncertainty can be reduced by gaining more knowledge through research (e.g., further measurement, literature research or consulting more experts) (Hauschild et al., 2018; Huijbregts, 1998; Igos et al., 2019; Walker et al., 2003).

In contrast, *variability* [also called "aleatory" or "ontic" uncertainty (Igos et al., 2019; Walker et al., 2003)] stems from inherent variations in the natural world (Hauschild et al., 2018; Huijbregts, 1998; Igos et al., 2019; Walker et al., 2003), leading to a spread in the data that will always be observed (Hauschild et al., 2018). Therefore, it cannot be reduced through further study (Hauschild et al., 2018; Igos et al., 2019). As Warmink et al. (2010) mention, the distinction between epistemic uncertainty and variability is not always very clear. One can argue that random variation in the natural world can also be seen as a lack of knowledge, which in turn can be reduced given enough resources. However, it is unrealistic to assume unlimited available resources and variability is therefore seen as a variety of system behaviors taking into account a realistic amount of available resources.

Life cycle assessment (LCA) is one of the research fields in which proper uncertainty reporting is becoming more and more important. LCA quantifies the potential environmental impacts (e.g., environmental consequences of resource use) throughout a product's life cycle, from raw material to final disposal. LCA outcomes should ensure that impacts are addressed at the point in the life cycle where they will most effectively reduce overall environmental impact and resource use (ISO, 2006a). ISO 14040/44 (2006a, 2006b) developed an LCA framework with four iterative phases: Goal & Scope Definition (defining the functional unit, system boundaries, etc.); Life Cycle Inventory (collecting relevant data with regard to the studied system); Life Cycle Impact Assessment [evaluating potential environmental impacts associated with the in- and outputs by classifying them into specific impact categories, e.g., climate change (kg CO_2 eq)]; and Life Cycle Interpretation.

Next to this framework, ISO 14040/44 (2006a, 2006b) also lists data quality requirements that should be addressed in an LCA. However, LCA results are still typically being reported as deterministic [e.g., Bosona and Gebresenbet (2018) and

Hajibabaei et al. (2018)]. Other studies do include an uncertainty analysis, but completely disregard the distinction between uncertainty and variability [e.g., Bautista et al. (2018) and Jiao et al. (2019)]. Data quality reporting is important to assess the reliability of the study results and to properly understand its outcome (ISO, 2006b). However, uncertainty is frequently used as a very broad concept, often including related concepts such as variability (Hauschild et al., 2018). This makes it difficult for LCA practitioners to clearly define and propagate uncertainty and variability in their analysis. Moreover, uncertainty and variability are often mentioned as factors complicating the interpretation of LCA outcomes (Huijbregts, 1998).

Huijbregts (1998) developed a classification system specifically for LCA to distinguish between different sources of uncertainty and variability, to which Björklund (2002) and Hauschild et al. (2018) extended upon. Huijbregts (1998) distinguished between six types of uncertainty and variability:

1. parameter uncertainty, uncertainty due to a lack of knowledge of the “true” data (e.g., inaccuracy, unrepresentativeness and lack of data),
2. model uncertainty, uncertainty due to a loss of information when modelling reality within the present LCA structure (e.g., assumption of linear relationships),
3. uncertainty due to choices, uncertainty caused by unavoidable choices when performing LCAs (e.g., definition of functional unit),
4. temporal variability, variations over time (e.g., seasons),
5. spatial variability, variations across locations (e.g., regional differences in emission factors), and
6. variability between sources and objects, inherent differences in a product system (e.g., different characteristics between factories).

Björklund (2002) added:

7. epistemological uncertainty, uncertainty caused by lack of knowledge on system behavior (e.g., ignorance about relevant aspects of the studied system), and
8. mistakes (e.g., using wrong units)

to which Hauschild et al. (2018) added:

9. relevance uncertainty, uncertainty of the representativeness of the used indicators for the decision at hand (e.g., completeness of relevant impact categories covered).

Hauschild et al. (2018) stated that these nine types are essentially sub-classes of a wider used classification of uncertainty i.e., parameter, model and scenario uncertainty. In that case, parameter uncertainty consists of both uncertainty and variability in the model input parameters, and is the most accessible type (though, not necessarily the most important one) to be assessed and addressed in LCA (Hauschild et al., 2018).

Thus, there are different viewpoints when it comes to classifying uncertainty (epistemic and aleatory), which are related to each other, but not completely compatible. Now, turning to the topic of this PhD thesis, the classification as defined by Huijbregts (1998) is used because when dealing with uncertainty and variability in LCA, this classification is often referred to (as of August 5, 2020, Huijbregts' article (1998) has been cited 275 times). To be able to compare the different methodologies, we look at the different viewpoints from the perspective of Huijbregts' classification (1998), without trying to reconcile them or develop a new overarching school of thought.

In this PhD thesis, the focus lies specifically on methodologies used to propagate '*parameter uncertainty*' and '*variability between objects and sources*' – as defined by Huijbregts (1998) – because those two types of uncertainty and variability are the most feasible to be quantified in the inventory analysis by the LCA practitioner (Huijbregts, 1998).

Through a systematic review, we aim to study which methodologies have already been used that allow to decide whether uncertainty or variability is dominating in LCA results. Quantifying uncertainty and variability separately in the same LCA study leads to the ability of distinguishing between them in the interpretation phase and making well-informed conclusions and decisions. A systematic review is a review that uses systematic and explicit methods to identify, select, and critically appraise relevant research to answer a clearly formulated research question, with the goal of minimizing bias (Moher et al., 2009).

There have been studies that surveyed [e.g., Lloyd and Ries (2007) who discussed the quantitative uncertainty analysis of 24 LCA studies] and discussed [e.g.,Groen et al. (2014), Heijungs and Lenzen (2014) and Igos et al. (2018)] methods for uncertainty analysis in LCA. In these articles, uncertainty and variability were quantified together (as if they were interchangeable) and not separately in the same LCA study. To our knowledge, there has been made no attempt to review all methodologies that allow to decide if either uncertainty or variability is dominating in the results. For each methodology identified and included in the systematic review, we will study which visualization options exist and what the limitations are. We aim to select the most appropriate one(s), which allow to clearly conclude whether uncertainty or variability is dominating in the results, for future use in LCA.

3.2 Methods

The search process and reporting of the systematic review is based on the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) statement (Moher et al., 2009). This statement was very well-received as a tool for conducting systematic reviews (the PLoS Medicine publication has 20265 citations as of August 5, 2020).

For this systematic review, relevant published articles were identified by searching through the Web of Science Core Collection database, while “articles in press” were identified within Scopus. No restrictions were set for language or publication date. The reference lists of the articles included in the review were also checked for additional relevant studies. The last search was run on August 31, 2018.

Four topics were defined that reflected the research question: uncertainty, variability, methodology and life cycle assessment. For each topic, a range of search terms was iteratively developed and tested. One search term of every topic had to be present in the title, abstract and/or keywords in order to be identified within the databases (Fig. 3-1).

Eligibility criteria were specified in advance. These criteria were designed in a way to consecutively narrow down the pool of identified articles (thus criterion 1 has a much broader scope than criterion 4). Studies were found eligible to be included in the review if they met all of the following four criteria:

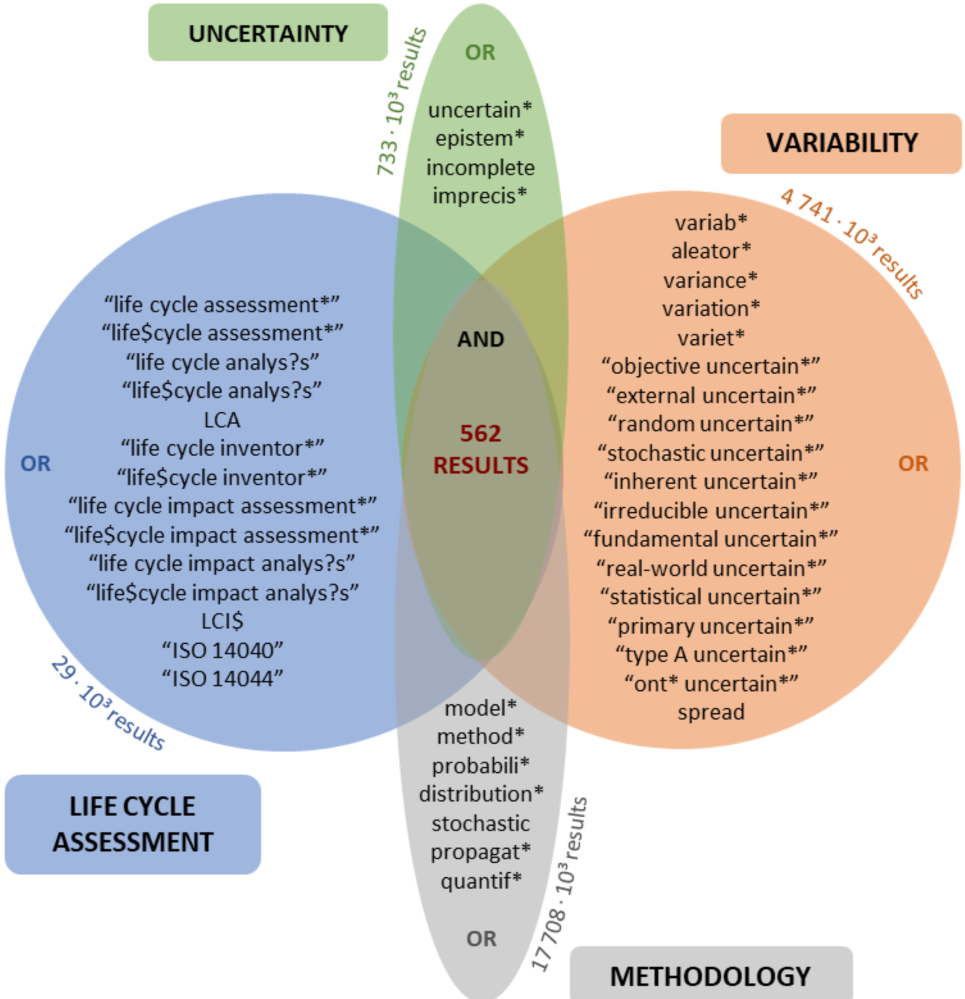


Figure 3-1 Search strategy of the systematic review.

562 records were identified through database searching by combining search terms related to four main concepts (* represents any group of character(s), including no character; ? represents any single character; and $ represents zero or one character).

1. An LCA was conducted. The methodology needed to be usable within the LCA framework, and a fully worked out case study would provide valuable insights with regards to possibilities and limitations. Therefore, review papers or other types of assessments, such as risk assessment and assessments of fate, exposure and effects models, were excluded.

2. A clear distinction was made between uncertainty and variability in the inventory phase. Some kind of difference needed to be notable based on the given definitions, descriptions, input tables and/or graphs. It had to be clear which – and possibly how – input data reflected uncertainty and/or variability.

3. The effect of 'parameter uncertainty' and 'variability between sources and objects' were both considered, because – as stated before – those two types are the most feasible to be quantified in the inventory analysis (Huijbregts, 1998). Though, keeping in mind the different viewpoints discussed in the introduction, it was not required for those specific terms to be used in the selected articles. However, it was required that there was a possibility to justifiably assume that those two types were included, even when a different viewpoint was taken or when the authors did not thoroughly specify the distinction.

4. The applied methodology allowed the reader to conclude whether uncertainty or variability is dominating in the results. Thus, even when the authors did not specifically discuss that such a conclusion could be made, the reader would still be able to deduce it from the results shown in tables and/or graphs.

Identified studies were consecutively read carefully and their eligibility assessed based on the title (e.g., LCA was also used as an abbreviation for "last common ancestor), abstract and, when the abstract did not lead to a clear judgment, the full-text. The information found was structured as will be shown in the results section. One author was contacted because of unclearly reported information on the used methodology in their study, for which we got a response.

3.3 Results

562 records were identified in Web of Science and Scopus based on the defined search strategy (Fig. 3-1 and 3-2). Not surprisingly, LCA was the limiting topic in the search strategy (Fig. 3-1). Four duplicates were excluded. Subsequently, 558 records were screened on title and abstract, of which 397 records were excluded because the studies clearly did not meet the eligibility criteria. 161 records were assessed based on their full-text. For some articles, it was very clear from the full-text if they needed to be excluded [e.g., Sastre et al. (2015) and Venkatesh et al. (2011) stated that even though uncertainty and variability are inherently different, they considered them jointly]. In other articles, it was not so clear if the authors used the two terms more as synonyms or if a clear distinction was made.

The full-text eligibility check is provided in the online supplementary material of the published article of this systematic review. It shows the main reason why an article was excluded from the systematic review and why in the end we could designate 11 out of 161 records as eligible. The three possible reasons, reflecting the eligibility criteria described in the methods section, were:

1. the article does not make a distinction between uncertainty and variability, or only in passing,
2. the article does not take both ‘parameter uncertainty’ and ‘variability between sources and objects’ into consideration, and
3. it cannot be concluded if either uncertainty or variability is dominating.

It should be noted that the supplementary material only indicates the main reason why an article was not included, but that these three reasons are not mutually exclusive. This limited number of final articles illustrates that researchers often treat uncertainty and variability alike, even when mentioning the importance of separating them. The reference lists of the eleven selected articles were checked for additional relevant studies, however none were found outside the defined search strategy.

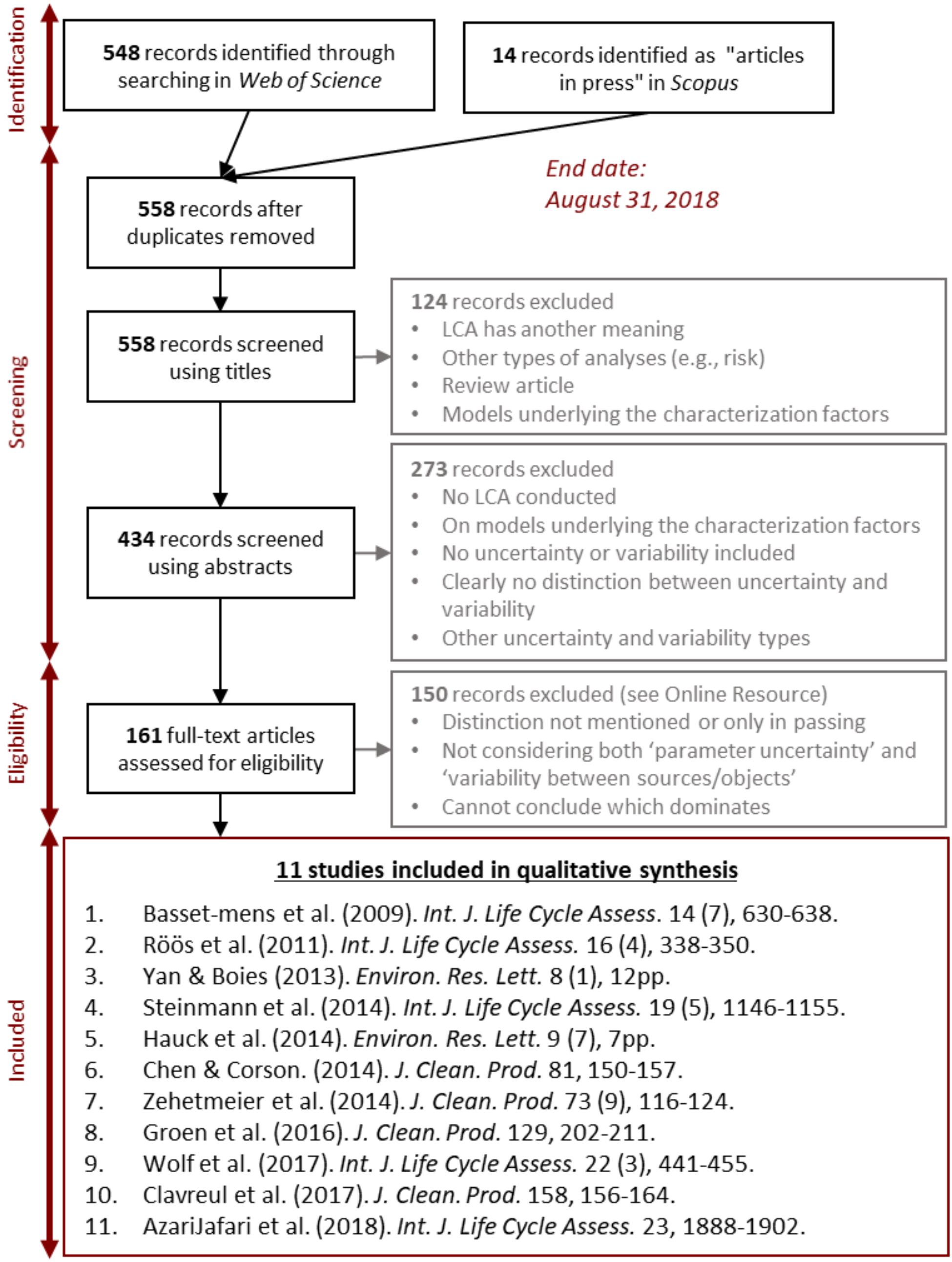


Figure 3-2 Flow of information through the different phases of the systematic review.

From the eleven included articles, eight studies conducted an LCA of an agricultural product and three on energy generation (Fig. 3-3). One of those articles (Yan and Boies, 2013) studied the environmental impact of a specific biofuel. The most recent article focused on pavements (AzariJafari et al., 2018). Hence, propagating variability seems especially relevant for LCAs of agricultural products, probably because of their inherently variable inventory data, e.g., different soil types, weather conditions, consumption patterns, etc. (Notarnicola et al., 2017).

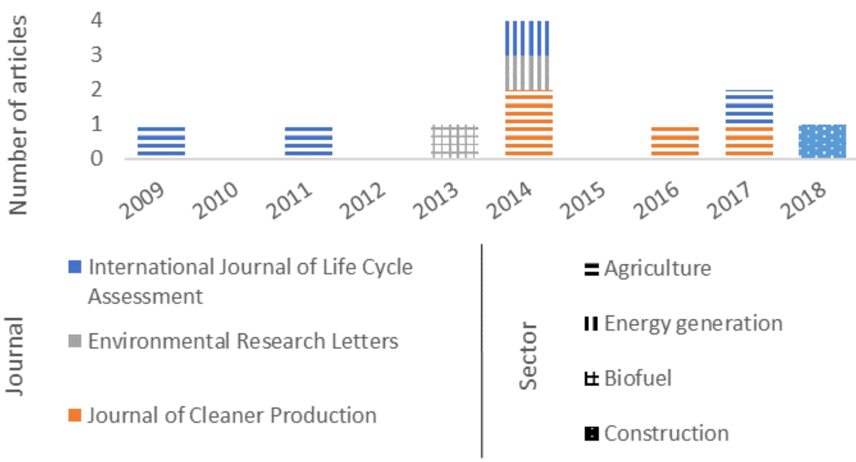


Figure 3-3 Classification of the eleven included articles.
The classification is done by year, journal (distinguished by color) and sector (distinguished by patterns).

Table 3-1 gives an overview of the eleven selected studies and their supplementary materials regarding their studied system, functional unit, system boundaries, geographical location, impact category, example sources of parameter uncertainty and variability between sources and objects, and on which information we could base the conclusion of whether uncertainty or variability is dominating. For readability, we will use the article ID's, as defined in Table 3-1, throughout the remainder of the manuscript. The terminology used by the authors themselves is used in the table, illustrating the lack of harmonization. Nine (except ID 6 and 11) out of the eleven articles focused exclusively on the impact category climate change, using terms such as "global warming potential", "carbon footprint", "greenhouse gas intensity" and "(life cycle) greenhouse gas emissions".

Table 3-1 Overview of the eleven selected articles (using the terminology of each individual paper).
The table lists (i) the identification number (ID) used in the review, (ii) the source, (iii) the researched system, (iv) the functional unit, (v) the chosen system boundary, (vi) the geographical location of the system, (vii) the considered impact categories, (viii & ix) where the sources of parameter uncertainty and variability between sources and objects can be found in the selected articles and a few examples of those, and (x) where we could find the information to base the conclusion of whether uncertainty or variability is more dominating in the results, followed after ":" with the actual conclusion made, either formulated or explicitly discussed in the text or deduced by combining information in the paper. Further information on why and which assumptions we had to make regarding the classification of uncertainty and variability is given in the results section. (Loc. = Location; GWP = Global Warming Potential; GHG = greenhouse gas; FU = functional unit).

ID	Source	System	Functional unit	System boundary	Loc.	Impact category	Sources of parameter uncertainty	Sources of variability between sources/objects	Uncertainty or variability dominating?
1	(Basset-Mens et al., 2009)	Milk production	1 kg of New-Zealand milk	Cradle-to-farm-gate	NZ	GWP	Table 1: milk yield, feed supplements, etc.	Table 1: milk yield, feed supplements, etc.	Fig. 1, Table 3, section 3.1: variability
2	(Röös et al., 2011)	Refined wheat products	1 kg of wheat before the milling process[a]	Cradle-to-mill	SE	Carbon footprint	Table 3: wheat yield, amount of N fertilizer, distance farm to mill, etc.	Table 3: wheat yield, amount of N fertilizer, distance farm to mill, etc.	Fig. 2, Table 5, section 3.2: uncertainty (for the scenario for which soil N_2O emission uncertainty was included), etc.

[a] The study also included a functional unit of "1 kg of KGI (Kungsörnens Gammeldags Idealmakaroner, a common Swedish pasta variety) in paper packaging available for sale in a supermarket in Stockholm" with a cradle-to-retail functional unit, but was not used in the reviewed methodology for propagating uncertainty and variability separately and therefore not included in the overview

Table 3-1 Continued

ID	Source	System	Functional unit	System boundary	Loc.	Impact category	Sources of parameter uncertainty	Sources of variability between sources/objects	Uncertainty or variability dominating?
3	(Yan and Boies, 2013)	Wheat ethanol	1 MJ of final fuel energy produced	Considered life cycle stages: agriculture, wheat transport and handling, biorefinery, ethanol distribution and potential land use change	UK	GHG intensity	Table S3 Run 4-6: embedded GHG in pesticide, transport distance, etc.	Table S3 Run 1: grain yield, N application rate, etc.	Fig. 2, section 3: uncertainty
4	(Steinmann et al., 2014)	Coal-fueled power generation	1 kWh of electricity generated at a plant or plants in a particular calendar year	Mine to wire	US	Life cycle GHG emissions	Table S1: electricity use for surface mining, diesel use truck, etc.	Introduction p. 1147: mine type, mode of transport, etc.	Fig. 2, Fig. 4, section 3.1: variability
5	(Hauck et al., 2014)	Gas power generation	1 kWh of electricity generated at the power plant	Well to wire	US	Life cycle GHG emissions	S3: well life time, gas turbine heat rate, etc.	Figure 1 caption: production practice, processing technology, etc.	Fig. 2, Fig. 3, Fig. 4, section 3.1: variability
6	(Chen and Corson, 2014)	Dairy farms	1 ha of on-farm usable agricultural area & 1000 kg of fat-and-protein-corrected milk sold	Cradle-to-farm-gate; with exclusion of all inputs, output and usable agricultural area of cash crops to retain only the milk-production subsystem for the “milk” functional unit	FR	Climate change, acidification, eutrophication	Table 1: NH_3 from manure spreading, mineral fertilizer application, etc.	Section 2.3: farm characteristics	Fig. 2, section 3.1, section 4.1: variability (for eutrophication, for FU per ha of usable agricultural land), etc.

Table 3-1 Continued

ID	Source	System	Functional unit	System boundary	Loc.	Impact category	Sources of parameter uncertainty	Sources of variability between sources/objects	Uncertainty or variability dominating?
7	(Zehetmeier et al., 2014)	Dairy cow production systems	1 kg of milk	Dairy farm gate & system expansion: dairy farm gate and fattening systems farm gate	DE	GHG emissions	Table 1: emission factor nitrogen input into soil and emission factor beef from suckler cow production	Table 1: calving interval/ replacement rate	Fig. 2, Table 4, section 3.1, section 3.2: uncertainty
8	(Groen et al., 2016)	Pork production	1 kg body weight of a growing pig	Processes considered in the pig chain: production of crop inputs, feed processing, piglet production, manure management, pig housing, and enteric fermentation from pigs	NL	GHG emissions	Section 2.5.4: N_2O emissions of feed-crop production, CH_4 emissions of manure management, etc.	Section 2.5.4: crop yield, feed intake, etc.	Fig. 7: uncertainty
9	(Wolf et al., 2017)	Milk production	1 kg of energy corrected milk	Cradle-to-farm gate	DE	GHG emissions	Fig. 5: direct N_2O crop cultivation, CH_4 manure, etc.	Fig. 5: milk yield, replacement rate, etc.	Fig. 5, Fig. 6: uncertainty

Table 3-1 Continued

ID	Source	System	Functional unit	System boundary	Location	Impact category	Sources of parameter uncertainty	Sources of variability between sources/objects	Uncertainty or variability dominating?
10	(Clavreul et al., 2017)	Open-field tomato production	1 ton fresh tomato	Farm gate	ES & PT	Carbon footprint	Table 2: N_2O direct emissions, GHG emissions from fertilizer production, etc.	Table 1: nitrogen input, diesel use, etc.	Fig. 5, Fig. 6, section 3.2: variability
11	(AzariJafari et al., 2018)	Pavements	Providing a path for traffic service for 20000 Annual Average Daily Traffic including 5% of the truck, over 1 km length of a two lanes road in Quebec urban area and for a 50-year lifespan	Cradle-to-grave	CA	Midpoint & endpoint impact categories of IMPACT 2002+	Table S7: equipment, electricity, etc.	Section 2.2.4.2: pavement lifetime, variation in materials, etc.	Fig. 4, Fig. 5, section 3.2: uncertainty (for ecosystem quality), etc.

Figure 3-4 shows in which of the included articles a conclusion can be drawn regarding specific type(s) of uncertainty and variability. The type is either (i) propagated on its own, (ii) propagated alongside another type because it was not feasible (or relevant) to separate the types, or (iii) the type was not considered. A type was only included if the type [as defined by Huijbregts (1998)] was explicitly mentioned by the article or if we could deduce it based on the given definitions. For example, the study done by Zehetmeier et al. (2014) (ID 7) presented a clear table showing how each parameter was classified to a certain type or several types of uncertainty and variability.

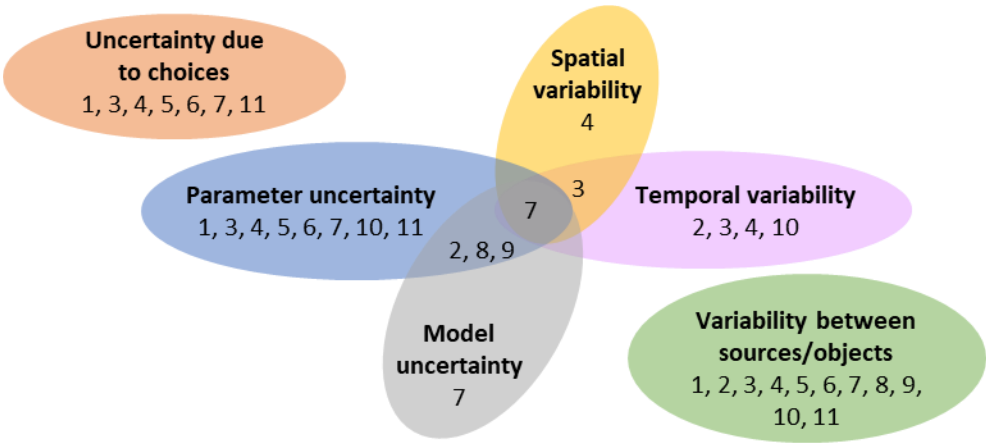


Figure 3-4 Diagram showing the specific type(s) of uncertainty and variability accounted for in each article.

The Venn-diagram shows in which articles (using article IDs as defined in Table 3-1) a conclusion can be drawn regarding specific type(s) of uncertainty and variability (note: an article ID such as 7, can appear more than once in a specific type depending on how the different input parameters are classified).

If the authors used a different viewpoint for the uncertainty classification, the sources of uncertainty and variability were interpreted from the perspective of Huijbregts' classification (1998). If no clear terminology or definitions were given, then it was deduced based on context and other information given in the study. Sometimes, some assumptions had to be made regarding the sources of uncertainty and variability to compare and assess the effectiveness of the methodology. For example, Clavreul et al. (2017) (ID 10) distinguished between the "primary data", described as the variability in farmer's inputs, and the "secondary data”, which they described using both “model uncertainties” and “uncertainty in model parameters”. However, they did not give an explicit definition about these terms. Even though the primary data can also include parameter uncertainty, in this systematic review they were classified as variability between sources and objects based on their given description. The secondary data were classified as having parameter uncertainty.

Yan and Boies (2013) (ID 3) refer to the uncertainty and variability classification shown in Lloyd and Ries (2007), where uncertainty and variability sources can be classified according to three possible LCA modeling components i.e., parameter (input date), scenario (normative choice) or model (mathematical relationships). However, they used an unreferenced subclassification for parameter uncertainty (consisting of both uncertainty and variability for this classification), i.e.: “statistical uncertainty”, “temporal/spatial variability”, “data limitation” and “scientific uncertainty”. Based on the used classification and the given definitions, we classified “statistical uncertainty” as variability between sources and objects; and “data limitation” and “scientific uncertainty” as parameter uncertainty. Groen et al. (2016) (ID 8) and Wolf et al (2017) (ID 9) based their classification on Walker et al. (2003), thus distinguishing between “epistemic uncertainty” and “variability uncertainty”.

Furthermore, Chen and Corson (2014) (ID 6) added uncertainty in emission factors to a study done by van der Werf et al. (2009) which already included variability in farm characteristics. Their aim was to assess how the inclusion of a different type of uncertainty to an already existing LCA study changes the interpretation. However, they stated that, because of the references they used, epistemic uncertainty and variability could not be clearly separated in the uncertainty ranges of the emissions factors. Nevertheless, seeing as they specifically wanted to separate the two sources of uncertainty and because, in this systematic review, we are especially interested to see which methodologies are used to propagate that separation, it was chosen to classify the emission factors as belonging to parameter uncertainty.

ISO 14040/44 (2006a, 2006b) did not provide specific definitions and classifications for uncertainty and variability. It is clear that since then, no consensus has been reached regarding the terminology and definitions for the different types of uncertainty and variability.

Typical parameter uncertainty sources were electricity use and emissions, while variability between sources and objects was often found in yield data and lifetimes (Table 3-1). Next to this, uncertainty due to choices was the most frequently assessed (fig 3-4). The most prominent source of that uncertainty type was related to the choice of the impact assessment method (ID 1, 4, 5 and 11). Especially the choice of the Global Warming Potential (GWP) time horizon, which varied between 20, 100 and 500 years (ID 1, 4 and 5), was often taken into account. While the LCA practitioner can deal with parameter uncertainty and variability between sources and objects through e.g., propagation, dealing with uncertainty due to choices is more study-specific and often related to following guidelines and standards.

3.4 Discussion

It is clear that the origin and implications of epistemic uncertainty and variability differ. By assessing the nature of uncertainty, we can know if the quality of the output can be improved by additional research, which is only the case for epistemic uncertainty (Walker et al., 2003). However, variability can also further guide system optimization, product development or policy (Steinmann et al., 2014). A clear distinction between epistemic uncertainty and variability may help decision makers to judge differences in product comparisons, options for product improvements or the assignment of ecolabels (Huijbregts, 1998).

For example, regarding options for product improvements, we noticed in Goossens et al. (2017a) that it is possible to produce 1 ton apples with low impacts across all impact categories, thereby illustrating the importance of assessing the variability in managerial influence. If variability would have been included within the broad concept of uncertainty, then this feature would not have been noticeable during the interpretation phase. Outliers would have been considered as inherent to the uncertainty and actors would not have known that it is caused by a real variation. Moreover, regarding product comparisons, separating uncertainty and variability is also especially relevant when comparing bio-based products, derived from natural systems, with abiotic ones, for which conditions are controlled and often standardized. Bio-based products are subject to environmental conditions, which can cause a lot of variability in the data (Milà i Canals et al., 2011). When comparing, for example, LCAs of biofuels with fossil fuels, it is likely that variability will dominate the biofuel's LCA results, while uncertainty will dominate the ones of fossil fuel. In that case, the distinction will only be noticeable after clear separation of uncertainty and variability, and suitable decisions can only be drawn after proper communication to decision makers. These examples illustrate the general need for quantifying uncertainty and variability in LCA.

3.4.1 Classification of parameters

As stated previously, the goal of this systematic review is to study which methodologies have been used in LCA to separately account for uncertainty and variability in the results. For this we will first discuss the classification of the parameters used by the eleven included articles because it impacts the review. Whereas people may expect that definitions are clear, it became obvious during our study that the classification of parameters as belonging to one or more of the different types of uncertainty and variability in the data inventory phase, is study-specific (see example sources of parameter uncertainty and variability between sources and objects in Table 3-1). It depends on goal and scope definition (Huijbregts, 1998) and data quality.

In the *goal definition*, researchers define the reasons for carrying out their study (ISO, 2006a). As can be seen in Table 3-1 and Figure 3-4, this has prominent consequences on which types of uncertainty and variability will be taken into consideration. For example, Basset-Mens et al. (2009) (ID 1) set out to calculate the Global Warming Potential (GWP) of New-Zealand milk, because decision makers seek to understand the significance of changing milk production due to refining New Zealand's agricultural management. By using national statistics, they explicitly propagated variability between sources and objects (i.e., farms), which inherently included spatial variability. However, rather than focusing on geographical location (e.g., compare the GWP caused by the milk production in the North Island with the South Island), only the inter-farm variability was relevant for their goal.

The *scope definition* comes into play by defining the back- and foreground system and the functional unit (ISO, 2006a). The foreground system is commonly defined as comprising those processes of a system that are specific to it, and are largely modelled using primary data i.e., data collected first-hand by the LCA practitioner. In contrast, the background system is commonly defined as those processes of a system that are not specific to it, and are typically modelled using life cycle inventory databases (Hauschild et al., 2018). This distinction influences the choice of classifying data as either deterministic, uncertain, variable or both uncertain and variable.

Data collected in the *foreground system* for one individual life cycle tend to be more easily accepted as being deterministic by LCA practitioners or are expected to have a very low uncertainty given that the LCA practitioner should have made sure that the collected data is reliable. Yet, data in the foreground system can also be uncertain and variable, though that information is often not considered or unavailable during collection. LCA practitioners can also use an extensive foreground system, containing different individual life cycles, which can be in itself an indication for variability. For example Steinmann et al. (2014) (ID 4) and Hauck et al. (2014) (ID 5) used the deterministic data of a relatively large number of plant-specific life cycles to calculate a variability ratio. Thus, their input parameters were either deterministic or had an uncertain distribution assigned to it, but not a variable one.

In contrast, the *background system* should – in theory – always include uncertainty and variability, seeing as it is not specific to the studied system. However, the data quality of the database determines if that kind of information is available. It might not be that relevant to even put in the time to find qualitative background data, since the decision maker will be more inclined to base their decision on results from the foreground data, since they can influence it more. The LCA practitioner also has more control over the foreground system to make it truly representative, which is less the case for the background system. Lastly, a lot of product/process comparisons have a common background system. By limiting the uncertainty there, one can effectively focus on the prevalent differences between the two product systems found in the foreground system.

The classification of parameters is also hampered by certain parameters that can be classified as parameter *and/or* model uncertainty. For example, emissions can either be measured relative to a specific functional unit and incorporated as parameters or they can be modeled mathematically in relation to input parameters (Lloyd and Ries, 2007). In the selected articles, Yan and Boies (2013) (ID 3) clearly define soil N_2O emission from fertilizer use as “scientific uncertainty” (i.e., parameters that are currently highly uncertain with the best available science) which they defined as being part of parameter uncertainty. Clavreul et al. (2017) (ID 10) considered direct N_2O field emissions as having “model uncertainties”. However, as stated in the results, due to unclear terminology and non-reported definitions, we classified it as parameter uncertainty. Zehetmeier et al. (2014) (ID 7) classified the emission factor of nitrogen input into soil as having both model uncertainty and parameter uncertainty.

It is clear that distinction between the different types of uncertainty is not straightforward, often because an input parameter can be considered as belonging to different types, or insufficient data is available. Several authors (ID 2, 4 and 6) stated that it was not feasible for them to clearly separate uncertainty and variability in their parameters, and the parameter was subsequently considered as uncertain.

It may be interesting to further subdivide variability between sources and objects in inter-individual [as defined by the U.S. EPA (Wood et al., 1997)] and technological variability [as used by Steinmann et al. (2014) (ID 4) and Hauck et al. (2014) (ID 5)], because technological variability can provide information on how processes can be improved, as opposed to inter-individual variability.

3.4.2 Propagation, visualizations and limitations

The chosen methodology has a big influence on how the distinction between uncertainty and variability can be made, how it can be propagated and analyzed, how it can be visualized and what kind of conclusions can be drawn regarding the dominance of either uncertainty or variability. All the included methodologies in this systematic review generally follow the different steps for treatment of uncertainty (which includes variability) of LCA models, as described by Igos et al. (2018):

1. *characterization*, i.e., the qualitative and quantitative description of uncertainties from the model and inputs,
2. *uncertainty analysis*, i.e., the propagation of uncertainty to the outputs,
3. *sensitivity analysis*, i.e., the analysis of the influence of input uncertainty on output uncertainty, and
4. *communication*, i.e., the ability to inform the audience about uncertainty.

Each methodology that was used in the articles to propagate the different types of uncertainty and variability – in particular focusing on parameter uncertainty and variability between sources and objects – is qualitatively analyzed in the following sections. Uncertainty analysis and sensitivity analysis are distinct but related disciplines and often conflated in literature (Saltelli et al., 2019). The different methodologies were therefore categorized as uncertainty and variability propagation, local sensitivity analysis, screening method and global sensitivity analysis; to clearly distinguish between the different types of analyses.

Since LCA results are becoming more and more disseminated [e.g., for the Product Environmental Footprint (European Commission, 2018), by companies (BASF, 2021; Unilever, 2021), etc.], clear communication of the uncertainty component (including variability) is required to avoid biased interpretations from non-experts (Igos et al., 2019). Therefore, a proper LCA study should communicate all different components related to the uncertainty and variability quantification, from defining the concepts and identifying the sources, to the propagation of these sources (Hauschild et al., 2018; Igos et al., 2019). The chosen communication form should be understandable and clear for the target audience. It should enhance the interpretation and lead to robust conclusions, keeping in mind that the same information can be interpreted differently depending on the audience's context and their familiarity with the concepts (Hauschild et al., 2018).

Hauschild et al (2018) list four different, complementary ways to present uncertainty information:

1. *qualitatively* (e.g., reporting sources of uncertainty/variability and their potential influence on results),
2. *descriptively* (e.g., summary statistics),
3. *graphically* and
4. *numerically* (e.g., ranges, probability distributions of results or statistical results).

In the following review, all these ways are considered, but the focus lies especially on graphical visualization, because it allows to show a lot of information in a concise and structured way. However, it also bears the risk of being suggestive and easily misinterpreted (Hauschild et al., 2018), or it might be too complex or conversely, too simple, depending on the degree of detail and nuance included. Figure 3-5 shows how the results were visualized in the selected studies for the specific methodologies used for all the considered types of uncertainty and variability. The data used in the visualization options, part of Figure 3-5, has no link with the data in the eleven included articles, only with their methodologies. These illustrative data were chosen to always have variability be the most dominating.

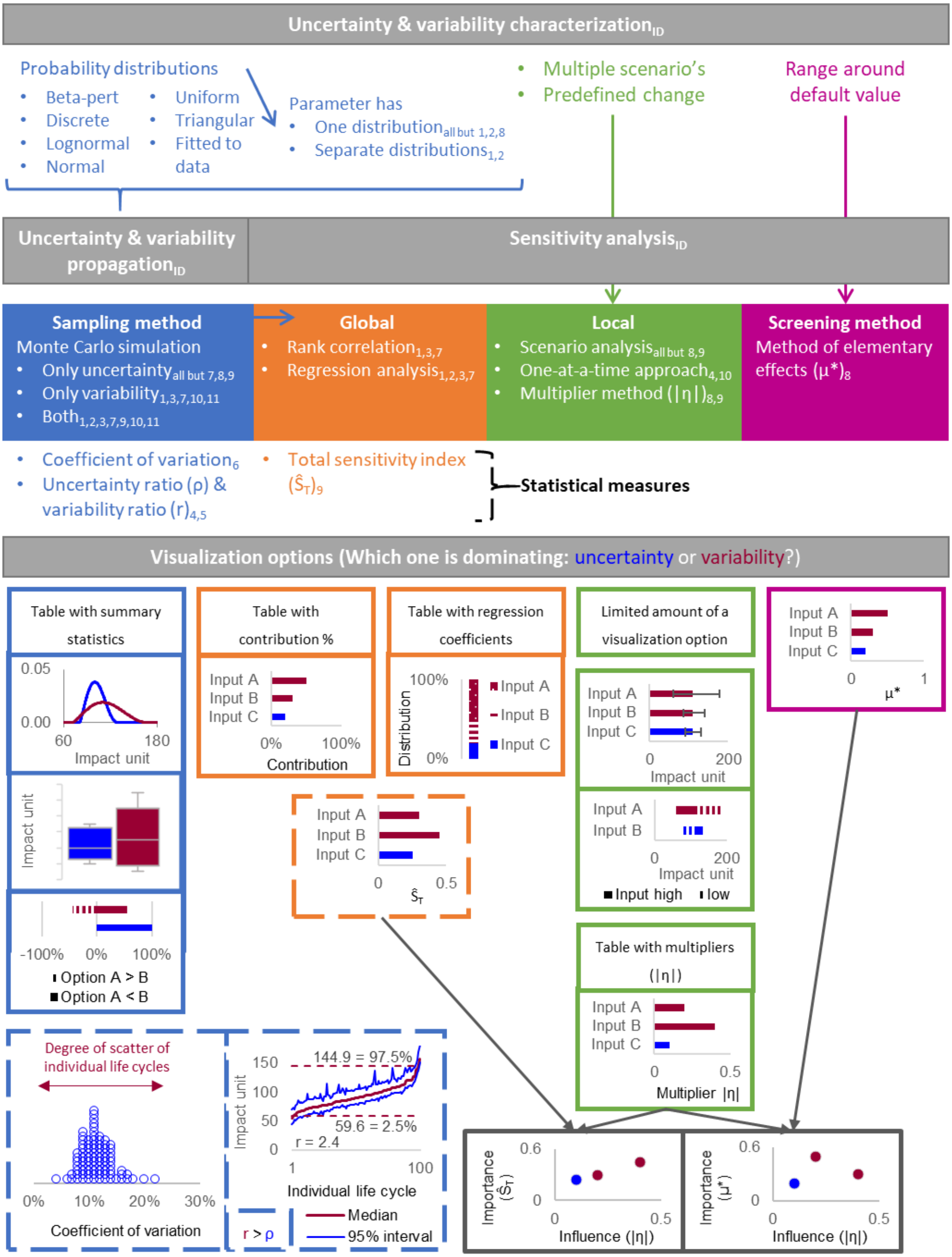


Figure 3-5 Overview of the steps taken by the different articles to visualize uncertainty and variability in the results.

The different articles are indicated by ID's as defined in Table 3-1. The used data in the visualization options is fictional and chosen to have variability dominating. Striped frames show visualizations where statistical measures are applied.

3.4.2.1 Uncertainty and variability propagation

Processing uncertainty in LCA is usually done by using either a sampling method or an analytical method (Heijungs and Lenzen, 2014; Igos et al., 2019), however other methods such as scenario analysis, interval calculations and fuzzy set theory were also occasionally used (Igos et al., 2019; Lloyd and Ries, 2007).

The aim with *sampling methods* is to simulate several result possibilities represented by a probability distribution, by sampling inputs from probability distributions (Hauschild et al., 2018; Igos et al., 2019). In contrast, in the *analytical approach* the first-order approximation of the Taylor series expansion is usually used to determine the variance of the output based on the variances of the uncertain inputs. Its main advantages are calculation speed and smaller data requirements. The drawback are that less uncertainty information can be obtained from the result and that it is predominately applicable for simple models with small uncertainties (Groen et al., 2014; Heijungs and Lenzen, 2014).

Scenario analysis for uncertainty analysis leads to a range of possible LCA results calculated from different model formulations (Igos et al., 2019). *Fuzzy sets* – which is an extension of *interval calculations* (Igos et al., 2019) – simulate the way an expert reasons by degrees of plausibility or possibility, rather than frequency, of an uncertain parameter value. This is mostly displayed by triangular or trapezoidal distributions, based on a lower and upper bound (support) and a most plausible value or interval (core), respectively. Narrower intervals of this distribution at any given degree of possibility α (from 0 to 1), are called α-cuts, which can be manipulated using interval arithmetic. The computational effort is limited, seeing as only a few α-cuts are needed (e.g., 20) to give insight into the output uncertainty. The result of this method is a possibility function – combining the inventory results at all α-cuts – with a core value (of height equal 1) and a lower and upper bound, for which the resolution is determined by the number of propagated α-cuts (Groen et al., 2014; Igos et al., 2019; Tan, 2008). In the selected articles, only sampling methods i.e., Monte Carlo simulations, were used to propagate uncertainty and variability separately. Therefore, the other possible methods for uncertainty propagation in LCA are not further discussed; more extensive overviews can be found in e.g., Groen et al., (2014), Hauschild et al. (2018), Heijungs and Huijbregts (2004), Igos et al. (2018) and Lloyd and Ries (2007).

Monte Carlo simulations

The most commonly used sampling method in LCA is Monte Carlo simulation (Groen et al., 2014; Hauschild et al., 2018; Igos et al., 2019), available in all major LCA software (Hauschild et al., 2018). The method was used in ten out of the eleven included studies (all except ID 8). The basic principle of this sampling method is conducting iterations of model calculations using values sampled from defined probability distributions for each input parameter. Therefore, the model output can be represented by a probability distribution as well (Hauschild et al., 2018; Igos et al., 2019) as illustrated in the first graph in light blue on the left of Figure 3-5.

Basset-Mens et al. (2009) (ID 1) highlighted the difficulty of defining appropriate probabilistic distributions for the input parameters. The lack of statistics for inventory data result in an additional and time-consuming phase for estimating their probabilistic functions based on a set of data, literature references or expert judgement. Moreover, the aggregated nature of available datasets make it difficult to define potential correlations between parameters (Yan and Boies, 2013).

Any Monte Carlo simulation has the same basic, iterative process, but the way values are randomly sampled from the probability distribution can vary (Hauschild et al., 2018). Sampling can be done using e.g., Monte Carlo sampling, Latin Hypercube sampling (Groen et al., 2014; Hauschild et al., 2018; Heijungs and Lenzen, 2014) and Quasi-Monte Carlo sampling (Groen et al., 2014; Igos et al., 2019); with the last two having a faster convergence rate (Igos et al., 2019). One of the selected articles (ID 1) specifically stated that they used Latin Hypercube, because the stratified sampling without replacement leads to a quicker stabilization of the results (Basset-Mens et al., 2009).

Characterization

Monte Carlo simulations are in the selected studies most often used to firmly separate the different types of uncertainty and variability, with scenario-like outcomes (ID 1 – 3, 10 and 11). One or more types are considered as deterministic, while the other considered types are sampled from during the iterations, and the combined effect of all types is often propagated as well (ID 10 and 11).

Propagating parameter uncertainty in the selected articles by means of Monte Carlo simulations was done by sampling exclusively from distributions reflecting uncertainty (ID 1 – 6, 10 and 11). A distinction can be made between studies that propagate specific parameters as only being uncertain (ID 3 – 6 and 10), and studies that assign uncertainty distributions and variability distributions to each parameter (ID 1 and 2). The assigned distributions are: uniform, triangular or beta-PERT, depending on available values (ID 3 – 5 and 10); normal or lognormal, using the standard error of the mean (ID 1); or lognormal, using arithmetic metrics (ID 5), using geometric metrics (ID 2, 4 and 5), or using the uncertainty factors of the pedigree matrix (ID 11).

Propagating variability between objects and choices is done similarly as parameter uncertainty. Monte Carlo simulations were conducted, sampling exclusively from distributions reflecting variability (ID 1, 3, 7, 10 and 11). The assigned distributions are: discrete (ID 10), uniform (ID 11), or normal or lognormal, using the standard deviation (ID 1, 3, 7 and 10) as opposed to using the standard error of the mean for propagating parameter uncertainty (ID 1).

Some studies *propagated parameter uncertainty and variability between sources and objects alongside each other* during Monte Carlo simulations. There are three distinct methods used:

1. sampling from both uncertainty distributions and variability distributions, after having conducted simulations for each separately (ID 10 and 11), which – of course – causes a larger spread in the results,
2. conducting two Monte Carlo simulations, sampling exclusively from uncertainty distributions and sampling from both distribution types (ID 2), and
3. conducting two Monte Carlo simulations, sampling exclusively from variability distributions and sampling from both distribution types (ID 7).

The impact of uncertainty and variability in method 2 and 3 is measured by how much the spread increases in the resulting probability distribution by also propagating variability and uncertainty respectively.

Visualization

Exclusively sampling from uncertainty distributions versus variability distributions leads to scenario-like outcomes. In this case, a choice needs to be made about which kind of statistic, based on the resulting probability distribution, is a proper indication to determine whether uncertainty or variability is most dominating. The resulting probability distribution of the Monte Carlo simulations are expressed in the selected articles using: median values (ID 3), standard deviation (ID 1 and 10), ranges [e.g., 5^{th} – 95^{th} percentiles (ID 1 and 3), 2.5^{th} – 97.5^{th} percentiles (ID 2), 0^{th} – 100^{th} percentiles (ID 1)] and skewness (ID 1).

For the graphical visualization, only one of the included articles (ID 1) visualized the results from the simulations with probability distributions and three (ID 3, 5 and 10) used box plots (first and second illustrative graph in light blue on the left of Fig. 3-5, respectively).

Pairwise analysis

AzariJafari et al. (2018) (ID 11) sampled exclusively from one type of uncertainty or variability, but had a slightly different approach. They conducted a pairwise analysis, meaning that they took the relative uncertainty and/or the relative variability of two products (option A and option B; see third illustrative graph in light blue on the left of Fig. 3-5) into consideration by subtracting their impacts from each other during the simulations (A-B). Instead of having two outputs (one for each product), only one is generated showing how many times option A performed better (negative values) or worse than B (positive values). They did this same analysis multiple times, once only propagating parameter uncertainty, once only propagating variability and once propagating all uncertainty and variability.

For each impact category, their analysis shows if relative uncertainty and/or relative variability is a dominating factor in the selection of the preferred product (i.e., in how many iterations has option A less impact than option B when considering only relative uncertainty or only relative variability). For example, in 100% of the iterations, option A had less impact on climate change than option B, when only considering uncertainty. In contrast, when only considering variability, option A was the preferred option regarding climate change in only a little more than 50% of the iterations.

Number of iterations

The accuracy of Monte Carlo simulations output increases when more iterations are conducted (Hauschild et al., 2018; Igos et al., 2019). However, the number of iterations performed is generally stated as being a trade-off between acceptable accuracy and needed computation time (Chen and Corson, 2014; Hauschild et al., 2018; Igos et al., 2019). An insufficient number of iterations will not give a reliable output, because the full range of possible input values will not be sampled from nor will the shape of the probability distribution be adequately represented. Yet, there is no specific amount of iterations that is generally large enough, rather it depends on when convergence is reached in the output of a specific model (Hauschild et al., 2018). Nevertheless, a rule of thumb of 10000 iterations is normally applied to ensure stable variance (Ciroth et al., 2004; Igos et al., 2019).

Hauschild et al. (2018) suggest repeatedly increasing the number of iterations until the difference of two subsequent uncertainty measures (e.g., mean or standard deviation) is acceptably low [i.e., numerical stability is reached (US EPA Technical Panel, 1997)]. This is however also a subjective measure and the question then arises, what is “acceptably low”? Robust estimators (e.g., median or extreme percentiles) might produce an “acceptably low” difference with a lower increase in iterations. Though, since skewed distributions are commonly used in LCA (e.g., lognormal), solely using robust estimators should be avoided. This illustrates how the choice of number of iterations is practitioner-specific as well as study-specific (Hauschild et al., 2018).

In the selected studies, the number of iterations varied from 1000 to 50000. One article (ID 2) did not mention the number of iterations that was used. Only two (ID 4 and 6) studies verified if increasing the number of iterations leads to an unacceptable difference compared to the smaller number. Steinmann et al. 2014) (ID 4) took a ten-fold of their chosen number of iterations (i.e., 10000 instead of 1000 runs) and concluded that the difference in uncertainty ratio (see section Statistical measure) was smaller than 1%. Chen and Corson 2014) (ID 6) specified that increasing their 1000 iterations to 5000 increased the computation time from 30 to 90 minutes for each farm, a difference considered unacceptable when compared to the corresponding increase in stability of estimates of the mean values.

In this context, it seems relevant to reflect on what a long computation time really looks like. Although computation time might appear long (say hours), it may in fact be relatively short compared to the time needed to complete, for example, the data inventory analysis. Hence, it seems unbalanced to limit computation time to hours, even days, given the importance of appropriate uncertainty and variability assessments. Lack of computational power and time should not be used to justify lack of convergence. For example, actual (super)computer capabilities exist able to solve thousands of parallel nonlinear differential equations for weather predictions. Therefore, the number of iterations should be increased accordingly to ensure that convergence is obtained (Hauschild et al., 2018). If needed, one can look for appropriate computational solutions at software or hardware level.

Communication

Monte Carlo simulations give a probability distribution as output, which might be challenging to disseminate to a broader audience. Communication can be simplified by using summary statistics or by taking specific values from the output distribution and using them to calculate a single value. Of the articles selected in this systematic review, Chen and Corson (2014) (ID 6) calculated coefficients of variations and Steinmann et al. (2014) (ID 4) and Hauck et al. (2014) (ID 5) calculated uncertainty and variability ratios to facilitate communication.

Statistical measure: Coefficient of variation

Chen and Corson (2014) (ID 6) conducted Monte Carlo simulations, only propagating uncertainty, for each individual life cycle [which together reflect variability and was already assessed in the study of van der Werf et al. (2009) on which Chen and Corson built further, see section 3.3] and calculated the coefficients of variation for each life cycle as a measure for uncertainty. The degree of scatter among the calculated coefficients of variations reflects the inter-individual variability in the coefficients of variations. Thus, the measure of variability is dependent on Monte Carlo simulations propagating uncertainty. It is difficult to conclude if either uncertainty or variability is dominating in the results, because two different, incomparable measuring systems (i.e., coefficient of variation and degree of scatter of individual life cycles) are used. Still, an indication is given by visualizing the strip plots (blue striped framed graph at the bottom left in Fig. 3-5).

Statistical measure: Uncertainty ratio (ρ) and variability ratio (r)

Steinmann et al. (2014) (ID 4) and Hauck et al. (2014) (ID 5) conducted Monte Carlo simulations, only propagating uncertainty, for each "individual" life cycle and for the "comprehensive" life cycle (encompassing all of the individual life cycles). They divided the 97.5th percentile by the 2.5th percentile, thereby creating an "*uncertainty ratio ρ*" for the comprehensive life cycle (equation 3-1):

$$\rho = \frac{q_{0.975}(\{Y\})}{q_{0.025}(\{Y\})} \qquad \text{(Equation 3-1)}$$

With the numerator being the 97.5th percentile of the Monte Carlo simulation results for the ‘comprehensive system’ {Y} and the denominator the 2.5th percentile of the same (Hauck et al., 2014). Steinman et al. (2014) (ID 4) also calculated that uncertainty ratio for each individual life cycle (see blue lines in the right blue striped framed graph in Fig. 3-5).

Subsequently, Steinman et al. (2014) (ID 4) and Hauck et al. (2014) (ID 5) calculated a “*variability ratio r*” (equation 3-2):

$$r = \frac{q_{0.975}(\{E(y)\})}{q_{0.025}(\{E(y)\})} \qquad \text{(Equation 3-2)}$$

by dividing the 97.5th percentile by the 2.5th percentile of a set of arithmetic means {E(y)} taken from the probability output distributions that were generated by conducting Monte Carlo simulations for each individual life cycle (though both used median values in their graphical visualization instead of arithmetic means; see red line in blue striped framed graph in Fig. 3-5).

The uncertainty ratio and variability ratio show whether uncertainty or variability was the primary cause of the range in the results. If the ratio equals 1, then there is no effect upon the LCA results of uncertainty or variability respectively. If the uncertainty ratio is the biggest ratio, then further research may reduce the range in the LCA results. If the reverse is true, then further research will not substantially reduce the range, rather physical changes must occur, if possible (Steinmann et al., 2014).

Only uncertainty and variability ratios make it possible for the reader to make a clear-cut conclusion regarding which is more dominating. Other methodologies are not as straightforward and can lead to more ambiguous conclusions [for example the incomparable measuring systems of Chen and Corson (2014) (ID 6)].

The variability ratio is based on an extensive database of deterministic values recorded for each included individual life cycle. Thus, calculating uncertainty and variability ratios is only possible if such widespread deterministic data is available for each individual life cycle. Moreover, Steinmann et al. (2014) (ID 4) pointed out that it was not always feasible to completely disentangle uncertainty and variability. They specified parameters as uncertain in their modeling approach, even though the influence of variability could not be fully excluded. However, even if they were able to completely distinguish between uncertainty and variability, their used methodology of calculating uncertainty and variability ratios does not seem to allow the presence of strictly variable parameters. Thus, even though variability and uncertainty ratios allow for a clear distinction and conclusion, it requires a high degree of quality of the data, which is often not available.

3.4.2.2 Local sensitivity analysis

ISO 14040/44 (2006a, 2006b) defines sensitivity analysis as: "systematic procedures for estimating the effects of the choices made regarding methods and data on the outcome of a study." However, sensitivity analysis is often used more broadly than how it is defined by ISO 14040/44 (2006a, 2006b). The sensitivity of a model also describes to which extent the variation of an input parameter leads to variation in the model result. Thus, a model is sensitive toward a parameter if a small change in the parameter results in a large change in the model result (Hauschild et al., 2018; Pianosi et al., 2016). A *local sensitivity analysis* can be considered as the effect of a certain predefined change in input on the output, while keeping the others constant (Björklund, 2002; Hauschild et al., 2018; Igos et al., 2019; Pianosi et al., 2016; Wolf et al., 2017).

Scenario analysis

Scenario analysis (first green visualization option in Fig. 3-5) is a typical sensitivity analysis as defined by ISO 14040/44 (2006a, 2006b), where possible changes to the LCA results caused by discrete choices are calculated (Hauschild et al., 2018; Igos et al., 2019). In the selected studies, it was only used to evaluate uncertainty due to choices [i.e., allocation procedures (ID 3 and 7), functional units (ID 6), Life Cycle Inventory assumptions (ID 11) and Life Cycle Impact Assessment methods (ID 1, 4, 5 and 11)], temporal variability (ID 2, 4 and 10) and spatial variability (ID 4). Not one specific visualization option exists, rather the visualization that is used to show the analysis results is repeated for each scenario. It is only feasible to maintain an overview when a limited amount of scenario's is being compared. Therefore, it is not an advisable method for considering parameter uncertainty and variability between sources and objects, because of their high number of possible scenarios.

One-at-a-time approach

Perturbation analysis with a one-at-a-time approach can be regarded as a local sensitivity analysis. Thus, interaction effects between parameters are ignored

(Saltelli and Annoni, 2010). Groen et al. (2016b) mention two weaknesses associated with this method, i.e., the number of inputs parameters assessed is usually a subset of all input parameters and the arbitrary choice of the predefined change may not reflect the actual uncertainty range.

This last issue is somewhat countered to by the two articles (ID 4 and 10) that used perturbation analysis with a one-at-a-time approach in their study. Steinman et al. (2014) (ID 4) used sequential perturbation analysis to assess the sensitivity of the results with respect to the uncertain parameters (since only those can be reduced by additional research), using the 2.5th and 97.5th percentiles of the assigned probability distribution as a predefined change. Similarly, Clavreul et al. (2017) (ID 10) used the minimum and maximum values of the assigned probability distribution as a predefined change for their one-factor-at-a-time perturbation analysis. Results were visualized with error bars on a bar plot, showing the minimal and maximal results obtained when testing each parameter (ID 10) or with a tornado diagram (ID 4), where the longer bars at the top represent the parameters with the largest influence on the output (first two green graphs in Fig. 3-5). Clavreul et al. (2017) (ID 10) underlined their primary data parameters (containing variability in farmer's input) in contrast with the secondary data parameters (classified as parameter uncertainty), in their bar plot allowing for a quick assessment for which the model output was most sensitive.

Multiplier method

Groen et al. (2016b) and Wolf et al. (2017) (ID 8 and 9) used the multiplier method (lowest green graph in Fig. 3-5) as a local sensitivity analysis. The multiplier method uses first-order partial derivatives to quantify the effect of a small change around the default value of each input parameter on the result. The obtained multipliers can be interpreted as how much and in which direction a 1% increase in the input will affect the output (in %) (Groen et al., 2016; Wolf et al., 2017). Groen et al. (2016b) (ID 8) chose the multiplier method because it includes all input parameters, which is not necessarily the case in a one-at-a-time approach. Both studies (ID 8 and 9) distinguished in the inventory between uncertainty and variability, making it possible to assess if the biggest multipliers (in absolute values) correspond to either uncertain or variable parameters. The visualization of this multiplier method was done in a table (ID 8) or bar plot (ID 9) (last two green visualization options in Fig. 3-5).

3.4.2.3 Screening method

Method of elementary effects

Next to the multiplier method, Groen et al. (2016b) (ID 8) also used the method of elementary effects, a kind of sensitivity analysis belonging to the area of screening methods (Igos et al., 2019; Saltelli et al., 2008). *A screening method* can be seen as an intermediate tool between local and global sensitivity analysis (see 4.2.2 and 4.2.4 respectively) to find approximate sensitivity information at a lower computational cost than global sensitivity analyses (Wei et al., 2015), and should be followed by a more detailed sensitivity analysis for the selected parameters (Mutel et al., 2013; Wei et al., 2015). The method is specifically convenient when there is a large number of parameters in the model (Saltelli et al., 2008). Local sensitivity analyses and screening methods can be used as a preliminary step to identify for which parameters the model is sensitive, and on which the focus should thus lie when gathering more representative data for more computationally intensive analyses [such as in Mutel et al. (2013)].

Characterization and method description

The method of elementary effects systematically varies all input parameters in series within their minimum and maximum values, instead of keeping all but one constant, to explore the full range of model outcomes (Igos et al., 2019; Mutel et al., 2013). Thus, the whole input space is explored rather than just a selection, as is the case in most local sensitivity analyses (Saltelli et al., 2008). It therefore gives more reliable and informative results than local sensitivity analyses (Igos et al., 2019). For this, trajectories are constructed in which each point represents a set of parameter values. One parameter value varies with each trajectory step between preselected values (Mutel et al., 2013).

The method calculates for each input parameter a number of incremental ratios, called “Elementary Effects” [i.e., the output variation divided by the input variation that is observed on each point of the chosen trajectories (Igos et al., 2019)], from which two sensitivity measures are computed: the average and the standard deviation (Campolongo et al., 2007). The average of an input’s elementary effects reflects how sensitive the model is to that parameter, while the standard deviation is an indication for the interaction or non-linear effects within the model (Campolongo et al., 2007; Igos et al., 2019; Saltelli et al., 2008). Groen et al. (2016b)

(ID 8) used the (absolute) mean of the average elementary effects [as refined by Campolongo et al. (2007)] to estimate the “importance” (see further) of a parameter, which they visualized in a bar plot (pink in Fig. 3-5).

Visualization

Generally speaking, while sensitivity analyses give information on the influence of a certain parameter on the result, an uncertainty analysis (including variability) shows how the spread in the input is reflected as spread in the output (Hauschild et al., 2018). It is possible that a highly uncertain input parameter has a negligible influence on the output uncertainty (i.e., the model output is insensitive to this parameter). Thus, changes within the uncertainty range will not lead to noteworthy changes in the result and improving the reliability of that parameter might therefore be redundant. Similarly, the fruitfulness of trying to improve the reliability of a very sensitive parameter is dependent on the degree of its certainty (Hauschild et al., 2018; Heijungs, 1996). Ideally, both types of information are studied to judge on which parameters the focus should lie.

Turning now to Groen et al. (2016b) (ID 8), these authors combined the results of *the multiplier method* ($|\eta|$) and the (absolute) mean of the average elementary effects (μ^*) obtained by *the method of elementary effects* in a graph to identify their so called “essential” parameters (dark grey at the bottom right of Fig. 3-5). This graph is adapted from Heijungs (1996), which distinguishes between data that is uncertain and data for which the final result is sensitive. The multipliers ($|\eta|$) are ranked on the horizontal axis as “influence” [which Heijungs (1996) called “contribution” and Hauschild et al. (2018) called “sensitivity”], while the elementary effects (μ^*), defined as “importance”, are ranked on the vertical axis [a.k.a. “uncertainty” (Hauschild et al., 2018; Heijungs, 1996)]. Four classifications of a parameter are identified, depending on where the parameter is ranked on the axes.

1. If a certain parameter ranks low for both sensitivity analyses, then those are defined as “*minor parameters*” [a.k.a. “not a key issue” (Heijungs, 1996) or “negligible parameters” (Hauschild et al., 2018)].
2. An “*influential parameter*” ranks low on the vertical axis and high on the horizontal axis [a.k.a. “perhaps a key issue” (Heijungs, 1996) or “possibly important parameter” (Hauschild et al., 2018)]. Those parameters could have the most impact if they are reduced (Groen et al., 2016).

3. An "*important parameter*" ranks high on the vertical axis and low on the horizontal axis [Heijungs (1996) and Hauschild et al. (2018) use the same terminology as for the "influential parameters"]. These are the most important parameters to the output uncertainty, caused by either variability or uncertainty (Groen et al., 2016).
4. Lastly, parameters that rank high on both axes (i.e., in the upper right corner) are defined as the "*essential parameters*" [a.k.a. "a key issue" (Heijungs, 1996) or "very important parameter" (Hauschild et al., 2018)], which can be used to identify mitigation strategies (Groen et al., 2016).

By distinguishing between uncertain and variable parameters in the inventory phase, it is possible to identify if the mitigation strategies for the essential parameters should focus on e.g., improving reliability or adapting management strategies respectively (Groen et al., 2016). Groen et al. (2016b) (ID 8) stated that the use of the method of elementary effects is limited because it is only based on minimum and maximum values, excluding a distribution function or an average value. They instead recommend using a global sensitivity analysis to rank the "importance" of a parameter, which was later done by Wolf et al. (2017) (ID 9).

3.4.2.4 Global sensitivity analysis

It is clear that Monte Carlo simulation is the preferred method for propagating uncertainty and variability in LCA, often in combination with a sensitivity analysis to quantify the contribution to variance of the input parameters. This is sometimes defined as *global sensitivity analysis* (Groen et al., 2016; Igos et al., 2019; Wolf et al., 2017), which evaluates the sensitivity of the outputs to the variability and/or uncertainty of the entire input space (Igos et al., 2019; Pianosi et al., 2016). These more data-intensive global sensitivity methods are suitable to include correlations among input parameters (Groen et al., 2016).

Rank correlation and standardized regression coefficients

A simple global sensitivity analysis consists of a correlation analysis (i.e., calculating Spearman's rank correlation coefficients or regression coefficients) based on the sampled results from uncertainty propagation (e.g., Monte Carlo sampling) (Igos et al., 2019). Because of this, full knowledge of the input parameters is required (Wolf et al., 2017) and the effect of uncertainty is included within the analysis (Hauschild et al., 2018). While correlation quantifies the strength of a linear relationship between two variables, regression expresses the relationship using an equation (Bewick et al., 2003).

Correlation methods use the correlation coefficient between the output and each of the input parameters as a sensitivity measure (Pianosi et al., 2016), which is calculated from the rank of values in the case of Spearman's rank correlation (Igos et al., 2019). For *regression analysis*, regression coefficients are calculated from the slope of the output in response to the input samples. The regression coefficients are standardized when input parameters have different units (Pianosi et al., 2016). For both methods, the *contribution to variance* of a specific parameter can then be obtained by dividing its squared correlation or its regression coefficient by the sum of all coefficients (Hauck et al., 2014; Igos et al., 2019).

After conducting Monte Carlo simulations, Yan and Boies (2013) [ID 3; using Crystal Ball (Oracle, CA, USA)], Hauck et al. (2014) (ID 5; using Crystal Ball) and Chen and Corson (2014) [ID 6; using R (R Foundation for Statistical Computing, Vienna, Austria)] used Spearman rank correlation coefficients to assess the contribution to variance of each *uncertain* parameter (orange in Fig. 3-5). The resulting statistics can be interpreted as the percentage of variance that may be explained by each uncertain input parameter (Hauck et al., 2014).

Standardized regression coefficients were calculated to assess the contribution to variance (orange in Fig. 3-5) by Zehetmeier et al. (2014) [ID 7; using @Risk (Palisade, NY, USA)] and Basset-Mens et al. (2009) (ID 1; using @Risk). A regression coefficient predicts a standard deviation change in the output for one standard deviation change in the input parameter. Zehetmeier et al. (2014) (ID 7) expressed those coefficients in contribution percentages. Basset-Mens et al. (2009) (ID 1) calculated regression coefficients for the uncertainty distributions and the variability distributions separately. Thus, they could assess if the key input parameters were ranked the same for both the "uncertainty" and "variability" analysis. Zehetmeier et al. (2014) (ID 7) calculated the regression coefficients based on the Monte Carlo sampling that was done when both uncertainty and variability were propagated alongside each other. Because they clearly showed which parameters had which type of uncertainty and/or variability in their inventory, the reader could decide which was dominating in the results based on their relative contribution to the variance.

Statistical measure: Total sensitivity index

Wolf et al. (2017) (ID 9) conducted Monte Carlo simulations, which they used to determine the output variance. Thereafter, they calculated the standardized regression coefficients (which they adjusted for correlated input parameters) to determine the parameters' contribution to the output variance, which they used as a proxy to calculate total sensitivity indices (orange striped framed graph in Fig. 3-5). The sensitivity index represents the sensitivity of each input parameter and is given by a ratio explaining how much each input parameter contributes to the output variance (Groen and Heijungs, 2017).

Wolf et al. (2017) (ID 9) used the same graphical visualization as Groen et al. (2016b) (ID 8). However, instead of using the vertical axis to show elementary effects, they identified their "important" parameters by using the total sensitivity indices ($\hat{S}_T$; dark grey in Fig. 3-5). Thus, their "essential" parameters have a big multiplier and a high total sensitivity index. Because Wolf et al. (2017) strictly distinguished in the inventory between uncertain and variable parameters, it was possible to assess if the most important or essential parameters are affected by either uncertainty or variability.

Identifying the essential parameters through the use of the multiplier method and sensitivity indices is a methodologically sound and visually appealing way to analyze uncertain and variable parameters separately, but evidently it is only possible if there is a clear distinction made in the inventory phase. The sensitivity indices do not necessarily have to be derived from standardized regression coefficients. According to Groen et al. (2016a) the sampling-based methods squared Spearman correlation coefficients and Sobol's indices (Sobol, 2001) or the analytical method key issue analysis (Heijungs, 1996) can also be used for global sensitivity analysis in LCA, in which case the choice depends on the available data, the magnitude of its uncertainties and the aim of the study.

3.5 Conclusions

A first observation made during the preparatory phase of this research is that even in this era, no consensus on definitions and viewpoints on the terms *uncertainty* and *variability* could be found in the selected articles. Classification of the different types of uncertainty and variability clearly depended on the goal and scope definition and on the quality of the data, and was on some occasions open for interpretation. Regardless, the most important thing is that uncertainty and variability are both considered and propagated in some way. While some studies effectively focused on separating uncertainty and variability, with others it seemed more coincidental or as an after-thought. Properly accounting for and dealing with uncertainty and variability should be a part of the LCA process from the very start.

A large number of studies combine a variety of methodologies to propagate and analyze uncertainty and variability through the different LCA phases, often following a multi-step approach as described by Igos et al. (2018). Based on the used methodologies in the included articles, the different steps for the treatment of uncertainty and variability (Igos et al., 2019) can be categorized as follows:

1. *characterization* using multiple scenario's, predefined changes, ranges around a default value or probability distributions,
2. *uncertainty and variability propagation* using Monte Carlo simulations,
3. (a) *local sensitivity analysis* using scenario analysis, one-at-a-time approach or the multiplier method,

   (b) *screening method* using the method of elementary effects, or

   (c) *global sensitivity analysis* by calculating rank correlation coefficients or regression coefficients, and
4. *visualization* using summary statistics, ranges, coefficients of variation, uncertainty and variability ratios, contribution to variance percentages, sensitivity indices and essential (i.e., both important and influential) parameters.

Regarding *characterization*, the challenge lies in representing the uncertain and variable data as realistically as possible. It is essential that uncertainty and variability are already sufficiently taken into consideration during the inventory phase, and not just as an after-thought once the assessment has been completed. While defining multiple scenarios can be effective for a limited number of scenarios, a clear overview can be lost quickly when that number increases. Moreover, a range around a default value can be useful to get a first impression of the results and to identify where the focus should lie. Still, using probability distributions is the most preferable of the four characterization options used in the included articles. Although it requires much effort and time to gather the required input information, rich information is returned, and correlations can be included. Local sensitivity analyses and screening methods can be used as a preliminary step to identify the most influential parameters on which the focus should lie for gathering more data for further analyses.

Regarding *uncertainty and variability propagation*, only the Monte Carlo method – a sampling method – was used in the selected articles of the systematic review. Monte Carlo simulation outputs – where either uncertainty, variability or both are propagated – can be used to conclude if either uncertainty or variability is dominating in the results. Output probability distributions and their statistics can be visualized and compared. However, each uncertain and/or variable input parameter should then have an appropriate probability distribution assigned to it during the inventory phase. It is advisable to combine uncertainty analysis with a sensitivity analysis. Sensitivity analysis can be used after the uncertainty and variability propagation to determine how much influence the highly uncertain parameters have, and thus where uncertainty reduction is most desirable.

In contrast, global sensitivity analysis is more of an extension of an uncertainty analysis. Hence, the conclusion of which is dominating can also be based on a global sensitivity analysis in combination with a local sensitivity analysis. Measures of sensitivity can be visualized and compared by clearly showing which input parameter is uncertain and which is variable. Thus, this method also requires a clear distinction to be made between uncertainty and variability in the inventory phase. Predefined changes, uncertainty ranges or probability distributions for Monte Carlo sampling need to be defined for each uncertain and/or variable input parameter.

3.6 Recommendations based on the selected articles

Based on the methodologies used by the eleven selected articles and keeping the need for clear communication in mind, we strongly recommend Monte Carlo simulations visualized in (i) uncertainty and variability ratios and/or (ii) total sensitivity indices through global sensitivity analysis for future use in LCA. On one hand, ratios allow to clearly decide whether uncertainty or variability is most dominating. The two ratios are clearly separated from each other, they can be easily compared because the outcome is a single value, and they are calculated based on probability output distributions from Monte Carlo simulations, making them representative towards the reality. On the other hand, total sensitivity indices (or another suitable index calculated by global sensitivity analysis) in combination with the results of a local sensitivity analysis (such as the multiplier method), allow to identify the essential parameters and whether these are predominantly uncertain or variable. Combining uncertainty/variability and sensitivity measures allows for a clear communication to the actors on which parameters the focus should lie in further decision making regarding e.g., uncertainty reduction and system improvement. Depending on the goal and scope of the LCA study, either methodology can be a good option, provided that the outcomes are interpreted within the study-specific choices made during classification.

3.7 Finding a solution for the shortcomings

In this systematic review, 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 both. It is however possible that a parameter is influenced by both. For example, sorting apples at the auction can be both uncertain and variable. It 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). It can be variable, due to the biological nature of apples, causing different percentages of apples to be spoiled 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 ID 4), 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 propagates them separately for that parameter.

Additionally, one of the recommended methods (visualizing Monte Carlo simulations through uncertainty and variability ratios) required the availability of a large dataset of individual systems. This kind of extensive data is often not available to the LCA practitioner, too time-consuming to construct themselves, or the LCA study might not even require this type of data source when it comes to the goal and scope of the study. An alternative method is needed that can be applied for both extensive databases that contain multiple individual life cycles *and* survey data from one life cycle only.

A solution to these two drawbacks 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 also 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 identify how 2DMC can be used for LCA, which might differ from its use in other domains. In Chapter 4 and 5, the applicability of this method for propagating uncertainty and variability separately in LCA is analyzed by conducting 2DMC simulations for a case study, using two types of data sources: surveys and large datasets, respectively.

Chapter 4

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

This chapter is based on: Michiels, F., Geeraerd, A. *(under review)* Two-dimensional Monte Carlo simulations in LCA: an innovative approach to guide the choice for the environmentally preferable option.

Author's contributions: Michiels F. performed the analysis and drafted the manuscript

4.1 Introduction

In Chapter 3, we extensively discussed the need to take uncertainty and variability separately into account in order to communicate about reality in a representative way, and to fully and correctly understand the study results and their reliability. (Epistemic) *uncertainty* refers to the imperfection of our knowledge, while v*ariability* represents the inherent heterogeneity of the natural world that will always be observed (Hauschild et al., 2018; Walker et al., 2003). In quantitative risk assessment, 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)]. Even if uncertainty is accounted for, variability is often treated alike or even left unacknowledged [e.g., Jiao et al. (2019)]. Because of this, when products or processes are compared in 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 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 chapter lies.

In this chapter, we aim to introduce a novel approach, two-dimensional Monte Carlo simulations (2DMC), in LCA that allows to decide if either uncertainty or variability is dominating in the results. We aim to clarify in full details the 2DMC procedure using a fully detailed proof of concept model, available on our website (Michiels and Geeraerd, 2021), and a realistic case study, comparing two products, with special attention on how data uncertainty and variability is assigned to different input parameters. Lastly, we aim to interpret the 2DMC results in an LCA context to see how it can influence decision making by reflecting on the above-mentioned questions.

4.2 Methods

Propagating uncertainty and variability separately can be done by conducting two-dimensional Monte Carlo simulations, which has been shown in the field of quantitative risk assessment [e.g., Wu and Tsang (2004), Vásquez et al. (2014) and Boué et al. (2017)]. 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 separately at the same time when a parameter is both uncertain and variable. Separate 1DMC simulations can be conducted each time in- or excluding either uncertainty or variability. However, the question then arises on which statistic measure the decisions on which is dominating, should be based. This is one of the shortcomings that was identified in Chapter 3 (Michiels and Geeraerd, 2020) when we reviewed which methodologies have already been used in LCA that allow to decide whether uncertainty or variability is dominating in the results.

2DMC does allow to propagate uncertainty and variability simultaneously as well as disentangle their influence on the results. 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). We have found no indication as of yet that 2DMC has been applied in an LCA study previously. Though, it has been applied in studies related to LCA, such as for the ecotoxicological impact assessment of down-the-drain products (Douziech et al., 2019) which can be used to calculate the ecotoxicological results of an LCA.

The first part of the Methods section describes the general 2DMC methodology, focusing on what kind of information is needed for it, how the calculations are performed and how the results can be synthesized. 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 realistic case study i.e., the post-harvest chain of apple in Flanders (Belgium), for which the 2DMC method was applied. In Chapter 5, 2DMC is applied for the apple cultivation chain.

4.2.1 Two-dimensional Monte Carlo simulations

2DMC consists of two 1DMC loops (Fig. 4-1), 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, however, separate distribution data is needed 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 sections 4.3.1. The uncertain parameters are randomly sampled from their respective distributions and considered as a set of fixed values while performing 1DMC simulations with random values from the variable parameters (*m* iterations). 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).

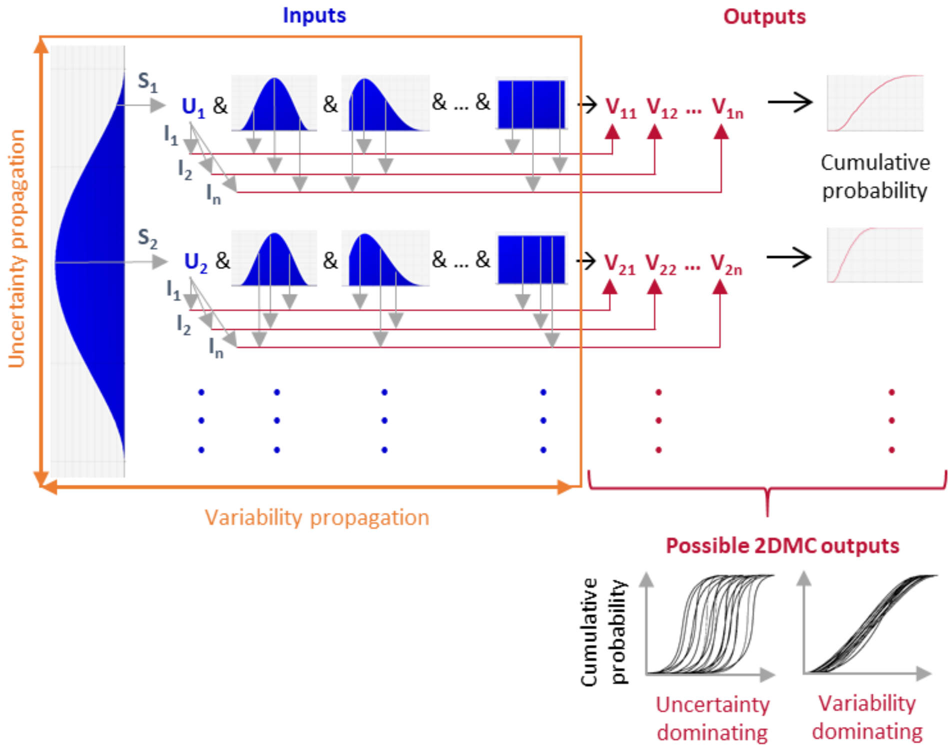


Figure 4-1 Diagram of how two-dimensional Monte Carlo simulations are conducted. This figure was adapted from Cummins (2016). S = simulation, I = iteration, U = unique set of fixed uncertainty parameters, V = possible LCA output.

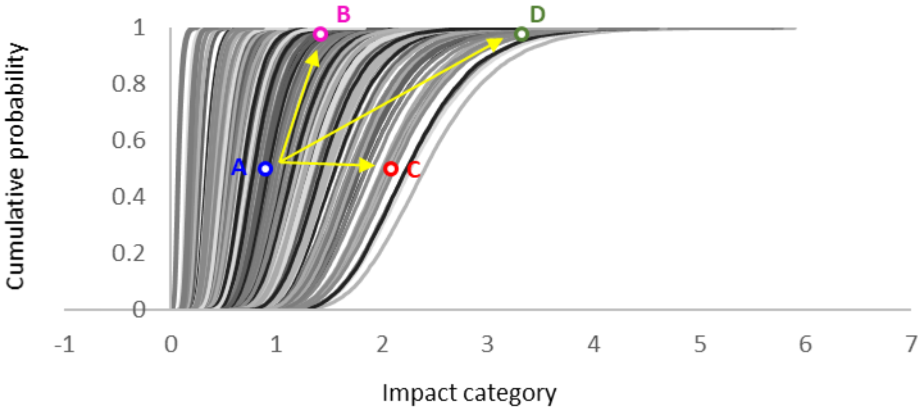
In this PhD thesis, 10 000 iterations and 250 simulations were conducted, leading to 2 500 000 possible LCA outcomes shown in 250 2DMC curves. The number of iterations was chosen because 10 000 iterations are often seen as a rule of thumb in Monte Carlo simulations (Ciroth et al., 2004; Igos et al., 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. A further discussion on an adequate number of Monte Carlo runs can be found in section 7.1.5. The Excel add-in @Risk (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 between different products and impact categories, a fixed initial seed value was used, which was different for each of the 250 simulations.

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) 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. 4-2):

- 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.

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).



A: median of uncertainty for the median of variability
B: median of uncertainty for the 97.5th percentile of variability
C: 97.5th percentile of uncertainty for the median percentile of variability
D: 97.5th percentile of uncertainty for the 97.5th percentile of variability

Figure 4-2 Graphical representation of the points needed to calculate ratios. Variability ratio = B/A, uncertainty ratio = C/A and the overall uncertainty ratio = D/A (Özkaynaka et al., 2009; Pouillot et al., 2016).

4.2.2 Life Cycle Assessment of the post-harvest apple chain

4.2.2.1 Goal and scope definition

We implemented 2DMC in an existing attributional LCA of the Belgian (Flanders) apple, developed by 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. 4-3). 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”.

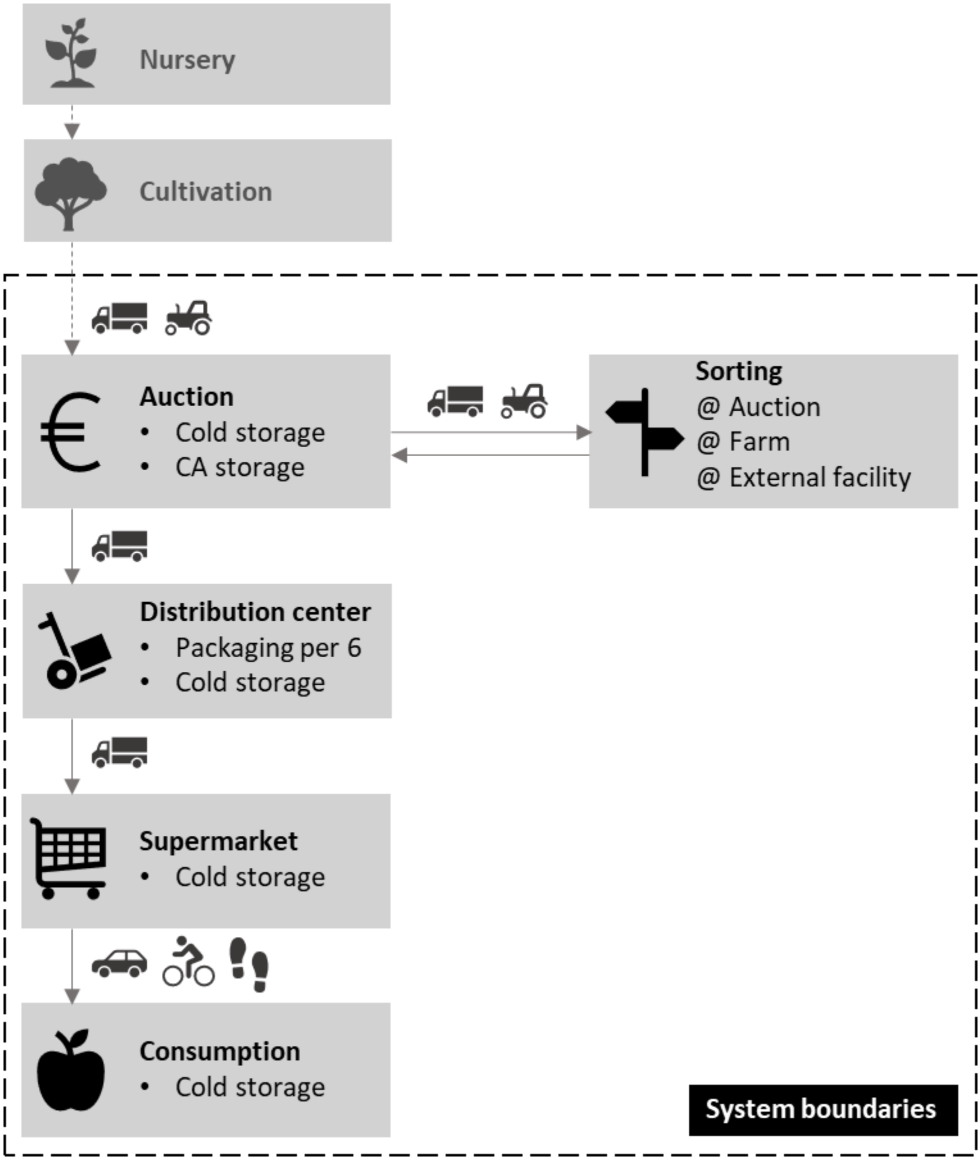


Figure 4-3 System boundaries of the post-harvest apple chain.
CA = Controlled Atmosphere.

4.2.2.2 Life Cycle Inventory

Goossens et al. (2019) gathered information on the apple post-harvest chain by interacting with two 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 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 uncertainty ratings based on the Product Environmental Footprint (PEF) quality criteria (European Commission, 2012), ranging from no uncertainty to very high uncertainty, which can be used to quantify uncertainty. With this data we can conduct a 2DMC analysis.

4.2.2.3 Input probability distributions for the post-harvest parameters

As we discussed in the 2DMC methodology (section 4.2.1), 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 and variable. Appropriate probability distributions need to be selected for the last three categories.

The parameters were categorized as deterministic, uncertain, variable and, uncertain and variable, depending on the kind of data that was provided and available in literature. A summary of the parameters, together with their categorization, is given in Table 4-1. 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 over the data of a variable parameter, making it uncertain and variable. If no variable or uncertain data were provided and that information could not be found in literature, then the parameter was considered deterministic. Thus, in this case study, the choice of a parameter being considered as deterministic is purely driven by data availability (this is further discussed in section 4.4.1).

For example, storage time at the shop is deterministic since no uncertain or variable data was provided. It is, however, quite possible that the amount of apples stored in the supermarket varies a lot. The same could be said for the storage electricity at the consumer. We could have guessed/estimated how much those parameters will vary, thereby introducing uncertainty ourselves. In the end we chose to exclusively use the available data, without making any expert opinions ourselves.

For the parameters for which the auctions and retailer did provide *variable* data, PERT (based on provided min, most likely and max data) or uniform (in case there was not a most likely value provided) distributions were constructed. The PERT (Program Evaluation and Review Technique[7]) distribution is similar to a triangular distribution but is preferred over it because of its curved density, emphasizing most likely values more (Palisade, 2016a).

Additionally, the data of both 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 both equally likely to occur. For example, both auctions provided deterministic data on their storage 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 (Bernaert et al., 2018; DEFRA, 2010; Johnson et al., 2008) 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,

[7] A statistical tool originally used in project management to analyze the time needed to finish the planned tasks.

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 consumers that compost at home or participate in a municipal collection of biowaste.

Packaging data was generally considered as *deterministic*, since the production of those has been fine-tuned [e.g. EPS size M and H plastic crate weight (Euro Pool System, 2017)]. However, the weight of apples transported by paloxes, cardboard boxes or plastic crates could vary. 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., 2007) was considered using a uniform variability distribution.

Uncertainty was taken into account by using the uncertainty ratings of the PEF quality criteria (European Commission, 2012). For example, the distribution center was not certain about how much electricity they needed during storage, 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 or a variable amount, 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%; for which 5% was used), has distribution [x*Pert(1-5%; 1; 1+5%)]. The parameter is then considered strictly uncertain. In the case where the given amount is variable, 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 and 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.

Table 4-1 Summary of the post-harvest parameters and their categorization. The parameters are categorized into deterministic, uncertain, variable and uncertain & variable, with a short explanation on how the type was reflected by the data and which source was used in case the data did not come from surveys. All information for each separate parameter can be found in Appendix A.1.

Input parameter	Type	Data (and literature source)
Apple consumption	Variable	Varies over the year
Apples loss along the chain		
Apple loss @ auction	Variable	Varies over the year & data from two auctions
Apple loss @ distribution center (only for pre-packed apples)	Uncertain & variable	Variable data with uncertainty rate
Apple loss @ shop	Uncertain	Deterministic value with uncertainty rate
Apple loss @ consumer	Variable	Consumer dependent, based on different sources (Bernaert et al., 2018; DEFRA, 2010; Johnson et al., 2008)
Storage and sorting		
Electricity mix	Deterministic	Deterministic wind, solar and grid percentages
Sorting data	Deterministic	Deterministic annual electricity, water use and apple weight
Storage electricity @ auction	Variable	Data from two auctions
Storage time @ auction	Variable	Variable data from two auctions
Storage electricity @ distribution center	Uncertain	Based on uncertain electricity data and deterministic storage space for apples
Storage time @ distribution center	Variable	Variable data
Packaging data	Uncertain	Based on uncertain annual electricity, uncertain share of machine used and uncertain apple weight
Storage electricity @ shop	Uncertain & variable	Based on variable share of cold room for apples, uncertain electricity data, uncertain annual apple sales and the amount of shops
Storage time @ shop	Deterministic	No uncertain or variable data provided
Storage electricity @ consumer	Deterministic	Based on electricity and storage volume from PEFCR (European Commission, 2018)
Storage time @ consumer	Variable	Consumer dependent
Packaging production, transport and waste		
Weight packaging material	Deterministic	Deterministic weights for palox, pallet (Barthel et al., 2007), cardboard box, plastic crates [EPS M & H (Euro Pool System, 2017)], pulpsheet, plastic bag, cardboard tray and plastic foil
Weight of apples that fit in packaging material	Variable	Weight varies when using palox, cardboard box and plastic crate

Table 4-1 Continued

Input parameter	Type	Data (and literature source)
Packaging production, transport and waste		
Weight of apples on pallet	Deterministic	No uncertain or variable data provided
Share of cardboard box vs. plastic crates used	Deterministic	No uncertain or variable data provided
Distance from packaging production sites	Deterministic	Set distances from the packaging production sites
Packaging production	Deterministic	Deterministic production processes
Washing water plastic crates	Deterministic	Based on Barthel et al. (2007)
Loss of packaging material	Variable	Variable reusability of plastic crates with a deterministic breakage rate (Barthel et al., 2007) and variable loss of plastic bags, cardboard trays and plastic foil
Waste of packaging material	Deterministic	Deterministic share of wasted packaging material when packaging apples per 6
% of packaging material used for apples	Deterministic	Deterministic share of plastic bag, cardboard tray and plastic foil, used for packaging apples
Distance to waste facilities	Deterministic	Set distances to the waste facilities
Distribution		
Transport distances	Variable	Location dependent (farm, auction, distribution center, shop, consumer) & data from two auctions
% of tractor vs. truck for farm-auction	Variable	Data from two auctions
% of apples sorted @ farm, auction or sorting facility	Variable	Data from two auctions
Volume consumer car	Deterministic	Based on PEFCR (European Commission, 2018)
% car use by consumer	Deterministic	Based on mobility data (FOD Mobiliteit, 2017)
Biowaste		
Distance to digestion facility after sorting	Variable	Depends on where the apples are sorted (farm, auction, external sorting facility) & data from two auctions
Distance to digestion facility from distribution center	Deterministic	Set distance to digestion facility
% to municipal biowaste collection @ consumer	Variable	Based on deterministic opportunity percentage (De Groof et al., 2015) and variable participation rate of consumers (Goossens et al., 2019)
% to compost @ consumer	Variable	Data based on two sources (Goossens et al., 2019; M.A.S. et al., 2012)
% to household waste collection @ consumer	Variable	Based on variable percentages of municipal biowaste collection and compost
Compost emissions	Deterministic	Based on Colón et al. (2010)

Regarding the (potential) *relationship* between different parameters, we envisioned three ways to include them in 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, which is not the case for the post-harvest chain but is for the cultivation chain (see Chapter 5).
- 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, 2006b). 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 Appendix A.1. Of the 145 parameters in total, 77 were categorized as deterministic, 41 as variable, 17 as uncertain and 10 as uncertain and variable. The POC model (Michiels and Geeraerd, 2021) shows how uncertainty and variability can be differentiated in the @Risk software, and how input probability distributions can lead to probability distributions in the LCA output.

4.3 Results

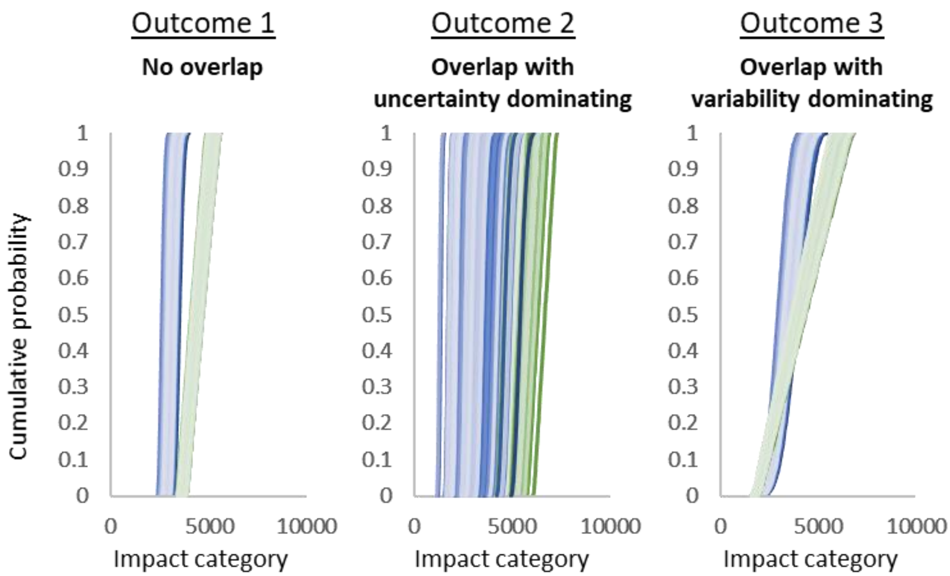
The results section is divided into two parts. In section 4.3.1, three hypothetical outcomes when using 2DMC for the comparison of two options within an LCA context are illustrated. These possible outcomes are further illustrated using real-life data for the apple post-harvest chain in section 4.3.2. The POC model and manual (Michiels and Geeraerd, 2021) explain how the 2DMC results can be visualized and synthetized using ratios.

4.3.1 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. 4-2.

In contrast, the comparison between two products or processes is an important LCA goal. For comparative LCAs, 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 were used instead of accurate measurements)? Does the decision stay the same?

2DMC can be used in LCA to make the choice between two products or processes more robust. Generally, there are three possible 2DMC outcomes in LCA. These are illustrated in Fig. 4-4 for fictitious data (based on the POC model), showing the cumulative probability of a specific impact category reaching a certain impact.



P1 preferred to P2

	P1	P2
UR	1.11	1.07
VR	1.09	1.18
OR	1.21	1.26

Inconclusive

	P1	P2
UR	**1.66**	**1.49**
VR	1.09	1.08
OR	1.81	1.61

Inconclusive

	P1	P2
UR	1.11	1.07
VR	**1.28**	**1.51**
OR	1.42	1.62

Figure 4-4 Three possible 2DMC outcomes when comparing two products/processes.
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), which causes the results to be inconclusive. 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).

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. This allows to base the decision on the central tendency comparison, namely, by looking at their respective positions, left or right, for that specific impact category. Secondly, the 2DMC could show overlap either due to high uncertainty (high uncertainty ratio) or, thirdly, it could show overlap due to high variability (high variability ratio) in the input data. This implies that the most environmentally friendly option, still with respect to that specific impact category, cannot yet be decided upon. Instead, the range of the input data needs to be reduced by reducing the uncertainty or variability, respectively. For uncertain data, this means collecting more information, for variable data, a change in the physical system is required (Vose, 2008).

4.3.2 2DMC results for the post-harvest apple chain

Almost all impacts of the post-harvest chain for bulk and pre-packed apples show clearly divided 2DMC curves when being compared in one graph (except for a small overlap in the tail ends), with bulk apples being environmentally preferable. This is illustrated in Figure 4-5a for Climate Change (the remaining impact categories can be found in Appendix A.2), clearly showing that the impact category can be categorized as a typical outcome 1 ‘No overlap’ of Figure 4-4. There is only one impact category, Ionizing Radiation (Human Health), for which the 2DMC curves do show an overlap (Fig. 4-5b). Variability has here the higher ratio compared to uncertainty; therefore, the impact category is categorized under outcome 3 ‘Overlap with variability dominating’ of Figure 4-4. 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 1.02. This means that the overall uncertainty ratio is dominated by variability.

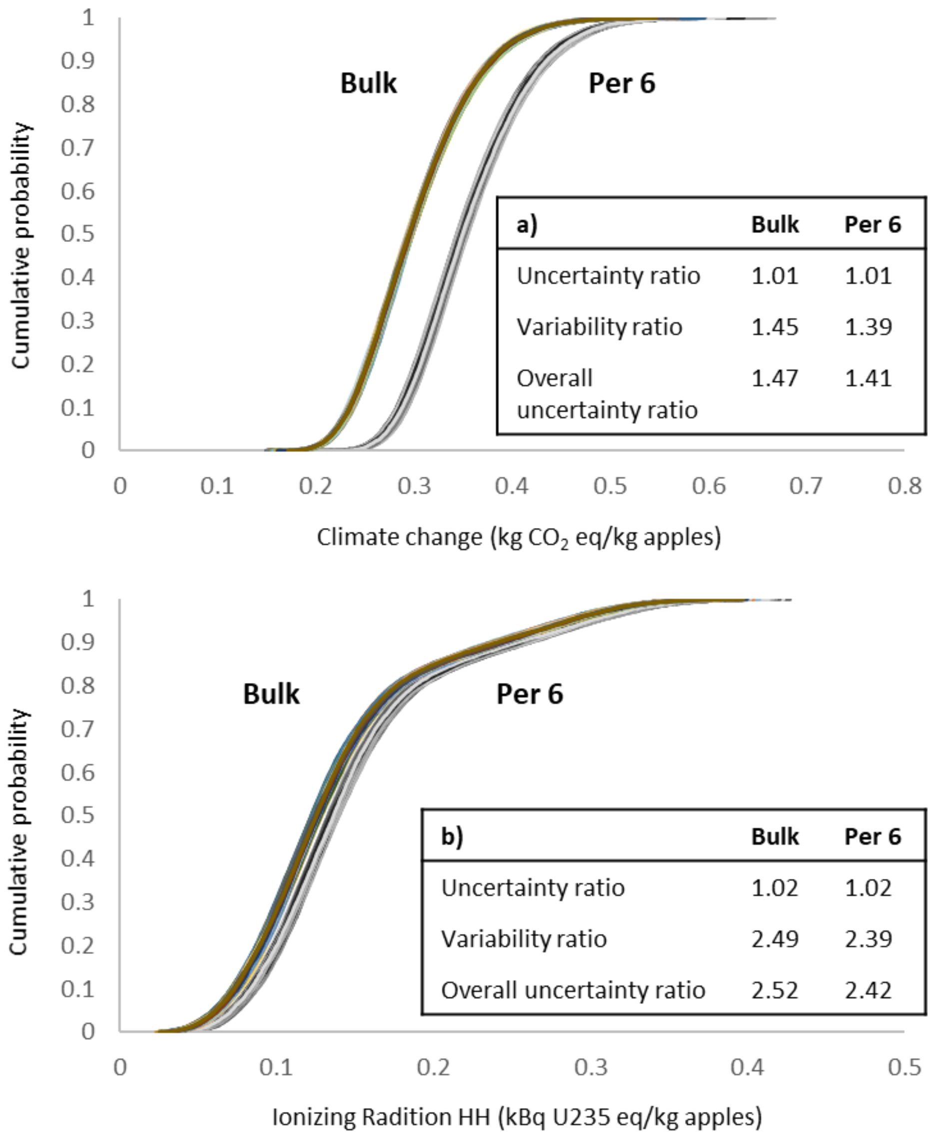


Figure 4-5 2DMC results for the postharvest chain.
The bulk apples are colored and the pre-packed are shown in greyscale.

It is interesting to put these results into the perspective of the original (deterministic) results, as calculated by Goossens et al. (2019). These deterministic results generally fall between 15% and 55% cumulative probability. For Climate Changes this was 0.28 kg CO_2 eq/kg en 0.35 kg CO_2 eq/kg for bulk and pre-packed respectively (cumulative probability of 39% and 51%); and for Ionizing Radiation (Human Health) this was 0.086 kBq U235 eq/kg and 0.094 U235 eq/kg respectively (cumulative probability of 17% and 16%).

4.4 Discussion

4.4.1 Assigning uncertainty and variability

The aim of this chapter was to *introduce 2DMC as a potential successful 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) for which we already had uncertain and variable data available. All parameters for which that information was not available and could not be readily found online, were considered as being deterministic. Though, this in itself is a kind of uncertainty. We are uncertain if these parameters are in fact deterministic, but we choose to analyze them that way based on data availability. We also run the risk of mislabeling either uncertainty or variability as being dominant, because an influential parameter was considered deterministic and therefore its variability or uncertainty range, respectively, was not accounted for.

In general, parameters were considered uncertain in this PhD thesis when the surveyed people (i.e., auction and retail) indicated being uncertain of the provided data. For example, when it came to sorting data (provided by the auction) and packaging data (provided by the retailer), similar data was provided (e.g., annual electricity use, apple weight that is sorted or packaged respectively, etc.). However, while the auction rated their uncertainty for these different inputs, the retailer did not; hence the packaging data were considered as deterministic. 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 apple yield to the auction) the distance is seen as variable.

This is not how an LCA practitioner would normally go about. When starting an LCA for a specific case study, the LCA practitioner will probably first focus on identifying which parameters are part of the life cycle. Then he/she might decide to use a *local sensitivity analysis or screening method* (Igos et al., 2019; Michiels and Geeraerd, 2020) to identify for which parameters the model is sensitive. Thereby identifying on which parameters the focus should lie when gathering uncertain and/or variable data for conducting 2DMC simulations. It is thus probable that first the highly influential parameters are categorized into being uncertain and/or variable, before starting to gather the necessary data. This is the reverse of what we did in this case study, namely categorizing parameters based on the already available data. The LCA practitioner would then most likely categorize the remaining, low influential parameters as deterministic. So, there would still be uncertainty connected to those parameters because they could still be uncertain and/or variable. However, the LCA practitioner would at least know that these parameters do not really influence the results that much.

To be able to actually propagate uncertain and/or variable parameters, data needed to construct probability distributions have to be available/provided. The definition of the *fore- and background system* can play an important role in that. On the one hand, foreground data is more easily accepted as being deterministic by the LCA practitioner (Michiels and Geeraerd, 2020). On the other hand, 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. Therefore, it is crucial that the LCA practitioner takes uncertainty and variability into consideration from the very start of the LCA process (Michiels and Geeraerd, 2020).

Data in the background system is generally more uncertain and variable, as it is usually not product, process or location specific. However, 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 (Bamber et al., 2020; Henriksson et al., 2015).

Moreover, the foreground system 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 more relevant that the focus lies on the foreground system since there they have more power to intervene (if necessary). Again with this, sensitivity analyses might be useful to see where the focus should lie, either on the foreground or background system.

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. However, we have to keep in mind that Monte Carlo simulations are a simplified model of reality and therefore never meant to be a perfect description of the real world (von Brömssen and Röös, 2020). 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.

A major advantage of 2DMC is the possibility of *categorizing a parameter as being both uncertain and variable*, provided that the necessary data is available for that. This was a possibility that was lacking when we reviewed in Chapter 3 which methodologies have already been used in LCA that allow to decide whether uncertainty or variability is dominating in the results. As stated in chapter 3, one of the most promising methodologies was used by Hauck et al. (2014) and Steinmann et al. (2014). They calculated uncertainty and variability ratios using one-dimensional Monte Carlo simulations. The limitations in their methodology were the need for an extensive database of deterministic values for different individual life cycles (in this case power plants) to account for variability and the impossibility for a parameter to be uncertainty and variability. It is clear that the 2DMC approach introduced here does not have these shortcomings.

4.4.2 Basing decisions on the central tendency

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). 2DMC can help in that regard because basing decisions on model outputs that are clearly separated is much more meaningful. This is what generally showed to be happening for the post-harvest chain in our case study. For each impact category, the 2DMC outputs show no crossing or overlap (except in the extremities of some curves) between the bulk and pre-packed apples, with buying bulk being consistently environmentally preferential. In this case, the central tendency or the deterministic impact are robust enough to base conclusions and decisions on, e.g., the median impact of the impact categories can be reduced by switching to a larger share of bulk apples.

4.4.3 Interpreting ratios

When 2DMC results of two products or processes do show overlap – as is the case for Ionizing Radiation (Human Health) in this case study – it is important to look at uncertainty and variability to make informative decisions. 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. 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. *Uncertainty* is everything we do not know and how far off we are from the truth (Hauschild et al., 2018). Therefore, if the range of LCA results is dominated by uncertainty (represented by a high uncertainty ratio), then gathering more knowledge through e.g., further measurements, literature research and expert consultations (Hauschild et al., 2018; Huijbregts, 1998; Igos et al., 2019; Walker et al., 2003), may be needed before two products or processes can robustly be compared.

In contrast, *variability* is the effect of chance (Vose, 2008). Thus, a high degree of variability (represented by a high variability ratio) implicates true differences between the two products or processes, and therefore cannot be reduced by further study (Hauschild et al., 2018; Igos et al., 2019). Collecting more information would just be a waste of time (Vose, 2008). However, 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).

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. In the case of apple post-harvest chain, it is the variability ratio that dominates the overall uncertainty of Ionizing Radiation (Human Health). This implies that it would be a waste of time to try to reduce uncertainty by collecting more information. This is an interesting and valid observation as it shows that gathering more data is not always the way to go. Instead, the results indicate that reducing the overall uncertainty could be achieved by examining and changing the physical system. When looking at the results of Goossens et al. (2019), it is not a surprise that overlap between the 2DMC results can be seen for this impact category. Goossens et al. (2019) considered a scenario in their LCA study where they examined how the impact of purchasing 1 kg apples evolved throughout the year for each packaging method. Ionizing Radiation (Human Health) turned out to be the only impact category (of the ones that were included in the results) for which pre-packed apples could lead to a lower impact than bulk apples, depending on the moment of purchase.

With the three possible outcomes (Fig. 4-4), the recommended decision can differ for each impact category due to differences in overlap and ratios. In this case, Ionizing Radiation (Human Health) is the only one for which a clear-cut decision cannot be made, and the overwhelming majority of impact indicators points at the selection of bulk apples as the environmentally preferable option.

4.4.4 Communication consensus

2DMC results can be visualized and communicated on in two ways: either by looking for overlap in the graphs *or* by comparing ratios. At least, that is how we propose to deduce conclusions from the results in this chapter. Of course, there are alternative ways to do this for both.

4.4.4.1 Comparing simulation results using statistical tests

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; Heijungs, 2021; Mendoza Beltran et al., 2018b). Heijungs (2021) reviews following approaches that can be used to single out the superior option of two (or more) products when uncertainty is propagated using (1D) Monte Carlo simulations:

- null hypothesis significance testing (e.g., comparing mean scores using the *t*-test or median scores using the Wilcoxon-Mann-Whitney test),

- standardized mean difference (measures how many standard deviations the two means are separated)
- "modified" null hypothesis significance testing (with a required minimum threshold difference similar to the standardized mean difference, in the H_0 hypothesis),
- nonoverlap statistics (measures the degree of overlap or the similarity between probability distributions; more information in section 7.1.5), and
- comparison indicator/discernability analysis (pairwise analysis that counts how many times one product is preferred to another; more information in section 7.1.5).

Yet, even more variations and measures are possible to assess the superiority of one product over another (Gregory et al., 2016; Heijungs, 2021; Mendoza Beltran et al., 2018b). In the end, 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.

The hurdle when it comes to these methods, is that they start with one output probability distribution for each product. Further analyses are thus needed to see to which degree these methods can be applied when each product has multiple output probability distributions, such as with 2DMC, and if they subsequently provide meaningful results.

4.4.4.2 Alternative uncertainty and variability ratios

To communicate about uncertainty and variability in a clear way, we used the *50^{th} and 97.5^{th} percentiles* to calculate uncertainty and variability ratios as described in Pouillot et al. (2016) and proposed by Özkaynaka et al. (2009). However, we could have chosen to use other ratios, such as the ones calculated from the 10^{th} and 90^{th} percentiles, as was done by Douziech et al. (2019) and Huizer et al. (2012). We could even have used the 2.5^{th} and 97.5^{th} percentiles, as to be more in line with the ratios calculated by Hauck et al. (2014) and Steinmann et al. (2014) (section 3.4.2.1).

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. Of course, in the future, there will need to come a consensus among LCA practitioners on which tests and ratios will be used for further communication. Once a communication consensus is established, distinguishing between uncertainty and variability in LCAs may help decision makers in judging the significance of the differences in product comparisons, options for product improvement or the assignments of ecolabels (Huijbregts, 1998). In the 2DMC method, Monte Carlo simulations were used for visualizing overall uncertainty and using this information in decision support when comparing the environmental impact of different products or services. According to von Brömssen and Röös (2020) this is one of the few correct ways to apply Monte Carlo simulations in LCA while it should not be used for inferential statistics [8].

4.5 Conclusions

To the best of our knowledge, this was the first time 2DMC was used in LCA to separately propagate data uncertainty and variability. 2DMC is a useful approach to integrate in LCA, allowing decision makers to judge the significance of the results and to make robust decisions. We recommend to always conduct 2DMC in an LCA when comparing two products or processes, provided that the data availability allows to do so and if time permits it. For this reason, uncertainty and variability should be taken into consideration from the very start of the LCA process. Sufficient

[8] Combining descriptive measures with probability theory to make generalizations about a population based on a data sample (von Brömssen and Röös, 2020)

data quality can only be attained if information on uncertainty and variability is collected already during the LCI and/or by collecting additional data. Both approaches were followed in this chapter.

2DMC outcomes allow to first see if the 2DMC curves of the two products/processes overlap in any way. If not, an unambiguous conclusion can be made on which would be environmentally preferable based on the central tendency. When the 2DMC curves de show overlap, it would be more advisable to first try to 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 thus reducing variability by making physical changes in the production process). For the results of this case study, the best general advice to give to a consumer – at this moment – would be to buy bulk apples.

In the next chapter, we conduct 2DMC for an LCA of the apple cultivation chain. To this end, the Farm Accountancy Data Network will be used, which is a large database containing data on cultivation in- and outputs. This will be in contrast with the case study on the post-harvest chain, which was reported on in this chapter, for which the inventory mainly consists of survey data.

Chapter 5

Comparing the environmental impact of an established and young apple cultivar by conducting two-dimensional Monte Carlo simulations for a large set of orchards

This chapter is based on: Michiels, F., Geeraerd, A. *(article in preparation).* Comparing the environmental impact of an established and young apple cultivar by conducting two-dimensional Monte Carlo simulations for a large set of orchards.

Author's contributions: Michiels F. performed the analysis and drafted the manuscript

5.1 Introduction

In Chapter 4, the possible added value of conducting two-dimensional Monte Carlo simulations (2DMC) in an LCA context is explained and illustrated. 2DMC was introduced using the apple post-harvest chain as case study. That part of the apple chain was based on surveys conducted by two auctions and a retailer, for which the answers were gathered during the study of Goossens et al. (2019). In contrast, the cultivation part of the apple chain in the study of Goossens et al. (2019, 2017a) was based on an extensive database of the in- and outputs of different apple orchards located in Flanders. It seems relevant to study how this type of inventory can be used for 2DMC in an LCA context.

Thus, our aim in this chapter is two-fold. First, we aim to complete the 2DMC analysis for the apple chain by conducting simulations for the cultivation part. The packaging method (i.e., bulk vs. pre-packed) was compared in Chapter 4. In this chapter, a comparative LCA for two different apple cultivars (i.e., Jonagold and

Kanzi) will be conducted. Second, we aim to illustrate the different approach that needs to be taken when using such a different type of inventory (i.e., an extensive database with individual records for each orchard).

5.2 Methods

5.2.1 Goal and scope definition

A 2DMC analysis was conducted for an updated version of an existing attributional LCA of the Belgian (Flanders) apple cultivation (Goossens et al., 2017a). The cultivation chain goes up to the farm gate (excluding the tree seedling nursery) and consists of all orchard management operations, including manufacturing, transport and use of energy, water, pesticides and fertilizers; and excluding construction, manufacturing and maintenance of farm buildings, infrastructure, machinery, equipment and materials (Goossens et al., 2017a). All orchards were based on dwarf rootstocks. Cultivation was done using Integrated Pest Management (IPM).

Direct field emissions from fertilizers, pesticide and energy use were calculated using the IPCC guidelines (Garg and Weitz, 2019; Hergoualc' et al., 2019), the Agri-footprint manual (Durlinger et al., 2017b), ecoinvent reports (Nemecek and Schnetzer, 2011), the Product Environmental Footprint Category Rules (European Commission, 2018) and the air pollutant emission inventory guidebook (European Environment Agency, 2016). The functional unit is 1 ton of apples leaving the farm. No distinction was made based on the quality or purpose of the apples; all apples were assumed to be consumed as whole fruit. The inventory includes all inputs to cultivate both harvested and lost apples, therefore field losses are accounted for.

Calculations were performed using SimaPro 9.0.0.49 (Pré Sustainability, the Netherlands), JMP Pro 15 (SAS Institute Inc., NC, USA) and 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 databases ecoinvent 3.5 and Agri-footprint 4.0., using "allocation, at point of substitution" and "economic allocation" respectively. For the 2DMC analysis, 10 000 iterations and 250 simulations are conducted, leading to 2 500 000 possible LCA outcomes shown in 250 2DMC curves (see section 7.1.5). The Excel add-in @Risk (Palisade, NY, USA) was used to conduct these 2DMC simulations.

5.2.2 Life Cycle Inventory of the cultivation chain

Cultivation data was obtained from the EU Farm Accountancy Data Network (FADN). The detailed cultivation data includes anonymized company data (e.g., area in production, yield, etc.) and orchard records. Each orchard record holds information on the yield and on the fertilizer, pesticide, energy, water and land use of a specific cultivar during a specific year in a specific farm. As stated above, the cultivation chain of apple in this PhD thesis is based on an updated version of the apple LCA conducted by Goossens et al. (2017a). More specifically, in the updated version reported on in this PhD thesis, the used FADN database contained cultivation data for a period of 11 years [from 2005 to 2015 instead of 2012 as in Goossens et al. (2017a)], the 2019 refinement to the 2006 IPCC guidelines was used, pesticide production was included, the European Commission's (2018) guidelines for pesticide emission was followed and newer, more relevant database input processes were used when possible.

Two apple cultivars were studied: Jonagold (and its mutants), an established cultivar (created around 1970) in Belgium, and the relatively young Kanzi (from 2004; a hybrid of Gala and Braeburn). 973 Jonagold orchard records spread over 70 farms and 36 Kanzi orchard records spread over 6 farms were selected, cultivated between 2005 and 2015. The yields ranged from 1 to 166 t/ha for the Jonagold orchards, and from 4 to 61 t/ha for Kanzi orchards, including low, full and mixed productive stages [as defined in Goossens et al. (2017a)]. For all field operations, the manufacturing, transport and use of energy carriers, water, pesticides and fertilizers, were considered.

The FADN database does not provide any indication of how certain the apple growers are when providing the amount of products that they used during cultivation. Therefore, a small survey was conducted among twelve Flemish apple growers asking them how big the maximum error would be when we would ask them to give the amount of specific energy, water, pesticide and fertilizer products or product groups used in their orchards. The apple growers were asked to rate their uncertainty according to the Product Environmental Footprint (PEF) quality criteria (European Commission, 2012), ranging from no uncertainty to very high uncertainty. Since the FADN database is completely anonymous and we could therefore not contact the farmers from the 76 selected farms, we surveyed apple growers during the "Open day pit fruit" of pcfruit (test center for fruit cultivation).

Five of those twelve apple growers indicated that they participate in the FADN database.

By combining all the information of the FADN database and the uncertainty ratings of the apple growers, we now have an inventory for the cultivation chain than includes quantifiable uncertainty and variability. With this data we can conduct a 2DMC analysis.

5.2.3 Input probability distributions for cultivation parameters

For the first step of the 2DMC analysis, the input data are categorized into four categories: deterministic, uncertain, variable and, uncertain and variable. Appropriate probability distributions are selected for the last three categories.

For the cultivation chain, the *amount of input products* used for energy, water, pesticide (considering active ingredients instead of products) and fertilizer could be considered as being both variable and uncertain. They are variable because the 1009 selected orchards all used different products and different amounts. This can, for example, be caused by the varying soil type underneath the different orchards, leading to different fertilizer and water needs. To account for this variability caused by the diverging management practices of the apple growers, distributions were fitted with @Risk for each product, during which the correlations between the different products are calculated and a correlation matrix is generated. That way, if there are specific product combinations being used, that will be accounted for during sampling. For the distribution fitting, the lower bound was set to zero and the Akaike Information Criterion (AIC) test statistic was used. This generally led to an exponential distribution being chosen, and occasionally a lognormal or logistic distribution.

On a sidenote, it could be argued that variability does not need to be accounted for in the cultivation chain, because the extensive FADN database actually provides a rather large amount of deterministic data on the management practices. However, here we look at the apple chain from the perspective of the consumer, who does not know from which orchard or orchards the apples come from. Stated differently, our approach for the energy, water, pesticide and fertilizer inputs illustrates how variability can be accounted for from a large dataset of deterministic values.

For the uncertainty aspect of the amount of input products, twelve apple growers provided data on how certain they would be when giving the amount of different energy sources, water, pesticide and fertilizer products or product groups used in their orchards. The uncertainty ratings were used to construct PERT distributions, which need a min, most likely and maximum amount. The most likely amount was the amount given in the FADN database, while the min and max were based on the provided percentage of uncertainty.

For example, the grower indicates that he would have a very low uncertainty (≤ 10%; for which 5% was used) when giving the amount of tap water that was used during cultivation. The amount of tap water is represented by a variable probability distribution (as explained above), which is consecutively sampled from generating x amount of tap water used. Just as explained in Chapter 4, this can be combined in following formula: [x*PERT(1-5%; 1; 1+5%)], where x represents the variable probability distributions and the PERT function represent the uncertain probability distribution. Thus, for the amount of input products used, the variable distribution (which was fitted based on the products used in the FADN database) and the uncertain distribution (which was based on uncertainty surveys) were derived separately, allowing multiplication and separate sampling later on.

Apple growers often chose different uncertainty ratings for the same product. If we consider tap water again, three apple growers rated it as having “no uncertainty”, four “very low uncertainty”, two “low uncertainty”, one “fair uncertainty, one “high uncertainty” and one blank (which was excluded). A discrete distribution was constructed to combine these estimates (i.e., the PERT distributions) from several people (Palisade, 2016b).

How uncertainty and variability was further taken into consideration is explained for each input category separately. An overview of all parameters is given in Table 5-1. More details on the methodology and used data can be found in Appendix B.1.

Energy: Manufacturing, transport and emissions of energy products used by the grower for farm equipment and transportation was accounted for. The units used in the FADN database for the different energy carriers were (usually) not the same as the ones used in the corresponding SimaPro processes. Since the FADN database always included the amount of MJ for each energy source, we decided to use that unit for the further calculation. Therefore, the units used in SimaPro needed to be conversed to MJ (if needed) to match with the FADN database. For some energy sources, the conversion factors already reported on within FADN database itself could be used, which were then deterministic (Table 5-1). For others, uncertain conversion factors from literature were selected (CREG, 2018; IFA, 2020; World Nuclear Association, 2018), leading to uniform input distributions. The emissions to air from energy use also included, where possible, uncertainty distributions based on data found in the IPCC guidelines (Buendia et al., 2019) and the air pollutant emission inventory guidebook (European Environment Agency, 2016). Emissions factors are generally classified as uncertain (Michiels and Geeraerd, 2020).

Water: Water is used in apple orchards for e.g., irrigation and frost protection. Four sources of water were used for these purposes i.e., groundwater, rainwater, surface water and tap water.

Pesticides: Plant protection and sanitation measures were accounted for, using 250 different active ingredients for Jonagold and 148 for Kanzi. Pesticide use was included as 90% active ingredient emitted to the agricultural soil compartment, 9% emitted to air and 1% emitted to water, following the Product Environmental Footprint Category Rules (PEFCRs) (European Commission, 2018).

Fertilizers: 786 fertilizers products for Jonagold and 125 for Kanzi were used during cultivation in the different orchards. The uncertainty of emission factors was propagated when calculating the emissions from fertilizer use to air from NH_3, N_2O and CO_2 and to water from NO_3^- and P (Durlinger et al., 2017b; European Commission, 2018). Uncertain PERT distributions were based on data from the IPCC guidelines (Hergoualc' et al., 2019), supplemented with deterministic data found in the Agri-footprint manual (Durlinger et al., 2017b). When calculating the emissions of heavy metals to soil and water (Durlinger et al., 2017b), the heavy metal content of the organic fertilizers was considered variable, where possible, for which distributions were based on various literature sources. Oftentimes minimum, default, maximum and standard deviation data was available, which lead to the construction of a normal distribution (using the default as a mean, and the standard deviation) which was truncated using the minimum and maximum values.

Table 5-1 Summary of the cultivation parameters and their categorization.

The parameters are categorized into deterministic, uncertain, variable and uncertain & variable, with a short explanation on how the type was reflected by the data and which source was used. All information for each separate parameter can be found in Appendix B.1.

Parameter	Type	Data and sources
Energy		
Conversion to MJ for gasoline, butane, charcoal, LPG and propane	Deterministic	Already present in SimaPro with MJ unit or deterministic data from the FADN database
Conversion to MJ for natural gas, diesel, fuel oil, methane gas and petroleum	Uncertain	Uncertain literature data (CREG, 2018; IFA, 2020; World Nuclear Association, 2018)
Emission factors for stationary combustion	Uncertain	Uncertain data from volume 2 chapter 2 of the IPCC guidelines (Garg and Weitz, 2019)
Emission factors for on-road diesel machinery	Uncertain	Uncertain data from 1.A.3 of the air pollutant emission inventory guidebook (Ntziachristos et al., 2018)
Emission factors for off-road diesel machinery	Deterministic	Deterministic data from 1.A.4 of the air pollutant emission inventory guidebook (Winther et al., 2017)
Amount	Uncertain & Variable	Uncertainty ratings from apple growers (this PhD thesis) & varying management practices (FADN)
Water		
Amount	Uncertain & Variable	Varying management practices (FADN) & uncertainty ratings from apple growers (this PhD thesis)
Pesticide		
Emission factors	Deterministic	Based on the PEFCRs (European Commission, 2018)
Amount	Uncertain & Variable	Varying management practices (FADN) & uncertainty ratings from apple growers (this PhD thesis)

Table 5-1 Continued

Parameter	Type	Data and sources
Fertilizer		
Emission factors	Uncertain	Uncertain data from volume 4 chapter 11 of the IPCC guidelines (Hergoualc' et al., 2019)
Fraction of fertilizer that volatilizes	Uncertain	Uncertain data from volume 4 chapter 11 of the IPCC guidelines (Hergoualc' et al., 2019)
Fraction of N that is lost due to leaching or runoff	Uncertain	Uncertain data from volume 4 chapter 11 of the IPCC guidelines (Hergoualc' et al., 2019)
Fraction of P that is lost due to leaching or runoff	Deterministic	Deterministic data from Agri-footprint manual (Durlinger et al., 2017b)
Heavy metal content of mineral fertilizers	Deterministic	Deterministic data from the Agri-footprint manual (Durlinger et al., 2017b)
Heavy metal content of the organic fertilizers animal manure and champost	Variable	Variable data for animal manure and champost[a] (Jordan et al., 2008; Klein and Roskam, 2018; Moreno-Caselles et al., 2002; Römkens and Rietra, 2008)
Heavy metal content of the organic fertilizers compost, digestate, green manure and sewage sludge	Deterministic	Only deterministic data found for compost, digestate, green manure and sewage sludge (Amlinger et al., 2004; Goossens et al., 2017a; Mels et al., 2008; Sager, 2007)
Deposition of heavy metals	Deterministic	Deterministic data from the Agri-footprint manual (Durlinger et al., 2017b)
Heavy metal content of apple	Deterministic	Deterministic literature data (Delahaye et al., 2003; Stefanut et al., 2007)
Heavy metal leaching to groundwater	Deterministic	Deterministic data from the Agri-footprint manual (Durlinger et al., 2017b)
Amount	Uncertain & Variable	Varying management practices (FADN) & uncertainty ratings from apple growers (this PhD thesis)

[a] The Hg content of champost is deterministic (Delahaye et al., 2003)

5.3 Results

5.3.1 2DMC results for apple cultivation

A representative selection of the 2DMC results reflecting the three possible outcomes (Fig. 4-4) is shown in Figure 5-1. The results for the remaining impact categories can be found in Appendix B.2.

The 2DMC curves for Jonagold and Kanzi cultivation are clearly separated (except for sometimes a small overlap in the tail ends) for half of the impact categories: Climate Change, Human Toxicity, Particulate Matter (Fig. 5-1a), Photochemical Ozone Formation, Freshwater Eutrophication, Freshwater Ecotoxicity and Land Use, with Jonagold being environmentally preferable. This corresponds with possible outcome 1 “No overlap” as shown in Figure 4-4 (section 4.3.2).

For some of the other impact categories where the 2DMC curves do overlap, one is still able to distinguish a certain tendency of Jonagold having a generally smaller impact than Kanzi, such as for Ozone Depletion, Acidification (Fig. 5-1b) and Terrestrial Eutrophication. However, for Water Resource Depletion and Mineral, Fossil & Renewable Resource Depletion (Fig. 5-1c) this is not the case. A pronounced overlap between the two cultivars can be observed here.

When comparing the ratios of Jonagold and Kanzi, the overall uncertainty ratio and the variability ratio is always higher for Kanzi than for Jonagold except for the impact categories Land Use and Mineral, Fossil & Renewable Resource Depletion. For the uncertainty ratio, there is an equal division of the impact categories being higher for either Jonagold or Kanzi. For Kanzi itself, variability is clearly always dominating the overall uncertainty. This is the same for Jonagold with Marine Eutrophication (Fig. 5-1d) being the exception of having a larger uncertainty than variability ratio.

Thus, for the impact categories that do show overlap, this is mainly dominated by variability (Fig. 5-1b and 5-1c) as in possible outcome 3 shown in Figure 4-4. The impact category Marine Eutrophication is the odd man out, since the overlapping 2DMC results are due to dominating uncertainty for Jonagold and dominating variability for Kanzi (Fig. 1d). It is therefore a combination of possible outcome 2 and 3 of Figure 4-4.

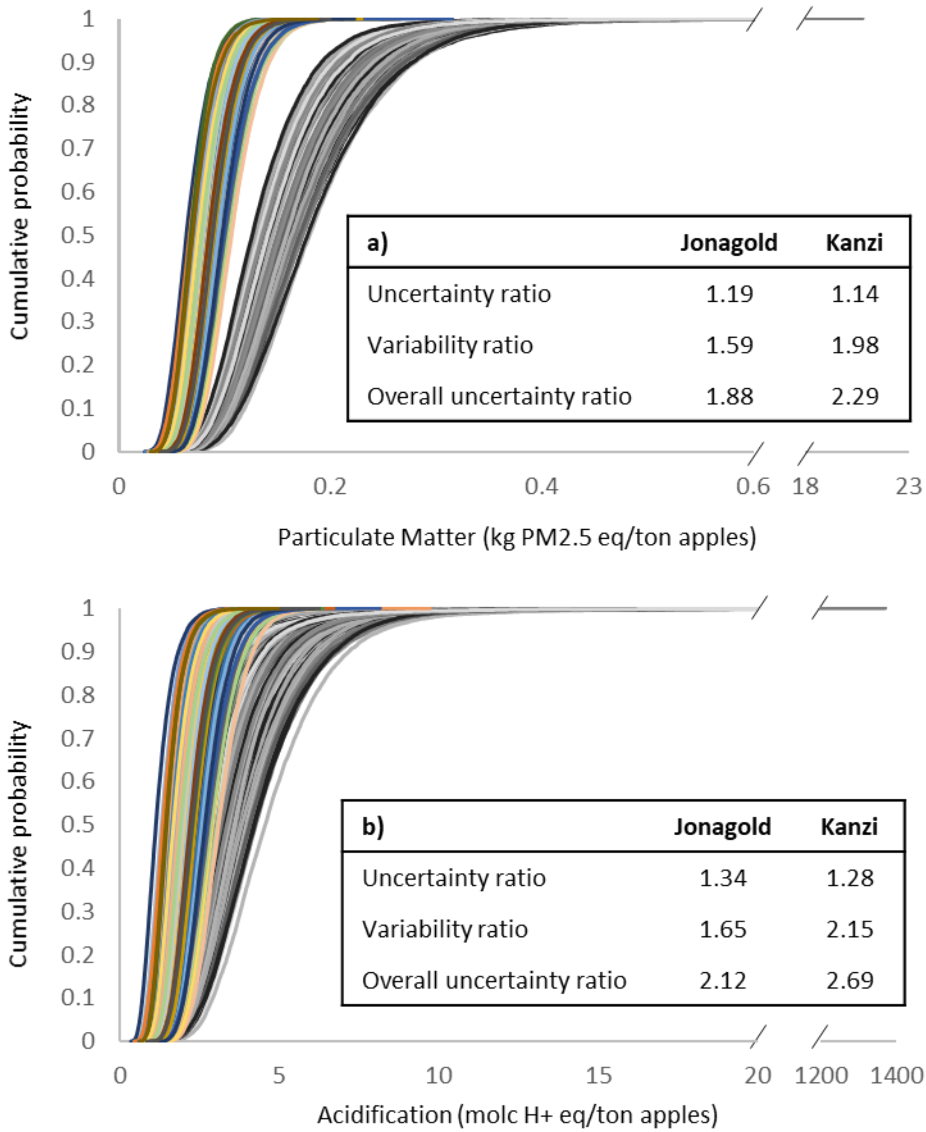


Figure 5-1 2DMC results for the cultivation chain.

The Jonagold apples are colored and the Kanzi apples are shown in greyscale.

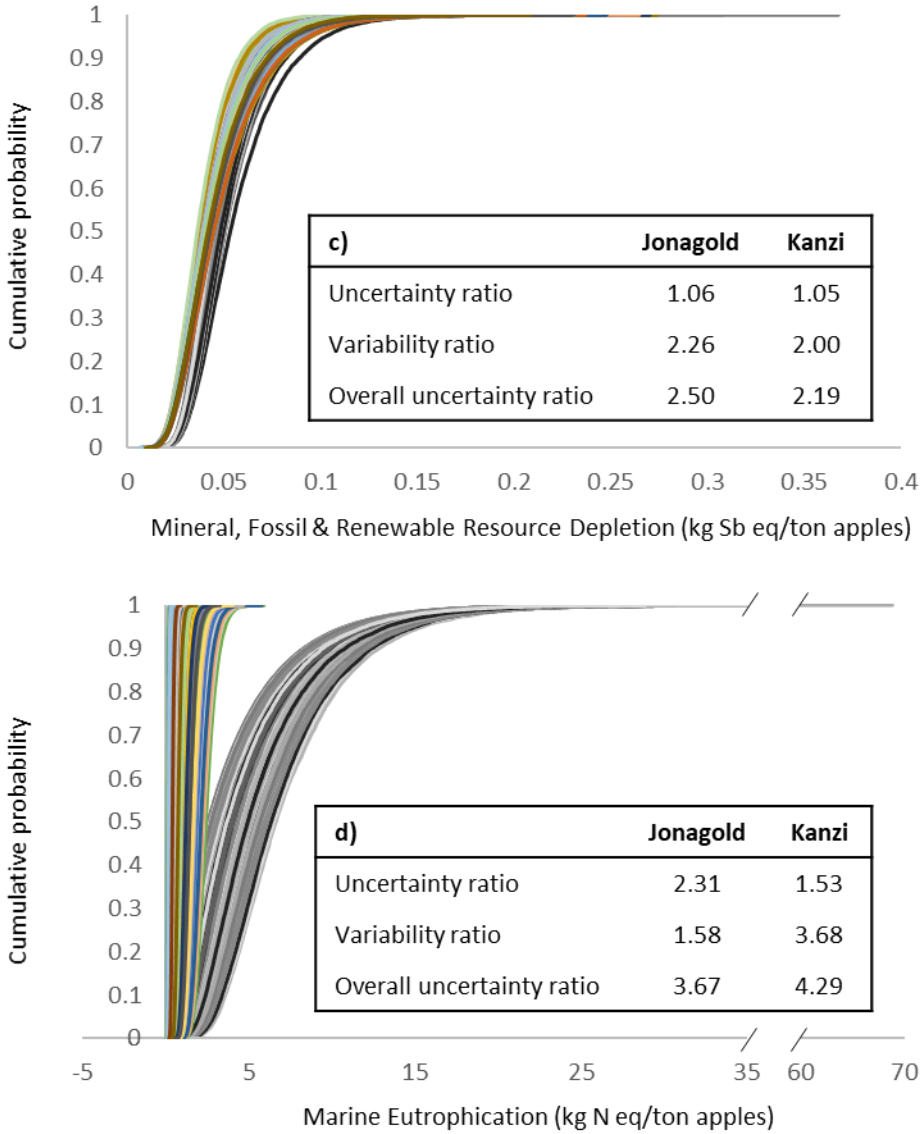


Figure 5-1 Continued

5.3.2 Comparing 2DMC with deterministic results

It is interesting to also study how impacts calculated using 2DMC and impacts calculated using solely deterministic input values approximate each other. Therefore, next to 2DMC, a separate scenario was considered were all uncertain, variable and uncertain ánd variable parameters were assumed to be deterministic. Instead of using probability distributions, the data in the FADN database was considered deterministic for each orchard record and default and most likely values were used for the remaining input values. We can then compare the 2DMC curves with the calculated deterministic impacts (973 for Jonagold and 36 for Kanzi, represented by respectively orange and black dots in Fig. 5-2).

For the Jonagold orchards, there are outlier impacts that are not represented by the 2DMC curves (Fig. 5-2a). In contrast, the 2DMC impact range for Kanzi is often much larger than its deterministic impact (Fig. 5-2b), except for Human Toxicity Non-Cancer Effects, Marine Eutrophication (Fig. 5-2c) and Mineral, Fossil and Renewable Resource Depletion, where 1 Kanzi orchard has a larger impact than simulated by 2DMC.

The 973 Jonagold orchards can give the most complete indication of how well the deterministic values approximate the 2DMC curves. The slope of the Jonagold deterministic impacts is generally steeper for the smaller probabilities, compared to the 2DMC results. Though, the curve of the deterministic impacts bends sooner, crossing the 2DMC results approximately between the 80% and 90% cumulative probability. This is illustrated in Figure 5-2d for Climate Change. However, when the uncertainty ratio is relatively high (around 1.20 and higher), the deterministic impacts follow the 2DMC curves more accurately (Fig. 5-2e).

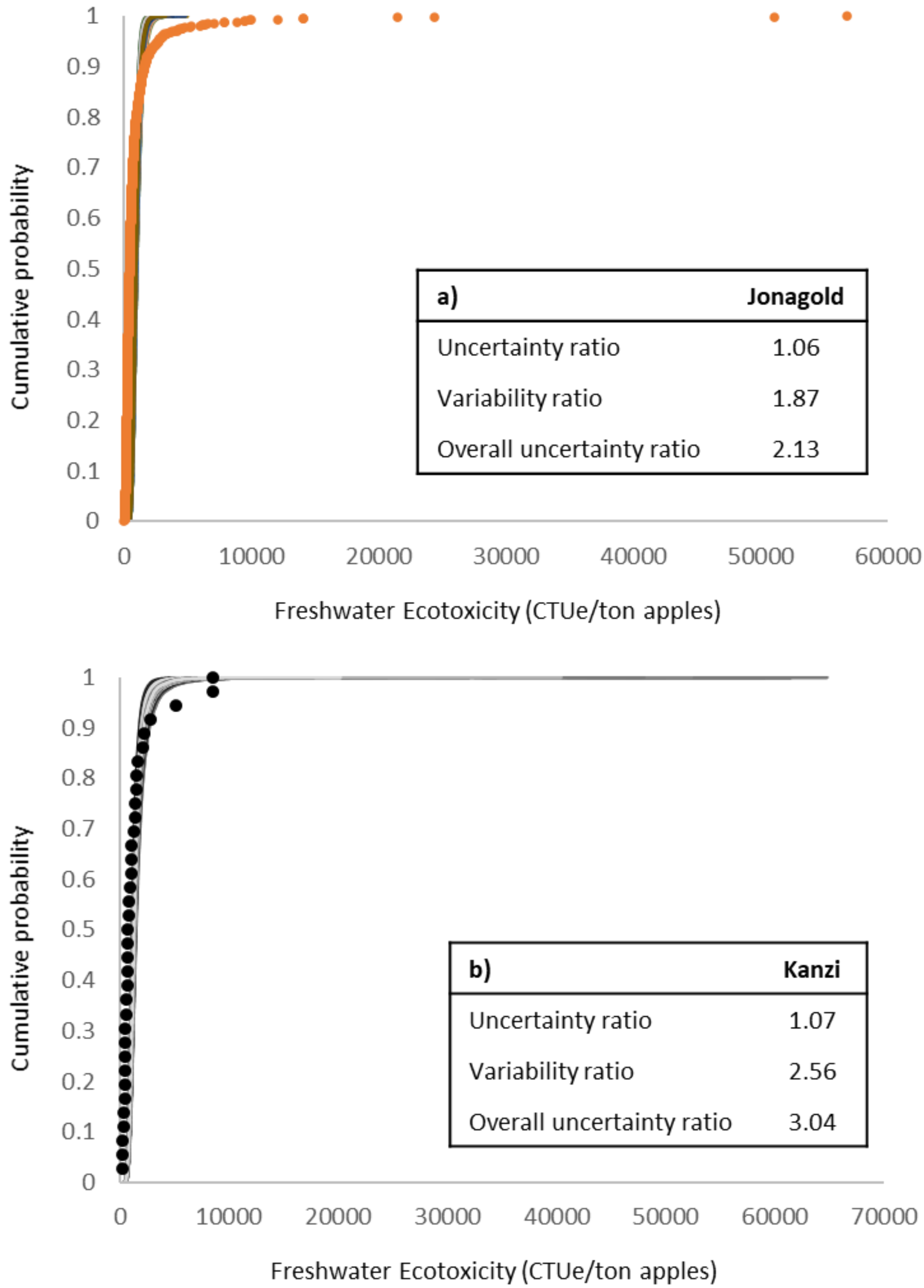
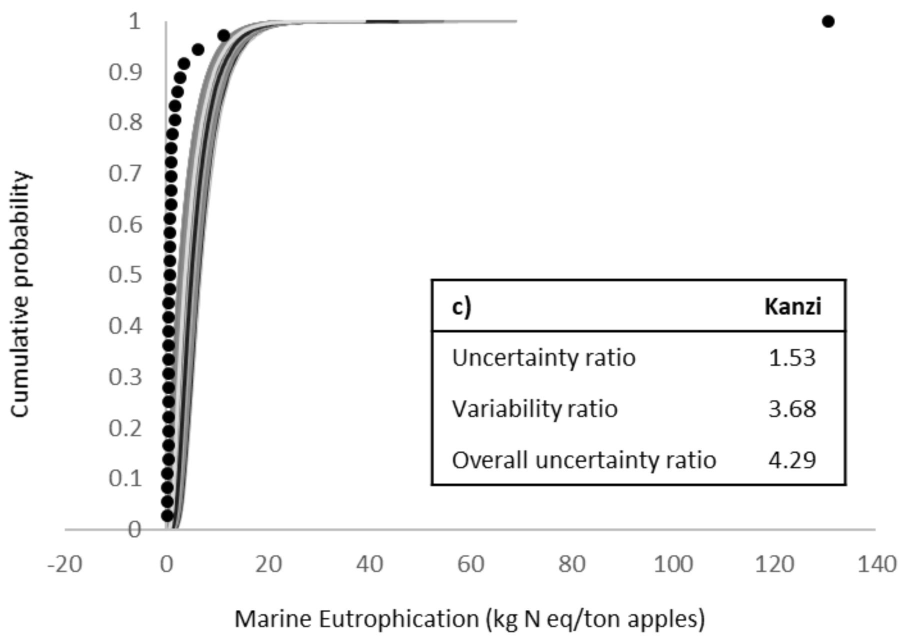


Figure 5-2 Deterministic (dots) and 2DMC (curves) results for Jonagold (colored) and Kanzi (greyscale) cultivation.



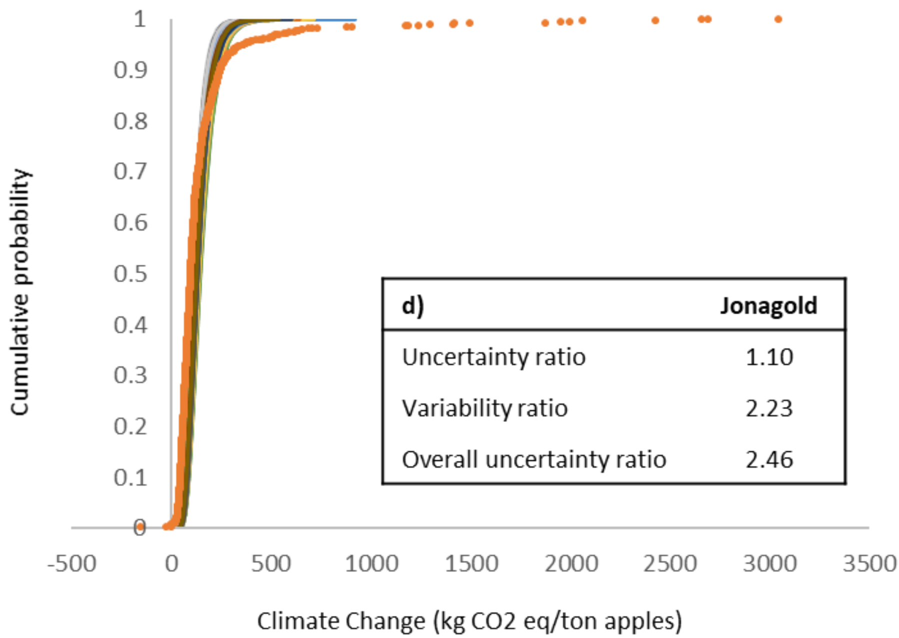


Figure 5-2 Continued

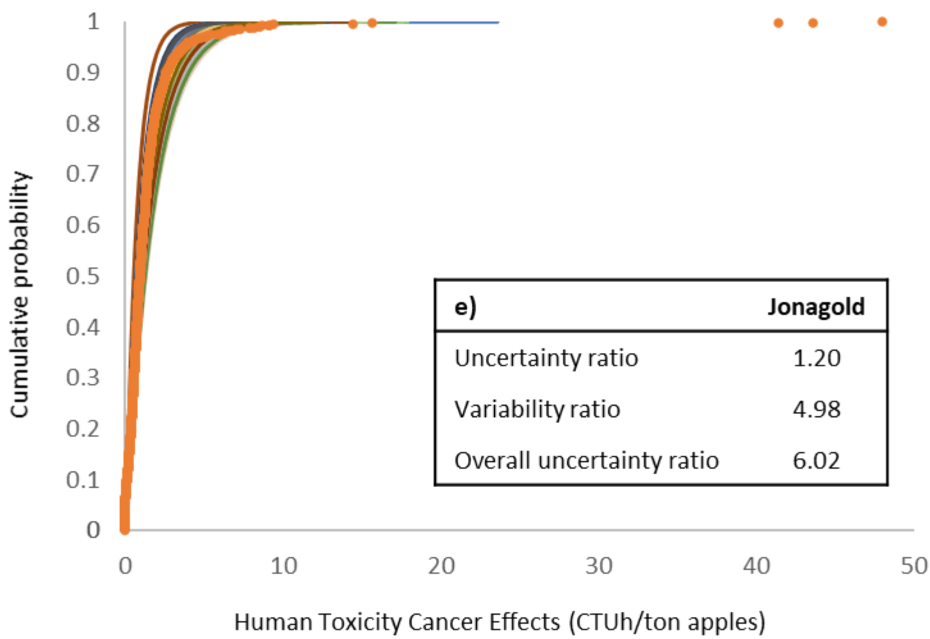


Figure 5-2 Continued

5.4 Discussion

5.4.1 From 2DMC results to decisions

A clear conclusion can be made for half of the impact categories of the cultivation chain, where it seems that the established Jonagold apple is preferable over the younger Kanzi cultivar when it comes to lowering environmental impacts. This can possibly be due to Kanzi having a higher economic value than Jonagold apples. In 2018, apple growers received an average of 93 eurocent per kg of Kanzi apples, while they only received 65 eurocent per kg of Jonagold apples. Additionally, Kanzi is a so-called “club breed”, meaning that growers need to have permission and pay a fee to be allowed to grow them (Vilt, 2018). It is possible that due to Kanzi being more exclusive and causing more financial gains, that the grower will be more inclined to invest more resources in its cultivation (e.g., fertilizers) and protection (e.g., against frost), compared to Jonagold. The 2DMC outcomes do show overlap for Jonagold and Kanzi apples for the other 8 of the 16 impact categories. In those cases, it is important to look at uncertainty and variability to make informed 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, even when there is still a clear general tendency of which might be preferable (such as in Fig. 5-1b). In the case of apple cultivation, it is almost always the variability ratio that dominates the overall uncertainty for both cultivars. This is in accordance with the results of the post-harvest chain in Chapter 4. Though, the variability ratios were generally smaller there, with a maximum of 2.49. The maximum variability ratio for the cultivation chain is 7.10. This difference probably stems – among other things – from the limited number of companies that were included in the post-harvest chain on the input side i.e., two auctions and one retailer. However, the analysis is still representative for the whole of Flanders since the post-harvest chain represents a standardized industrial process. For example, the storage of fruit is maintained using an optimized controlled atmosphere – depending on the fruit quality – which is generally applied by the auctions.

In contrast, apple growers generally have small businesses and are more inclined to use their own management strategies and techniques, which are less optimized. Additionally, they are much more dependent on biological processes, making standardization a challenge. The FADN database does not allow to identify different management techniques (except for integrated vs. organic farming), otherwise it would have been possible to further select on the different variations in the production techniques, thereby reducing variability and introducing scenario uncertainty (see Chapter 3).

Because variability is dominating, it implies that it would be a waste of time to try to reduce uncertainty by collecting more information. Instead, the results indicate that reducing the overall uncertainty could be achieved by examining and changing the physical system. The variability shows that apples could be produced at a low impact, but for some reason this does not always happen. However, it depends on the source of the variability if changing the system is possible.

For example, variability could be reduced by making changes to the management strategies of Kanzi cultivation. It is plausible that the management of the new Kanzi apple is not as uniform and efficient yet as it is for the established Jonagold apple, leading to more variability and a generally larger impact. Optimizing the management strategies for pruning, fertilizer, pesticide, energy, etc. could reduce this variability. There are, however, also sources of variability that cannot (realistically) be reduced. For example, variability due to weather occurrences, differences in the productive stage of the orchards (see section 1.4.2), or the location (and thus soil type) of the orchard.

The only case where gathering more knowledge would lead to more conclusive results, is for Marine Eutrophication. For Jonagold apples, more precise emission factors, more accurate measurements, etc., should be gathered to lower the overall uncertainty ratio for that impact category.

For the cultivation chain, the recommended decision differs for each impact category, due to differences in overlap and ratios. Therefore, it might be advisable to focus on those impact categories that are deemed important or noteworthy for the studied product or process. For example, Marine Eutrophication shows high overlap between Jonagold and Kanzi 2DMC curves (Fig. 5-1d) and it is recommended to trying to reduce the overall uncertainty for Jonagold and Kanzi. However, Helmes et al. (2020) suggest in their proposal for Hortifootprint Category Rules (based on representative product studies), that the most important impact categories for apples are: Climate Change, Particulate Matter, Photochemical Ozone Formation, Acidification, Terrestrial Eutrophication and Mineral, Fossil and Renewable Resource Depletion. Since Marine Eutrophication is not part of this list, the decision maker might decide to discard the recommendation because the impact category is not relevant enough.

Another way to select relevant impact categories is by looking at the goal and scope of the LCA study. In this LCA, we studied the environmental impact of Flemish apple cultivation, so we could decide to select impact categories that are relevant for Flanders on a local scale. In that case, eutrophication would probably be chosen because there is too much nitrogen deposition in the region. In 2018, 64% of the area protected under Natura 2000 had a nitrogen deposition exceeding the critical deposition value[9] (Flemish Government, 2021). If we did a study that was more

[9] The critical deposition value is the amount of nitrogen deposition (kg N per ha per year) for a certain ecosystem below which, according to the current scientific knowledge, no meaningful change in biodiversity will occur in the long term (Flemish Government, 2021).

focused on the global scale, other impact categories might be more relevant, such as Climate Change.

5.4.2 Influence of the data source

The outcome of the Monte Carlo results - just as with LCA results - needs to be interpreted considering the quality of the input data (von Brömssen and Röös, 2020). To account for uncertainty and variability in the post-harvest chain (Chapter 4) and some parts of the cultivation chain, distributions were based on lower tendency, most likely and higher tendency data, gathered through surveys or literature. In contrast, the amounts of the used energy, water, pesticide and fertilizer products in the cultivation chain was taken into consideration through distribution fitting using individual orchard data from a large database. While in the first case, outliers are generally not included in the distributions, this was not the case when fitting distributions for the cultivation chain, sometimes leading to higher-than-expected outcomes.

For example, when calculating the environmental impacts for the impact category Freshwater Ecotoxicity for Kanzi using only deterministic input values [such as in Goossens et al. (2017a)] – completely disregarding uncertainty and variability – we see that 3 of the 36 orchards can be identified as "far out" outliers (using Tukey's fences[10]), which is 8% of the results (fig. 5-2b). For Jonagold on the other hand (fig. 5a), only 58 of the 973 orchards are shown as being "far out" outliers (6%). The difference of "far out" outlier percentages can be even higher, with for example only 4% (39 "far out" outliers) for Jonagold and 14% (5 "far out" outliers) for Kanzi for the impact category Freshwater Eutrophication. A high degree of outliers can influence the 2DMC results because more "extreme" results will have larger influence when fitting input probability distributions, possibly leading to right-skewed probability distributions and over-sampling of higher input values.

In such cases, we have to keep in mind that Monte Carlo simulations are a simplified model of reality and therefore never meant to be a perfect description of the real world (von Brömssen and Röös, 2020). A possible solution to counteract these outliers is by excluding the outlier simulations and only showing the simulations between 2.5% and 97.5% [as in Vásquez et al. (2014)]. These percentiles are used

[10] A "far out" outlier is any observation lying outside the range $[Q_1 - 3(Q_3 - Q_1); Q_3 + 3(Q_3 - Q_1)]$, with Q_1 and Q_3 being the lower and upper quartiles respectively.

when calculating the ratios which do not show to be much influenced by the outlier inputs.

Another possibility is to exclude the orchards that have “far out” deterministic impacts, before proceeding with distribution fittings. It is possible that these outliers had low yields due to bad weather or because the orchards were very young and therefore not fully productive yet (this is further discussed in section 5.4.3). However, such outliers might just lead to valuable information and insights on how the process can be improved and the impacts lowered and, therefore, we did not omit them from our 2DMC simulations. We specifically chose to use all available inputs and to show all results in order to be as transparent as possible (see section 1.2). Especially, since we aim to introduce the 2DMC method to other LCA practitioners. When communicating the results to stakeholders, a simplification of the results might be more fitting.

In conclusion, 2DMC is more suitable for large datasets. When using a relatively small dataset to account for variability, 2DMC results can be unexpectedly large. We therefore advise to look at the results more critically when such a dataset is being used and to identify if any outliers are present in the input data. It would be relevant to conduct further research on the effect of using 2DMC for small datasets and the different outlier treatment options.

5.4.3 How do the 2DMC results fit in the current literature?

Finally, we look at how our 2DMC results and deterministic results compare with the state-of-the-art when it comes to apple cultivation impact. We compare the literature results for the Climate Change impact category for the Jonagold results (Fig. 5-2d). The large orchard dataset for Jonagold includes a wide range of possible management strategies. Do keep in mind that the system boundaries between the discussed studies and the one reported on in this chapter are not completely equivalent and that different LCIA methods might have been used.

Jonagold cultivation has a *deterministic* Climate Change impact between -150 and 3045 kg CO_2 eq per ton apples with an average of 153 kg CO_2 eq/t and a median of 99 kg CO_2 eq/t, while the *2DMC* results range between 1 and 920 kg CO_2 eq/t, and had an average of 133 kg CO_2 eq/t and a mean of 122 kg CO_2 eq/t. This range of results included impacts for all low productive and the full productive stages (see section 1.4.2). The wide range of deterministic values can be caused by multiple reasons:

- there might be a loss of yield due to extreme weather events resulting in high impacts,
- the orchard might still be very young or very old, only providing a minimum of yield,
- negative impacts can be caused by using a lot of inputs for which the chosen (sometimes proxy) input processes in SimaPro have a negative Climate Change impact, such as:
    - "Nitrogen fertiliser, sludge from pulp and paper production, landfarming" to account for the impact of paper sludge,
    - "Biogas, from grass" to account for the impact of digestate,
    - "Nitrogen fertiliser, nutrient supply from vinasse, from fermentation of sugar beet" to account for the impact of Monterra (see Chapter 6), and
    - "Rapeseed oil methyl ester" to account for the impact of the growth regulator
- the apple grower might have incorrectly registered their data in the FADN database,
- etc.

These results are further compared to results published in apple LCAs in the last few years. Longo et al. (2017) calculated an impact of 125 kg CO_2 eq/t for apples grown in Northern Italy. They based this on data from an experimental field and expert opinions, and focused on the full production stage. Bartzas et al. (2017) conducted interviews to gather the primary data of 28 fully productive orchards covering multiple production years to calculate the Greek apple impact, leading to 89 kg CO_2 eq/t using average weighted input data. Vinyes et al. (2017) considered a multiyear approach for a specific Spanish orchard, leading to an impact of 111 kg CO_2 eq/t for the agricultural stage.

Alaphilippe et al. (2015) focused on two specific French orchards, which had an impact of 89.8 kg CO_2 eq/t for the intensive one and of 75.2 kg CO_2 eq/t for the semi-extensive one. They considered the full orchard life cycle including the nursery and destruction phases. Basset-Mens et al. (2016) also considered the full orchard life cycle in France and found an impact of 67.8 kg CO_2 eq/t. They mostly used expert knowledge as a source supplemented with a large sample of field survey data for crop protection.

For the conventional Canadian (Nova Scotia) apple production, Keyes et al. (2015) send surveys to thirty farmers, of which ten completed it. The authors stated that the received data represented around 15% of the total conventional apple growing area in Nova Scotia. They calculated an impact of 64.1 kg CO_2 eq/t using the weighted average of the input data, which included inputs for land preparation, infrastructure and farm equipment. These were not included in the study reported on in this chapter. Excluding those inputs led to an impact of 51.4 kg CO_2 eq per ton Canadian apple.

Bamber et al. (2020) calculated impacts ranging between 122 and 192 kg CO_2 eq/t depending on the apple production treatment (with or without bark mulch as a soil amendment) in a Canadian orchard. They considered parameter uncertainty using Monte Carlo simulations in their assessment which led to higher mean results, ranging between 250 and 360 kg CO_2 eq/t. Their lowest possible result was -577 and their highest 1473.

In general, we see that just as in our results, there is a wide range of Climate Change results among the published studies, however their range is generally not as broad. This is most probably due to them oftentimes using survey data/expert opinions, only studying full productive orchards, limiting the study to a limited number of orchards and mostly not including any uncertainty or variability. Only Bamber et al. (2020) conducted an uncertainty analysis, leading to a wide range of possible impacts, just as was the case for our apple cultivation study. Variability could have been included in a couple studies (Bartzas et al., 2017; Keyes et al., 2015) but weighted average input data was used instead.

5.5 Conclusions

This assessment completes the apple chain by calculating the environmental impacts of the cultivation part of the chain. It is shown that 2DMC can – next to input values from surveys – also be used when the data source consists of a large database with individual deterministic input values. Though, care needs to be taken when interpreting the 2DMC results, especially for small datasets that contain outlier input values.

The shape and location of the 2DMC curves lead to different conclusions and thus have a different implication on decision/policy level. The 2DMC results indicate that for half of the impact categories a first conclusion can be made on which would be environmentally preferable based on the central tendency. For the results of this case study, the conclusion might be to cultivate more Jonagold apples. However, this might be a too general conclusion seeing as for the other half of the impact categories, the 2DMC curves of the Jonagold and Kanzi apples do overlap. When the 2DMC curves show overlap, it would be more advisable to first try to reduce the overall uncertainty. The ratios indicate that such a thing can mainly be achieved by examining the system more closely (and thus reducing variability by making physical changes in the production process). Seeing as the different impact categories lead to different results and thus, different future steps to take, the decision maker might have to decide which impact categories are relevant enough to retain to base their final conclusions on.

PART III

Accounting for organic fertilizers

Chapter 6

Why mass allocation with representative allocation factor is preferential in LCA when using residual livestock products as organic fertilizers

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6.1 Introduction

Life Cycle Assessment (LCA) is a standardized method to calculate the potential environmental impact arising throughout the life cycle of a product or process. Each production system has a primary function, but secondary functions can emerge throughout the life cycle. These secondary functions to the determining function are often of low relevance, however, they can be of high relevance when used as input (material or energy) in other processes (European Commission et al., 2010; Hauschild et al., 2018; ISO, 2006a). These production systems are called *multifunctional* because they provide more than one good/service.

A typical example is animal husbandry, where meat is the primary output in the beef system or milk in the dairy system. Secondary products of these systems include hides, bones, blood and manure, which can also lead to economic gains, but are not the primary/determining function of the systems. Multifunctionality causes a challenging methodological issue in LCA, since LCA is based on analyzing a single system to determine its environmental impacts, and such isolation becomes problematic as soon as a secondary product emerges. When the secondary product is used in other systems, the original system becomes part of another process as well. The environmental impact can then no longer reasonably by ascribed to the original system only (European Commission et al., 2010; Hauschild et al., 2018), instead, a proper assignment (allocation) of shared inputs and emissions are needed between the different products of the multifunctional process (FAO, 2016).

This multifunctionality causes especially a problem for agricultural products. When looking at cultivation, organic fertilizers such as manure or compost are typically seen as residual products of which the future use is considered as having no impact on the production of it (Durlinger et al., 2017a; Notarnicola et al., 2015). Because of this, the impacts of producing such organic fertilizers are usually not accounted for within agricultural and horticultural LCAs where the application of these organic fertilizers is considered [e.g., Goossens et al. (2017) and Spångberg et al. (2011)]. This is in accordance with the “default option” when it comes to exporting manure from a livestock farm (European Commission, 2018). In those cases, manure is seen as a *residual* product where the manure does not lead to economic gain at the farm gate. The emissions related to manure management up to that point are allocated to the other outputs of the livestock system (European Commission, 2018; FAO, 2016) whereas the subsequent transformation of the manure in a useful product (e.g., organic fertilizer) and the emissions on the field are assigned to the crop production system (FAO, 2016).

Alternatively, manure can be seen as a *waste* product if it has to be disposed of or when it is applied as an organic fertilizer in excess of crop nutrient requirements (FAO, 2016; Leip et al., 2019), for which mineral fertilizers are considered as a “wasteful” application before organic material is considered to be in excess as well if nutrient requirements are still exceeded (FAO, 2018a). In those cases, all the extra emissions are ascribed to the other products within the livestock system (FAO, 2016).

Lastly, manure can be considered a *co-product* of the livestock system when it leads to economic gain at the farm gate, in which case part of the environmental impact of the livestock system should be allocated to it (European Commission, 2018; FAO, 2016). These three categories (residual, waste and co-product) can be extended to include other organic fertilizers originating in the livestock system, such as blood meal. ISO 14044 (ISO, 2006a) designed an allocation hierarchy to solve these kinds of multifunctionality problems for co-products. FAO’s decision tree (FAO, 2016) based on this hierarchy for large ruminants is shown in Figure 1-6.

Firstly, allocation should be tried to be avoided by dividing the unit process into two or more sub-processes. This *subdivision* should clearly separate the production between the different co-products, which is often not possible.

Allocation can also be avoided by doing *system expansion* (ISO, 2006a). This can be interpreted by adding another, not provided function to the system to make it comparable; or by crediting the product system with the impacts of an alternative product/process which is avoided because of the emergence of the secondary function (European Commission et al., 2010; Hauschild et al., 2018). These avoided impacts have also been used to substitute/replace the impact of the co-product, especially when the use of the co-product elsewhere is considered (Bier et al., 2012; Nguyen and Hermansen, 2012). Notarnicola et al. (2015) specifically proposes to use the quantity of avoided mineral fertilizers to account for the production impact of organic fertilizers used during fruit production.

If allocation cannot be avoided, ISO (2006) advices to partition the system between the different co-products in a way that reflects the underlying *physical relationships* between them [such as mass or energy content (European Commission et al., 2010)] or – as a last resort – based on another relationship such as the *economic value* of the products. The choices made when allocating impacts is crucial since each allocation procedure produces different results and thus different interpretations and comparisons (Martínez-Blanco et al., 2014; Nguyen and Hermansen, 2012).

ISO's allocation hierarchy has since been interpreted in general (European Commission, 2018; European Commission et al., 2010) and in focused [e.g. pigs (FAO, 2018b), animal feed (FAO, 2014), large ruminants (FAO, 2016), dairy (IDF, 2015) and livestock (FAO, 2018a)] LCA guidelines, and the sensitivity of the results to the different approaches has been tested in several case studies, such as:

- thermoplastic production from blood meal comparing five approaches (Bier et al., 2012),
- ethanol production from molasses comparing four approaches (Nguyen and Hermansen, 2012),
- biodiesel production from soybean comparing three approaches (Esteves et al., 2018) or from waste cooking oil comparing five approaches (Caldeira et al., 2016),
- lignin production comparing twelve approaches (Hermansson et al., 2020),

- compost application in crop sequence comparing two approaches (Quirós et al., 2015),
- the dairy sector comparing four (Battini et al., 2016) and seven approaches (Gac et al., 2014; Rice et al., 2017), and
- the meat sector comparing three (Vergé et al., 2016) and four approaches (Cherubini et al., 2018).

Even this year, Wilfart et al. (2021) found that despite the many guidelines and scientific articles that have been published since the release of the ISO standard, no consensus has been reached regarding a preferential allocation rule.

The fact that manure is generally seen as a residual product, with no production impacts ascribed to it, raises questions on how realistic comparisons are between conventional crop production systems that use mineral fertilizers and organic systems that use organic fertilizers such as manure and blood meal. The flows of resources and associated impacts are not represented equivalently in both systems. It is, therefore, relevant to review the different allocation procedures that could be used to include the environmental impact of organic fertilizers in the organic production system.

The aim of this study was to conduct sensitivity analyses for the possible allocation procedures – and the choices within each procedure – that can be used for organic fertilizers stemming from a livestock system. We will address these questions using the cultivation of organic apples in Flanders (Belgium) as a case study. We aim to select the most preferable allocation procedure, leading to a realistic approximation, for future use in organic cultivation LCAs. This study might also be of interest for other LCAs where agricultural residues/waste/co-products are used as a resource for, e.g., feedstocks for value-added products such as biofuels and bioplastics.

6.2 Methodology

6.2.1 Goal and scope definition

The goal of this LCA is to evaluate the effect of different allocation procedures on the environmental impact of organic fertilizer production within organic apple cultivation. We intend to assess the influence of the chosen procedure on the total environmental impact and will identify difficulties and uncertainties associated with each procedure.

An attributional cradle-to-gate LCA (excluding the nursery) of the organic apple cultivation in Flanders was conducted based on an updated version of the study of Goossens et al. (2017). The functional unit is 1 ton of organically cultivated apples leaving the farm. All annual orchard management operations are included using data on energy carriers, water, pesticides and fertilizers use, unless otherwise specified.

Calculations were performed using SimaPro 9.0.0.49 (Pré Sustainability, the Netherlands), JMP Pro 15 (SAS Institute Inc., NC, USA) and Excel 2016 (Microsoft, WA, USA). The ReCiPe [2016 Midpoint (H) V1.03 / World (2010) H] method was used as impact assessment method, and all of its 18 impact categories were considered. Input processes were collected from the databases ecoinvent 3.5 and Agri-footprint 4.0., using “allocation, at point of substitution” and “economic allocation” respectively, as a standard. Other choices made because of the different allocation procedures are specified in section 6.2.3.

6.2.2 Life Cycle Inventory

Cultivation data for the apple orchards was obtained from the EU Farm Accountancy Data Network (FADN). In Flanders, 650 agricultural holdings are part of FADN (Departement Landbouw en Visserij, 2018). Approximately 1.4% of the Flemish agricultural area in 2019 was organically cultivated or in transition (Timmermans and Van Bellegem, 2020). The detailed primary production data in FADN includes anonymized company data and orchard records, which refers to all areas within a farm where the same apple cultivar is grown. One orchard record holds the information on the yield and on the fertilizer, pesticide, energy, water and land use of a specific cultivar during a specific year on a specific farm.

Four organic apple orchard records were selected in which Jonagold or its mutants (i.e., Jonagored, Decosta and Novajo) were cultivated in 2011, with yields ranging from 2.4 t/ha to 72.8 t/ha, including both low and full productive tree stages [as defined in Goossens et al. (2017)]. Due to this high variability in yield, median impacts are reported on for the purpose of the allocation study reported on in this article.

The grower uses fossil energy and lubricants for farm equipment and transportation. Only the cumulative amounts of specific energy categories were included within the FADN dataset. Thus, energy use cannot be subdivided between field operations and transportation steps (which will have implications as shown below). Twenty fertilizer products including blood meal, solid cow manure and semiliquid cow manure were used in the different orchards. Allocation procedures for the organic fertilizers are described in detail in section 2.3.

Direct field emissions from fertilizers and energy use (including pesticide and fertilizer application) were calculated using the IPCC guidelines (Garg and Weitz, 2019; Hergoualc' et al., 2019), the Agri-footprint manual (Durlinger et al., 2017b), ecoinvent reports (Nemecek and Schnetzer, 2011), the Product Environmental Footprint Category Rules (European Commission, 2018) and the air pollutant emission inventory guidebook (European Environment Agency, 2016).

For the sake of transparency and data traceability, detailed descriptions of the input processes and emission calculations for the energy, water, pesticide and fertilizer use can be found in Appendix B.1.

6.2.3 Allocation procedures and sensitivity analysis

A scenario analysis, which is a kind of local sensitivity analysis (Hauschild et al., 2018; Michiels and Geeraerd, 2020), was conducted for the methodological choice of the allocation procedures for the three organic fertilizers stemming from a livestock system. Considering the organic fertilizers as residual products was taken as the base scenario (see 6.2.3.1), to which system expansion (see 6.2.3.2), mass allocation (see 6.2.3.4) and economic allocation (see 6.2.3.5) were compared. For those last three allocation procedures, the organic fertilizers are considered as co-products of the livestock system.

6.2.3.1 Excluding organic fertilizer production (residual product)

In this base scenario, the impact of the production of the organic fertilizers is not included because they are seen as residual products pertaining to the life cycle of their original system (Notarnicola et al., 2015). This approach has also been called the "*waste assumption*" [as in Bier et al (2012)]. No impacts of farming and meat processing are attributed to blood meal and manure. However, the transformation of blood into blood meal through blood drying is taken into consideration (Bier et al., 2012; Goossens et al., 2017a). The management and use phases of the manure and blood meal are included within the main boundaries of the apple cultivation system as energy inputs and as emissions from fertilizer use (see 6.2.2). In Figure 6-1, the processes belonging to the base scenario are indicated by the blue area (the input processes used in SimaPro can be found in Appendix C.1).

6.2.3.2 System expansion

In system expansion through substitution, the impacts of an equivalent, alternative product are allocated to the studied system. Two possible substitution products were selected for blood meal and manure. A mineral fertilizer, in accordance with the suggestion of Notarnicola et al. (2015), and an organic plant-based fertilizer. For the mineral fertilizer, a general NPK compound was selected from Agri-footprint. For the organic fertilizer, the 100% vegetable fertilizer Monterra Bio Malt NPK 4.5-2.5-8 (MeMon, 2019; Servaplant, 2018) was chosen. The product is composed out of malt sprouts, corn gluten, vinasse and molasses (Servaplant, 2018); the exact subdivision not being a fixed value (composition in Appendix C.1). Because of its availability in the databases, vinasse was chosen as the NPK supply source.

To ensure the relevance of our calculations, the amount of active N supplied to the orchards by the mineral and organic plant-based fertilizer needed to be equivalent to the amount of active N that was actually supplied by blood meal and the two kinds of manure (active N percentages can be found in Appendix C.1). It was impossible to completely align the composition (e.g., P, K and C) of the substitute fertilizers to the organic fertilizers. A discussion on this can be found in section 6.4.3. Fertilizer transports by the grower were already considered within the energy use. Packaging was not considered since that was also the case for the other fertilizer products.

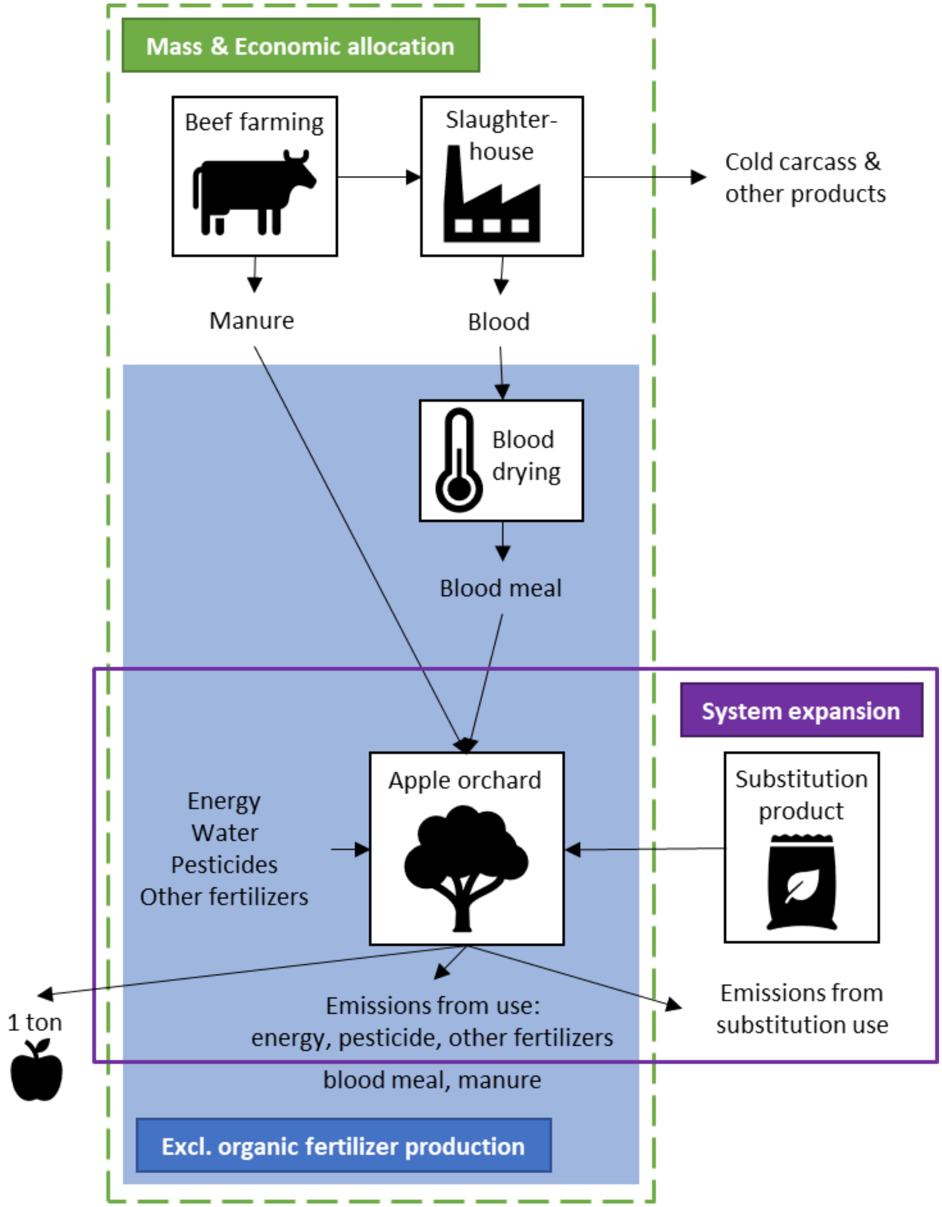

Figure 6-1 System boundaries and associated inputs and outputs of the different allocation procedures.

"Other fertilizers" are fertilizers not stemming from the livestock system.

The impacts of the use of the substitution products were calculated using the same methodology as the other fertilizer products (see 6.2.2). The transformation of blood into blood meal and the field emissions due to the use of blood meal and manure are not considered in this scenario. All impacts related to blood meal and solid and semiliquid cow manure are replaced by impacts from a substitute product (purple in Fig. 6-1). We assume here that system expansion would also be used for the livestock system, meaning that the system would be credited for the avoided impacts of the substitution products by subtracting them there. That way, there is no double-counting.

6.2.3.3 Allocation based on a relationship: the background beef system

For allocation based on a relationship (green in Fig. 6-1), the organic fertilizers are seen as co-products of the livestock system and a fraction of the impacts of the livestock system is thus added to the impacts of the base scenario (see section 6.2.3.1). Regarding allocation based on a physical relationship, we only use mass allocation in our case study. Other physical relationships exist and will be discussed in section 6.4.4.

Amount of organic fertilizer used in Flemish agriculture

Agri-footprint's input processes using mass and economic allocation are respectively used for the mass and economic allocation conducted in this research. As mentioned previously, three kinds of organic fertilizers were used in the apple orchards: solid cow manure, semiliquid cow manure and blood meal. The same livestock system could be used for both manure and blood, since we assumed that the blood supplied for the production of blood meal originated from beef cattle. We assumed that only 68% of the manure production was kept as manure, while the rest was spread on the pasture during grazing, following ERM and Universiteit Gent (2011).

Additionally, the Flemish manure report of 2019 (VLM, 2019) states that 92% of all produced bovine manure is used in Flemish agriculture in 2018. This was equivalent to 65 million kg N and 26 million kg P_2O_5. We assume that the same percentage can be extended to the usage of the manure produced in one beef farm. For the remaining 8%, the impact of anaerobic digestion for biowaste was added to the beef system. Thus, when calculating allocation factors, only 63% of the total manure production is considered as a possible co-product (Fig 6-2). For blood meal, the impact of the slaughterhouse was also accounted for.

A representative beef farm

To represent the impact of the beef system, Agri-footprints' process "*beef cattle for slaughter*" (Durlinger et al., 2017b) was used, which was built using the Irish beef study of Casey and Holden (2006). The beef system was based on a specialist beef farm with a herd consisting of 60 bovines (including calves, cows, bulls and heifers) with the intention to produce beef. Each year, the herd produces 616000 kg manure (Table 6-1, Fig. 6-2) and 18 animals from the beef farm are slaughtered, equivalent to a total live weight of 11700 kg (Durlinger et al., 2017b). Irish beef production systems are predominantly grass based (Casey and Holden, 2006), while in a typical Belgian beef system the female bovines are kept outside for long periods of time while the males are kept inside (ERM and Universiteit Gent, 2011). Although the Irish beef system is not completely equivalent to the Belgian beef system, we identified it as the best proxy available in LCA databases. Further details can be found in Appendix C.1.

It was assumed that the manure and blood meal, produced on that beef farm, were used in the organic apple orchard. The impacts of the beef system are expressed in "per kg live weight for slaughter". By multiplying this with the annual amount of live weight that is slaughtered for the beef farm, we know the total annual impact of the specific beef farm used in Agri-footprints' process. Using mass or economic allocation factors, a part of that impact is then ascribed to the organic fertilizers that are produced by the beef farm during one year (Fig. 6-3).

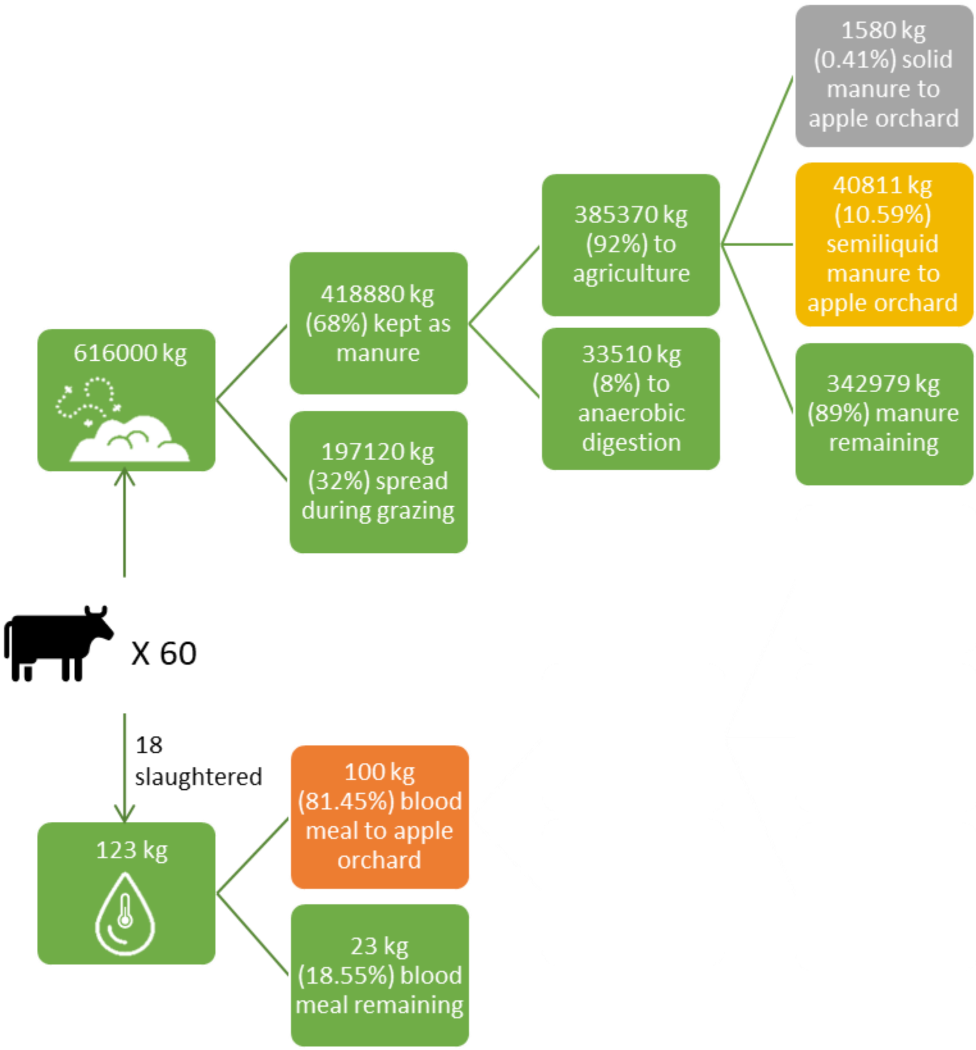

Figure 6-2 Schematic overview of the amount of manure and blood meal that is produced by the representative beef farm in one year and used as fertilizer on the apple orchards.

Amount of organic fertilizer needed for apple cultivation

Not all manure and blood meal produced by the considered beef farm in one year is needed to fertilize the apple orchard. Of the 63% of the total manure production that ends up being used in agriculture, 0.41% of the solid manure and 10.59% of the semiliquid manure would have been sufficient for apple cultivation, while of all the blood meal that could be produced from the considered beef farm in one year, 81.45% would have been sufficient (Fig 6-2). These percentages are based on the median amount of organic fertilizers that were applied on the four orchards (on which combinations of solid manure, semiliquid manure and blood meal were used). Therefore, only those parts of the impacts ascribed to the organic fertilizers are allocated to organic apple cultivation (Fig. 6-3).

Since we don’t know what happens with the surplus of blood meal and kept manure produced on the beef farm, it can either be considered as residual (in which case all production impacts are allocated to the beef farm) or as a co-product used as a resource in another system (in which case part of the production impacts is allocated to that system). Since there are several allocation factors that could be used for mass and economic allocation, ISO 14044’s recommendation (ISO, 2006a) of assessing the consequences of using different appropriate allocation factors by conducting a sensitivity analysis, was followed.

We now know how much manure and blood meal is produced and subsequently applied on the apple orchards. In the following sections, we will use this in our calculations of mass and economic allocation factors, which will divide the impact of the beef farm among its co-products.

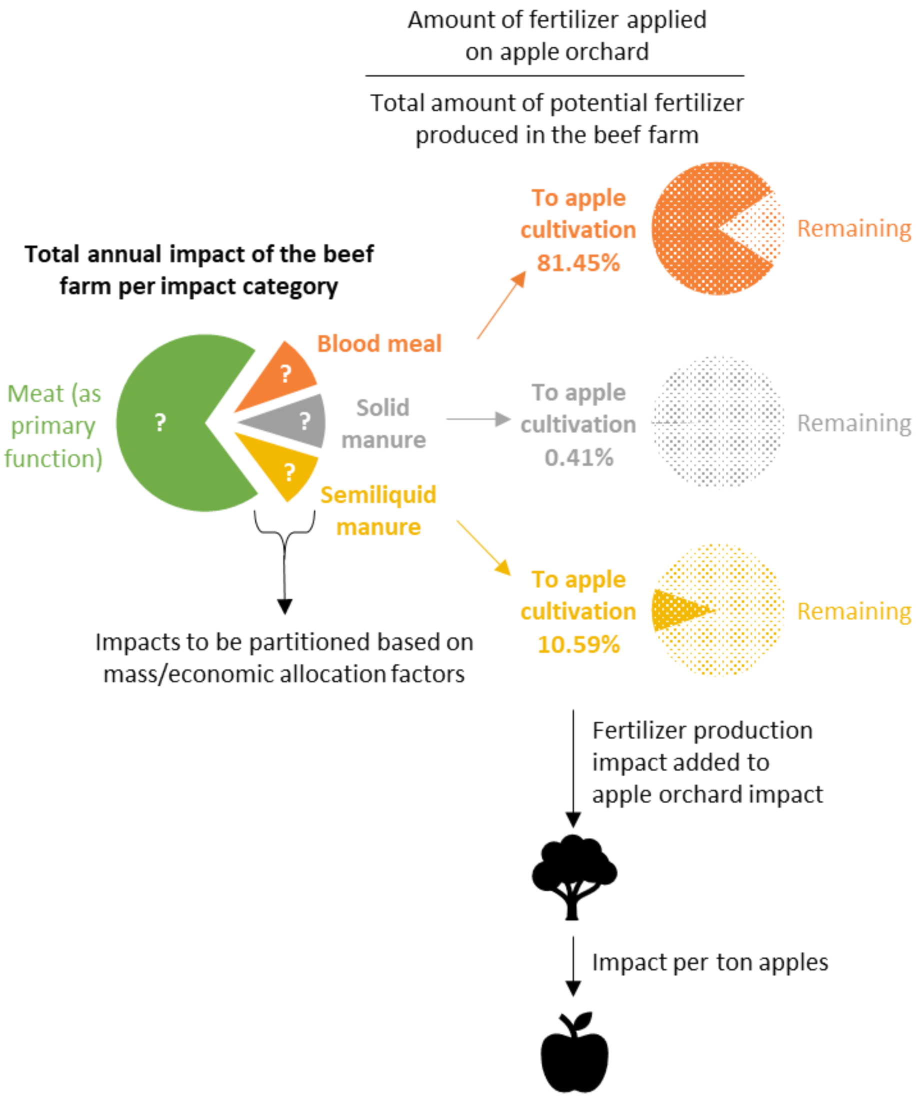

Figure 6-3 Schematic overview of the methodology used for allocating production impacts of organic fertilizers from the beef farm to an organic apple orchard.
The calculation of the allocation factors is the focus of this research. The remaining organic fertilizers (and their impact) can be handled as either a residual product or a co-product.

6.2.3.4 Allocation based on a physical relationship: mass allocation

In mass allocation, the associated environmental impacts are quantified based on the mass proportions between input and output variables. There are multiple masses from the livestock system that could be considered as valid options for calculating mass proportions. Several were considered in this case study with, on the side of the organic fertilizer, two possibilities:

- either the mass of the fertilizer [“*kg fertilizer*”; which is especially relevant for blood meal (Bier et al., 2012), but less so for manure], or
- the mass of N in the fertilizer (“*kg N in fertilizer*”);

and on the side of the beef cattle system four possibilities:

- the mass of the total live weight for slaughter and the mass of the annual manure production used in agriculture [“*kg (live weight + manure)*”], or
- the mass of the total live weight for slaughter (“*kg live weight*”), or
- the mass of the live weight and the mass of N in the manure (“*kg live weight + kg N in manure*”), or
- the mass of N in the live weight and the N in manure [“*kg N in (live weight + manure)*”].

Only the realistic mass allocation factors will be considered, where the allocation percentage turns out to be less than 100%. Otherwise, more than the total impact that is normally ascribed to the total beef cattle system would be allocated to the organic cultivation system. The mass allocation factors will be visually represented in section 6.3.1. Depending on the outcomes, a first selection on which factors are representative will be made there. For example, the partitioning of the beef system impact should still reflect that the determining function of the system is beef production and not organic fertilizer production. The necessary data for all the mass proportions can be found in Table 6-1 (calculations underlying the allocation factors can be found in Appendix C.1).

Table 6-1 Parameters and assumptions needed for calculating the mass and economic allocation factors.

Parameter	Value	Unit	Source
Blood meal related			
Amount blood produced by cattle	0.055	L blood/kg live weight	(Reynolds, 1953)
Blood density	1.06	kg blood/L blood	
Amount of blood meal produced from blood	180	kg blood meal/t blood	(Luske and Blonk, 2009)
N content in blood meal	0.13	kg N/kg blood meal	FADN database
Price of blood meal	0.49	€/kg blood meal	FADN database
Manure related			
Annual manure production in the beef farm	616000	kg/year	See Table C-3 in appendix C.1
Manure distribution	32	% spread during grazing	(ERM and Universiteit Gent, 2011)
	60	% kept as solid manure	
	8	% kept as semiliquid manure	
Kept manure used in Flemish agriculture	92	%	(VLM, 2019)
N content in semiliquid manure	0.0048	kg N/kg semiliquid manure	FADN database
N content in solid manure	0.0071	kg N/kg solid manure	FADN database
Price of manure	10.74	€/t manure	(Wageningen University & Research, 2020): 2018
Price of mineral fertilizer (for N)	1037	€/t product	as published in the European CAPRI database and used by FAO (2018) and Leip et al. (2019)
Animal related			
Age at slaughter	24	Months	(Durlinger et al., 2017b) based on the breeds Charolais, Simmental and Limousin as studied by (Casey and Holden, 2006)
Final live weight of 1 animal	650	kg live weight/animal	
Annual live weight for slaughter in the beef farm	11700	kg live weight/year	
Cold carcass weight	66.37	% of live weight	(Ministry of the Flemish Community, 2002)
N content of beef cattle ≥ 454 kg	2.4	%N of bodyweight	(FAO, 2018a)
Price of live animal	210.72	€/100 kg live weight	(Department of Agriculture and Fisheries, 2020): 2019 average for a “well-formed” bull

Table 6-1 Continued

Parameter	Value	Unit	Source
Animal related			
Price of cold carcass	363.25	€/100 kg cold carcass weight	(Department of Agriculture and Fisheries, 2020): 2019 average for a bull carcass classified as "very good"

Four orchards used both manure and blood meal for fertilization purposes and are discussed in this article. However, there were eight other orchards that only used blood meal as an organic fertilizer stemming from the livestock system. An additional analysis of the mass allocation factors that are possible when solely using blood meal is included in appendix C. An LCA practitioner might still consider manure as a residual product while considering blood as a co-product of the beef system, especially since – according to the FADN database – manure can often be received for free in Flanders, which is not the case for blood meal.

6.2.3.5 Allocation based on another relationship: economic allocation

In economic allocation, the associated environmental impacts are quantified based on the economic value of input and output variables. Four possible allocation factors were considered, using the annual output data of the beef farm. For the first three, the allocation factor is based on the price of the fertilizer ("*€ fertilizer*") versus:

- the price of the live weight at farm gate ["*€ live weight*"; option I (European Commission, 2018)],
- live weight and manure ["*€ (live weight + manure)*"; option II], or
- cold carcass weight ["*€ carcass*"; option III; as in Bier et al (2012)].

The fourth allocation factor (option IV) was calculated using the *nutrient value* of the organic fertilizers (FAO, 2018a; Leip et al., 2019). The nutrient value of the organic fertilizer is estimated by the amount of mineral fertilizer that the farmer would have to purchase in case the manure was not available to provide the required nutrients. The so-called pragmatic approach (Leip et al., 2019) was followed in which this "nutrient equivalent" is calculated based on the losses of nutrient – in this case N – to the atmosphere and hydrosphere of the mineral fertilizer versus the organic fertilizer, while also taking manure management practices into consideration. It was assumed that the organic fertilizers were not used in excess of crop nutrient needs and were therefore not considered as waste. The nutrient equivalent turned out to be 89% for blood meal and 38% for manure (calculation details in Appendix C-1). This means that for manure 38% of its total amount of nutrient is needed for a mineral fertilizer to be equivalent.

A mineral fertilizer (for N) price was then used of € 1037 per ton product [as published in the European CAPRI database and used by FAO (2018) and Leip et al. (2019)] to calculate the monetary value related to the nutrient value of the organic fertilizers. It should be kept in mind that this price can vary a lot depending on the considered mineral fertilizer, but for consistency sake, we use the same one as in the case study of FAO (2018) and Leip et al. (2019). If this allocation factor ends up being used as a standard, a consensus would have to be reached about the source of the mineral fertilizer price.

The economic allocation factor for each organic fertilizer is calculated by dividing its nutrient value by the nutrient values of all organic fertilizers and the price of a carcass. The methodology was developed specifically to account for manure as a co-product and was adapted in this case study to also include blood meal as a co-product. All economic allocation calculation details can be found in Appendix C.1. The necessary data for the economic allocation factors are also shown in Table 6-1.

Finally, to consider the effect of *price variations* (using a recent, minimum and maximum scenarios), a sensitivity analysis was conducted for two of the four allocation factors: price of the fertilizer as a fraction of the price of a live animal on one hand, and as a fraction of the price of a carcass on the other hand. For blood meal, the prices as found in the FADN database (2005-2011) were used. Using the database was not an option for manure, since oftentimes growers can get manure for free. Therefore, Dutch published prices from 2002-2018 were used, with the most recent price being € 10.74 per ton cattle manure (Wageningen University & Research, 2020). For the live adult animal and cold carcass, the price variation between 2011 and 2019 was considered (Department of Agriculture and Fisheries, 2020). Calculation details can be found in Appendix C.1.

6.3 Results

6.3.1 Mass and economic allocation within the beef cattle system

Figure 6-4 and 6-5 show respectively the possible mass and economic allocation factors that were considered and how the total impact of the beef cattle system would be allocated to organic apple cultivation when manure and blood are co-products. As indicated already higher, two additional options were also initially considered ("kg organic fertilizer/kg live weight" and "kg N in organic fertilizer/kg N in live animal"), however, these lead to an allocation factor bigger than 100% for manure. They were thus unrealistic and therefore excluded from the analysis. Additionally, it would not make sense to put "kg fertilizer" in the nominator and "kg N in fertilizer" in the denominator or vice versa.

Furthermore, using "the mass of the organic fertilizer" seems appropriate for blood meal (Bier et al., 2012), but this cannot be said for manure since the amount of manure that is generated in the farm largely outweighs the amount of meat and blood that is produced, causing disproportionate allocation factors. For two allocation options in Fig. 6-3 [option A "kg organic fertilizer/kg (live weight + manure)" and option B "kg N in organic fertilizer/kg N in (live animal + manure)"] less than 13% of the beef cattle system impact is allocated to meat. Since the determining function of the beef system is to produce beef, these two mass allocation factor do not seem like a good representation of the real world. They are therefore not considered anymore in the remainder of the results section. Instead, only the two final mass allocation factors [option C "kg N in organic fertilizer/kg live weight" and option D "kg N in organic fertilizer/(kg live weight + kg N in manure)] are considered as realistic options to allocate the impacts within the beef cattle system, resulting in less than 16% of the impact being allocated to organic fertilizers.

The four possible allocation factors for economic allocation are shown in Fig. 6-5. They all have a maximum of 12% of the beef farm impact allocated to organic fertilizers. The one option that is not further considered in the results section is option II "€ organic fertilizer/€ (live animal + manure)", because – according to the FADN database – manure can be freely available for Flemish apple growers. Therefore, manure does not always lead to an economic gain at the farm-gate and the allocation would become unrealistically large.

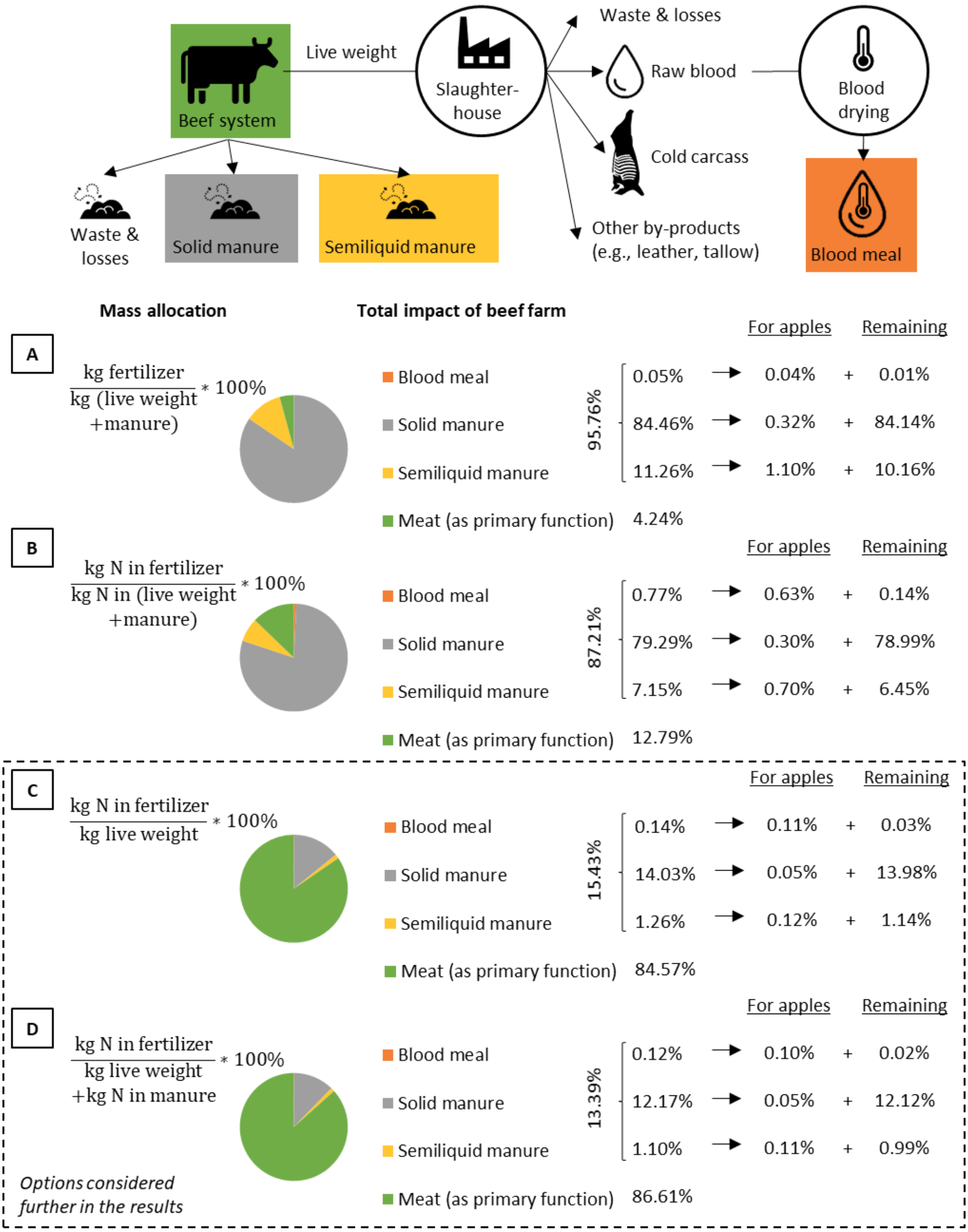

Figure 6-4 Representation of the farming and meat processing chain and how the beef farm impacts are allocated to blood meal and manure using mass allocation factors. The impacts allocated to the organic fertilizers can be divided into the parts that are allocated to the organic apple orchard (this study; see Fig. 6-3) and the remaining impacts that can be considered as residual or as a co-product used in another system. The options in the striped frame are withhold as realistic option.

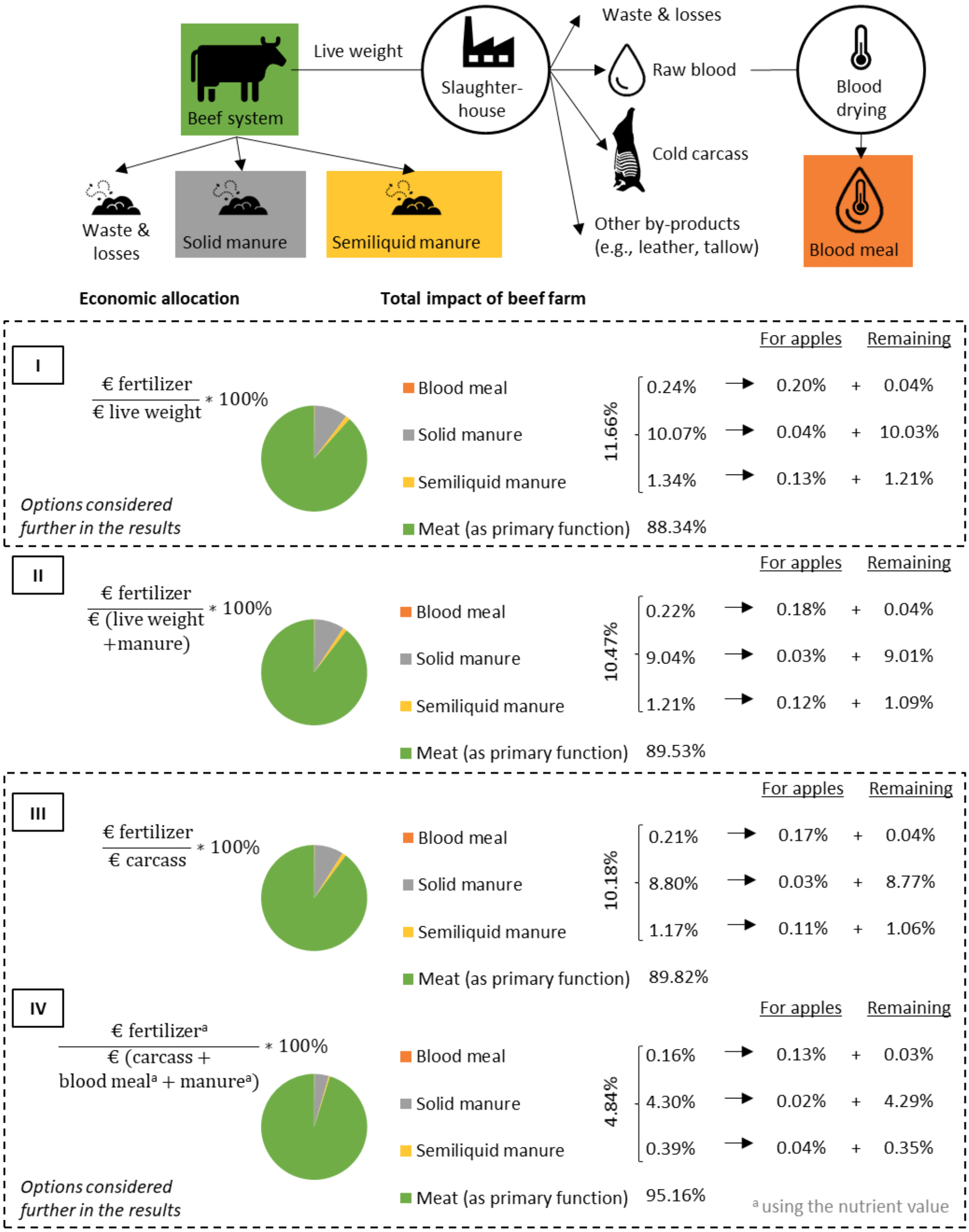

Figure 6-5 Representation of the farming and meat processing chain and how the beef farm impacts are allocated to blood meal and manure using economic allocation. Option IV is calculated based on the fertilizers' nutrient equivalence and the mineral fertilizer price (FAO, 2018a; Leip et al., 2019). The impacts allocated to the organic fertilizers can be divided between the apple orchard (this study; see Fig. 6-3) and the remaining impacts that can be considered as residual or as a co-product used elsewhere. The framed options are withheld as realistic option.

6.3.2 Effect of all allocation procedures on apple cultivation

Figure 6-6 shows the impact for the organic apple cultivation when manure is considered a residual product, or when manure is considered a co-product. For the last option, the effect of mass allocation, economic allocation and system expansion is shown. The allocation factors for mass (option C and D) and economic allocation (option I, II and IV) that were selected in 6.3.1 are used and for system expansion, an organic plant-based fertilizer and a mineral fertilizer were considered as possible substitute products.

When looking at the overall results in Figure 6-6, a first observation from the Global Warming impact is that the apple cultivation excl. organic fertilizer production always shows a smaller impact than mass and economic allocation. This is an evident observation: parts of the impacts of the beef cattle system (see pie charts in Fig. 6-4 and 6-5) are added to the impact of apple cultivation excl. organic fertilizer production for mass and economic allocation. Figure 6-6 shows this by stacking the impacts of blood meal, solid manure and semiliquid manure on top of the impact obtained for apple cultivation excl. organic fertilizer production. The impacts of the two possible substitute products are shown stacked upon the impact of apple cultivation excl. organic fertilizer production as well as use, meaning that this time, all impact related to blood meal and manure (i.e., use emissions and blood drying) was excluded.

The following two graphs in Figure 6-6 show the impact categories (ICs) where using an allocation procedure would lead to the biggest changes compared to when organic fertilizer production is excluded. For Land Use, blood meal and manure contribute the most to the total impact, more than 94%. It needs to be kept in mind here that no land transformation was considered for the apple orchards [as in Goossens et al. (2017a) see Appendix B.1]. Marine Eutrophication is where the substitute products in system expansion contribute the most to the total impact, more than 98%. The graphs of the other ICs are shown in appendix C.2.

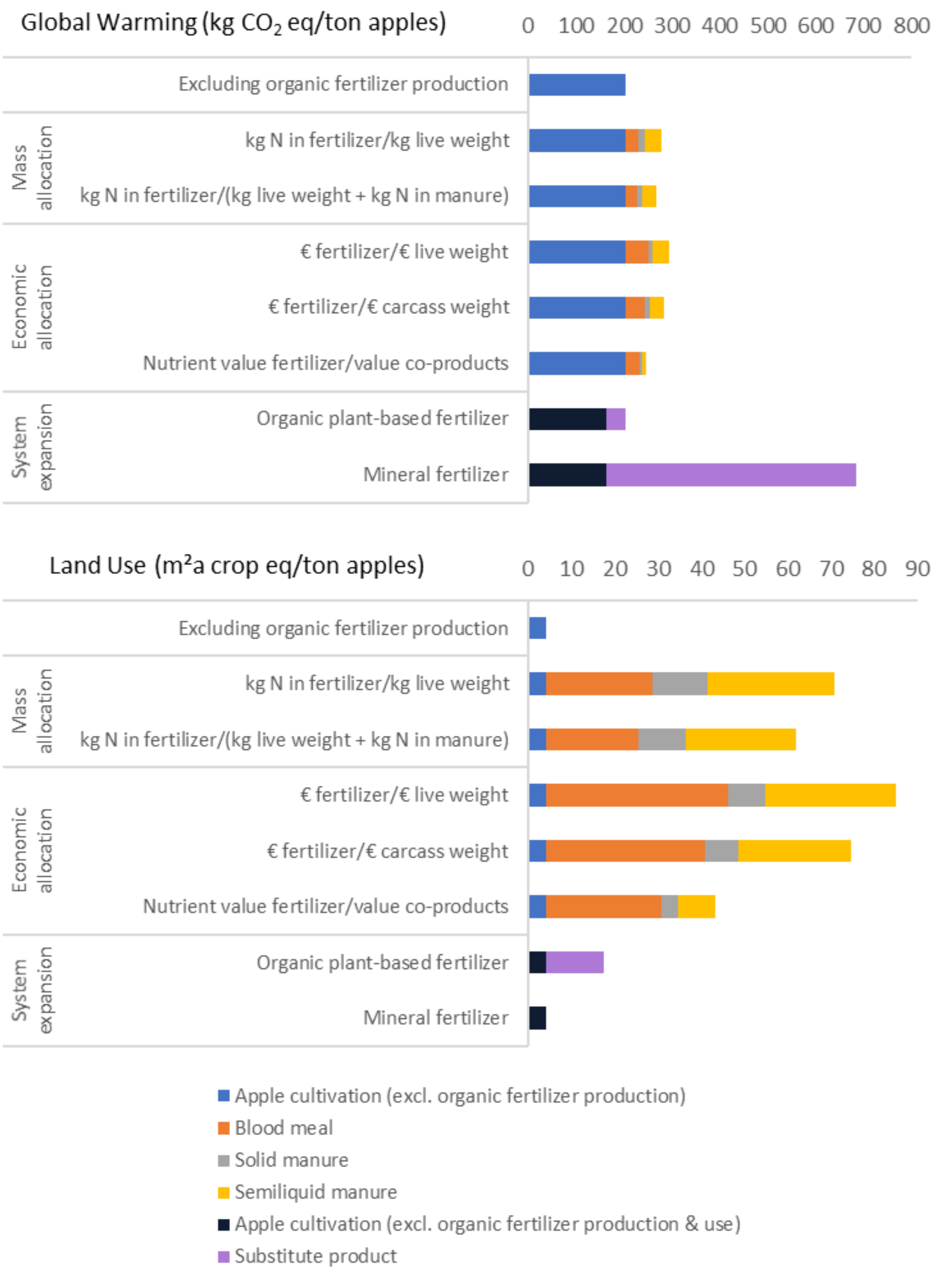

Figure 6-6 Median impacts of three impact categories for organic apple cultivation with the different considered allocation procedures.

The considered allocation procedures are shown for the four apple orchards using blood meal, solid and semiliquid manure.

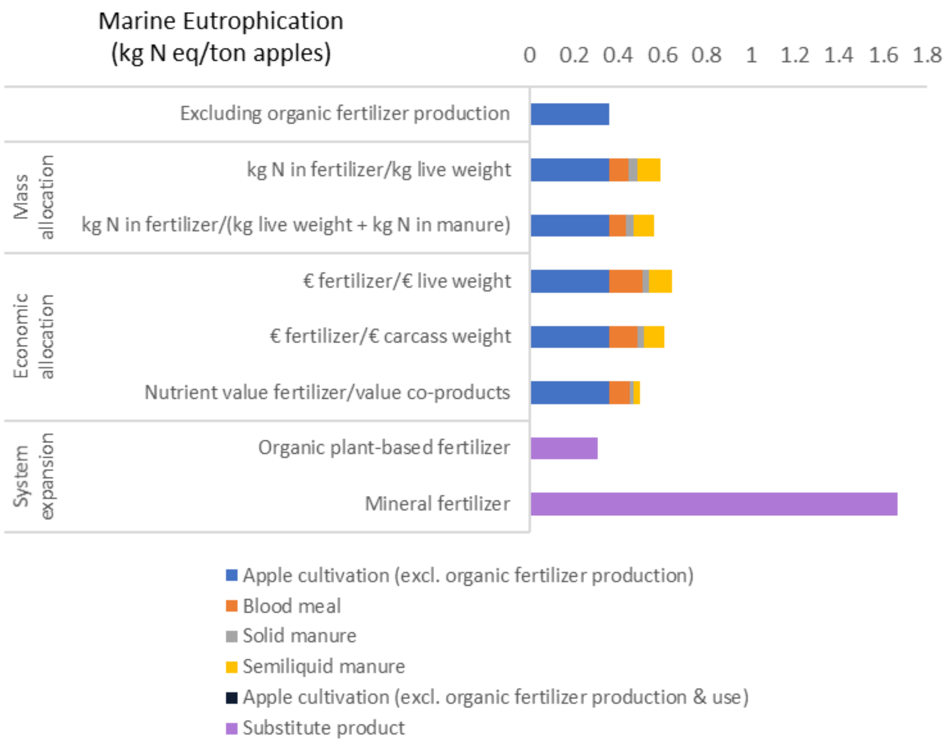

Figure 6-6 Continued

System expansion generally (11 of the 18 ICs) leads to the highest total impact, with the substitute option mineral fertilizer mainly (8 ICs) having the largest total impact. For the impact categories Ozone formation, Freshwater ecotoxicity, Marine ecotoxicity, Human non-carcinogenic toxicity, Land use and Water consumption, mass and economic allocation cause the higher total impact. For those ICs, the economic allocation option I "€ organic fertilizer/€ live weight" consistently lead to the largest total impact. This illustrates how the ranking associated with the chosen allocation procedure varies between the different ICs and how important the choice of the allocation factor is. Different factors may lead to very different results.

Additionally, the amount of the fertilizer used determines how big the impact is. While the allocation factors for solid manure is higher than those of semiliquid manure, the amount of semiliquid manure used on the orchards is approximately three times bigger. Blood meal was used in the lowest amount.

6.3.3 Price variations for economic allocation

Prices can vary over the year, and this needs to be considered when determining economic allocation factors. Figure 6-5 shows the allocation factors when recent prices for the fertilizers, live animal and cold carcass (which is economically more valuable) are considered. Figure 6-7 shows the results for possible price variations for Global warming, comparing a minimum and maximum scenario with the recent scenario (see Table C-8 in Appendix C.1 for the allocation factors). While the allocation factors for blood meal are almost equal for all six scenarios (ranging from 0.21 to 0.25%), relatively big differences can be observed when it comes to manure (ranging from 1.50% to 10.63% for solid manure and from 0.20% to 1.42% for semiliquid manure). Manure is cheaper than blood meal, however, much more is produced per live weight or per carcass. Therefore, manure's allocation factors are generally larger than those of blood meal. In Figure 6-7, the difference due to the price variation is mostly visible for semiliquid manure because this fertilizer is applied in the highest amount on the apple orchards. The recent prices lean more towards the maximum scenario of the price variations.

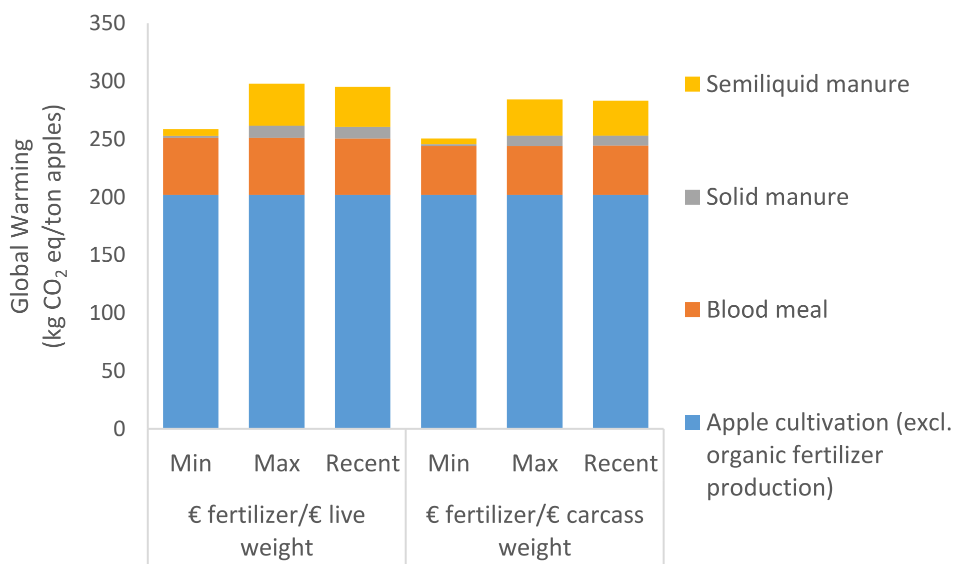

Figure 6-7 Median Global Warming impacts for the four orchards that use blood meal, solid manure and semiliquid manure as organic fertilizers.
Price variations (minimum, maximum and recent scenario) for economic allocation are taken into consideration.

6.4 Discussion

The results show that the choice of an adequate multifunctionality solution cannot be arbitrary but should be based on a clear motivation related to the goal and scope of the studied system (Pelletier et al., 2015; Vergé et al., 2016). Transparency is key when it comes to making these decisions (Pelletier et al., 2015). We have to keep in mind that allocation procedures are an artificial construct and therefore, none is perfect (Wilfart et al., 2021).

6.4.1 Organic versus conventional apple cultivation

For Global Warming, the median impact of the Belgian organic apple cultivation ranged between 202 and 684 kg CO_2 eq per ton (Fig. 6-6), depending on which allocation procedure was chosen. We compared this result to published LCA studies, though, keep in mind that the system boundaries between all the different studies are not completely equivalent.

Longo et al. (2017) calculated that organic apple cultivation in Northern Italy had an impact of 102 kg CO_2 eq per ton apples, while for conventionally cultivated apples this was 125 kg CO_2 eq/t. They stated that nitrogen organic fertilizers and mineral fertilizers were used in the organic and conventional farms, but they did not specify anything further. These results are lower than the results reported on in Fig. 6-6, however, Longo et al. (2017) only focused on the full production orchard stage. The study reported on in this chapter also included orchards in their low productive stage. For apple cultivation excl. organic fertilizer production, the four considered organic orchards had Global Warming potentials of 38, 39, 364 and 938 kg CO_2 eq/t.

For the Canadian apple production (Keyes et al., 2015), 64.1 kg CO_2 eq/t was attributed to conventional cultivation and 73.2 kg CO_2 eq/t to organic cultivation. It was not clear if this included the production impacts for manure. Alaphilippe et al. (2013) did state that the production of organic fertilizers (compost and feather manure) were included in their study on the French apple cultivation, though they did not specify how. They calculated results ranging from 32 to 38 kg CO_2 eq/t for conventional cultivation and from 50 to 84 kg CO_2 eq/t for organic cultivation in different regions and for different varieties for the full production orchard stage. Thus, only in the study of Longo et al. (2017) was the impact of organic apples lower than conventional ones.

6.4.2 Excluding organic fertilizer production (residual product)

When it comes to the different allocation procedures studied in this chapter, apple cultivation excl. organic fertilizer production could be justified if the total impacts from a unit process depend solely on the demand for the main product. Thus, it assumes that the amount of beef cow farming is independent of the demand of blood meal (Bier et al., 2012) or other organic fertilizers.

However, what would then happen if the demand of the main product decreases? What if we looked at for example co-produced animal foods within the hypothetical scenario where everyone decides to eat less meat? This would cause a change in beef production which would also affect milk production since beef can evidently also be from the dairy type (Barré et al., 2018). Barré et al. (2018) calculated that the reduction of ruminant meat would be limited in the hypothetical diet due to co-production constraints since the dairy consumption stayed stable. In that scenario, meat becomes the residual product that is eaten because of its availability. Not using it would in the end be introducing a new form of waste. This illustrates that as long as other bovine (derived) products, such as gelatin, hides, rennet, blood meal and manure are commonly used, the co-production constraints prevent completely detaching the demand of the main product from that from a residual product. It would be another story if all bovine (derived) products are substituted such as agar-agar for gelatin, faux leather, etc. While more and more of such kinds of alternatives are getting commercially available, it is not realistic (yet) to assume this as the “new normal”.

Additionally, excluding organic fertilizer production does not allow for a clear distinction when it comes to environmental impact, between processes where a low-value residual product is used instead of disposed of (Bier et al., 2012). This could possibly curtail waste-avoiding incentives. Also, when excluding organic fertilizer production, organic growers have an advantage over growers using more conventional mineral fertilizers for which fertilizer production is being included in the system boundaries. Organic growers do not carry any of the burdens of the production of something they clearly regularly use and require for a successful yield.

Though, it needs to be noted that organic agriculture does provide services for which they are (at the moment) not rewarded. These (ecosystem) services include biological control of pests, mineralization of plant nutrients, soil formation, carbon accumulation, nitrogen fixation, pollination, aesthetic, etc. (Sandhu et al., 2008). Conventional agriculture also provides those services but to a (much) lesser extent. Ideally, all the different kinds of products and services are included when the sustainability of two systems are compared. Boone et al. (2019) proposed a procedure to divide the environmental impact over the whole set of delivered agricultural outputs, meaning between the harvested product and other (such as regulating, maintaining and cultural) ecosystem services. That way the environmental impact of organic and conventional farming could potentially be compared more fairly.

6.4.3 System expansion

6.4.3.1 Choosing a substitute product

In system expansion, instead of the originally used organic fertilizers (i.e., blood meal and manure), the impacts of a substitute are attributed to the studied system (i.e., the apple orchard). Often, several substitution possibilities for the co-product are available, leading to multiple scenarios and different results (Heijungs and Guinée, 2007). Though, finding a true, representative replacement is difficult.

Notarnicola et al. (2015) proposed to consider the quantity of avoided mineral fertilizers in system expansion. A *mineral fertilizer* is not a perfectly suitable substitute, since the growers are (generally) not allowed to use it in organic cultivations. Though, it is possible that the organic fertilizers originate from conventional livestock farms, meaning that the bovines are fed with conventionally grown crops. Moreover, while mineral fertilizers are soluble and thus rapidly available to the plants, the nutrient release of organic fertilizers is rather slow. Mineral fertilizers also have a much higher nutrient content, so a smaller supply is needed to fertilize the plant than with an organic fertilizer (Chen, 2006; Roba, 2018).

The LCA results (section 6.3.2) show that ICs for which organic fertilizers have a relatively high contribution to the total impact (e.g., Land use, Human non-carcinogenic toxicity and Water consumption) are generally different from those where the mineral fertilizer has a high contribution (e.g., Stratospheric ozone depletion, Freshwater/Marine eutrophication, Human carcinogenic toxicity and Fossil/Mineral resource scarcity). Thus, using a mineral fertilizer for system expansion does not lead to realistic results for organic cultivation and can even distort decisions for reducing the environmental impact.

Since we are dealing with organic cultivation in this case study, we also searched for a clear-cut organic fertilizer (i.e., an *organic plant-based fertilizer*) as replacement. If a suitable replacement is found, the necessary data also must be available or has to be obtained for its impact to be included in the system. In this study, Monterra Bio Malt was used which consists of an unspecified composition of malt sprouts, corn gluten, vinasse and molasses (Servaplant, 2018). However, only vinasse was available in the LCA databases as an input process, and we were unable to find applicable data in literature for the other ingredients. Therefore, it was assumed that all NPK was supplied by vinasse. This assumption causes the impact of Monterra to be more of a rough estimate, illustrating how lack of data can be a serious hindrance when choosing for system expansion. Additionally, malt sprouts, corn gluten, vinasse and molasses are all by-products as well. For example, molasses, a by-product of the sugar production, is used as feed and in ethanol production (Nguyen and Hermansen, 2012). System expansion can therefore lead to further multifunctionality problems and system expansions (European Commission et al., 2010).

Just finding a suitable alternative is often not sufficient, transportation, energy use and equipment need to be considered as well. The FADN database did not allow us to distinguish for which purpose the energy was used. This probably led to an overestimation of energy use in the system expansion scenario, since less machine operations are needed when applying the substitute products to the orchards vs. spreading manure, given the difference in N-content (15% N for the mineral fertilizer and 4.5% for Monterra versus 0.71% and 0.48% for solid and semiliquid manure respectively). On the other hand, blood meal has an N-content closer to that of the mineral fertilizer (13% N), which may cause the difference in energy use to be more balanced.

6.4.3.2 Aligning the product quantities

Nitrogen was chosen as the common denominator to align the quantities of the original fertilizer products with the replacement products (Knudsen et al., 2010), since N was a common quantitative element in all fertilizer products and the right amount of N is crucial for a good apple yield (Bloksma, 2003). N also had the largest content percentage in manure and blood meal. Alternatively, P or K could have been used, however, blood meal does not contain those elements according to the FADN database (in reality, it might contain low amounts of P and K), and all fertilizer products need to contain the chosen element. This means that the amount of P and K provided by the substitute products were not equivalent to those of the original fertilizers.

Additionally, the use of organic fertilizers can affect soil organic carbon dynamics. For example, Aguilera et al. (2015) assumed, in their LCA of Spanish fruit tree orchards, that 30.5% of the carbon contained in external organic inputs (e.g., manure and manufactured organic fertilizers) is incorporated in the soil, thereby contributing to the net carbon accumulation. This effect on soil quality and thus on apple yield, was also not taken into account when selecting substitute products and amounts. Though, this aspect might become more relevant when the impact of soil organic carbon is incorporated into LCA (see section 1.4.2) or when carbon farming (EU, 2021) is introduced (see section 7.2.2).

It is clear that it is virtually impossible to find a substitution product for which the composition can be aligned to the original product, and that we have to make peace with the fact that – when choosing system expansion – the overall fertilization will never be completely equivalent.

6.4.3.3 Attributional vs. consequential approach

Knudsen et al. (2010) found no markedly different results for their three studied ICs when using system expansion compared to considering manure as a livestock waste in their consequential LCA on organic soybean. However, in our study, substantial differences were found. When looking at the organic plant-based fertilizer, a realistic substitute product for organic cultivation, system expansion led to the largest total impact of all possible allocation procedures (excluding mineral fertilizer as a substitute) in only 4 of the 18 ICs. This illustrates why system expansion is especially useful in consequential LCAs, while its appropriateness for attributional LCAs is questionable (Bier et al., 2012; Pelletier et al., 2015). Those results raise the question if growers should not permanently switch to more use of Monterra as their main organic fertilizer. However, the cost for the grower for replacing the original fertilizers with Monterra needs to be taken into account. According to the FADN database, the Flemish apple grower was frequently able to use manure for free and the price for blood meal was between 0.35 and 0.75 €/kg, giving a max price of 11.54 €/kg active N. Meanwhile, the price for Monterra Bio

Malt is 0.89 €/kg (Servaplant, personal communication, June 2020) or 30.43 €/kg active N, which could cause an unacceptable price increase for the grower.

The main problem of system expansion, according to Heijungs and Guinée (2007), is the accumulation of 'what if' argumentations. System expansion relies on factors that lie outside the coverage of the studied system (Bier et al., 2012). In contrast, allocation methods require fewer data and not a whole new system of avoided processes (Heijungs and Guinée, 2007).

6.4.4 Allocation methods based on a relationship

6.4.4.1 General observations: from the ideal situation to realism

With mass and economic allocation, manure and blood are not considered as residual products but rather as valuable co-products. Therefore, part of the impacts of the livestock system is ascribed to the system that uses the co-product as a raw material. It can be argued that when manure is freely available for the apple grower, it cannot be seen as a co-product. In regards to this, it is bizarre that allocation based on physical relationships is ranked above economic allocation, while still using an economic criterium to determine wheter a product can be classed as a co-product (Mackenzie et al., 2017; Wilfart et al., 2021).

The ideal situation would be for the LCA practitioner to consider the livestock system as part of the foreground system and collect all the necessary data to calculate the related impacts first-hand. However, this is often not realistic due to time-constraints and data unavailability. Different databases or published studies can, in that case, be chosen as the source of the impacts of the livestock system, if those are in fact available. In this study, the livestock system of all three organic fertilizers was the same (which might not necessarily be the case), making it rather straightforward to align system boundaries and LCIA methods. It goes without saying that when LCIA methods don't align, then the results of different studies cannot readily be combined.

Furthermore, choosing an adequate livestock system is crucial. In this study, the beef cattle system was chosen because of its high supply in blood that can be used for blood meal. Alternatively, the dairy cow system would also have been a realistic option because of its relatively higher supply in manure per animal. Milk would then be considered as part of the valuable co-products. We tested the influence of this in appendix C, which generally led to smaller total impacts for mass allocation and diverging total impacts for economic allocation.

Next to mass and economic allocation, biophysical allocation is also often used for meat and dairy farming systems, which is based on the feed energy required to produce the milk and meat (IDF, 2015). When manure is a valuable output of the farm, the FAO (2016) proposes to also apply a biophysical approach based on the energy for digestion needed to utilize the nutrients and create manure. In their example, they calculated an allocation factor of 77.5% for milk, 7.2% for meat and 15.3% for manure. For this study, we were unable to find how the consumed feed could also be transformed into an adequate allocation factor for blood meal. We could consider using the mass of blood per kg live weight to partition part of the impact biophysically allocated to beef, to blood meal. However, mass and biophysical allocation would then be combined, which may lead to inconsistencies in the methodology [as FAO (2016) also warns about when biophysical and economic allocation are used for different parts of the system].

6.4.4.2 Mass allocation

Choosing representative functions

Mass allocation requires the choice of appropriate masses to be used in the mass allocation factors (Bier et al., 2012). The chosen physical characteristics should relate to the use or purpose of the product. This characteristic should be relevant and common between the different low-value co-products, making it possible for competing products delivering the same function to be compared (Pelletier et al., 2015). Fig. 6-4 shows that depending on which masses are chosen, the results can differ between 13.39% and 95.76% of the beef farms' impact allocated to the organic fertilizers.

When only blood meal is used as an organic fertilizer, there are more mass allocation factors possible that could lead to credible results (analyzed in appendix C). For manure, however, they would lead to unrealistic results of allocating more than 100% of the beef farms' impact to the organic fertilizers, since their total mass would be used as basis. Thus, even though several mass allocation factors can be appropriate for different organic fertilizers, it might be a challenge to find a common one that leads to realistic results. Ideally, this would in the future by provided by guidelines such as the Product Environmental Footprint Category Rules (PEFCRs) for fertilizers, livestock and fruit products (European Commission, 2021).

Just as for system expansion, N was in the end chosen as a common quantitative element of which the right amount is crucial for a good apple yield (Bloksma, 2003). Thus, providing N is a representative function of the organic fertilizers. When looking at the possible mass allocation factors (Fig. 6-4), three options use the *N content of the organic fertilizer* as a basis. The first option, where the N content in the live animal and manure is used as the denominator is not considered as a realistic allocation factor for two reasons.

First, 87.21% of the beef cattle systems' impact would in that case be allocated to the organic fertilizers, which we interpret as not being an appropriate reflection of the real world seeing as beef production is the determining function of the beef system. Additionally, the organic fertilizers are secondary products which would (probably) be wasted if they were not used for organic cultivation. Allocating such a high percentage to the organic cultivation system could be unacceptable for the growers, possibly leading to the adverse effect of them avoiding the use of organic fertilizers from livestock systems.

Second, while the N content is a representative function of fertilizers, this is not the case for the beef cattle system. If we solely look at the beef cattle system (excluding any processing steps), the representative function of the beef cattle system is the mass of the live animal. A representative function for the beef system might also be "the mass of the meat" or "the protein available in the meat", if the slaughterhouse system is included within the system boundaries. Additionally, when the agricultural residues would be used in other systems, for example as feedstocks for biofuels, the approach we propose in this manuscript would be valuable as well, pending the search for another basis representative of the biofuel function.

In this study, we considered the mass of the live animal as being the most representative function for the beef cattle system. However, we need to keep in mind that for mass allocation, manure is considered a co-product of the beef cattle system and should therefore be included within the representative function (the N in blood meal is already included within the live weight). We therefore consider option D "kg N in organic fertilizer/(kg life weight + kg N in manure)" as the allocation factor which will lead to the closest approximation to the real world.

Mass allocation as the (un)preferred method in literature

When allocation procedures are scored objectively, allocation based on a physical relationship often comes out on top. Mass allocation using liveweight or carcass weight in a milk-meat system were preferred in the study of Rice et al. (2017) because those had the best pedigree scores. Wilfart et al. (2021) found that while literature and stakeholders of the meat supply chain generally do not prefer physical allocation, when the stakeholders scored the allocation rules on six criteria (i.e., ISO compliance, recognition, consistency, use of the results, applicability and stability of the results), physical allocation had the highest score.

FAO (2016) does not recommend basing allocation on physical parameters (but rather economic value) when the functions on the market differ between the different co-products (e.g., beef for nutrition and manure for fertilization). Indeed, physical relationships do not necessarily reflect the reason of existence of a process. Bier et al. (2012) argue that mass allocation does not take into account that meat production is the incentive for the existence of a beef system and not a low-value co-product such as blood meal. However, in the end they concluded that mass allocation based on blood meal as a fraction of all slaughter products excluding waste and losses, together with the option of excluding organic fertilizer production (or “waste assumption” as they call it), was the most appropriate method to consider the impact of blood meal in the production of a renewable thermoplastic.

Vergé et al. (2016) also recommend using mass allocation, because the individual animal is at the origin of the environmental impact and this way it is an “indivisible” component in the agricultural system. It does not make sense to assume that either meat, manure or hides cause a larger environmental impact, rather it is the animal “as a whole” that causes it.

It is important here to reflect on the perspective of different LCA practitioners. Either the allocation problem stems from having to allocate the impact of a studied system between different co-products, or the LCA practitioner uses a co-product from another system and introduces it in their studied system (as was the case in this study). FAO’s recommendation (FAO, 2016) is especially relevant for the first case. In our study, finding a common function for the different beef system products is less of an issue than finding a common function for the organic fertilizers. The question arises if these two perspectives could be aligned in some way. It is essential that all burdens are accounted for, without omitting or double-counting, when several LCAs are combined to obtain an aggregated view of a larger system (FAO, 2016). A clear consensus on the used methods and models is needed for this.

The methodology in the PEFCR (European Commission, 2018) using the relative economic value of manure on the one hand, and the methodology in Leip et al. (2019) using nutrient value on the other hand, consider to first allocate a part of the livestock systems' impact to manure after which a biophysical allocation is applied for allocating the remaining impact between the other co-products (i.e., milk and live animals). This can be a good first step to a consensus. Though, FAO (2016) warns for inconsistencies that may arise in the methodology when biophysical and economic allocation are used for different parts of the system. Additionally, both methods focus on manure specifically and more study is needed for allocating other organic fertilizers and co-products.

6.4.4.3 Economic allocation

Economic allocation makes sense in the way that production is stimulated by an incentive of financial income. As such, a low-value co-product should be allocated an equally low share of impacts compared to the primary product with high market value (Hauschild et al., 2018; Vergé et al., 2016). That way, economic allocation can be an incentive to ascertain that secondary products generate economic gains, and consequently reduce/avoid waste, because the more impacts allocated to the those products, the less impacts are allocated to the determining function or main product (Vergé et al., 2016). However, allocating impacts this way is questionable since the production of the by-products are dependent on the demand of the main product.

A difficulty encountered with economic allocation is the selection of an appropriate price for each related product (Bier et al., 2012). Unlike with allocation based on a physical relationship (using units such as kg, J, etc.), economic allocation uses monetary units (such as euro, dollar, etc.) which have no universal value. In addition to this, the value of an output often changes from region to region. It will probably be easier, and thus cheaper, to get animal-related fertilizer products in regions with a high livestock density. Results are therefore very much location dependent. However, economic allocation does allow to reflect the changing value and even status of a product (from waste to co-product or vice versa). For example, when the increase in livestock density of a country leads to price reductions for animal-related fertilizer products. Yet, the economic revenue may also be an artefact of regulatory policy (Leip et al., 2019). This is why Leip et al. (2019) used the price of a mineral fertilizer instead and took the nutrient equivalent of manure (which defines the amount of mineral fertilizers that provides the same amount of nutrients) into consideration, when calculating the nutrient value of the organic fertilizer.

This also means that economic allocation is (evidently) sensitive to market fluctuations. Prices vary based on various external factors, independent from the manufacturing process (e.g. subsidies, climatic events, etc.) and economic fluctuations can vary between co-products (Bier et al., 2012; Martínez-Blanco et al., 2014; Vergé et al., 2016), making it challenging or even impossible to do comparisons or research trends (Vergé et al., 2016). However, Cherubini et al. (2018) researched the effect of an arbitrarily ±50% price variation, causing only a little variation in the mean and standard deviation of their results. In this study, while the choice of mass allocation factor leads to big differences in impact (Fig. 6-4), the differences in results from economic allocation are relatively more contained (Fig. 6-5 and 6-7).

Economic allocation assumes a positive correlation between environmental impact and market price (European Commission et al., 2010), essentially saying that something cheap equals environmentally benign (Pelletier and Tyedmers, 2011) or even friendly, and thus has a low or no environmental impact. The danger connected to this is that relative ecological efficiency of alternative systems providing the same product, might be overlooked (Pelletier et al., 2015), and there would be less incentive for a company to introduce impact-reducing measures. The function of the product needs to be considered from an environmental perspective and not from their use in human society (Vergé et al., 2016). Therefore, using monetary values for allocating the impact of organic fertilizers does not seem like a good fit. Of course, this statement would need to be revised if it would become common practice to include the cost of the environmental impact of a product into its price, as has recently been experimented with in the German supermarket Penny (REWE Group, 2020). Next to the selling price, they also advertised the real cost of the product (including environmental end climatological damage) making meat, for example, 188% more expensive and apples 12%.

6.5 Conclusion

The diverging results of the different allocation procedures underline the importance of avoiding arbitrary choices and selecting an appropriate method. Each procedure has its pros and cons and leads to different results for the same product.

Excluding organic fertilizer production does not allow the livestock system from receiving the environmental benefits of valorizing its waste as a co-product. When looking at the system that uses the residual product, organic growers do not carry any environmental burden for a product they need for fertilization, unlike more conventional growers. Excluding organic fertilizer production is therefore not advised as a realistic allocation method, especially when different crop production systems are compared.

System expansion causes too many uncertainties in attributional agri-food LCAs. Speculative scenarios and subjective choices of factors that lie outside the studied system, can lead to distorted results. *Economic allocation* implies that the impact of an output changes with its price, while in practice, the manufacturing process stays the same. Next to the choice of which possible economic allocation factor should be considered, prices also vary within the factor.

In the end, we selected *mass allocation* using a representative allocation factor [such as "kg N in organic fertilizer/(kg live weight + kg N in manure)"] as the least bad option for allocating production impacts to organic fertilizers. Following the allocation hierarchy of ISO (ISO, 2006a), we conclude that there are possible allocation options using "a physical relationship" as a basis, so there is – in theory – no reason to go to the last tier option of using an economic value instead. Additionally, mass allocation will lead to the most stable and closest approximation of the real world, since no parameters from outside the system are needed. This approximation of reality is crucial when looking for impact-reducing solutions. Yet, it is clear that more research needs to be done when it comes to finding an appropriate allocation procedure that can be harmonized for all systems – if it exists at all.

PART IV

Finishing up

Chapter 7

General conclusions and future perspectives

The need for sustainable production and consumption is strongly present in todays' society. To achieve this goal, an accurate quantification of environmental sustainability is needed. LCA results can guide the way for making decisions without the risk of burden shifting, but only if those results are robust and unambiguous. The aim of this PhD thesis was to lift LCA to a higher scientific level with the goal of generating more representative results and making the choice of the most environmentally friendly option more conclusive, and this specifically with a focus on the agri-food sector. Two methodological shortcomings were tackled, the methodological ignorance towards uncertainty and variability in part II and the inconsistency between the system boundaries of organic and more conventional cultivation in part III.

7.1 Acknowledging both uncertainty and variability

7.1.1 Identifying the methodological shortcomings

Making conclusive decisions on what product or process is environmentally preferable is not possible when only using deterministic data. Yet, LCA results based on this kind of data is still being widely disseminated. 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. Uncertainty and variability have a different origin and therefore also a different implication. While uncertainty shows lack of knowledge, which can be reduced, variability reflect the natural heterogeneity in the world, which will always be observed.

It is clear that including uncertainty and variability in LCA results could lead to a wealth of information. However, including them is only possible if data quality and quantity allows it, and if defined methods are available and known to the LCA practitioner. A first step was therefore, to identify the different attempts that had been made in the past to separately account for uncertainty and variability in LCA. A systematic review was conducted for this and the results were discussed in Chapter 3.

A first observation from the systematic review was the lack of consensus on viewpoints, definitions, terminology and classification of uncertainty and variability. As it turned out, of the 562 records that were identified through database searching, only for 11 studies it was possible for the reader to conclude whether uncertainty or variability dominated the LCA results. While some studies effectively focused on separating uncertainty and variability, in others it seemed more as an after-thought, making it more of a happy accident that the reader could deduce which was dominating. Properly taking uncertainty and variability into account should be a part of the LCA process from the very start.

In general, (one-dimensional) Monte Carlo simulations were conducted to propagate uncertainty and variability, often in combination with some kind of sensitivity analysis. Two methods were specifically recommended in the end: (i) Monte Carlo simulations visualized in either variability and uncertainty ratios to identify which is dominating or (ii) Monte Carlo simulations extended with global sensitivity analysis to identify the most essential parameters. Each of the recommended methods still had its advantages and shortcomings, but the final choice between the methods depends on the goal and scope of the LCA study at hand.

The focus in this PhD thesis was on how uncertainty and variability can be propagated separately in LCA with the goal of identifying the dominating one in the results. Therefore, I specifically looked deeper into the methodological shortcomings associated with the first recommended method. In this method, the ability to characterize a parameter as both uncertain and variable was lacking and the visualization of uncertainty and variability in the results could be improved upon. The data source could also be limiting, since the method required a large dataset of individual systems, which is not always available or is not required for the goal and scope of the study. Thus, LCA practitioners in all research fields urgently need a method for propagating uncertainty and variability separately, in order to have more representative results. Two-dimensional Monte Carlo simulations (2DMC) was identified as a possible approach that allows to improve upon these shortcomings.

7.1.2 Decision guidance through two-dimensional Monte Carlo simulations

2DMC was applied in an agri-food LCA. This, because the agricultural sector is largely influenced by variability, while this is less the case for industrial processes in the secondary sector due to optimizations and standardizations. Nevertheless, 2DMC is a useful method and applicable in all LCA fields. In this thesis, 2DMC was used in the LCA of the Belgian apple chain where it was illustrated how it can be applied using different kinds of data sources, with (post-harvest) data mainly stemming from surveys in Chapter 4 and (cultivation) data from a large dataset in Chapter 5.

2DMC allows to separately portray uncertainty and variability in LCA studies in a clear and representative way. This can help decision makers in judging the robustness of differences in product comparisons, while also indicating how the overall uncertainty can be reduced. In Chapter 4, possible 2DMC outcomes for comparative LCAs are demonstrated. In contrast to risk assessment for which the absolute values of the 2DMC results are of utmost importance, the relative 2DMC results of several options are of more significance for LCAs. The shape and location of the 2DMC curves lead to different conclusions and thus have a different implication on decision/policy level.

When comparisons are being made between two (or more) products or processes, 2DMC first allows to check if the model outputs are clearly separated or not. Basing decisions on clearly separated model outputs is much more meaningful. When this is the case, a decision maker could robustly conclude that one option is preferable over the other. However, whenever the model outputs do show overlap, the overall uncertainty should first be reduced before making any definite decisions. Here, the uncertainty and variability ratios, that can be calculated from the 2DMC results, come into play. This means, when the uncertainty ratio is high, and uncertainty is thus dominating the results, more knowledge should be gathered before making any decisions. In contrast, if the variability ratio is high, and variability is thus dominant, this can – in theory – not be reduced. Even when more information is gathered, the variation will always be observed. The only way to possibly reduce the overall uncertainty would be by examining the production system and making physical changes in the system itself. However, the latter is not always possible or wanted.

7.1.3 Keeping the bigger picture in mind

Decision makers might conclude from Chapter 5 that a switch should be made from the cultivation of Kanzi to Jonagold apples, seeing as Jonagold is clearly environmentally preferable for half of the impact categories. Caution is advised when drawing such ill-considered conclusions. Instead of drawing the conclusion that only Jonagold should be cultivated, another conclusion could be that there is an opportunity for improving the cultivation of Kanzi apples. From its high variability, it is clear that cultivating Kanzi apples with a low environmental impact is possible, it just does not always happen for some reason. Those reasons should be identified first. Below, I will discuss five sources of variability that can either be reduced or where reduction is not possible or wanted.

Since the cultivation of Kanzi apples is dominated by variability, it is possible that the *management strategies* of Kanzi is not as optimized and uniform yet as it is for the Jonagold apples. In that regard, it could be advised to look into possible improvements of the pruning, fertilizer, pesticide, water and energy strategy used during cultivation. This would make it possible to reduce variability by making changes in the different management strategies.

The variability in Kanzi cultivation might also be due to the difference in *productivity related to tree age* between the different orchards. Since the Kanzi apple is not as old yet as the Jonagold apple and less orchards (only 36 in comparison to 973) were included in the assessment, it is probable that a higher percentage of trees are still in their young and low productive years, which is related to a general higher environmental impact (Goossens et al., 2017a). I specifically chose not to exclude those orchards, as to not contribute to the practice of excluding low productive orchards from agri-food LCAs and because I consider the impact of apples from the viewpoint of the consumer, who does not know from which orchard the apples originate. Variability due to age cannot be reduced, unless by waiting several years for the orchards to reach full productivity without establishing any new orchards in the meantime. Moreover, variability due to *weather circumstances* can also not be reduced.

Variability can also be caused by differences in *soil type*. The soil type could influence the productivity of the orchard and the amount of inputs that an apple grower needs to make for an optimal yield, since it determines – among other things – the presence of water and nutrients in the soil and their availability to the orchard. This variation due to soil type could theoretically be reduced by uprooting and replanting all orchards in one spot. This change in the physical system is, however, unwanted and unrealistic.

Finally, a difference in *legislation* between regions and countries can be a source of variability. For example, legislation dictates the maximum allowed fertilization dose per hectare and per year, for which a distinction is made between sandy and non-sandy soils (VLM, 2021). Given the complicated decision process at legislative or policy level, reducing variability through legislation might be unrealistic as well.

As a final note, I also want to emphasize that when it comes to making policy decisions regarding the preference of one variety over another, *consumer preference* cannot be disregarded. Uniformity should not be strived to when it comes to fruit varieties.

7.1.4 A second illustrative case study: local vs. imported food products

In this thesis, I used the apple agri-food chain as a case study to "try out" the studied methodological improvements. I will now use a second case study to illustrate the wider applicability of the methodologies, and how they can be used for solving specific problems. The second part of the case study, regarding allocation, is discussed in section 7.2.4.

"Buy local" is an often-used slogan these days. People generally perceive local food as being more healthy, safe and good for the environment (Feldmann and Hamm, 2015). We can look at the environmental aspect of buying our foods locally since this can be measured by using LCAs, which is increasingly being done (Frankowska et al., 2019a, 2019b; Goossens et al., 2019; Loiseau et al., 2020; Stoessel et al., 2012; Webb et al., 2013). Preliminary research in our research group (Ghysen, 2020) has for example shown that when it comes to fruit and vegetables bought in Belgium, it might be environmentally preferable to buy products that are produced in Belgium or its neighboring countries.

What our preliminary study especially highlighted was that to truly compare a local and imported product, all different agricultural areas, management practices, post-harvest processes, transportation routes and transportation modes, and seasonality should be taken into account and this for both the home country as well as the country from which products are imported. It is clear that this already inherently entails a lot of uncertainty and variability. Yet, the overall uncertainty in this case is often even larger since local, qualitative data from each origin country is often lacking, especially in case more products and origin countries are included in one study. Finding good sources (such as farmers), with which there is no language barrier, can be quite difficult. LCA practitioners frequently use general data instead, often from a published database. If the practitioner is lucky, the studied origin country is at least available in the database, however these land-specific processes are often based on single-point values or central tendencies, assumed to be applicable for the whole country. If the country is as big as the United States of America, China or Brazil, with their variety of different climates and soils within one country, one can already deduce that a lot of variability will be ignored. If the LCA practitioner is not so lucky, and proxy data needs to be used for the product (e.g., apple cultivation represents pear cultivation) or the origin country (e.g., the United Kingdom is substituted by The Netherlands), additional uncertainty will also be introduced.

Such a study requires extensive and thorough research, which is not always possible. In case the study is more focused and limited in time, the LCA practitioner first has to identify which part of the life cycle chain is responsible for the order of magnitude of the potential environmental impact. That would be the part where including uncertainty and variability will be most relevant. It depends on the question which part of the chain that is. For example, if Belgian apples are compared to imported New Zealand apples, then the focus could lie on the mode of transport, since that is a big contributor to the New Zealand apple impact (Goossens et al., 2019). In contrast, if Belgian apples are compared to imported French ones, the emphasis will most probably lie on including overall uncertainty for the agricultural part of the chain.

Nauta (2000) illustrated for risk assessment that improperly quantifying the separation of uncertainty and variability may be better than not separating them at all. The same might be true for LCAs. Meaning that, even introducing a small indication of uncertainty and variability, might already lead to more conclusive results. 2DMC offers the opportunity to propagate this uncertainty and variability through the LCAs of the studied products and countries, leading to more conclusive results on if higher yields compensate the added impacts due to transport.

7.1.5 Finetuning 2DMC for LCA

In this PhD thesis, 2DMC was introduced as an innovative approach to propagate uncertainty and variability separately in LCA. While the basic methodology and outcome possibilities are shown in Chapter 4, the method could still be improved upon and finetuned for LCA. The topics that will be further discussed are shown in Fig. 7-1.

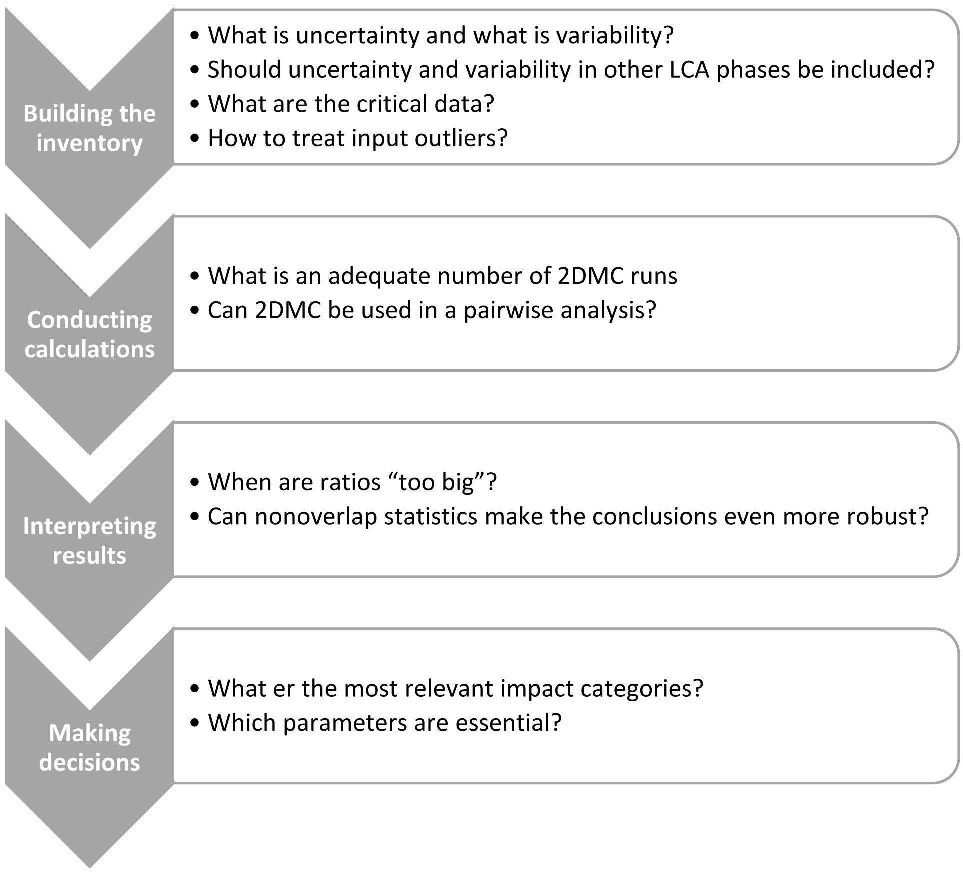

Figure 7-1 Flowchart showing different questions that can arise during the LCA process regarding 2DMC.

What is uncertainty and what is variability?

In Chapter 3, we identified the lack of uniformity and consensus when it comes to viewpoints, terminology and classification of uncertainty and variability. This lack of harmonization should be rectified to facilitate future product comparisons and communication, preferably in a focused session with LCA experts from all the different fields.

Should uncertainty and variability in the other LCA phases be included?

In this thesis, I focused on uncertainty and variability of the inventory phase, because this is the data that is (usually) gathered first-hand by the LCA practitioner and (usually) represents the bulk of their work. However, there is also uncertainty and variability in the other phases, such as the chosen time horizon for Global Warming Potential and the uncertainty of the lifetime of substances during the LCIA phase (Hauschild et al., 2018). For a complete list of examples for each LCA phase, I refer to Hauschild et al. (2018).

It would be interesting to see how broad the range of potential environmental impacts would be if all sources of uncertainty and variability in all LCA phases were included within one study. Though, in general, this would often not be very relevant or useful. If it would be done, there should still be a way to separate the different phases from each other, because they each give information to different stakeholders. If the LCA is being conducted for a client, such as a company or an association, the results from the inventory phase are relevant since they can directly influence that through improvements in the chain. In contrast, results from the LCIA phase would probably lead to confusion and miscommunication. Those results would, however, be very relevant for LCA database developers and the researchers concerned with the environmental mechanisms that underlies each impact category. It could be an incentive for them to focus on improving specific models or principles that are being used. So, it depends on the stakeholders which LCA phase should be studied regarding uncertainty and variability; one, two, or maybe even all of them.

What are the critical data?

2DMC is only possible when enough data is available to construct input probability distributions and when there is enough time to do so. It is therefore advised to take uncertainty and variability into consideration from the very start of the LCA process. Sufficient data can only be obtained if information on uncertainty and variability is collected already during the LCI and/or by collecting additional data. When there are limitations to gathering all the necessary data, and to be time-efficient, a LCA practitioner might wish to focus on only gathering the truly critical data. We have to keep in mind that we are constructing a relatively simple model to represent a very complex reality. Decisions need to be made on which data can be left out as insignificant, perhaps without sufficient evidence to back this up (Vose, 2008). Local sensitivity analyses and screening methods could in that case be used as a preliminary step to identify the most influential parameters on which the focus should lie for gathering more data. It would be interesting to study if doing this preliminary step truly leads to equivalent results and where the border lies for gathering the sufficient amount of additional data.

How to treat input outliers?

In Chapter 5, the cultivation of Kanzi apple showed some unexpectedly large 2DMC results. This was caused by the small dataset of “only” 36 orchards that was used. The smaller dataset caused input outliers to have a larger influence, leading to right-skewed input probability distributions when those distributions are fitted. Outliers can, for example, stem from data that was incorrectly registered in the database or from small yields. Several outlier treatment options were proposed such as removing those outliers beforehand, or only showing a limited part of the 2DMC results. However, in each of those cases possibly valuable data is being omitted and some transparency is lost. Therefore, the different outlier treatment methods should be tested out (and potentially more identified) to analyze how small datasets can still lead to adequate 2DMC results.

What is an adequate number of 2DMC runs?

In this PhD thesis, 10 000 iterations and 250 simulations were conducted, leading to 2 500 000 possible LCA outcomes shown in 250 2DMC curves. This total number of runs was chosen after some preliminary tests to have a good sampling of the full range and shape of each input probability distribution and for compatibility with

Microsoft Excel (Excel can only plot a maximum of 255 data series per graph). R could have been used to solve this restriction. However, the chosen settings seemed large enough to get a full representation of all possible LCA results.

The accuracy of Monte Carlo simulations output increases when the number of iterations increase, up to an unknown plateau level. There is no general specific number of iterations that is large enough, rather it depends on when convergence is reached in the output of a specific model. Though, this differs for each model and there is a lack of consensus of when convergence is actually reached (i.e., when a subjective measure is acceptably low). Von Brömssen and Röös (2020) state that "it is easy to get significant results by doing enough simulation runs, even though no new information is added and no generalizations can be made from the results." In this regard, Heijungs (2020) suggests to limit the number of Monte Carlo runs to a number not greater than the sample size of the input parameters, because an excessive amount of Monte Carlo runs will optimize precision while ignoring inaccurate inputs. However, this very recent suggestion would mean that in Chapter 5 for the Kanzi orchards, we should only have conducted 36 Monte Carlo runs (for the iterations or simulations or in total), ignoring the fact that distributions by themselves should be identified based on their representativeness and link with reality. Von Brömssen and Röös (2020) blatantly call Heijungs' suggestion incorrect since the simulations are a theoretical construct and therefore there is no way to determine the right number of simulation runs. Vose (2008) recommends to use the carnal rule that to produce a model that is both accurate and realistic, every iteration should be a scenario that could be observable in real life. It is clear that there is still some controversy going on when it comes to the adequate number of Monte Carlo runs; and that what applies for 1DMC, cannot necessarily be applied for 2DMC.

In the end, the chosen number of iterations is often a trade-off made by each LCA practitioner individually between acceptable accuracy and needed computation time (Hauschild et al., 2018; Igos et al., 2019). In Chapter 3, we argued that even though computation time might appear long, it may be relatively short compared to the time needed to complete, for example, the data inventory analysis. Additionally, computational power is increasingly improving, and solutions exist on software and hardware level. Further research is needed to find a clear balance between computation power, convergence, precision, accuracy and realism, when it comes to the number if iterations and simulations in 2DMC.

Can 2DMC be used in a pairwise analysis?

LCA is most frequently used in a comparative analysis. There are several ways to do this. In Chapter 4 and 5, we compared the absolute results (i.e., the two-dimensional cumulative probability distributions) of two products. In Chapter 3, we saw that AzariJafari et al. (2018) used a pairwise analysis for their comparative LCA. They took the relative uncertainty and the relative variability of two products (option A and option B) into consideration by subtracting the results of option B from option A. That way, the results showed in how many of the (one-dimensional) Monte Carlo iterations, option A had less impact than option B. This method has the advantage that 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). According to Hauschild et al. (2018), there are two frequently used methods for this, either subtracting (A-B) or dividing (A/B). Thus, option A has a lower impact than option B when A-B<0 or A/B<1, respectively. It would be interesting to conduct such pairwise analysis using 2DMC, to see if uncertainty and variability can still be visualized the same way and if the ratios show a noteworthy change.

When are ratios "too big"?

In Chapter 4, we advised that the uncertainty and variability ratio should be looked into when the 2DMC results of the product or processes that are being compared, overlap. It might also be relevant to look into the data uncertainty and variability when the ratios are "too big". The question then arises: when is a ratio "big"? In Chapter 4, for the apple post-harvest chain, the maximum uncertainty ratio was 1.02 and the maximum variability ratio 2.49. In Chapter 5, for the cultivation chain, the maximum uncertainty ratio was 2.31 and the maximum variability ratio 7.10. It might be interesting to look into a possible maximum limit for each ratio that indicates when definite choices cannot be made (even when the 2DMC results do not overlap) without looking into the source of the uncertainty and/or variability first.

Can nonoverlap statistics make the conclusions even more robust?

In this thesis, cumulative probability plots were used to visualize 2DMC LCA results. The cumulative probability plots of the two options could either show no overlap or overlap. We judged that the first scenario leads to a robust conclusion and the second one indicates which steps to take – based on the ratios – to reduce the overlap. We need to reflect here that if the 2DMC output was shown as histograms, all impact categories for both comparisons (bulk vs. pre-packed and Jonagold vs Kanzi) would show overlap. It's not because there is no overlap of the cumulative probability curves, that a randomly chosen 2DMC LCA result from option A and from option B cannot be equal. The probability that the randomly chosen bulk or Jonagold result is lower than their counterpart is – of course – higher, but it is still for example possible that a Kanzi orchard performs better when it comes to Particulate Matter impact than a Jonagold one (Fig. 5-1). In our studies in Chapter 4 and 5, we thus focused on the difference in cumulative probability of the options. It is possible that conclusions can be made even more robust by calculating nonoverlap statistics of the histogram outputs.

Cohen (1988) defined three such measures for the degree of nonoverlap (U_1, U_2 and U_3; Fig. 7-2) for cases where the histogram distributions being compared are normal with an equal standard deviation. U_1 is the area that does not show overlap. Thus, when $U_1 = 0$ there is 100% overlap or 0% nonoverlap between option A and B. U_2 is defined as the percentage of the higher distribution that exceeds the same percentage in the lower distribution. For example, the highest 60% of option B exceeds the lower 60% of option A. Lastly, U_3 is the percentage of the lower distribution that is exceeded by the upper half of the cases of the higher distribution. This means that the upper 50% of option B exceeds, for example, 90% of the values of option A.

Variations of Cohen's measures (1988) have been published since (Grice and Barrett, 2014; McGraw and Wong, 1992). In case of non-normal distributions, Bhattacharyya coefficient might be used (the coefficient is 0 for perfectly separated distributions and 1 for distributions that perfectly coincide) or variations thereof (Heijungs, 2021; Qin and Suh, 2018). Though, Heijungs (2021) argues that the decision maker might have difficulty interpreting those results.

It will have to be studied how these kinds of nonoverlap statistics can be adapted for 2DMC [e.g., which curve(s) should be used] and if these statistics can actually contribute to the robustness of 2DMC LCA results. If that is the case, meaningful thresholds should be defined that indicate when a certain measure shows a significant difference between the two alternatives. It should then also be researched if/how the measures can be used when more than two options are being compared.

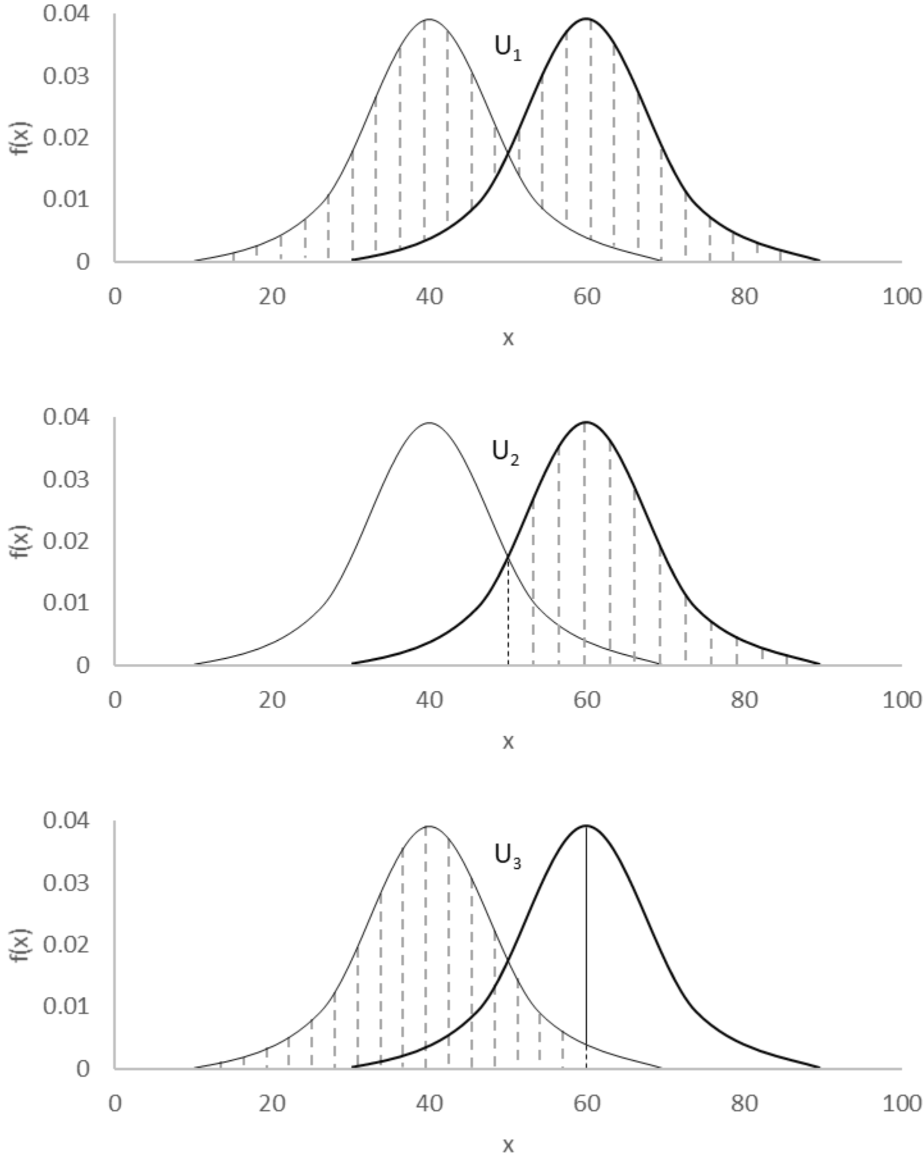

Figure 7-2 Nonoverlap statistics U_1, U_2 and U_3 as defined by Cohen (1988).
The two distributions represent option A and option B, with B having a larger line width. The grey indicated areas represent consecutively U_1, U_2 and U_3. Graphs are adapted from the supplementary material of Heijungs (2021).

What are the most relevant impact categories?

In Chapter 4 and 5, we saw that the overall uncertainty should be reduced before taking definite decisions for 1 out of the 16 impact categories for the apple post-harvest chain and for 8 out of the 16 for the cultivation chain, respectively. One might wonder if it is really worth the effort and resources of looking into the overall uncertainty of those select few impact categories, when a definite decision can already be made on which product is environmentally preferable from the majority of all impact categories. In such cases, it could be beneficial to identify the most relevant impact categories first. For the Product Environmental Footprint (European Commission, 2018), the most relevant impact categories are defined as all impact categories (at least three) for which the normalized and weighted results contribute to at least 80% of the total environmental impact. However, 2DMC provides a range of results, making this method not so straightforward. Further research is needed to find a suitable method for the identification of relevant impact categories using 2DMC results or a consensus needs to be reached on which impact categories are relevant for each product/process separately. Normally, this should be achieved when Product Environmental Footprint Category Rules are provided for all products (European Commission, 2021).

Which parameters are essential?

Determining the output variance, using 2DMC, is much more meaningful if it can be combined with a sensitivity rating. As we saw in Chapter 1 and 3, the parameters towards which the model output is sensitive and that are highly uncertain, are the essential parameters to look further into. Wolf et al. (2017) identified those respectively by combining a local and a global sensitivity analysis. For the global sensitivity analysis, they first conducted (one-dimensional) Monte Carlo simulations to determine the output variance. Then they calculated the standardized regression coefficients to determine the parameters' contribution to the output variance, which they used as a proxy to calculate total sensitivity indices. They used this to explain how much each input parameter contributes to the output variance (Groen and Heijungs, 2017). Further research is needed to determine how 2DMC can potentially be used in a global sensitivity analysis and how it can be combined with a local sensitivity analysis, in order for the essential parameters to be determined.

7.2 Connecting systems through allocation

In this section, the second methodological shortcoming regarding the allocation issue arising when organic fertilizers are used, is discussed. First, the inconsistency in LCA between organic and conventional cultivation for fertilizers is clarified. In the following section, I explain why mass allocation is preferred to other allocation methods. Third, the second case study on local vs. imported food products is used to illustrate how the different allocation procedures can cause issues in a broader context. Fourth, I focus on the need for harmonization and regulation when it comes to using these allocation procedures to connect different systems. In the fifth section, I question if allocation should and can be included into Monte Carlo simulations. In the final section, organic fertilizers are compared to recycled materials.

7.2.1 Inconsistency between system boundaries due to multifunctionality

Comparing options to reduce environmental impacts is only effective when the system boundaries of the different options are consistent. That is often not so straightforward, seeing as most processes are multifunctional, while LCA is based on analyzing single systems. Several methods exist to have different multifunctional systems approximate each other's system boundaries i.e., subdivision, system expansion and allocation.

Equivalent system boundaries are lacking when organic crop production systems are compared to more conventional ones. Generally, when residual products from livestock systems get a second life as organic fertilizers, the impact of producing those residual products are ascribed to the livestock system, thus the system where it originates from. Meaning that no production impacts of those organic fertilizers are allocated to organic cultivation, the system where it is used and very much needed. This is in contrast with mineral fertilizers, used in conventional crop production systems, for which the production impact is allocated to the system where it is used. This inconsistency between organic and conventional crop production can lead to skewed LCA results. To solve this issue, more insight is needed on how to handle issues concerning system boundaries, multifunctionality and allocation in agricultural systems.

7.2.2 A preferential method for residual products from livestock systems

In Chapter 6, we studied the effect of excluding versus including the production impacts from blood meal and manure (residual products from the beef system), and how the different allocation procedures can lead to very diverging results for organic apple cultivation in Flanders. Next to subdivision, which was not possible for this case study, ISO (2006a) proposes system expansion to avoid having to use allocation for such a multifunctionality problem. It was clear that this method leads to too many subjective choices and arbitrary assumptions for attributional LCAs. For organic cultivation specifically, an alternative product that could realistically be used during crop production is a plant-based fertilizer. However, these kinds of fertilizer are often themselves created from residual products, causing again problems regarding multifunctionality.

Alternatively, a mineral fertilizer could be assumed as a possible substitute, but this product would not be allowed for fertilizing organic orchards. The mineral fertilizer also often led to opposite results when compared to the plant-based fertilizers or the results obtained using the allocation methods. For example, the Global Warming impact for organic apple cultivation using a mineral fertilizer as substitute led to an impact of twice as large compared to all the other considered procedures. This is contradictory to the goal of approximating reality.

The next method recommended by ISO (2006a) in their allocation hierarchy, is allocation based on a physical relationship. Several possible relationships were studied, based on different mass flows. When choosing a mass allocation factor, it is most important that it is representative for the function performed by the residual products. This to guarantee that comparison of similar products from other systems is possible. The mass allocation should also not cause any burden shifting from the primary function to the co-product. Thus, the chosen mass allocation factor should still reflect that beef production is the purpose of the beef farm and not fertilizer production; again with the goal of generating representative results.

No parameters from outside the studied systems were needed to calculate the mass allocation factors, thereby reducing the influence of unrelated factors. This is not the case when conducting economic allocation, which is the last tier option of ISO’s allocation hierarchy (2006a). In theory, this option did not even need to be explored seeing as mass allocation lead to reasonable results. However, it was included seeing as it is one of the most used methods for solving multifunctionality problems. Economic allocation implies that the price of a product is somehow a valuation of its environmental impact, which is clearly not true. For example, when comparing two pig farms, one who uses a low ammonia emission stable system and one who has not, the first farm will have a lower (among others) acidification impact than the latter. Yet, the price for pork remains the same. The most important here to remember is that we strive towards the most accurate calculation of environmental impacts and – at the moment – mass allocation seems the best way to do that.

In mass allocation, the N content of the organic fertilizers was used to calculate the allocation factor, since it represents the function of the fertilizers. However, this could potentially change in the future if carbon farming is introduced. Carbon farming is a new way of farming to sequestrate carbon[11] in the soil (EU, 2021). There are several ways to do this, from small adjustments on farm level, such as applying fertilizers rich in carbon, to big changes in the entire farming system, such as agroforestry. With carbon farming, farms would be able to receive certificates that allow to emit greenhouse gasses, which they can use themselves or sell to other companies (EU, 2021). If this system is introduced, not only the N supply to the orchard, but also the C supply to the soil (if it is supplied well, ensuring carbon sequestration), would represent a relevant function of the organic fertilizers. In that case both the N and C content of the organic fertilizers could be seen as representative functions of the organic fertilizers and the mass allocation factor would need to be adapted.

7.2.3 A second illustrative case study: local vs. imported food products

Another example of a possible incompatibility of the defined system boundaries is when local food products are compared to imported ones. The same skewed LCA results can occur when comparing the cultivation impact of different countries. The management strategies in both countries will most probably substantially differ based on which resources are available and fits the farmers' budget. It is possible that the export country mainly relies on manure for fertilization. If organic fertilizer production is then excluded during the impact assessment, it could lead to skewed results when comparing with conventional crop production in the home country.

[11] Carbon sequestration is the long-term storage of carbon in plants, soils, geologic formations and the ocean. It typically refers to carbon that has the immediate potential to become carbon dioxide gas (Selin, 2019).

System expansion would in this case lead to even more subjectivity and assumptions, since multiple substitute fertilizers are needed/possible. It would not be realistic to assume that both countries have the access to and need for the same substitute fertilizer.

In Chapter 6, we argued that the value of an output can change between regions. This is definitely the case for manure, for which the price – among other things – depends on the livestock density of the region. This means that in one country the farmer might be able to get manure for free, while in the other country the farmer has to pay for it. In the case of economic allocation, this would lead to 0% allocation factor for the first country which would not be the case for the second. Or it might even go further than that. It could mean that in one country, the manure would be considered as residual while in the other country, it would be a co-product. Different allocation approaches would then be used for the same product. The recommended procedure in this thesis would solve this issue. By using mass allocation for which the allocation factor represents the function of the fertilizers, a representative comparison can be guaranteed. It is possible that the impact of the livestock system differs substantially between the two countries, and by using the proposed mass allocation procedure, this can be taken into account as well.

As a side note, it should be mentioned that it is also quite possible that organic and mineral fertilizers are used alongside each other. *Organic fertilizers* increase the organic matter content in the soil which improves the soil structure and the exchange capacity of nutrients. They also – among other things – enhance soil biological activity, colonization of mycorrhizae, root growth and the growth of beneficial micro-organisms and earthworms. However, they have a comparatively low nutrient content, which is slow to release, and which might not contain all necessary plant nutrients in the sufficient quantity for maximum crop growth. Their composition is highly variable, making accurate application of nutrients to match crop needs difficult (Chen, 2006; Roba, 2018).

Mineral fertilizers, on the other hand, have a high nutrient content which is usually immediately available for the plants, causing a fast effect. This can also lead to negative effects if the fertilizer is overapplied, possibly resulting in leaching, pollution of water resources, acidification, increased crop susceptibility to disease attacks, destruction of soil organisms, etc. Mineral fertilizers enhance the decomposition of soil organic matter, causing a degradation of the soil structure and a reduced fertilizer efficiency (Chen, 2006; Roba, 2018).

Different studies have shown that the combined application of the fertilizers can be a sustainable and cost-effective way to increase soil fertility and productivity, while reducing the negative impact of mineral fertilizers on the environment. The long-term benefits of organic fertilizers are then combined with the short-term ones of mineral fertilizers (Chen, 2006; Roba, 2018). Again for this example, if a combined application is the case in an LCA study, then both production impacts should ideally be accounted for to be consistent.

7.2.4 Further harmonization opportunities

LCA practitioners typically focus on the system that is being studied when solving multifunctionality problems. This means that the perspective when the multifunctionality problem stems from one system producing different co-products, is different from the perspective when a co-product from another system is introduced in the studied system. For example, allocating impacts between different co-products in the dairy farm (e.g., meat and milk) versus introducing manure, a co-product from the livestock system, in the apple cultivation system. For the first, a common function for the different dairy system products is needed and for the second a common function for the fertilizers. The difficulty also lies in the lack of data. Typically, when researching the beef system, there is no real data available on where the different co-products are used. The same goes for the orchard system. It is not clear from what type and which livestock system the organic fertilizers originate. Connecting these two systems is therefore very challenging, with a lot of assumptions as a consequence.

Further research must therefore focus on finding suitable and realistic allocation procedures that can be used for each possible co-product a system produces. Oftentimes, the focus still lies on the high-value co-products in multifunctional systems, such as meat and milk in dairy systems. However, the low-value by-products must not be dismissed, and the procedure must also be applicable for e.g., manure, blood, hides, tallow, etc. Ideally, a uniform LCA for each system in each agricultural region will eventually be available that can be used as a standard system data source when certain co-products of that system are needed but the real origin is unknown. At the same time, general assumptions for each co-product destination are needed for each region as well. Clear regulations are needed on where the system boundaries should lie for each system to ensure that proper comparisons can be made.

7.2.5 Combining allocation with Monte Carlo simulations

In Chapter 5, we saw that integrated cultivation for Jonagold led to 2DMC results ranging between 1 and 920 kg CO_2 eq/t. In Chapter 6, the organic cultivation of Jonagold apples excluding organic fertilizer production caused a potential impact of 202 kg CO_2 eq/t. The recommended mass allocation method would have led to 267 kg CO_2 eq/t. One might wonder how relevant the application of an appropriate allocation method is, when there is already such a range of potential impacts by included uncertainty and variability in the inventory phase. Is the extra 65 kg CO_2 eq/t resulting from the recommended allocation method really where the focus should lie in the grand scheme of things? Though, to be consistent, one should not then just add the absolute production impact, but also consider the uncertainty and variability in the livestock system. This in turn could also lead to a wide range of potential impacts that then have to be added to the range of impacts of the apple orchard. So, the difference might not be that small after all.

Moreover, the maximum impact for the organic apple cultivation would have been received by using system expansion with mineral fertilizer as substitute product, leading to 684 kg CO_2 eq/t. This is a substantial difference from the 202 kg CO_2 eq/t from the "excluding production impact" approach. Should we then include the uncertainty due to choice caused by the different allocation possibilities in our assessment?

In the past, this has been done by Mendoza Beltran et al. (2018a, 2016) using (one-dimensional) Monte Carlo simulations. For each applicable allocation procedure that could be used in their LCA, they assigned a "methodological preference". If only one procedure is applicable for a multifunctional process, then the preference is 100%. If three procedures are applicable then they each get a percentage p_1, p_2 and p_3, all adding up to 100%, which represent three ranges [0 to p_1; p_1 to $p_1 + p_2$; $p_1 + p_2$ to $p_1 + p_2 + p_3$]. Then, during the Monte Carlo simulations, a uniform distribution (from 0 to 100) is sampled alongside the probability distributions from parameter uncertainty. If, for example, the sampled value is smaller than p_1, the first allocation procedure is used; otherwise, one of the other two is used, depending on in which range the sampled value belongs. This leads to a Monte Carlo output probability distribution that shows the effect of both choice and parameter uncertainty. Other discrete choices could also be included in the Monte Carlo simulation this way (for example, the choice of different time horizons for Global Warming Potential). The contribution of the choice uncertainty versus parameter uncertainty to the overall uncertainty could potentially be identified through a global sensitivity analysis (Mendoza Beltran et al., 2016).

Again here, as in section 7.1.5, it depends on the stakeholder how useful and relevant this information is. Just as with the data inventory phase, an LCA practitioner has a lot of influence when it comes to choosing the allocation procedure, as it is part of the goal and scope definition phase (by using the method, two LCA phases would be mixed). However, the influence of the allocation procedure does not provide relevant information to the stakeholder, since it is not something they can control, rather it is something on which a consensus should be reached by the LCA community. This consensus might be to keep using the method proposed by Mendoza Beltran et al. (2016) or to use one allocation approach instead.

7.2.6 What about recycling?

In this thesis, I specifically focused on methodological improvements for agri-food LCAs, and in the case of allocation, the focus was on organic fertilizers. One might wonder how applicable the considered allocation procedures are for other sectors. The applicability for feedstocks for biofuels was already mentioned in Chapter 6, though, this is still related to the agricultural sector. When looking broader to more industrial multifunctional processes in the secondary sector, the recycling(/reuse/recovery) of end-of-life products and of waste is a prevalent allocation issue. A product to be recycled has two functions: first the function(s) the product is primarily made for and secondly the function of providing secondary resources for use in subsequent life cycles or systems (European Commission et al., 2010).

The question thus arises for products such as wastepaper, waste glass, scrap steel, etc., if production impacts are allocated to them, how many recycling rotations should then be considered and for how long? The recycled products are (generally) not usable forever, there are always some losses in quality and/or quantity that should be accounted for. For example, wastepaper fibers keep getting shorter and more damaged each time they are recycled. Regarding the time aspect, it is possible that, for example, metal based products (e.g., aluminum windows) will only be recycled in ten, twenty or even more years, assuming that the material will even still be in demand by then (Frischknecht, 2010). Allocating impacts to such “waste” products would mean introducing a lot of assumptions and subjectivity. So, there is ground for allocating all impacts to the original production and considering recycled material as burden-free. Though, from the perspective of attributional modelling, it is appropriate to assign a share to both the system that generates the end-of-life product or waste and to the one that uses it as a secondary good (European Commission et al., 2010).

A clear distinction here between organic fertilizers and products to be recycled, is that organic fertilizers are only used once and (normally) very soon after its production (depending on which fertilizer). Thus, the question of how many times it is recycled and when is not relevant here. This makes allocating impacts much more straightforward. And yet, theoretically, one might say that the nutrients resident in manure actually are recycled. They are the same nutrients that were applied to the crops that were fed to the livestock. Crop production and manure are thus linked via the nutrients available in feed. Applying manure could, in that case, be regarded as a recycling situation. Should manure then also be allocated an impact share from the fertilizer that was applied on the feed crop? And how far back should that go? This would differ based on the kind of fertilizer that was assumed to be used to fertilize the feed crop. If a mineral fertilizer is assumingly used, then only the one-time impact of producing the mineral fertilizer would be relevant. However, if it would be assumed that manure is used, then this could lead to a loop of “feed leading to manure leading to feed leading to manure” … This can occur between farms or within the same farm, applying an integrated crop-livestock farming system (FAO, 2021).

Looking further forward, since we considered apple cultivation as a case study, the recycling would stop since the apples – and thus the nutrients – are (presumably) eaten by humans and human feces are (in Belgium) not used as a fertilizer. Human feces are treated at sewage treatment plants, where the nutrients end up in the sludge. It is prohibited in Belgium to use this sludge on agricultural land (VLM, 2021). Thus, it would not be necessary to account for future recycling of the nutrients since they don’t end up on agricultural soil again, only for past ones. But again, this would mean introducing a lot of assumptions and subjectivity.

Frischknecht (2010) argues that the allocation modelling approach should also be chosen based on it representing *weak or strong sustainability*[12]. He uses climate change emissions of aluminum manufacture as a case study and explains that the end-of-life recycling approach (which is equivalent to the "crediting" approach of system expansion i.e., the livestock system is credited for avoided burdens of a mineral fertilizer product) would represent weak sustainability since the concentrated metal that is potentially recycled in the future is considered equivalent to the natural capital represented by the avoided climate change impacts. Meanwhile, the recycled content approach (or cut off approach, which is equivalent to considering organic fertilizers as residual products) accounts for the environmental impacts at the time they occur and is, thus, in line with strong sustainability since natural capital (climate change credits) is not replaceable by man-made capital (concentrated aluminum). The recommended approach for organic fertilizers, mass allocation, would then also be seen as strong sustainability, since the production impacts are also accounted for at the time they occur.

To sum up, I believe that for organic fertilizers we should account for the production impacts at the moment they occur since they are not a typical recycled product and to avoid making too many assumptions. Thus, use the recommended mass allocation method. The same conclusion could potentially hold for other processes, like scrap steel. Nevertheless, separate and focused research is advised to come to robust approaches that lead to representative results for the secondary sector.

In conclusion, I have shown that with the discussed methodological improvements, comparing products and processes to assess their relative environmental impacts will be much more robust and conclusive. Though, further research is needed to finetune 2DMC for LCA and to further harmonize the system boundaries and allocation methods when multifunctional processes come into play. Nevertheless, every improvement that is made for approximating reality has an added value when choices have to be made regarding sustainability. Clear decisions are much needed on industry, consumer and policy level to guide the way to sustainable production and consumption.

[12] *Weak sustainability*: total capital shall remain constant, depletion of natural capital can be compensated by a surplus in man-made capital vs. *strong sustainability*: natural capital shall remain constant, independent of man-made capital (Frischknecht, 2010; Neumayer, 2013).

PART V

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PART VI

Appendices

Appendix A

A.1 Apple post-harvest inventory

Please refer to the electronic supplementary material.

A.2 2DMC results for the post-harvest chain

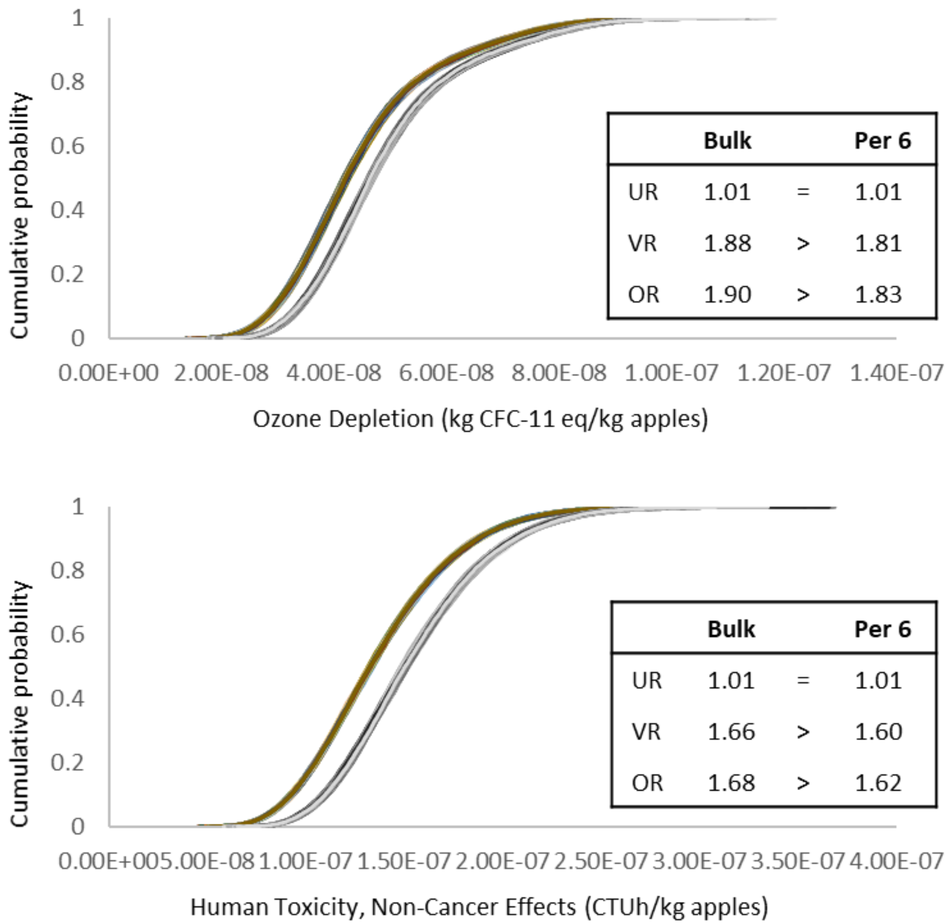
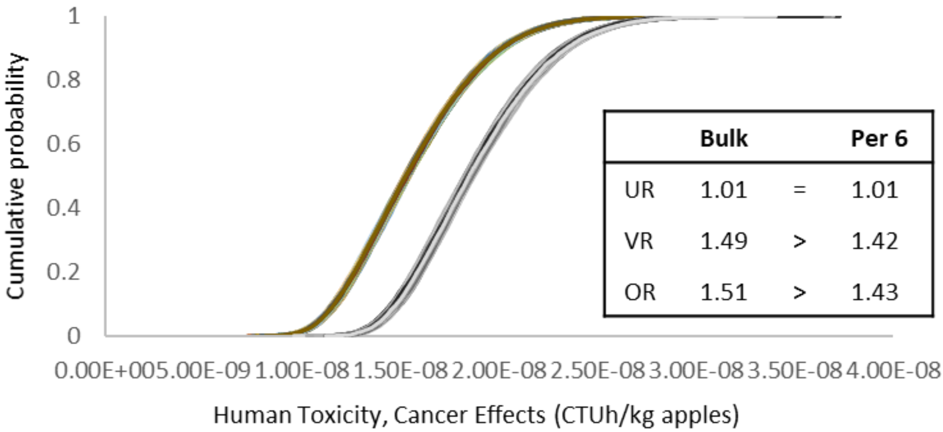
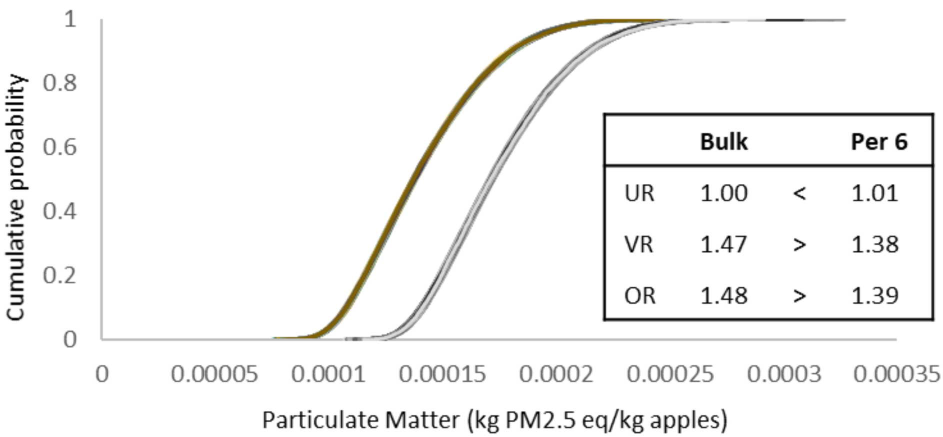


Figure A-1 2DMC results for the post-harvest chain.
The bulk apples are colored and the pre-packed apples are shown in greyscale. UR = uncertainty ratio, VR = variability ratio and OR = overall uncertainty ratio.





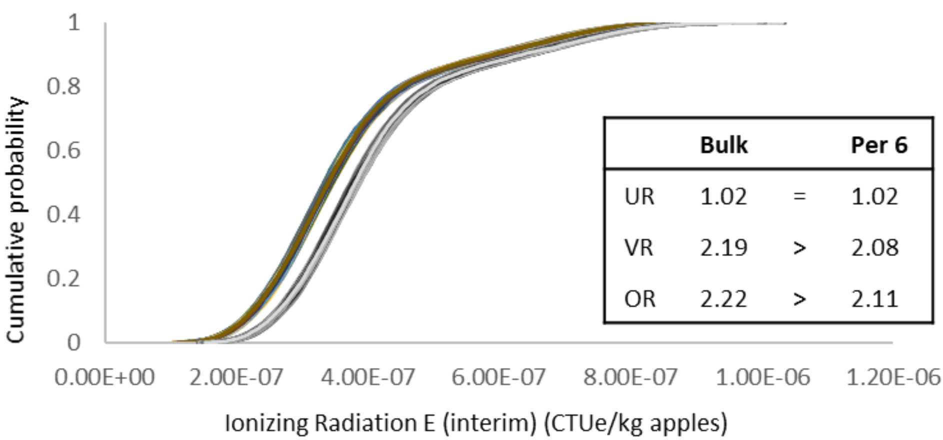


Figure A-1 Continued

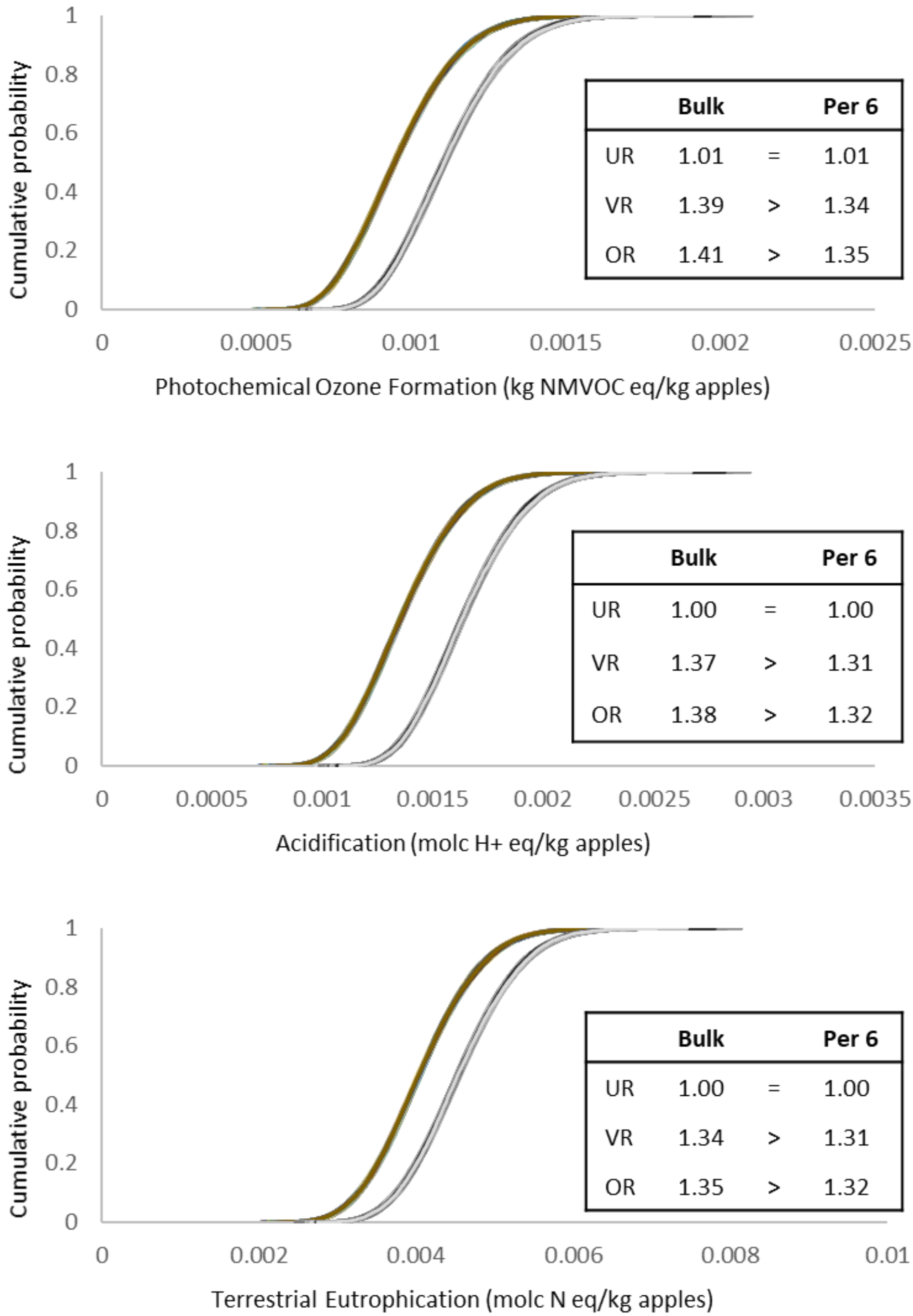
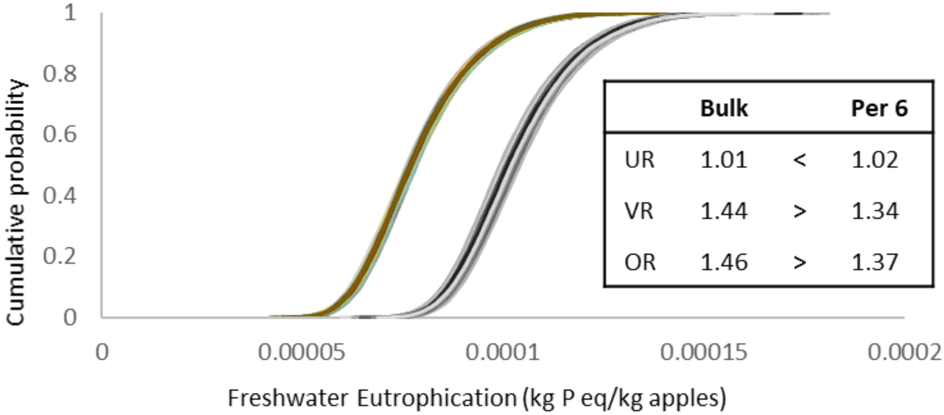
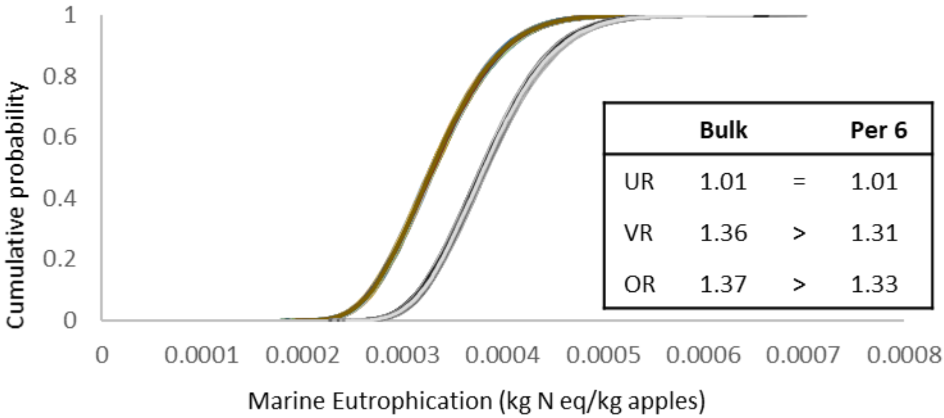


Figure A-1 Continued





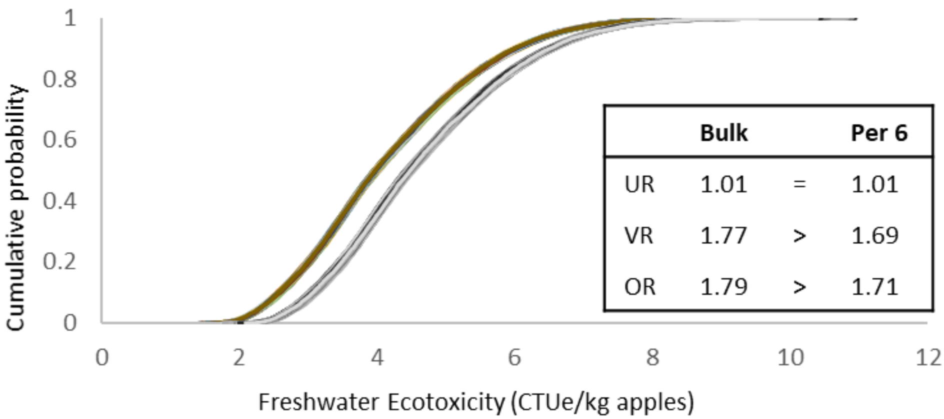
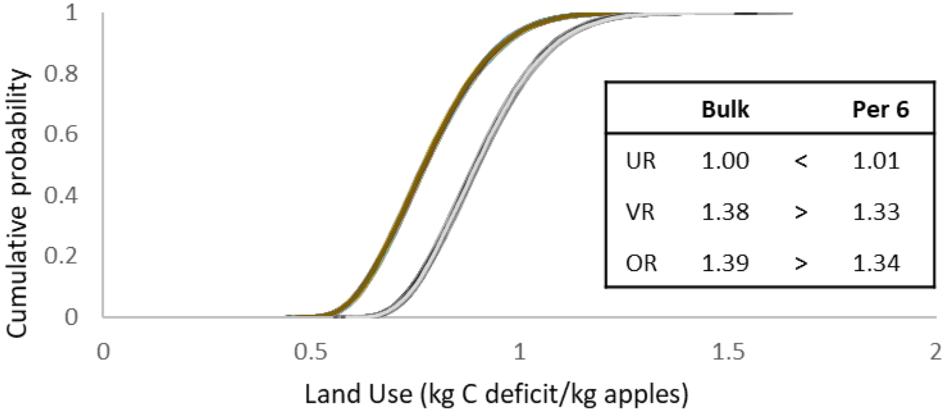
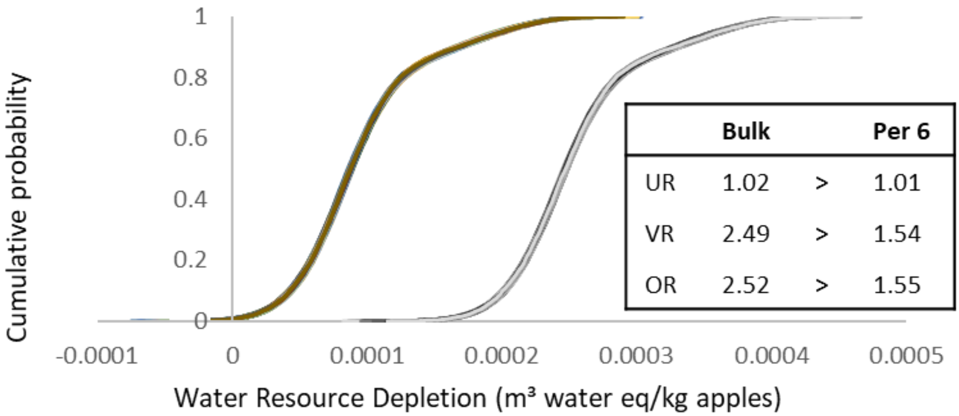


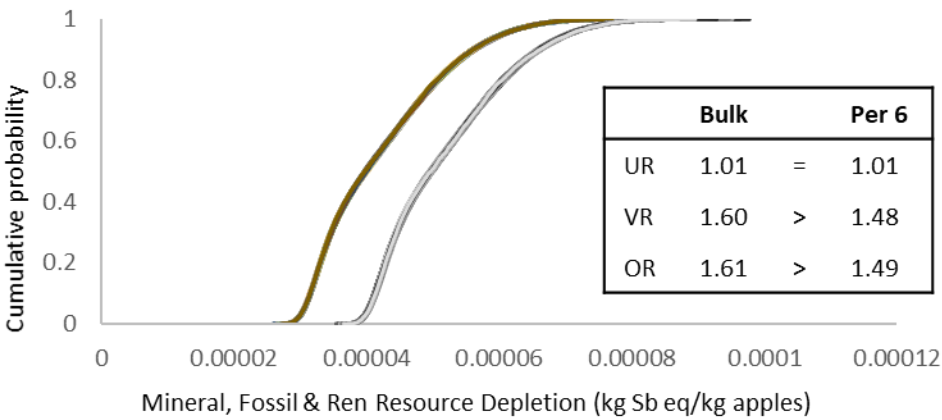
Figure A-1 Continued



	Bulk		Per 6
UR	1.00	<	1.01
VR	1.38	>	1.33
OR	1.39	>	1.34



	Bulk		Per 6
UR	1.02	>	1.01
VR	2.49	>	1.54
OR	2.52	>	1.55



	Bulk		Per 6
UR	1.01	=	1.01
VR	1.60	>	1.48
OR	1.61	>	1.49

Figure A-1 Continued

Table A-1 Deterministic impacts of the total post-harvest apple chain as reported on in the supplementary material of Goossens et al. (2019).

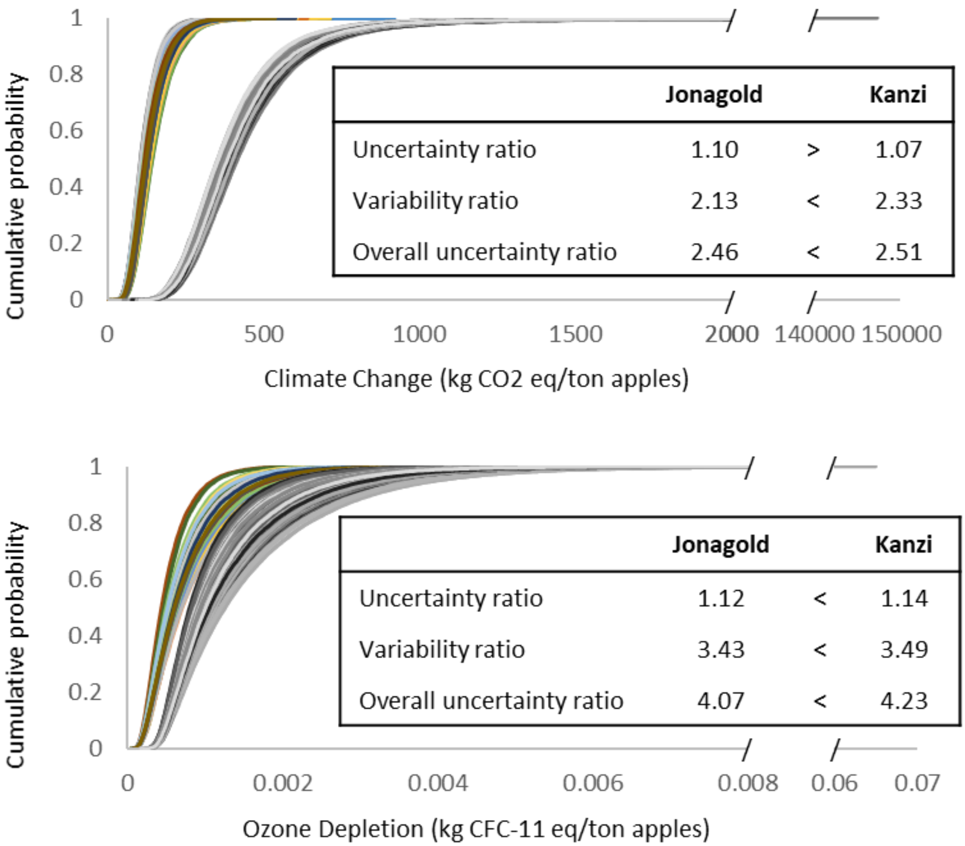
LCA impact category	LCA unit	Bulk	Per 6
Climate change	kg CO_2 eq	2.77E-01	3.49E-01
Particulate matter	kg PM2.5 eq	1.59E-04	2.04E-04
Ionizing radiation (Human Health)	kBq U235 eq	8.58E-02	9.39E-02
Photochemical ozone formation	kg NMVOC eq	9.53E-04	1.16E-03
Acidification	molc H+ eq	1.30E-03	1.67E-03
Terrestrial eutrophication	molc N eq	3.45E-03	4.14E-03
Freshwater eutrophication	kg P eq	7.72E-05	1.11E-04
Marine eutrophication	kg N eq	3.23E-04	3.92E-04
Mineral, fossil & renewable resource depletion	kg Sb eq	4.44E-05	5.35E-05

Appendix B

B.1 Apple cultivation inventory

Please refer to the electronic supplementary material.

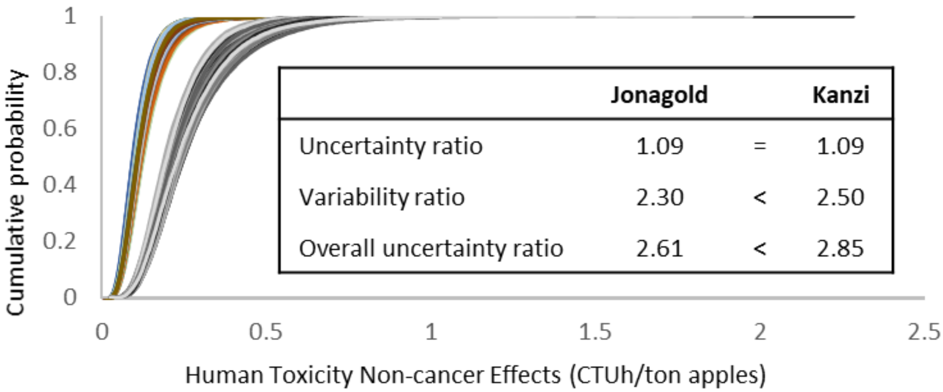
B.2 2DMC results for the cultivation chain

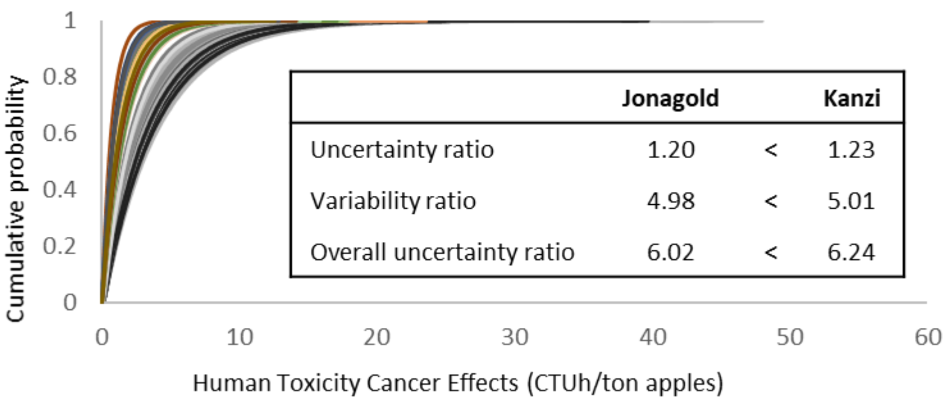


	Jonagold		Kanzi
Uncertainty ratio	1.10	>	1.07
Variability ratio	2.13	<	2.33
Overall uncertainty ratio	2.46	<	2.51

	Jonagold		Kanzi
Uncertainty ratio	1.12	<	1.14
Variability ratio	3.43	<	3.49
Overall uncertainty ratio	4.07	<	4.23

Figure B-1 2DMC results for the cultivation chain.
The Jonagold apples are colored and the Kanzi apples are shown in greyscale.





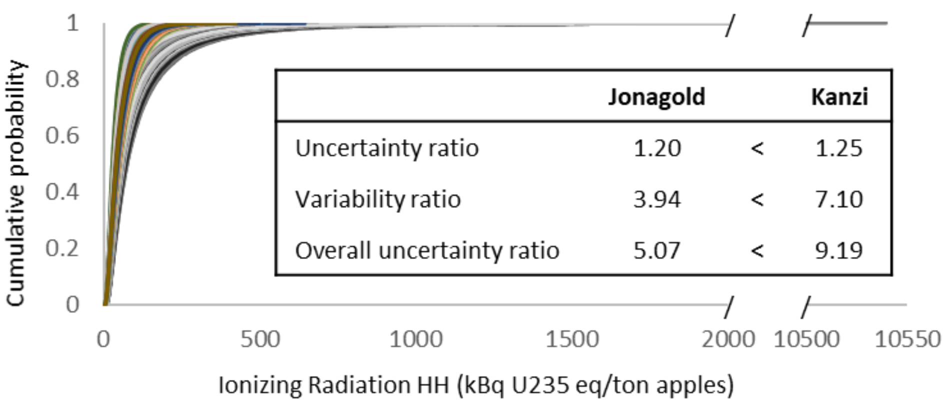


Figure B-1 Continued

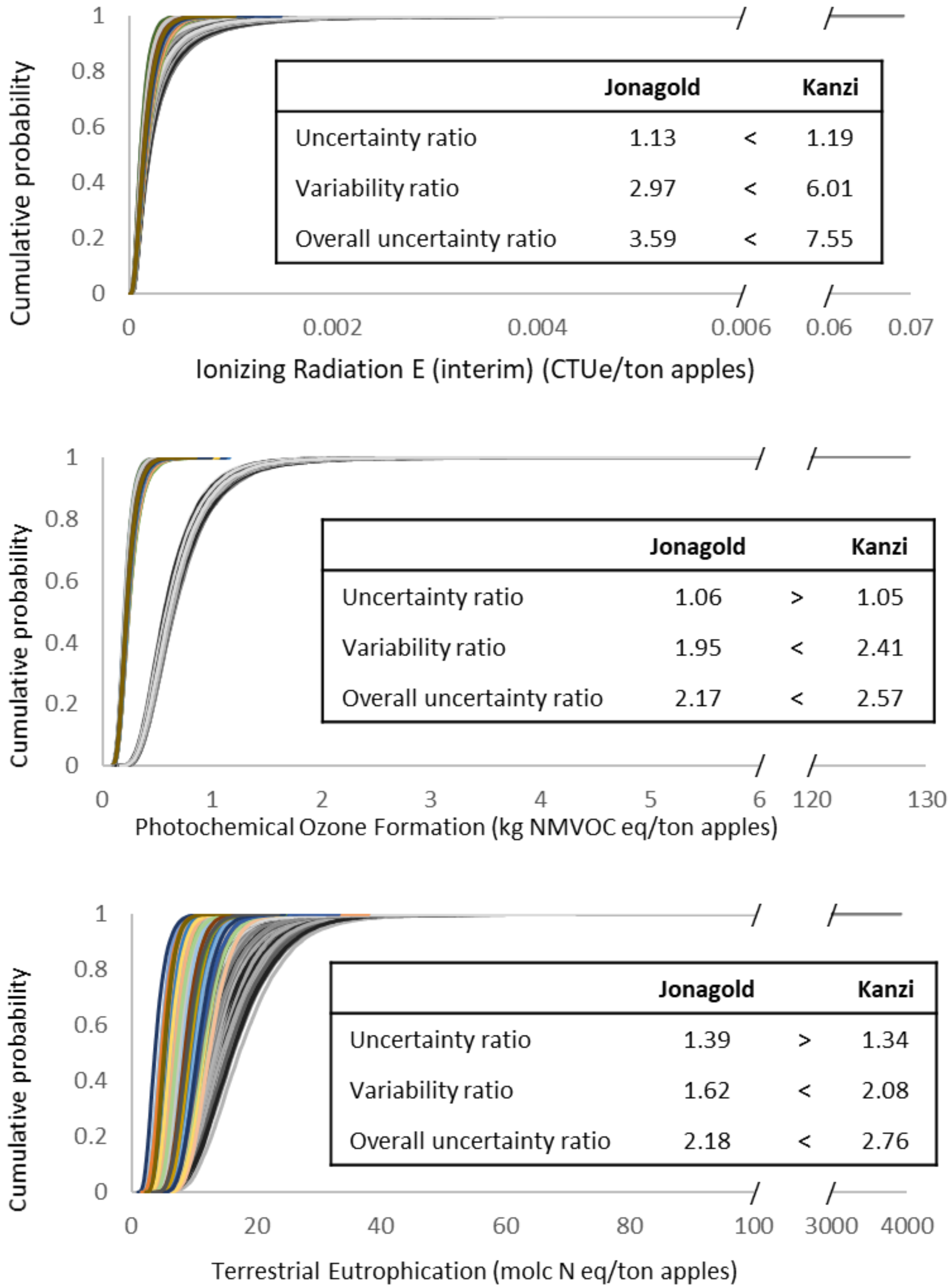


Figure B-1 Continued

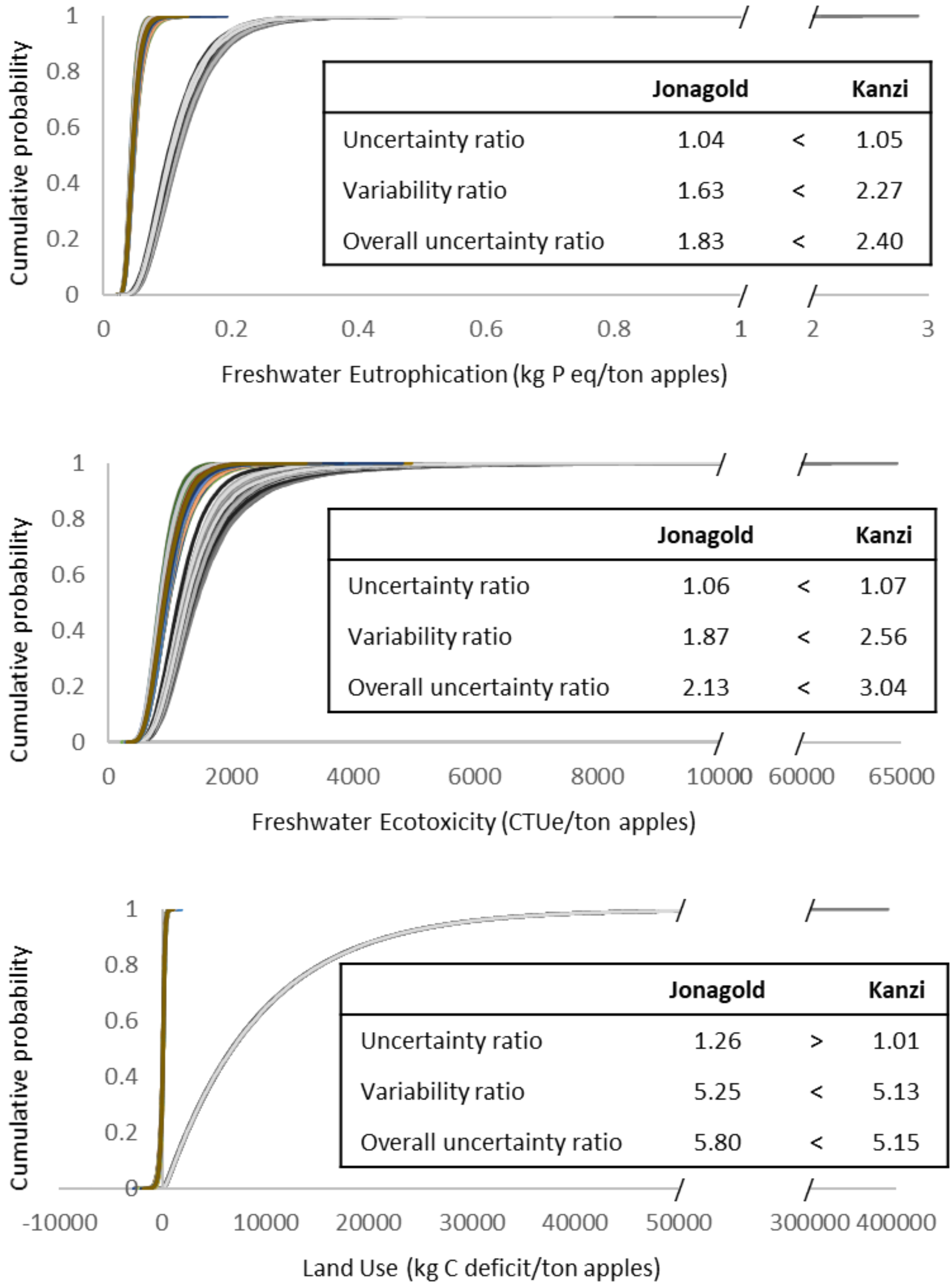
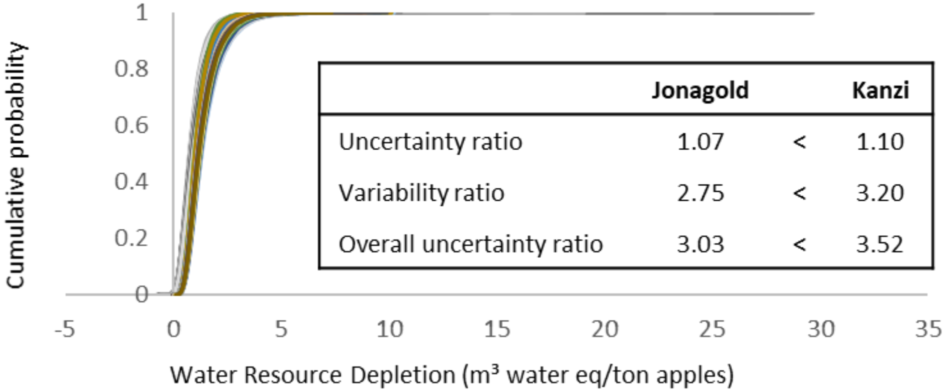


Figure B-1 Continued



	Jonagold		Kanzi
Uncertainty ratio	1.07	<	1.10
Variability ratio	2.75	<	3.20
Overall uncertainty ratio	3.03	<	3.52

Figure B-1 Continued

Appendix C

C.1 Organic fertilizer allocation methodology

Please refer to the electronic supplementary material for details on the chosen SimaPro processes, the assumptions and the calculations for the different allocation procedures. It also contains the methodology that was used for calculating mass allocation factors when only blood meal is used (results shown in Fig. C-2) and for assessing the influence of choosing a different livestock system (dairy instead of beef; results shown in Figures C-3 to C-6).

C.2 Median cultivation impacts for all allocation procedures

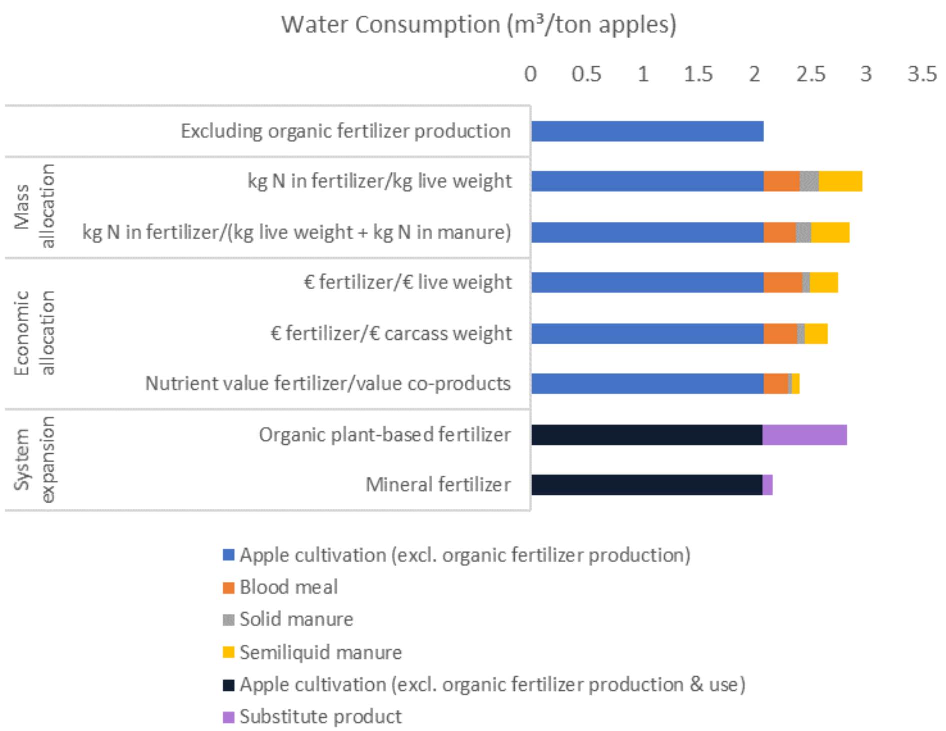


Figure C-1 Median impacts of organic apple cultivation with different allocation procedures. The considered allocation procedures are shown for the four apple orchards using blood meal, solid and semiliquid manure.

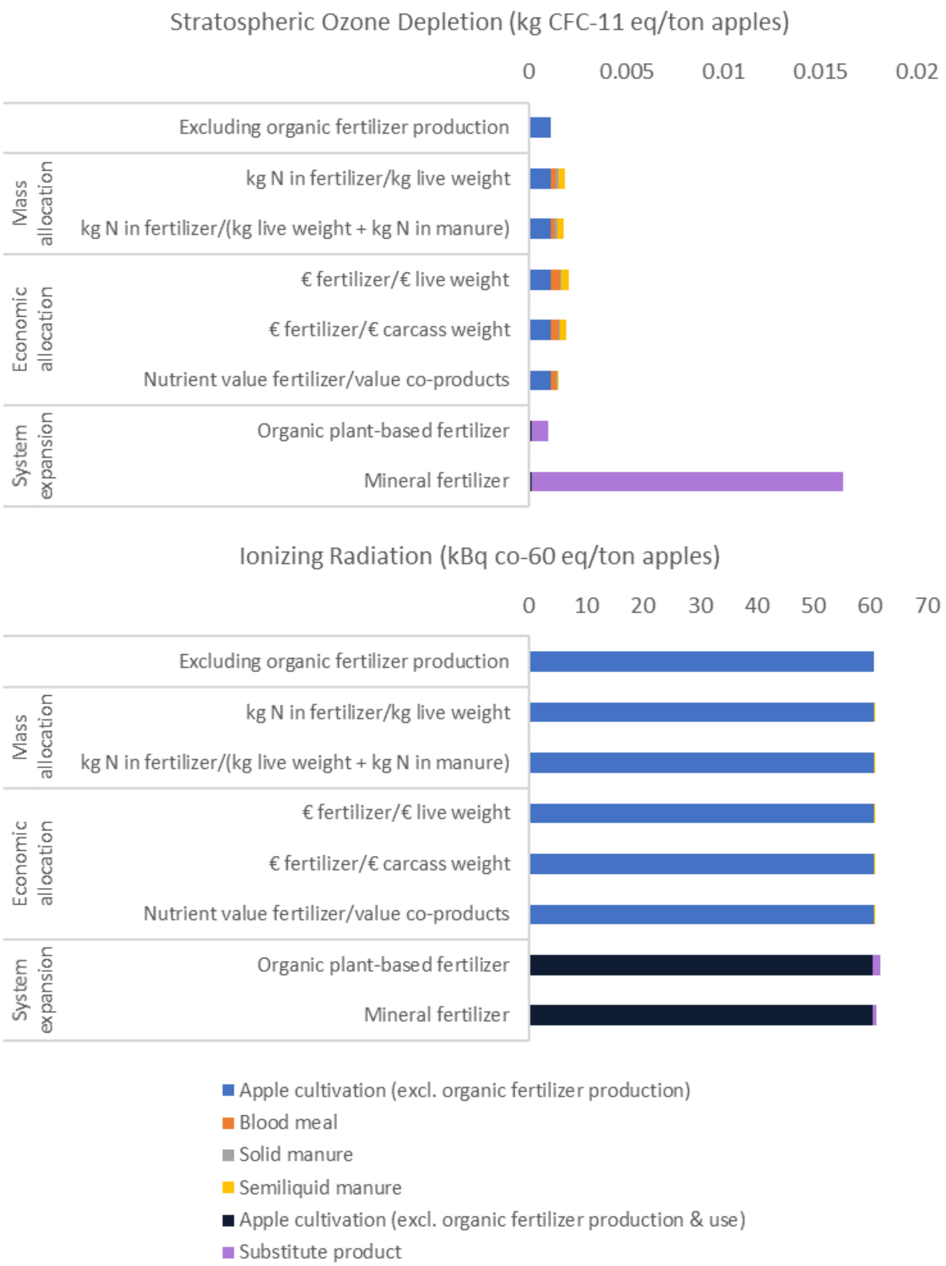


Figure C-1 Continued

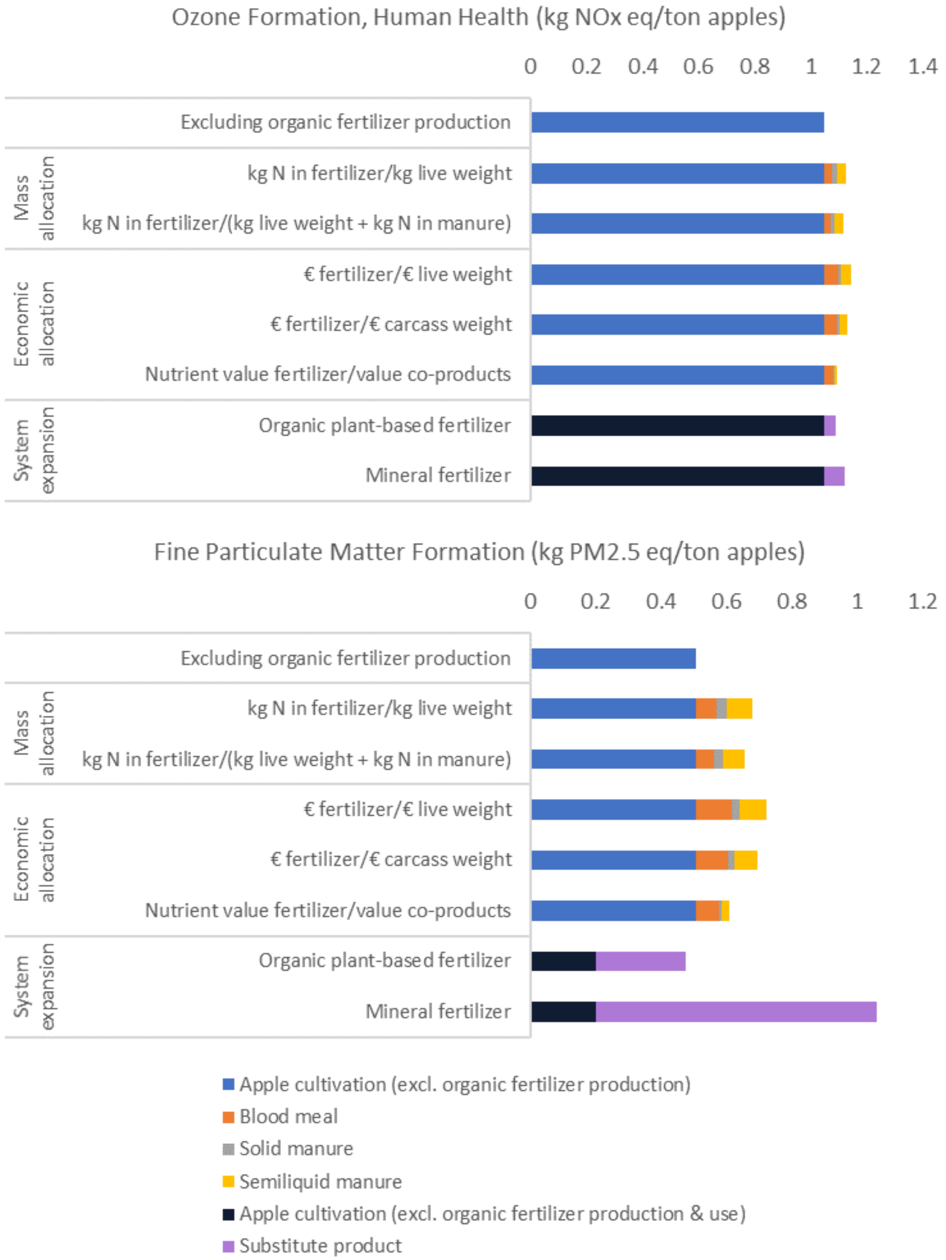


Figure C-1 Continued

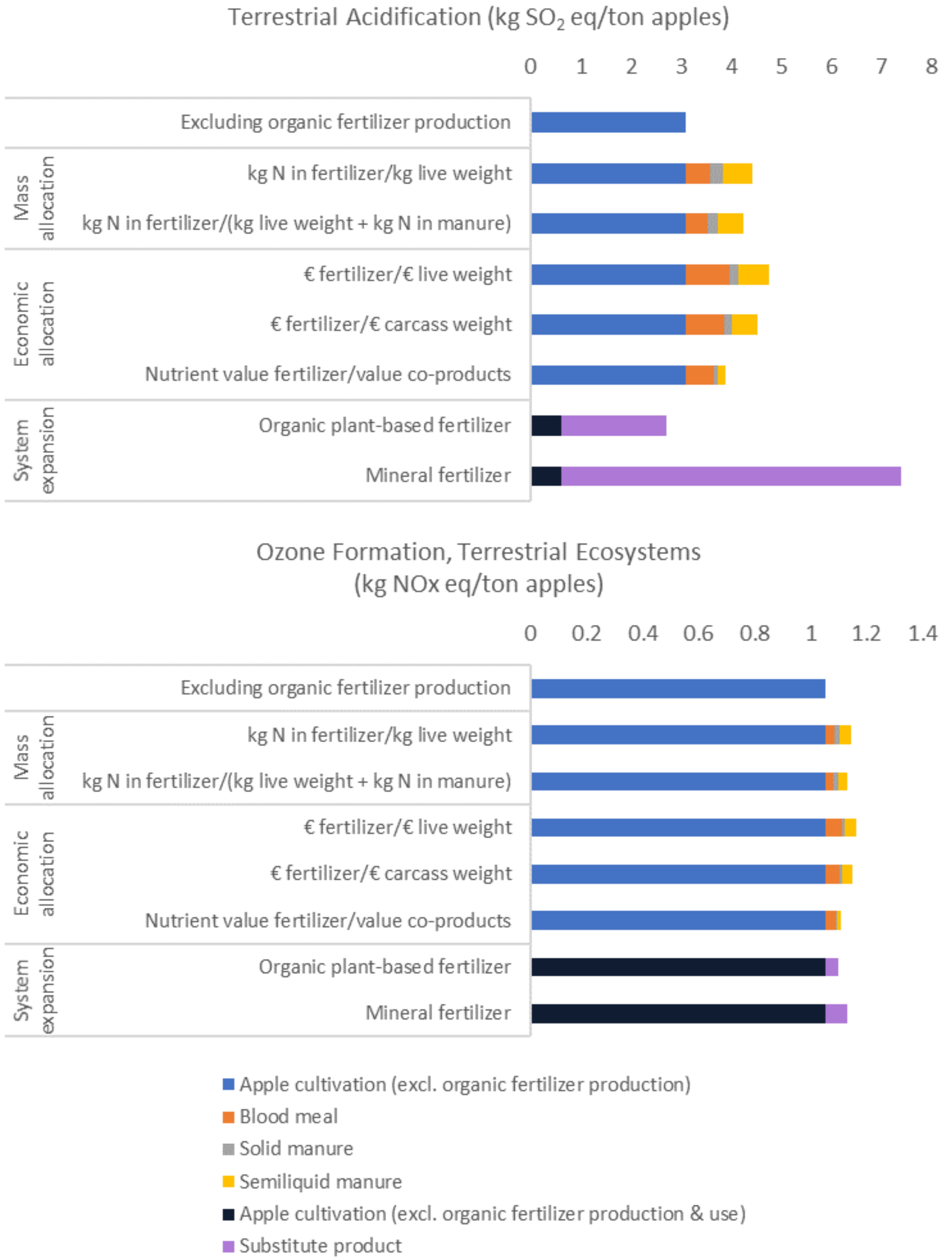
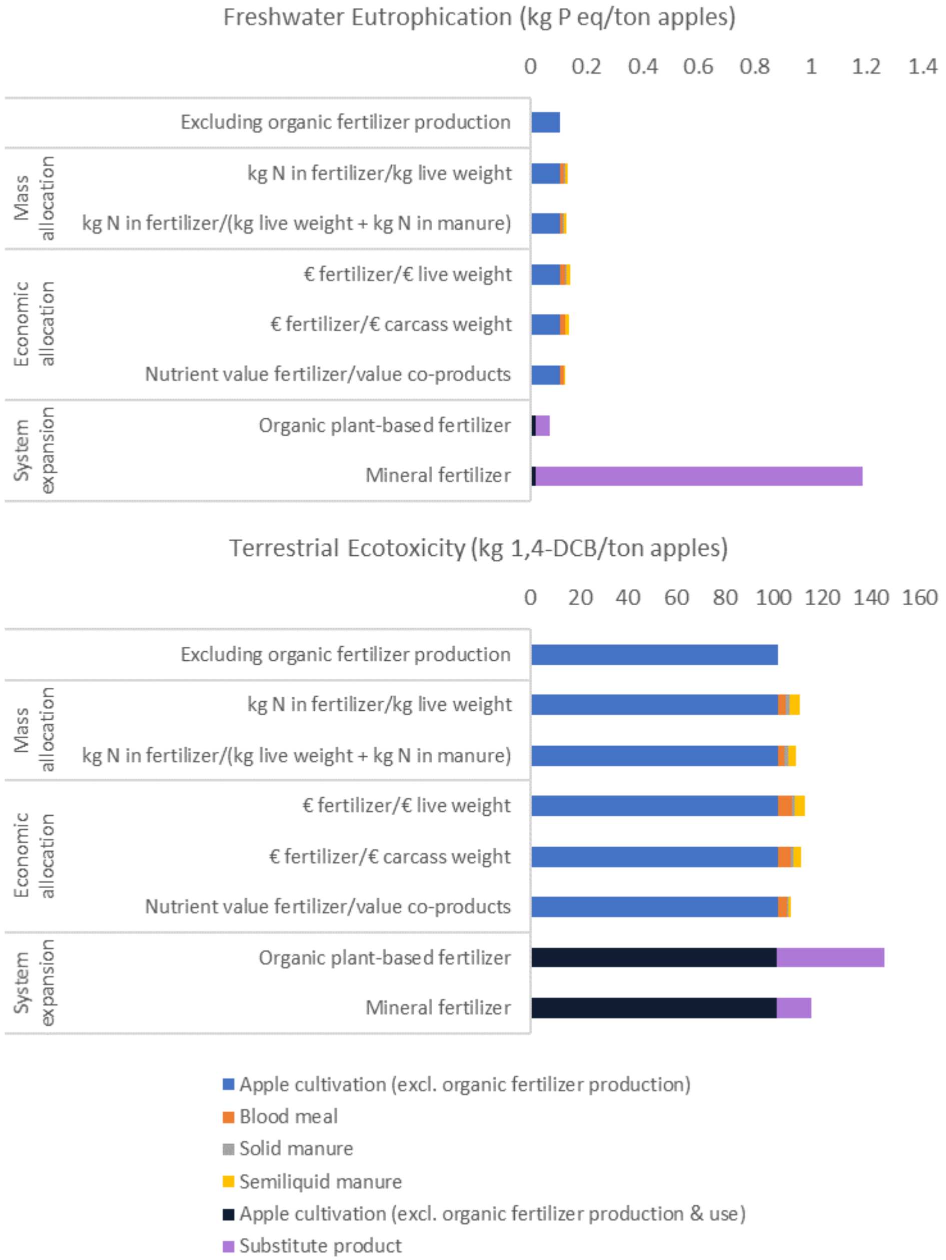


Figure C-1 Continued



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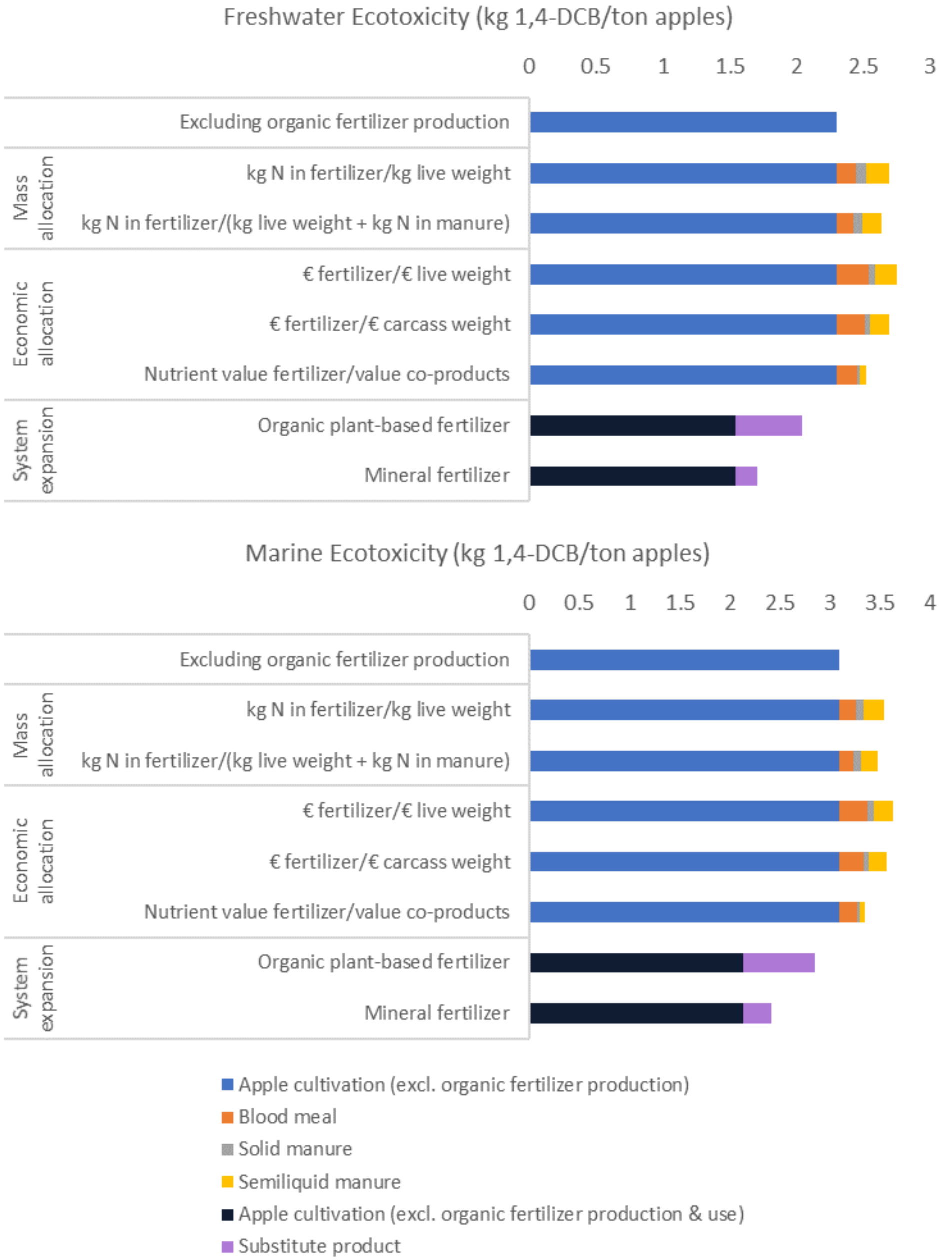

Figure C-1 Continued

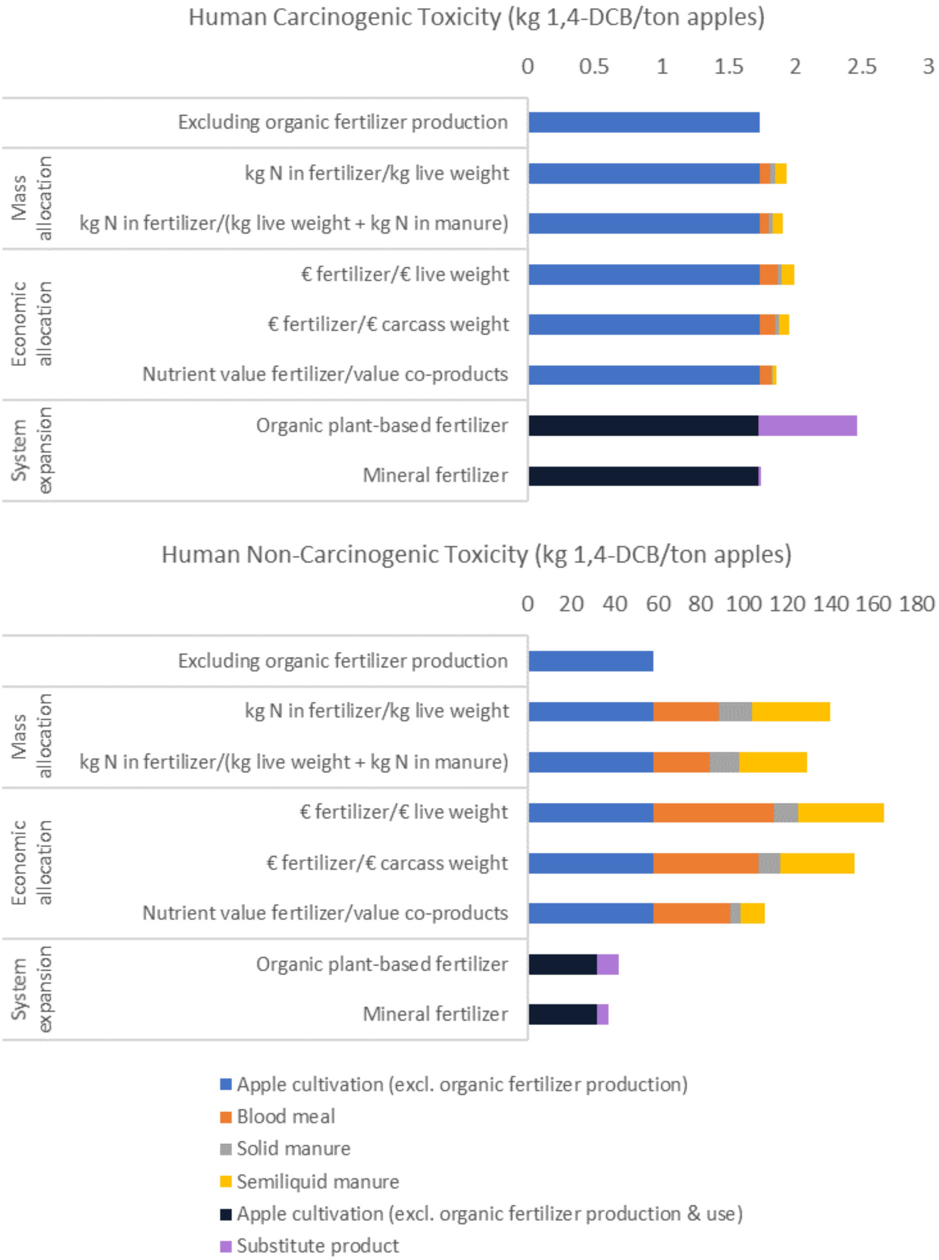

Figure C-1 Continued

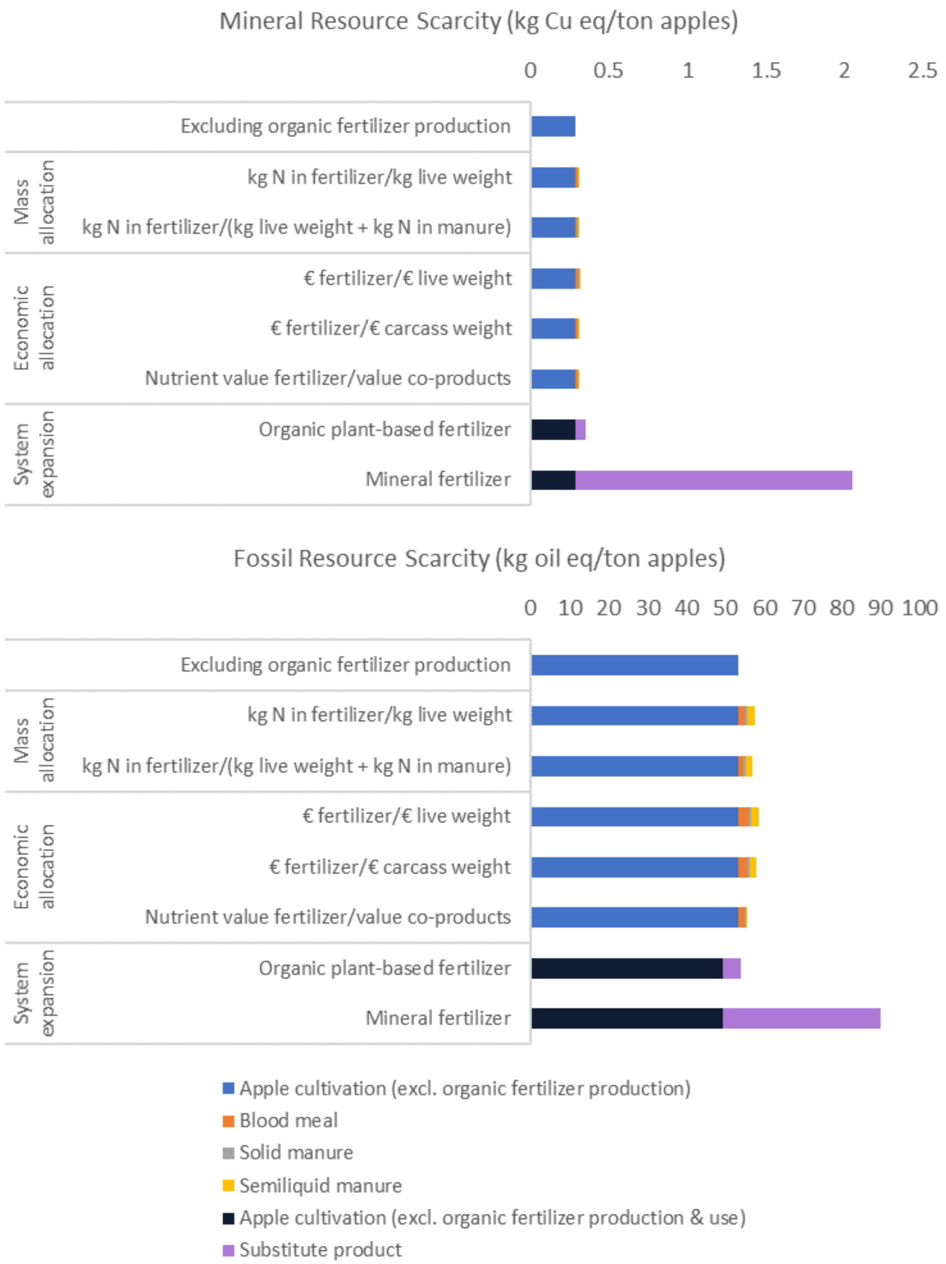

Figure C-1 Continued

C.3 Results of mass allocation for only blood meal

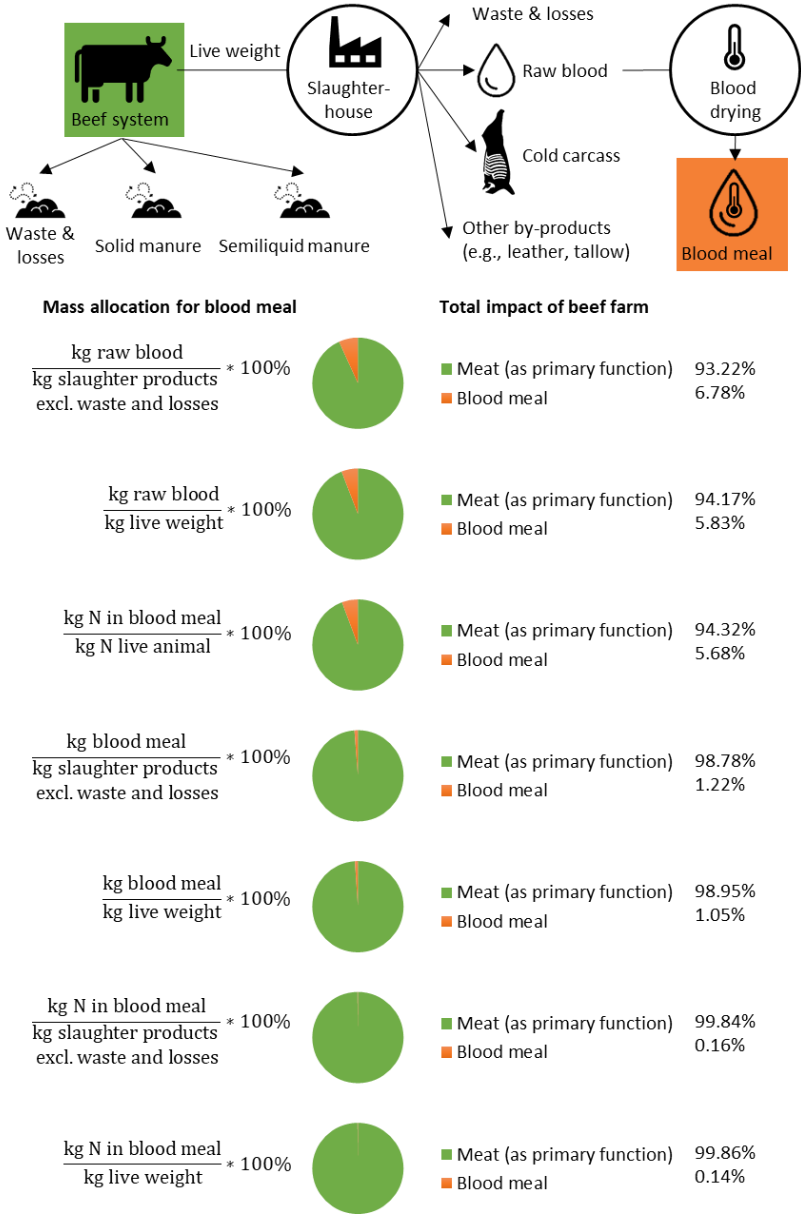

Figure C-2 Representation of the farming and meat processing chain and how the beef farm impacts are allocated to blood meal only using mass allocation factors.
A median of 487% of the total annual blood meal production of the beef farm is used to fertilize the apple orchards, meaning that five beef farms are needed to supply the required blood meal. All blood from the considered beef farm is thus assumed to be used for fertilizing the apple orchard.

C.3 Results of the influence of the livestock system

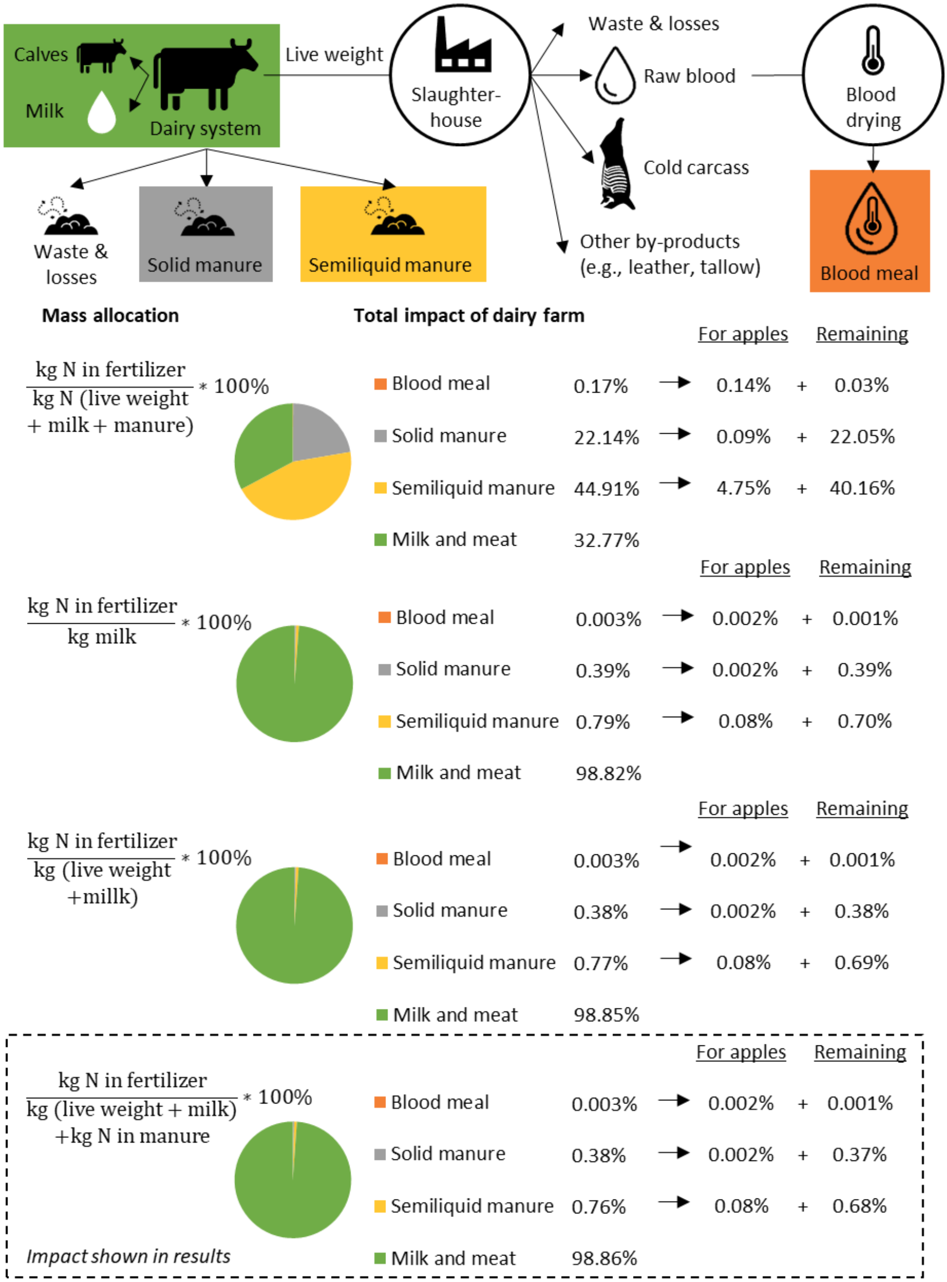

Figure C-3 Representation of the farming, dairy and meat processing chain and how the dairy farm impacts are allocated to blood meal and manure using mass allocation. The impacts allocated to the fertilizer can be divided into the parts that are allocated to organic apple cultivation (see Fig. 6-3) and the remaining impacts. The options in the striped frame are withhold as realistic option.

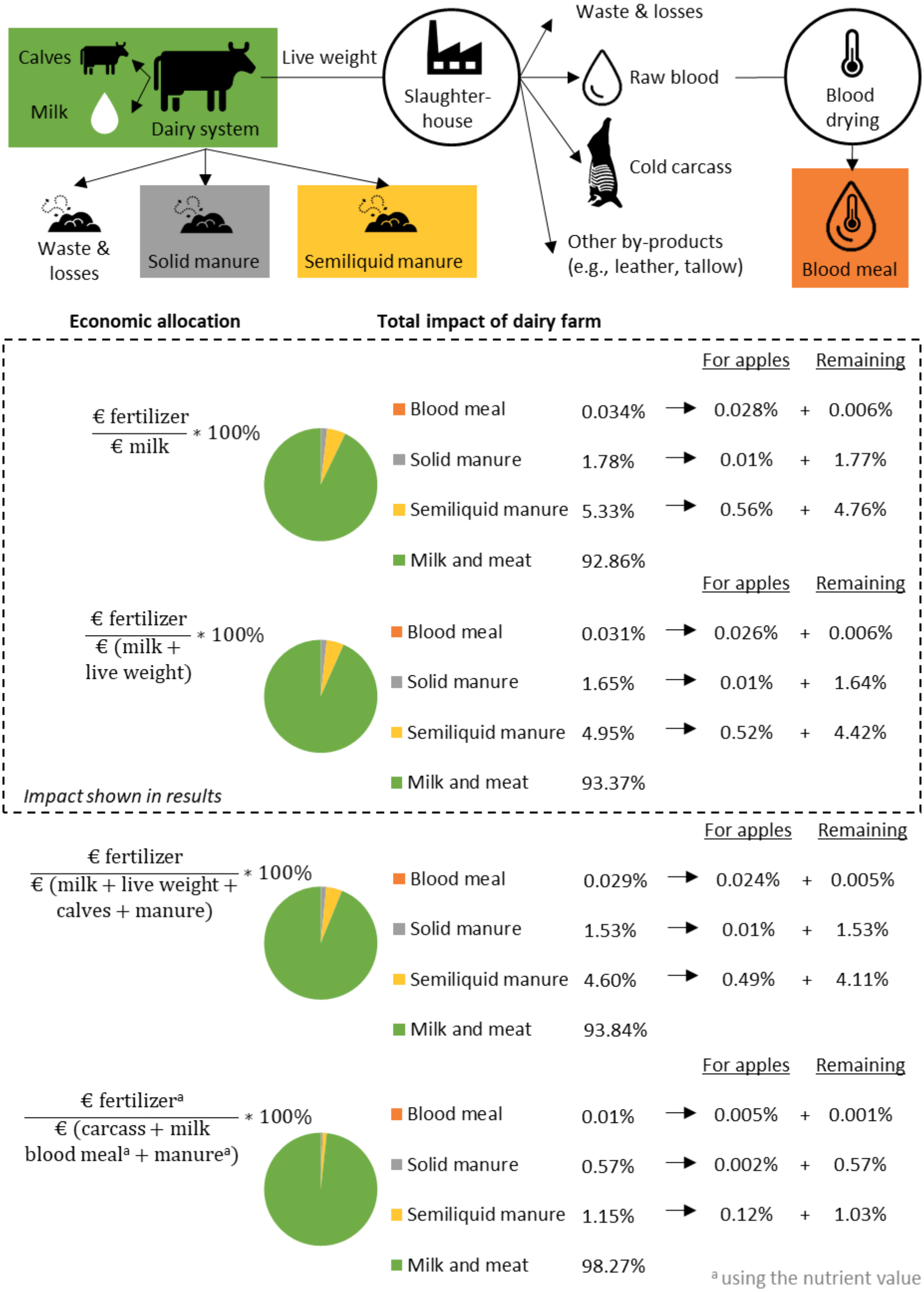

Figure C-4 Representation of the farming, dairy and meat processing chain and how the dairy farm impacts are allocated to blood meal and manure using economic allocation. The impacts allocated to the fertilizer can be divided into the parts that are allocated to organic apple cultivation (see Fig. 6-3) and the remaining impacts. The options in the striped frame are withhold as realistic option.

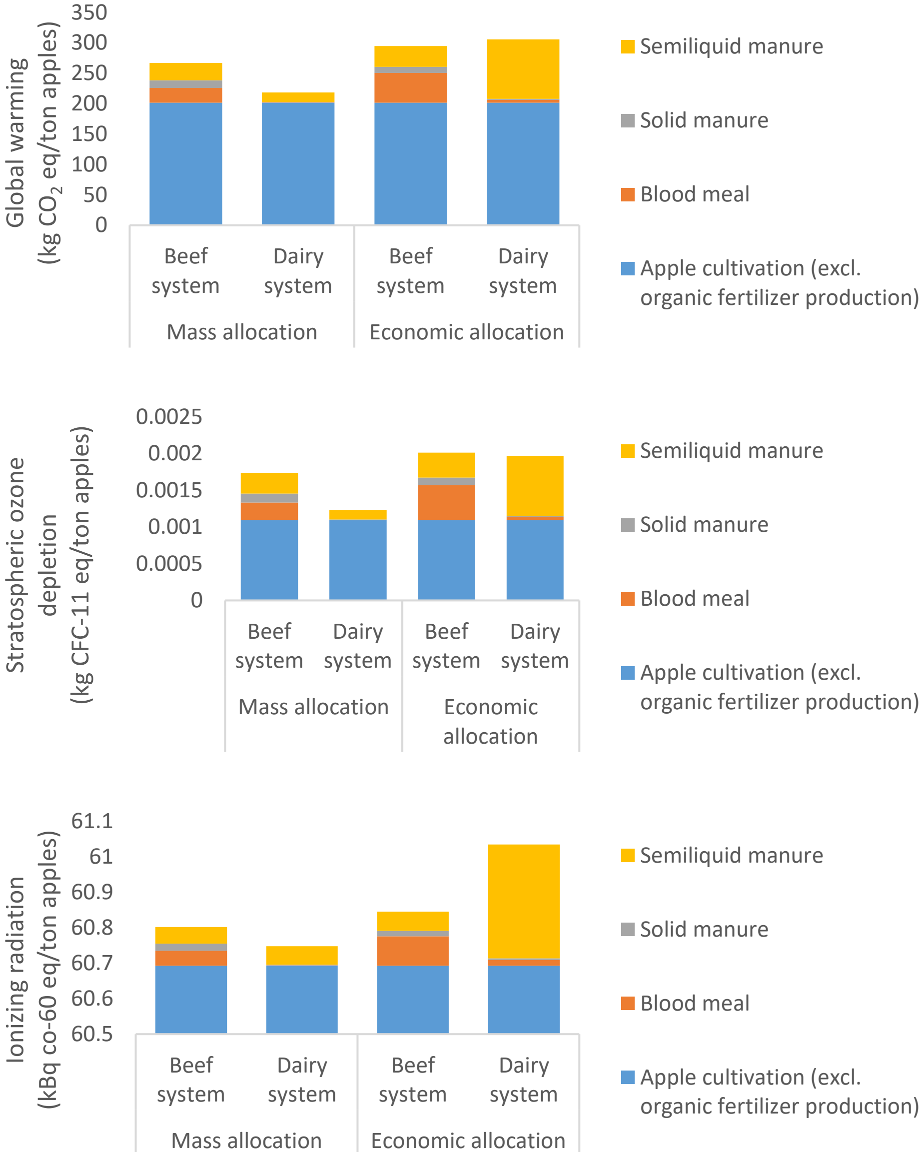

Figure C-5 Median impacts of apple cultivation showing the influence of using a different livestock system (dairy instead of beef).

For the beef system, “kg N in fertilizer/kg (live weight + N in manure)” was used as mass allocation factor and for the dairy system, “kg N in fertilizer/kg (live weight + milk + N in manure)”. For economic allocation for the beef system, “€ fertilizer/€ live weight” was used as allocation factor and for the dairy system, “€ fertilizer/€ (live weight + milk)”.

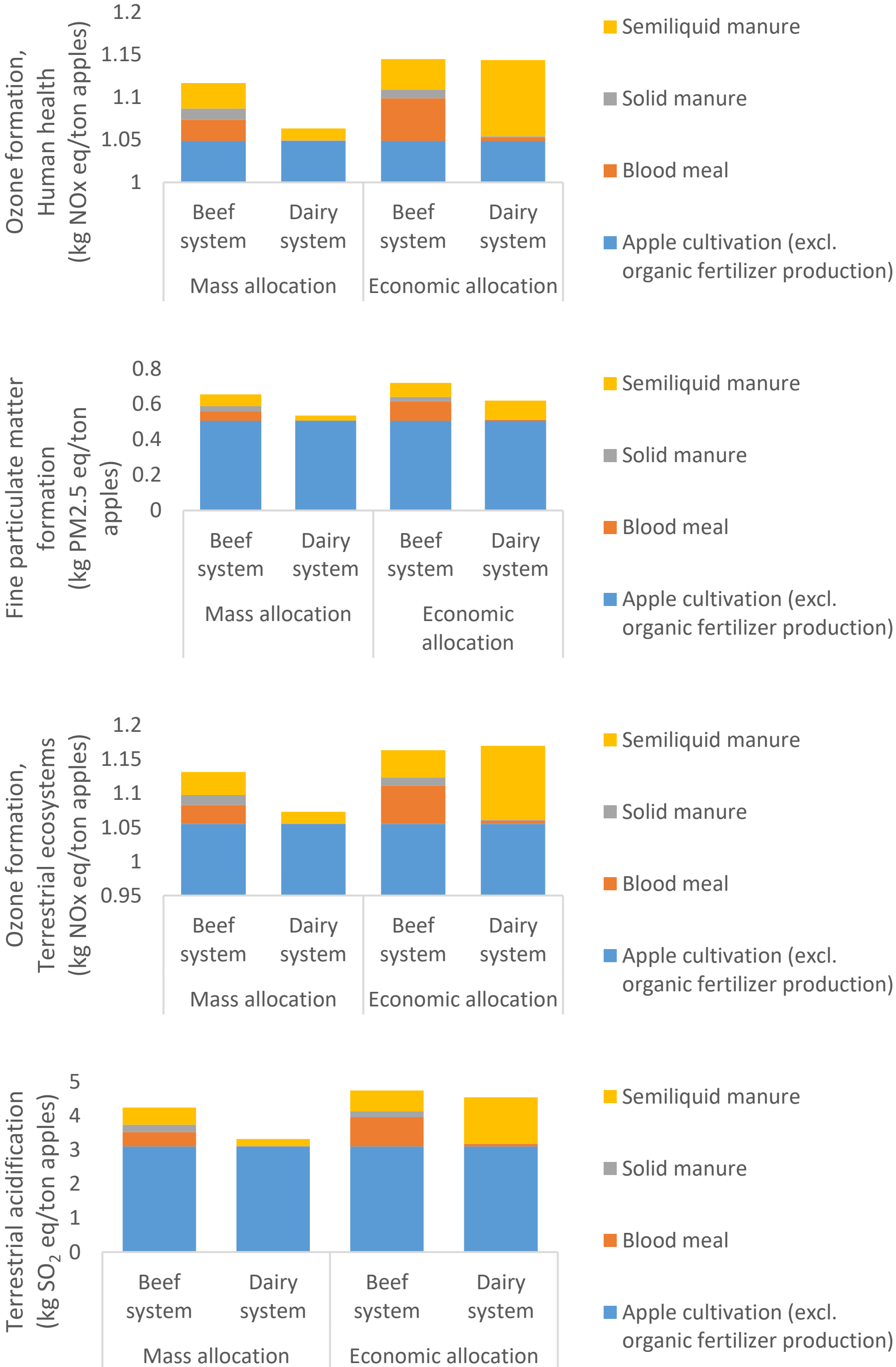

Figure C-5 Continued

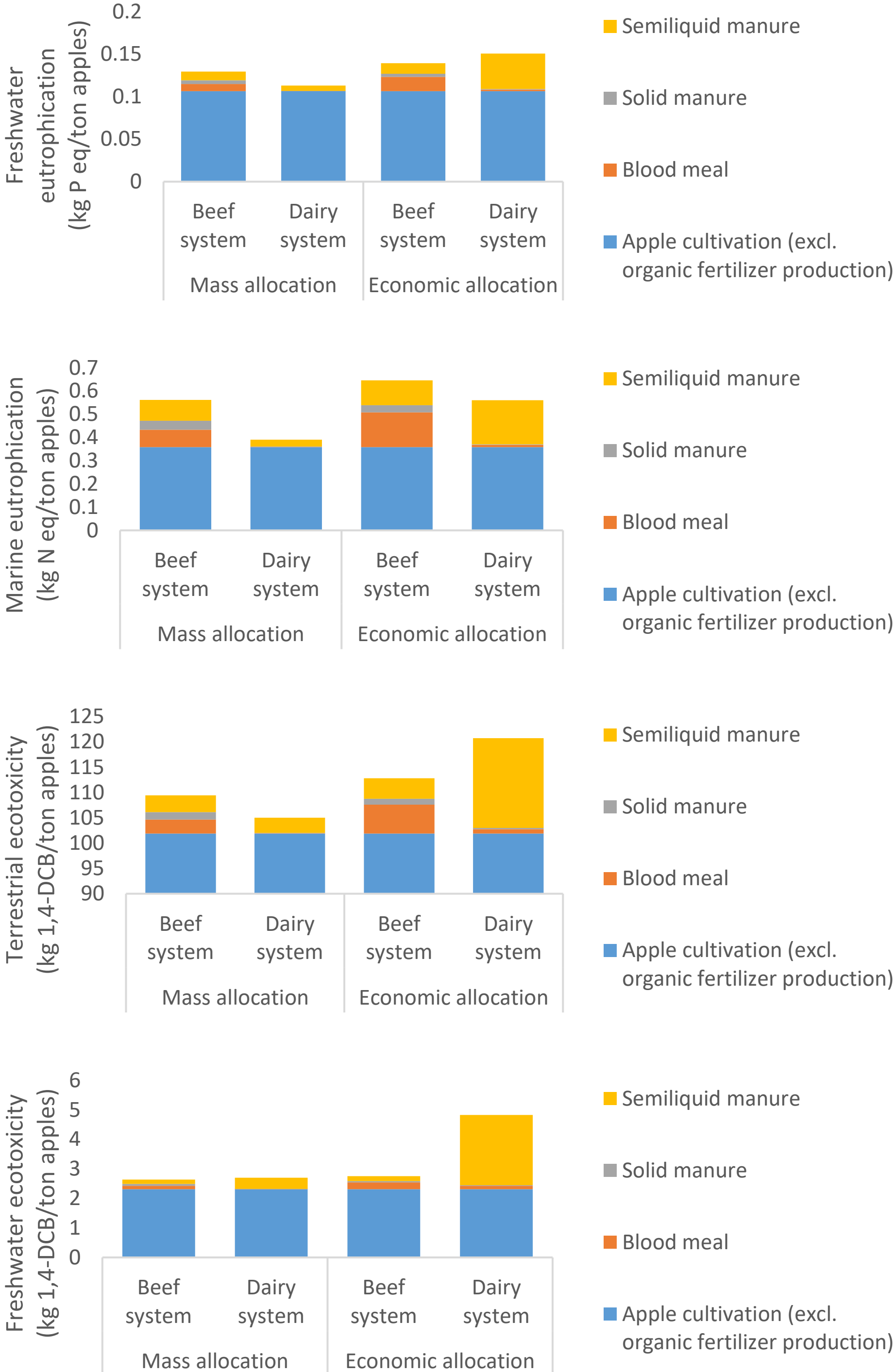

Figure C-5 Continued

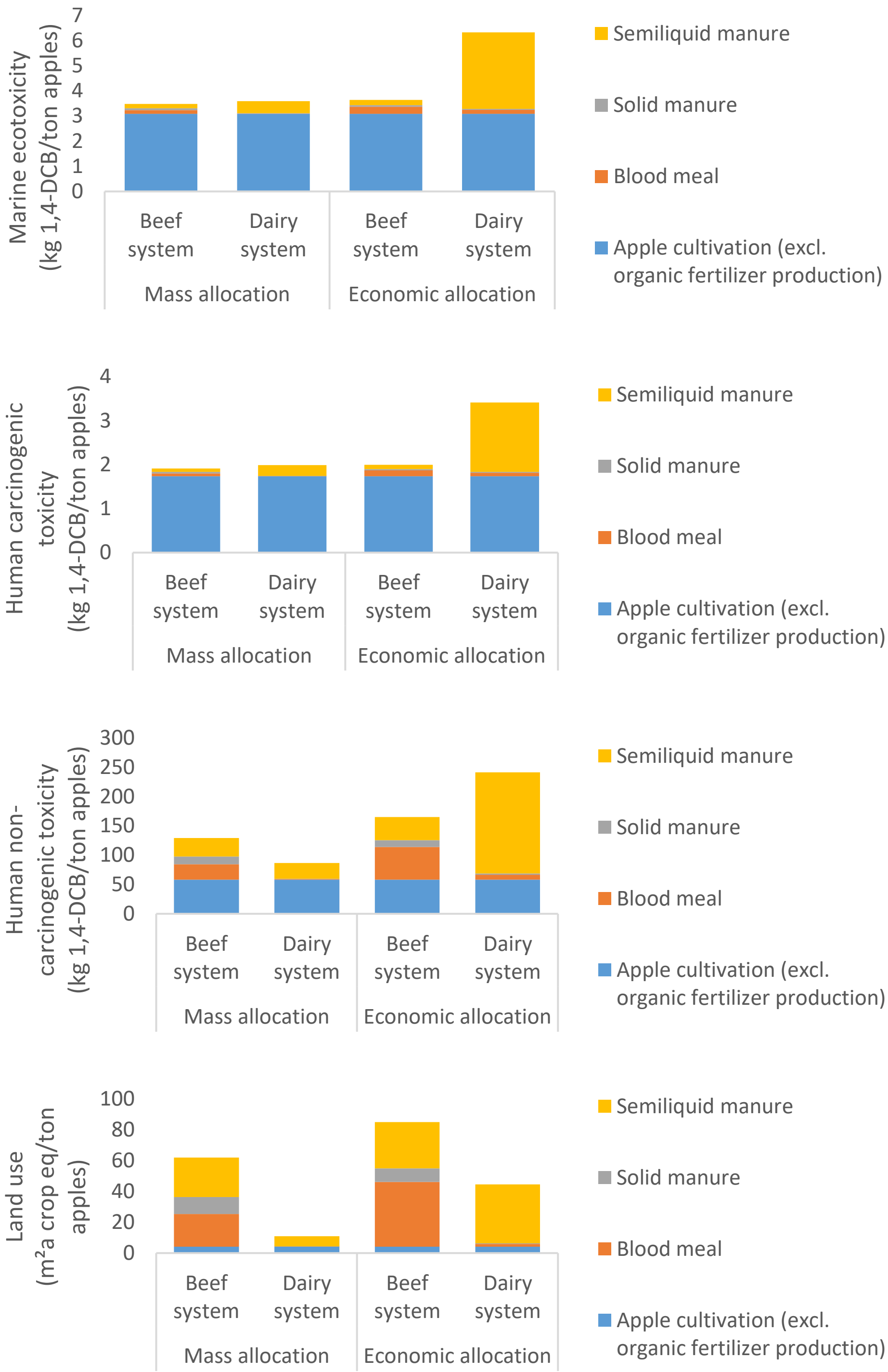

Figure C-5 Continued

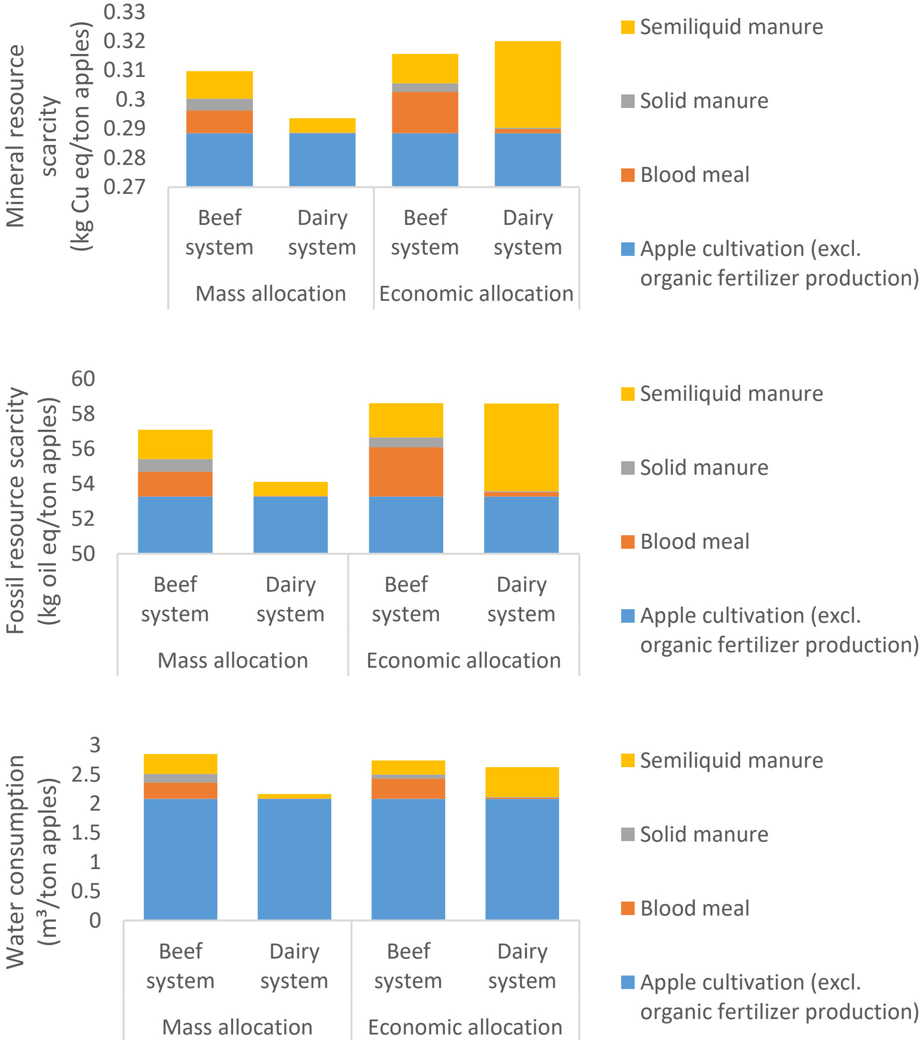

Figure C-5 Continued

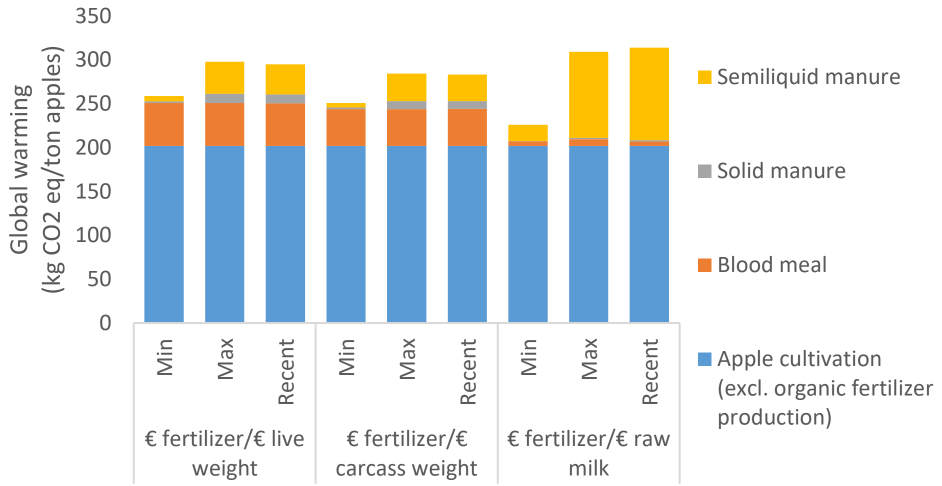

Figure C-6 Median Global Warming impacts of apple cultivation showing the influence of price variations for economic allocation comparing beef to the dairy system.

The beef system is represented by "€ fertilizer/€ live weight" and "€ fertilizer/€ carcass". For the dairy system, the allocation factor "€ fertilizer/€ milk" is considered.

PART VII

List of publications

Peer reviewed academic journals

Michiels, F., Hubo, L., Geeraerd, A. 2021. Why mass allocation with representative allocation factor is preferential in LCA when using residual livestock products as organic fertilizers. *Journal of Environmental Management*, 297, 113337. https://doi.org/10.1016/j.jenvman.2021.113337.

Michiels, F., Geeraerd, A., 2020. How to decide and visualize whether uncertainty or variability is dominating in life cycle assessment results: A systematic review. *Environmental Modelling and Software,* 133, 104841. https://doi.org/10.1016/j.envsoft.2020.104841

International scientific conferences

Michiels, F., Stalmans, A., Goossens Y., Geeraerd, A., 2021. Possibilities for sustainable reduction of apple losses at packaging level. In: Vieir, M., Pittia, P., Silva, C.L.M., Dubois-Brissonnet, F., Chrysanthopoulou, R.C.F. (Eds.). *Sustainable Development Goals in Food Systems: challenges and opportunities for the future*. 6th International ISEKI-Food Conference (ISEKI-Food 2021). Online. 23-25 June 2021. Abstract #310, pp 70.

Michiels, F., Geeraerd, A., 2020. Introducing a novel approach in life cycle assessments: propagating uncertainty and variability separately using two-dimensional Monte Carlo simulations. In: Eberle, U., Smetana, S., Bos, U. (Eds.). *Towards Sustainable Agri-Food Systems*. 12th International Conference on Life Cycle Assessment of Food (LCAFood2020). Berlin Virtually, Germany. DIL, Quakenbrück, Germany. 13-16 October 2020. pp. 353–356. Winner of the *Springer Award for the Best Young Scientist Presentation*.

Michiels, F., Hubo, L., Geeraerd, A., 2020. Life Cycle Assessment of Belgian organic apple cultivation using different allocation options for organic fertilisers. In: *Open Science for Enhanced Global Environmental Protection.* SETAC Europe 30th Annual Meeting (SETAC SciCon). Dublin Virtually, Ireland. 3-7 May 2020. Abstract No. 5.05P.5.

Michiels, F., Geeraerd, A., 2018. Methodologies for separating uncertainty and variability in Life Cycle Assessments: a systematic review. In: *The Role of LCA in Shaping the Future; Food, Fibre, Feed, Fertiliser, Fuel and Other Resources*. SETAC Europe 24th LCA symposium. Vienna, Austria. 24-26 September 2018. Abstract No. WE001.

Science popularization

Geeraerd, A., Van Mierlo, K., Michiels, F., 2021. Eating sustainably: beyond the myths. *Bio-ingenieus*, 24 (3), p. 26.

Michiels, F., Houben, G., Roose, D. De, Vancampenhout, K., Muys, B., 2017. Stadsbossen laten zich niet verplanten: Ontwikkelingen in het omstreden Sint-Annabos. *Natuur.Focus*, 16, 67–7