Deepening the uncertainty dimension of environmental Life Cycle Assessment: addressing choice, future and interpretation uncertainties.

Mendoza Beltran, M.A.

Author: Mendoza Beltran M.A.
Title: Deepening the uncertainty dimension of environmental Life Cycle Assessment: addressing choice, future and interpretation uncertainties.
Issue Date: 2018-10-09

Deepening the uncertainty dimension of environmental Life Cycle Assessment

Addressing choice, future and interpretation uncertainties

Maria Angelica Mendoza Beltran

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Addressing choice, future and interpretation uncertainties

María Angélica Mendoza Beltrán

Colophon

Maria Angélica Mendoza Beltrán
Deepening the uncertainty dimension of environmental Life Cycle Assessment. Addressing choice, future and interpretation uncertainties

PhD Thesis Leiden University, The Netherlands

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Lay-out: SVDH Media | www.svdhmedia.nl
Printed: ProefschriftMaken | www.proefschriftmaken.nl
ISBN: 978-94-6380-017-4

Chapter 2 and 3 of this thesis were carried out under the IDREEM project (Increasing Industrial Resource Efficiency in European Mariculture, www.idreem.eu) and have received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° 308571.

Deepening the uncertainty dimension of environmental Life Cycle Assessment

Addressing choice, future and interpretation uncertainties

PROEFSCHRIFT

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden,
op gezag van Rector Magnificus prof.mr. C.J.J.M. Stolker,
volgens besluit van het College voor Promoties
te verdedigen op dinsdag 9 oktober 2018
klokke 13.45 uur

door

Maria Angélica Mendoza Beltrán

geboren te Bogota D.C., Colombia

in 1983

Promotie commissie

Promotor:	Prof. dr. Arnold Tukker (Leiden University)
Tweede promotor:	Prof. dr. Detlef P. van Vuuren (Utrecht University)
Co-promotor:	Dr. Jeroen B. Guinée (Leiden University)
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To my mother Clemencia and my grandmother Isabel,
the women of my life

Table of Contents

1. General Introduction

This chapter contains several extensive quotations from:

Mendoza Beltran, M.A., F. Pomponi, J.B. Guinée, and R. Heijungs. 2018. Uncertainty Analysis in Embodied Carbon Assessments: What Are the Implications of Its Omission? In Embodied Carbon in Buildings Measurement, Management and Mitigation, ed. by F Pomponi, C De Wolf, and A Moncaster, 3–21. Springer. doi/10.1007/978-3-319-72796-7

1.1 On Life Cycle Assessment

Over time, the importance of addressing environmental problems has become evident. For instance, a key moment evidencing the ecological impacts of pesticides used in agriculture took place in 1962 with the publication of "Silent Spring" (Carson 1962). Also after 1962, the evidence continue to grow, for instance by the work of the Club of Rome (Meadows et al. 1972), the subsequent environmental assessments (such as the Millenium Ecosystem Assessment 2005) and the work on specific problems such as the assessments by the Intergovernmental Panel on Climate Change (IPCC 2014) and by the United Nations Environment Programme (UNEP) on biodiversity (CBD 2012). In order to formulate effective response strategies, tools are needed to assess the impact of human activities on the environment. Such tools deal with relevant aspects such as the different temporal (e.g. past, present and future), geographic (e.g. local to global) and economic scales (e.g. product, sector). An important tool is Life Cycle Assessment (LCA) that emerged as a method to assess environmental impacts along value chains of products in the 1970s. The LCA tool, however, really developed in the past 30 years (Guinée et al. 2011). LCA is nowadays a standardized and broadly accepted method to understand and address the environmental impacts associated with the life cycle of a product (ISO 2006). The method, however, continuous to evolve in response to new societal questions.

LCA addresses different questions related to the potential environmental impacts through a product's life cycle. This includes extraction of natural resources, production of materials and the product itself, the use of the product, and the end-of-life treatment when it is discarded (Guinée et al. 2002). An essential element of LCA is the cradle-to-grave coverage of the product life cycle, although in some cases the scope can be different. In general, LCA can help to identify improvement opportunities in relation to the environmental performance of products (ISO 2006). Performing an LCA can also support the selection of relevant indicators and measurement techniques to track environmental performance of product-systems as well as support the implementation of marketing schemes by providing an evidence basis for claims related to product environmental performance (ISO 2006). Finally, LCA can also be useful in comparing alternatives of similar products (Guinée et al. 2002), which is one of the most popular applications of LCA.

An LCA study has four phases: a) the goal and scope definition, b) the life cycle inventory analysis, c) the life cycle impact assessment and d) the interpretation phase (ISO 2006). During the goal and scope the aim, topics, basis for comparison and calculation (the functional unit) and intended use of the study are defined. Also, the scope including the product-system boundaries and the level of detail are defined. The life cycle inventory (LCI) analysis phase is the most data intensive and consists of collecting the inventory data, i.e. the inputs and outputs of each unit process related to the product-system analyzed. The result of the inventory analysis is typically a table with the quantified inputs from and output to the environment for each of the alternatives. The life cycle impact assessment (LCIA) aims to convert the inventory results to contributions to selected impact categories such as climate change, acidification, human toxicity, etc. Finally, the interpretation is the phase in which the results calculated in the LCI and LCIA are analyzed and synthetized in the light of the goal and scope of the study. As part of this phase techniques like contribution, perturbation, and uncertainty analysis can be applied. According to the Handbook on Life Cycle Assessment (Guinée et al. 2002 p.116), uncertainty analysis helps to "…assess the robustness of the overall LCA results with respect to variations and uncertainties in the methods and data used". LCA can suffer from uncertainty introduced by different sources, a topic that will be elaborated in detail in the following sections as it is the core of this thesis.

1.2 On the uncertainty dimension of Life Cycle Assessment

Certainty is the idea of confidence, assurance and accuracy about our knowledge of the truth. "Certainty and truth exist" (Briggs 2016, p.2), evading discussions on philosophical skepticism that are self-defeating as denying their existence is already accepting a truth with certainty (Briggs 2016). The idea of uncertainty is based upon the existence of truth by acknowledging there is something that is but cannot be fully known. Uncertainty does not exist in objects themselves, aside from the sense of existence, but only in our mind or intellect (Briggs 2016). Therefore, it is our incapacity to know the truth that underlines uncertainty. For a further discussion about the philosophical basis of uncertainty, we here refer to Box 1. The theme of this thesis is about how to deal with different sources of uncertainty in LCA, recognizing, acknowledging and quantifying as far as possible, different sources of uncertainty currently not yet properly captured by LCA (Box 1).

Uncertainty has been researched for about 30 years in LCA. The increased attention that LCA received during the 1990s as a tool to describe environmental impacts of products in the broad sense, came along with criticism about the drawbacks of this decision support framework used by governments and companies (Udo de Haes 1993). One of the major limitations is the importance of uncertainty (Finnveden 2000; Ross et al. 2002), which threats the reliability of decision makers on the results and recommendations from LCAs. Guinée et al. (1993 p.89) mentioned that: "A valuation of environmental profiles without an assessment of the reliability and validity of the results, is of little value". There are many ways to treat uncertainty but probability is one of the most used ones. Probability is the language of uncertainty that explains the limitations in our knowledge of the truth (Briggs 2016). This is why many fields of knowledge have relied on probability to help treat this limitation and the field of LCA is no exception.

Some of the first publications dedicated to uncertainty treatment in LCA appeared during the 1990s. Uncertainty analysis in LCA was defined by Heijungs (1996 p.159) as “the study of the propagation of unintentional deviations” in order to understand “those areas where product and process improvement lead to the highest environmental gain”. Similarly, Huijbregts (1998) identified the usefulness of uncertainty analysis in LCA to help decision makers judge the significance of the differences in product comparisons, options for products improvements or the assignment of eco-labels. Weidema and Wesnæs (1996) were the first to describe and apply Data Quality Indicators (DQI), semi-quantitative numbers providing information about the quality of the data, and Data Quality Goals (DQG), the desired quality of the data, in an LCA context. This methodological development known as the “pedigree-matrix” in LCA jargon, inspired by the purely qualitative proposal of Funtowicz and Ravetz (1990), is one of the most widely applied techniques to semi-quantitatively address uncertainty of data in LCA. This method was later incorporated in the ecoinvent database (Frischknecht et al. 2007). DQIs enabled early probabilistic approaches to account for data uncertainties and LCA models evolved from deterministic, point-value models to stochastic models characterized by probability distributions (Kennedy et al. 1996).

Box 1. Broad framework of definitions for uncertainty types

Broad kinds of uncertainty have been recognized in literature. Wynne (1992 p114), identified four kinds of uncertainty in environmental sciences departing from risk assessment:

- Risk – “The system behavior is well known” as well as the chance of different outcomes.
- Uncertainty as conventionally described – Parameters are well known but not their distributions. Uncertainties are recognized and explicitly included in the analysis.
- Ignorance – It is a characteristic of the linkage between knowledge and commitments based on it. “It bets on the completeness and validity of that knowledge.”
- Indeterminacy – Emerging from the question of “whether knowledge is adapted to fit the mismatched realities of application situations, or whether those situations are reshaped to ‘validate’ the knowledge.”

Such different types, particularly, ignorance and indeterminacy are specified to emphasize that uncertainties are not always due to incomplete scientific knowledge. Uncertainty can also emerge from indeterminacies, sometimes socially driven, which can lead to questions around the validity of a theory or model under new realities such as new conditions and situations (Wynne 1992; Compare also: Ravetz 1999; Stirling 2010; Castree et al. 2014). Related to the indeterminacies, Rotmans et al. (1994) and Tukker (1998) identified paradigm uncertainties which are related to the fact that a problem may be defined and analyzed from different scientific perspectives, an issue particularly important in the context of policy support. Further, Walker et al. (2003) identified three dimensions of uncertainty each of which has its own related sources of uncertainty some of which are recognized in Van Asselt and Rotmans (2001):

- Location of uncertainty – where does uncertainty manifest within the model?
- Level of uncertainty – at what level does uncertainty manifest within the spectrum from deterministic to total ignorance?
- Nature of uncertainty - is uncertainty due to imperfect knowledge or due to inherent variability?

This thesis is placed within the space of risk and uncertainty, recognizing, acknowledging and quantifying (where possible) sources of uncertainty for LCA models beyond the deterministic and total ignorance extremes of the level of uncertainty, and refers to uncertainty manifested in the parameters, choices and imperfect knowledge of the future in LCA. This means that total ignorance and indeterminacies and their related types of uncertainties, are not explicitly studied and discussed in this thesis, which does not mean that these do not exist. In fact, as the underlying principle of this thesis is recognition and acknowledgement, we emphasize that not all can be known neither quantified.

Yet only until the end of the 1990s and beginning of the 21st century, a general framework that distinguished various types of uncertainty and variability in LCA was proposed and further studied (Huijbregts 1998a; Björklund 2002). These frameworks are of particular importance as they differentiate various types of uncertainty and variability in LCA as well as recognize that different types of uncertainty and variability might require different treatment. The types of uncertainty and variability are (according to a combination of Huijbregts, 1998 and Björklund, 2002 and excluding those types of uncertainty not further treated in this thesis as explained in Box 1):

- Parameter uncertainty: data inaccuracy, data gaps and unrepresentative data
- Uncertainty due to methodological choices
- Model uncertainty
- Epistemological uncertainty
- Spatial variability
- Temporal variability

- Sources and objects variability
- Mistakes

While uncertainty refers to a lack of knowledge about the truth (Briggs 2016), variability makes reference to inherent differences within a population attributable to natural heterogeneity of values (Björklund 2002). Therefore, while uncertainty can be reduced, variability cannot be reduced but only better estimated for instance, with better sampling (Björklund 2002).

1.2.1. Types of uncertainty in LCA

There are different uncertainty types which have their origins in different unknowns within LCA. In this thesis the definitions and classifications of Björklund (2002) for the different uncertainty types are used.

- Parameter uncertainty has been associated to data inaccuracy (Huijbregts et al. 2001), unavailability and to unrepresentative data (Björklund 2002). This is uncertainty due to for example, wrong inventory data, missing data or the use of data that refers to different technologies, places or temporal resolutions other than the intended one. This is the most known source of uncertainty in LCA as well as the most treated in the literature.
- Methodological choice uncertainty is due to the unavoidable choices of practitioners along the phases of LCA. For example, the choice of functional unit, product-system boundaries (Tillman et al. 1994), allocation methods (Weidema 2000; Guinée and Heijungs 2007), environmental impact categories, and characterization methods and factors (Huijbregts 1998b; Finnveden 1999) are typical examples of practitioners' choices while undertaking an LCA. It has been shown for various applications that different choices lead to different, and in some cases significantly different LCA results.
- Model uncertainty refers to simplification aspects of LCA such as aggregation, and the modelling aspect of LCA for example linear and non-linear models (Heijungs and Sun 2002), derivation of characterization factors (Björklund 2002) or estimation of emissions with exogenous specialized models. Model uncertainty has not been widely addressed in LCA.
- Epistemological uncertainty emerges from the lack of knowledge on system behavior for instance, when modelling future systems (Björklund 2002). The word epistemology has its origins in the Greek epistanai which means "to understand", "to know" and it has been defined as "the study or a theory of the nature and grounds of knowledge especially with reference to its limits and validity" (Merriam-webster 2015). This is probably the least addressed source of uncertainty in LCA.

- Variability refers to intrinsic fluctuations of a numerical property (Björklund 2002) such as the yield of a hectare of arable land. Variability has been widely addressed in literature mostly in relation to input and output data used in LCA. Variability is also referred to as ontic uncertainty i.e. natural randomness often expressed with means and their ranges likelihood (van Vuuren 2007)

1.2.2 Approaches to deal with uncertainty in LCA

Different types of uncertainty in LCA may require different types of treatment. There are different approaches to deal with uncertainties in LCA. In certain cases, the aim is to reduce uncertainty in order to generate a more reliable assessment and therefore, better support for decision-making. In other cases, the aim is to reflect the uncertainty of the result as an extra piece of information to the decision-maker. In general, the main approaches to different types of uncertainty are (Heijungs and Huijbregts 2004): the scientific, the constructivist, the legal and the statistical approaches. These approaches use additional research, consensus or agreement, authority, and probability and statistics to deal with uncertainty. From these approaches, only the statistical approach explicitly incorporates uncertainty in the outcomes of LCA (Heijungs and Huijbregts 2004).

Statistical approaches to parameter uncertainty have led, in the past decade mostly, to sophisticated methods to characterize input uncertainties (Heijungs and Frischknecht 2004; Bojacá and Schrevens 2010; Ciroth et al. 2013; Henriksson et al. 2013; Muller et al. 2016; Qin and Suh 2016), to propagate such uncertainties through the LCA model (Imbeault-Tétreault et al. 2013; Groen et al. 2014; Heijungs and Lenzen 2014; von Pfingsten et al. 2017), to interpret outputs with uncertainty (Heijungs and Kleijn 2001; Prado-Lopez et al. 2014, 2016; Henriksson et al. 2015a; Cucurachi et al. 2016) as well as to approaches that deal with all the above (Hung and Ma 2009; Andrianandraina et al. 2015; Gregory et al. 2016; Wei et al. 2016). Statistical and mathematical approaches to treat methodological choice uncertainty have been proposed too (Cruze et al. 2014; Jung et al. 2014; Hanes et al. 2015). These incorporate in the outcomes, the effects of uncertainty due to the different choices. Statistical and scientific approaches have also been published for model uncertainties (Padey et al. 2013; Andrianandraina et al. 2015). Typically, these treat parameter and model uncertainty simultaneously.

The composition approach (i.e. constructivist approach in Heijungs and Huijbregts, 2004) and legal approach are based on consensus among stakeholders on the choices or on predefining (ISO 2006) or mandating the choices. This reduces uncertainty in the outcomes (Heijungs and Huijbregts 2004) and increases comparability of studies yet no information on the likelihood of the results can be provided. Environmental Product Declaration (EPD) schemes as well as Product Category Rules (PCRs) are examples of such approaches to deal with uncertainty due to choices (Del Borghi 2013).

Dealing with uncertainty due to methodological choices in LCA has mostly been handled by the legal approach.

The scientific approach has mostly focused on scenario modelling as a tool to deal with different sources of uncertainty. Among these there are uncertainty due to choices (Guinée and Heijungs 2007), epistemological uncertainty (Spielmann et al. 2005; Dandres et al. 2012; Hertwich et al. 2015; Gibon et al. 2015) and parameter variability and model uncertainty (van der Harst and Potting 2014; van der Harst et al. 2014). Further, there is a large body of literature in LCA that focus on sensitivity analysis which is a way to address uncertainty due to different assumptions for parameters, methodological choices, models, etc. usually assessing their change one at the time.

In summary, within the different approaches, varied tools to deal with different sources of uncertainty in LCA are available (Table 1).

Table 1. Main sources of uncertainty in LCA and some techniques and methods to treat them. Adapted from Huijbregts (1998), Björklund (2002) and Heijungs and Huijbregts (2004).

Tools \ Type	Parameter uncertainty	Model uncertainty	Uncertainty due to choices	Epistemological uncertainty	Spatial variability	Temporal variability	Sources and objects variability
Scientific Approach							
Additional measurements	x						x
Scenario modelling		x	x	x	x	x	x
Non-linear modelling		x					
Multi-media modelling		x			x		
Composition Approach (Constructivist approach in Heijungs and Huijbregts, 2004)							
Expert judgements/ peer review	x		x				x
Rules of thumb	x						
Legal Approach							
Standardization	x		x				
Prescription of specific methods	x		x				
Statistical Approach							
Probabilistic simulation	x		x				x
Data quality indicators	x				x	x	x
Uncertainty importance analysis (Global sensitivity analysis)	x	x	x		x	x	x
Classical statistical analysis	x				x	x	x

Bayesian statistical analysis	x				x	x	x
Sensitivity analysis	x	x	x	x	x	x	x
Interval arithmetic	x				x	x	x
Correlation and regression analysis	x						x

1.3 Problem identification and aim

1.3.1 Deepening the uncertainty dimension in Life Cycle Assessment

In general, it is widely-agreed that dealing with different sources of uncertainty in LCA is a vital step to increase reliability of LCA results (Ross et al. 2002; Lloyd and Ries 2008). It has also been recognized that there is a need to further develop, within the LCA community, protocols for characterizing, propagating, and interpreting uncertainty (Lloyd and Ries 2008). However, to date the most common approach in LCAs is deterministic (Wei et al. 2015), excluding any specification of any type of uncertainty. Most recent efforts have been in the direction of recognizing and increasing the community's understanding of the different sources and of the implications of uncertainty for different LCA applications.

This thesis extends knowledge in the same direction - towards a clearer understanding of the implications of different sources of uncertainty in LCA – and further develops methods to treat them. Such effort is referred to as deepening the uncertainty dimension in LCA. The term deepening has its origins in the Life Cycle Sustainability Assessment (LCSA) framework proposed by Guinée et al. (2011). In LCSA, current LCA deepens to include other than just technological relations such as economic and behavioral relations (Guinée et al. 2011). In this thesis, current LCA deepens to deal with some sources of uncertainty which have not yet been widely or at all addressed in the state-of-the-art literature, and new tools are developed, within the approaches previously described (see Box 2 for the sources of uncertainty addressed in this thesis). These sources of uncertainty have been selected as they relate to some of the most pressing topics for the LCA community: 1) allocation method choice, 2) accounting for future socio-technical changes in prospective LCA and 3) interpretation of LCA results including uncertainty estimates. These are the specific issues addressed in this thesis.

Box 2. Source of uncertainty to be further addressed in this thesis

Source of uncertainty	Issues addressed	Approach used	Tool
Methodological choice uncertainty together with parameter uncertainty	Allocation method <u>choice</u> together with uncertainty due to missing data, data that refers to different technologies, places or temporal resolutions than the intended one	Statistical approach	Probabilistic simulations
Epistemological uncertainty (The future is unknown)	Accounting for <u>future</u> socio-technical changes in prospective LCA	Scientific approach	Scenario modelling
Methodological choice during interpretation phase of LCA	Choice of the <u>interpretation</u> method of uncertainty analysis results	Legal approach	Guidance/ Prescription of specific methods

1.3.2 Research questions

The aim of this thesis is to deepen the uncertainty dimension of current LCA in order to increase the reliability of LCA results for specific applications by means of addressing different sources of uncertainty not yet addressed, with methods not yet available. On the basis of the identified sources of uncertainty to be addressed, the following research questions will be answered in this thesis:

RQ1: How can parameter uncertainty and uncertainty due to methodological choices in a single alternative LCA be quantified and propagated to the results?

RQ2: What are the implications for uncertainty analysis in a comparative LCA context of quantifying and propagating parameter uncertainty and uncertainty due to methodological choices?

RQ3: How can epistemological uncertainty for prospective LCA be systematically and consistently addressed?

RQ4: Which statistical method(s) should LCA practitioners use to interpret the results of a comparative LCA, under the light of its goal and scope, when considering uncertainty?

1.4 Thesis outline

Following the research questions this thesis has been organized in four content chapters **(chapters 2-5)**, one introductory chapter **(chapter 1)** and one concluding chapter **(chapter 6)**. Figure 1 shows the outline of this thesis as well as the source of uncertainty, the LCA application, the approach and the tool developed or used in each chapter.

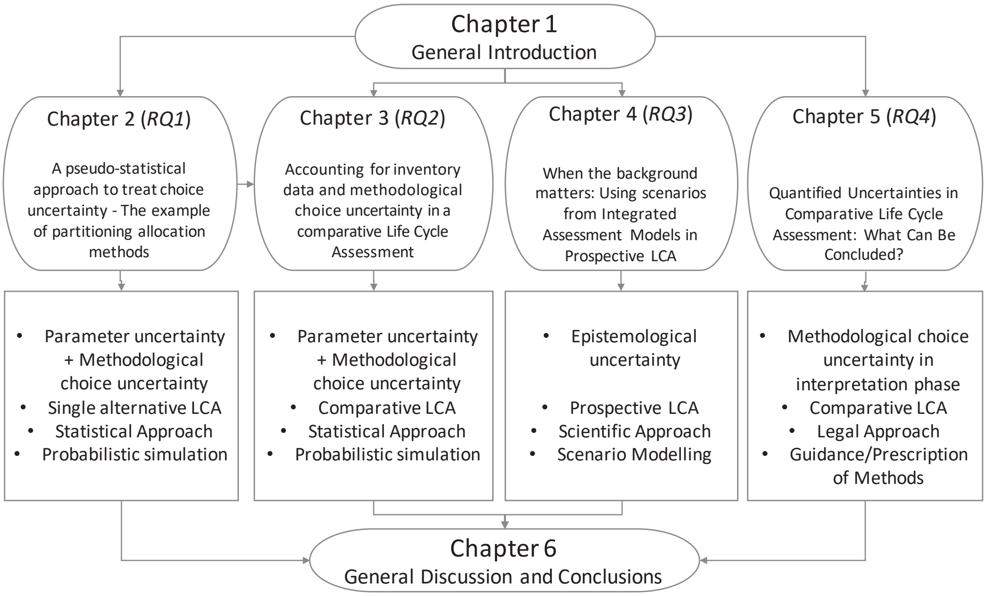


Figure 1: Outline of this thesis.

Chapter 2 develops, implements and tests a method to simultaneously propagate through LCA, uncertainty in unit process data and due to the choice of allocation methods of more than one process in the product-system. This chapter focuses on the particular example of the choice of partitioning methods for solving multi-functionality in LCA. The method developed can be used in LCA calculations and software. We assigned a methodological preference to the partitioning methods applicable to solve each multi-functional process in the foreground of the product-system, to enable pseudo-statistical propagation of uncertainty due to allocation (not strictly statistical as it is applied to choices). To illustrate the developed method and its outcomes it is applied to a single alternative LCA.

Chapter 3 broadens the application of the method developed in chapter 2 to a comparative LCA instead of a single alternative LCA. We identify the implications of broadening the scope to two alternatives with the same function. The case used in this chapter compares two aquaculture alternatives to produce fish. One of the two systems, co-produces fish with oysters, therefore, allocation of impacts becomes very relevant in this assessment to achieve comparability between the alternatives.

Chapter 4 explores a systematic and consistent approach for scenario development in prospective LCA. This approach is considered as a way to acknowledge and address epistemological uncertainty due to future socio-technical changes influencing the background of the LCA. A novel approach to systematically change the background processes in a prospective LCA is developed. It consists of deeply embedding scenarios from an Integrated Assessment Model (IAM) in the LCI of a product-system to derive future inventories based on the scenarios. The approach is applied to a prospective LCA case study comparing an internal combustion engine vehicle (ICEV) and an electric vehicle (EV) as mobility alternatives for the future. The background system addressed is the electricity production sector.

Chapter 5 conducts a critical review of methods to interpret uncertainty analysis results, particularly uncertainty-statistics methods (USM). The implications of the use of these methods for interpretation of comparative LCA results is investigated. Guidance is provided to help LCA practitioners select the most appropriate method to interpret their LCA uncertainty analysis results according to the type of goal pursued in the LCA study.

Chapter 6 reflects back on the research questions which are answered in chapters 2-5. Finally, a general discussion and a research agenda for the future are provided as part of this closing chapter

2.

A pseudo-statistical approach to treat choice uncertainty – The example of partitioning allocation methods

Angelica Mendoza Beltran
Reinout Heijungs
Jeroen B. Guinée
Arnold Tukker

Re-print with minor changes from:

The International Journal of Life Cycle Assessment (2016) 21: 252–264.
doi/ 10.1007/s11367-015-0994-4

Abstract

Despite efforts to treat uncertainty due to methodological choices in LCA such as standardization, one at the time (OAT) sensitivity analysis, and analytical and statistical methods, no method exists that propagate this source of uncertainty for all relevant processes simultaneously with data uncertainty through LCA. This chapter aims to develop, implement and test such a method, for the particular example of the choice of partitioning methods for allocation in LCA, to be used in LCA calculations and software. Monte-Carlo simulations were used jointly with the CMLCA software for propagating into distributions of LCA results, uncertainty due to the choice of allocation method together with uncertainty of unit process data. In this chapter, a methodological preference is assigned to each partitioning method, applicable to multi-functional processes in the system. The allocation methods are sampled per process according to these preferences. A case study on rapeseed oil focusing on three GHG emissions and their global warming impacts is presented to illustrate the method developed. The results of the developed method are compared with those for the same case similarly quantifying uncertainty of unit process data but accompanied by separate scenarios for the different partitioning choices. The median of the inventory flows (emissions) for separate scenarios varies due to the partitioning choices and unit process data uncertainties. Inventory variations are reflected in the Global Warming results. Results for the approach of this chapter vary with the methodological preference assigned to the different allocation methods per multi-functional process and with the continuous distribution of unit process data. The method proved feasible and implementable. However, absolute uncertainties only further increased. Therefore, it should be further researched to reflect relative uncertainties, more relevant for comparative LCAs. Propagation of uncertainties due to the choice of partitioning methods and to unit process data into LCA results is enabled by the proposed method, while capturing variability due to both sources. It is a practical proposal to tackle unresolved debates about partitioning choices increasing robustness and transparency of LCA results. Assigning a methodological preference to each allocation method of multi-functional processes in the system enables pseudo-statistical propagation of uncertainty due to allocation. Involving stakeholders in determining this methodological preference allows for participatory approaches. Eventually, this method could be expanded to also cover other ways of dealing with allocation and to other methodological choices in LCA.

Keywords: uncertainty, methodological choices, allocation, Monte-Carlo, LCA

2.1 Introduction

Methodological choices are unavoidable in all phases of LCA and are a source of uncertainty (Björklund 2002). Methodological choices in LCA refer, among others, to choices about system boundaries (Tillman et al. 1994), functional units, characterization factors (Huijbregts 1998) and methods to solve multi-functionality of processes (allocation methods). The latter is one of the most debated topics in the field of LCA (Weidema 2000; Pelletier et al. 2014; Ardente and Cellura 2012). According to the International Standardization Organization (ISO) 14044 guidelines, the choice of allocation method involves a stepwise procedure (ISO, 2006): 1a) avoid allocation by dividing multi-functional unit processes; 1b) avoid allocation by expanding the system; 2) divide the system (partitioning) using physical relations between products; or 3) divide the system (partitioning) by other relations of products. The application of this procedure to solve multi-functionality constitutes a source of variability in LCA results of many product-systems (Ayer et al. 2007; Weidema and Schmidt 2010; van der Harst and Potting 2014; Luo et al. 2009; Svanes et al. 2011; Guinée and Heijungs 2007) and may pose problems in different decision making situations (Wardenaar et al. 2012). Hence, the importance of this specific methodological choice in LCA is evident.

The ISO procedure aimed to create consensus and standardization (Björklund 2002) thus increasing the inter-comparability of LCAs dealing with the same topics. Despite the fact that ISO guidelines are widely applied by practitioners, the consensus reached in practice has been limited (Pelletier et al. 2014; Weidema 2014). Besides following standards and guidelines, LCA practitioners may opt to show the influence of different allocation methods on LCA results through sensitivity analysis. If more than one allocation method is applicable to a multi-functional process, one at the time (OAT) local sensitivity analysis is mostly performed. The influence of the choice of allocation method on the LCA results is investigated by adopting different sets or combinations of allocation methods in scenarios (Björklund 2002). This approach is very common when partitioning methods are used to solve multi-functionality (Ayer et al. 2007; Weidema and Schmidt 2010; van der Harst and Potting 2014; Luo et al. 2009; Svanes et al. 2011; Guinée and Heijungs 2007).

Another approach to treat the choice between methods to solve multi-functionality is based on mathematical arguments. To provide a solution for the system of linear equations of an LCA (Heijungs and Suh, 2002), the use of the least-squares technique has been investigated (Marvuglia et al., 2010; Cruze et al., 2014) . In this sense, particularly Cruze et al., (2014) favor avoiding allocation over partitioning regardless of the principle arguing that, “since the number of solutions to choose from is infinite, even consensus… would not necessarily lend validity to an LCA study”.

More recently, the study by Hanes et al. (2015) developed an analytical approach dealing with the choice of allocation method: the Comprehensive Allocation

Investigation Strategy (CAIS). This approach considers all possible combinations of partitioning methods in a comparative LCA, therefore it systematically explores the allocation space of various systems. CAIS helps determine whether comparisons between various systems are robust as far as the allocation space is concerned.

In a similar line of research, Jung et al. (2013) developed a method for integrating uncertainty of allocation factors in matrix based LCA calculations and propagating it to LCA results using an analytical approach (i.e. first-order approximations). This method considers the allocation factors themselves as uncertain input parameters that have a variation, and therefore lead to variability in the LCA outputs. It is thus not a method for choosing between allocation methods.

Besides the analytical method of Hanes et al. (2015), there is the statistical approach of Andrianandraina et al. (2015) .They apply local and global sensitivity analyses to determine the influence of uncertainty in unit process data, methodological and modelling parameters to the total uncertainty in LCA results. Technical, environmental and methodological parameters are treated as variables and using a detailed LCA model for the foreground system, they calculate scenarios dependent on the values of these parameters. Particularly, the partitioning method is treated as a qualitative methodological parameter with a uniform discrete distribution and two possible values that correspond to economic and mass partitioning. Moreover, of the available literature, only Andrianandraina et al. (2015) treat variability of LCA results due to unit process data uncertainty as well as due to the choice of allocation method.

Despite that the cited references address the uncertainty or variability introduced by the choice of allocation method, no method has yet been developed to simultaneously propagate uncertainty in unit process data and the sensitivity due to the choice of allocation methods of more than 1 process to LCA results, without requiring a detailed, parameterized foreground model and with the potential to be applied to other methodological choices. In this chapter, we develop such a method to be used in LCA calculations and software. Data uncertainty and sensitivity due to methodological choices together determine the total range of LCA results for a specific system. Only propagating their influence simultaneously will provide the full total range of results. As we strive towards circular economies, multi-functional processes will be encountered more often in LCA systems, increasing the importance of this simultaneous approach, the development of which is the aim of this chapter.

2.2 Methods

For the development of the method of this chapter, it is first important to place it in the space of methods that have a similar purpose (see Table 2). For each reviewed method, Table 2 also lists: allocation methods considered, the result after applying each approach and the sources of variability accounted for. The most sophisticated methods include uncertainty in unit process data, choice uncertainty and other sources of uncertainty, leading to results that account for these sources of variability.

Table 2. Approaches to choose among allocation methods and to deal with other sources of uncertainty and variability.

Approach to choose allocation methods	Reference	Uncertainty and variability sources explicitly included in the results			Allocation methods considered	Resulting allocation method
		Data	Choice	Other		
Standard / Guideline	ISO (2006)	-	✓	-	All	One method per multi-functional unit process in the system depending on standard hierarchy and OAT sensitivity when more than one allocation method apply
Differentiated standard	Pelletier et al. (2014)	-	✓	-	All	One method per multi-functional unit process in the system depending on standard hierarchy and OAT sensitivity when more than one allocation method apply
Mathematical based choice	Cruze et al. (2014)	-	-	-	All	Avoid allocation
One at the time (OAT) Sensitivity Analysis/ Scenario Analysis	Many studies	-	✓	-	All	Set of combinations of allocation methods for all multi-functional unit processes in the system
Comprehensive Allocation Investigation Strategy (CAIS)	Hanes et al. (2015)	-	✓	-	Partitioning	All possible robust allocation combinations using reformulated matrix algebra
Statistical method	Andrianan-draina et al. (2015)	✓	✓	✓	Partitioning	All possible combinations using detail foreground LCA model
Pseudo-statistical method	This chapter	✓	✓	-	Partitioning for illustration. Possibly all	All possible combinations using methodological preference and Monte Carlo simulations

In this chapter, for propagation of the uncertainty of unit process data, we use Monte Carlo simulations as propagation method. Within this sampling-based approach, we now include the discrete choice of allocation method as another element. Of course, uncertainty of process data and uncertainty of allocation method are distinct. There is a wide natural variability for process data, and a probability distribution properly reflects this, so that a sampling method is appropriate. For the discrete choice of allocation method, this is different. There is no natural variability. Nevertheless, we treat it in a similar way, because the effect is similar: in a given situation we are not sure of the precise process data and we are not sure of the precise choice of allocation method. Therefore, combining the uncertainty of data and the spectrum of choices in one probabilistic set-up is defendable. Notice that the usual terms that are appropriate for data uncertainty (uncertainty, probability, statistical, etc.) are not entirely suitable for describing choices. We will therefore in some cases avoid using such words, in other cases add a qualifier (like in "pseudo-statistical"), and in some cases just use them, tacitly acknowledging the changed usage. A short reflection around the – admittedly debatable – terminology used in this chapter will be provided at the end of the discussion section.

The application of this pseudo-statistical method, poses an additional question: is our method a local or global sensitivity analysis or rather an example of an uncertainty analysis? We argue that our method is closer to the realm of uncertainty analysis because, the way we treat unit process data uncertainty is an example of a true uncertainty analysis propagating input uncertainties into output uncertainties (Figure 2b). Moreover, contrary to common OAT practice (Figure 2c) the choice of allocation method is also propagated using Monte Carlo simulations. The latter is clearly beyond an OAT sensitivity analysis and also constitutes the main reason why we consider the method of this chapter to be more closely related to uncertainty analysis than to OAT sensitivity or scenario analysis. The aim of our method is to simultaneously propagate data and choice uncertainty to LCA results for all relevant processes of a product-system (Figure 2d).

Finally, to illustrate the development and implementation of the method, we use the choice among partitioning methods as an example of methodological choice in LCA. This means that methods to avoid allocation will not be considered. In the discussion section the possibilities of broadening up the application of the method to other ways of dealing with allocation and to other methodological choices is addressed.

2.2.1 Implementation of a pseudo-statistical propagation method for uncertainty due to the choice of partitioning method

For a multi-functional unit process, one or several partitioning methods can be applied in order to solve multi-functionality. Partitioning factors are defined as the fraction that divides the non-functional economic (i.e. the input products and the output wastes) and environmental flows to the functional flows (i.e. the product of interest) of a multi-functional process (Guinée et al. 2004). For each multi-functional unit process in the system, partitioning factors are defined and applied to enable the calculation of the inventory table. Typically, the sum of all partitioning factors for each partitioning method is equal to 1 (Heijungs & Guinée 2007). This is, in very general terms, the working procedure for partitioning methods using different physical and non-physical principles such as mass, energy content and economic value.

To be able to introduce pseudo-statistical propagation of the choice of partitioning method in an LCA system, the *methodological preference* (p) (as a percentage) is introduced for each applicable partitioning method per multi-functional process. This

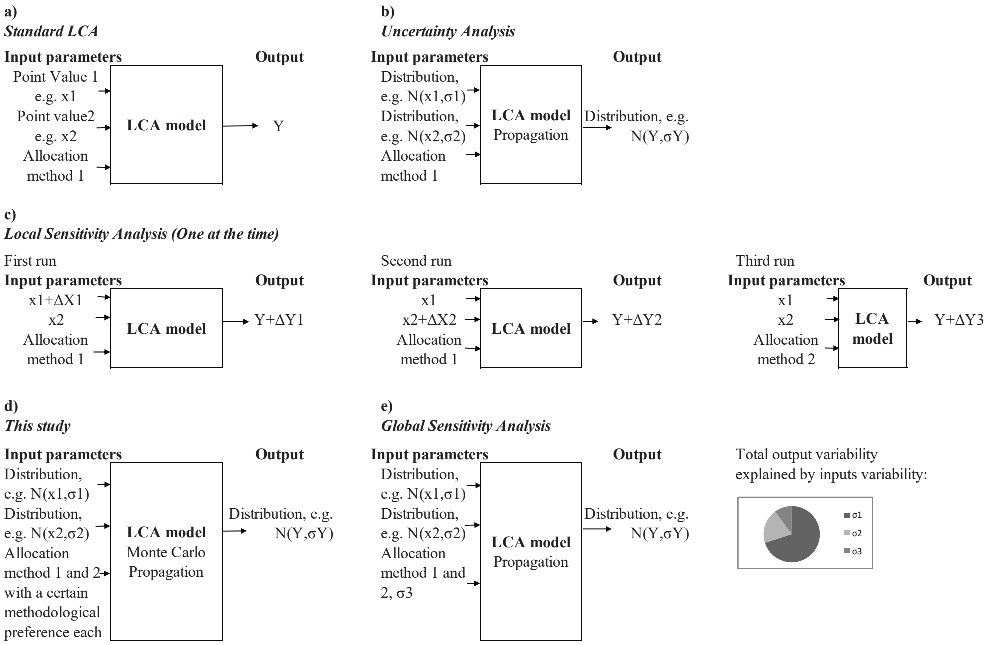


Figure 2. a) Schematic representation of a standard LCA using point values for unit process data as input as well as one allocation method per multi-functional process; the output corresponds with a point value for an environmental impact category or inventory flow. b) Uncertainty analysis, using ranges, standard deviation and distributions of unit process data instead of point values as inputs together with one allocation method per multi-functional process to calculate distributions of outcomes. c) Local OAT sensitivity analysis, varies a certain percentage the inputs (one at the time) to see the influence in the outcomes. d) The method of this chapter propagates both data and allocation method choice uncertainty to the outputs e) Global sensitivity analysis starts with an uncertainty analysis and then calculates how much of the variability of the output is due to variability of each input.

parameter corresponds to a discrete methodological parameter and has been set to a value between 0 and 100%. The assignment of a methodological preference is a subjective choice offering a possibility to more actively account for different views by involved scientists and stakeholders or perhaps accounting for patterns in the partitioning choices already made by relevant literature. For instance, if only one partitioning method is applicable for a multi-functional process then p equals 100% for that method and process, and if for example, for another multi-functional process, three partitioning methods are applicable then p_1, p_2 and p_3 should equal a value between 0 and 100%, all together adding up to 100%. These methodological preferences define the *ranges of methodological preference* such that for each range one partitioning method takes place. The value of a random number from a uniform distribution between 0 and a 100 is then generated and evaluated for the ranges of preference, and in this way a partitioning method is determined for each multi-functional process in the system.

In mathematical terms every time a multi-functional process is encountered in a system the following action takes place: a random deviate x is drawn uniformly between 0 and 100, and depending on its value, a certain allocation choice (partitioning in this case) is implemented.

$$\text{Allocation method} = \begin{cases} \text{Method 1} & \text{if } x \in [0, p_1] \\ \text{Method 2} & \text{if } x \in (p_1, p_1 + p_2] \\ \text{Method 3} & \text{if } x \in (p_1 + p_2, p_1 + p_2 + p_3] \\ \ldots & \\ \text{Method n} & \text{if } x \in (p_1 + p_2 + p_3 + \ldots + p_{n-1}, 100] \end{cases}$$

$$x \sim U(0,100)$$

After definition of the parameters introduced above, a method to propagate uncertainties to the LCA results is selected. For this, several methods exist and have been used in LCA (Groen et al. 2014; Heijungs and Lenzen 2014). Among the most widely-used ones are sampling methods such as Monte-Carlo (MC) simulations that rely on determining the probability distribution of the results by brute computing force progressively increasing in time (Heijungs & Huijbregts 2004). Other methods such as Latin Hypercube simulation, which uses a more efficient random sampling, could be used for propagation too (Groen et al. 2014). However, given the aim of the paper, we focused on the most widely-used and intuitively easiest approach: MC.

To propagate the uncertainty due to the choice of partitioning method using the described parameter definitions, MC simulations were adopted for the repeated random sampling. The larger the number of runs, the more combinations of partitioning choices could be taken into account in the results.

In case the same number of partitioning methods apply for all processes, the total number of partitioning scenarios for a system with multi-functional processes and several partitioning methods applicable to each process, would be equal to the total amount of multi-functional processes to the power of the number of partitioning methods possible. For instance, Guinée & Heijungs (2007) found 54 "multi-output" processes linked to passenger car and diesel systems in the ecoinvent v1.1 database (Swiss Centre For Life Cycle Inventories 2004). From these, only 7 were selected for the study by means of a contribution analysis. The study looked at the influence of economic partitioning, physical partitioning and the ecoinvent default partitioning on the LCA results. A full scenario analysis for all partitioning methods would have implied 54^3 i.e. 157464 possible partitioning scenarios, nonetheless only 3 were considered i.e. the 7 selected multi-output processes using either economic, physical or ecoinvent v1.1 default partitioning.

With the method proposed here, the analysis of a system with a relative large number of multi-functional processes and/or partitioning methods, such as that of Guinée & Heijungs (2007), would become computationally feasible, by capturing most (if not all) possible partitioning scenarios by means of MC simulations without actually having to define scenarios.

2.2.2 Case study

The approach described in section 2.2.1. has been implemented in the CMLCA software (CML, 2014) version beta 5.2 and has been tested with a simple system: rapeseed oil production in Northern Europe, as shown in the flow diagram of the system in Figure 3. The system is similar to the one implemented by Wardenaar et al. (2012) however, here it stops at rape seed at mill in order to concentrate on the really important novel aspect. The focus of the case study is on the only two multi-functional processes: [P1] rapeseed cultivation and [P3] rapeseed oil extraction by cold pressing of rapeseed. Process [P1] produces straw and rapeseed and process [P3] produces rapeseed oil and rapeseed cake at mill. Thus, both processes are multi-functional and require allocation. The functional unit is 1 kg of rapeseed oil at mill and the system includes the production, storage and transport of the main inputs to the three foreground processes shown in Figure 3. The entire background system is specified using ecoinvent data version 2.2 (Swiss Centre For Life Cycle Inventories 2007) which is already allocated. The background system remains constant for all the scenarios analyzed in this chapter. Scenarios result from combinations of the partitioning methods selected for process [P1] and process [P3], as will be further specified. A detailed description of the implementation of the system is available as supplementary material in the online version of this chapter.

For the two multi-functional processes, two partitioning methods are identified as applicable. In the case of [P1] (rapeseed cultivation), 100%-partitioning i.e. assuming the straw is ploughed through the soil and therefore all flows should be allocated to the rapeseed is the first option (Wardenaar et al. 2012). The second partitioning principle identified is based on the mass of straw and rapeseed which is found for the typical production of rapeseed and straw in Northern Europe in van der Voet et al. (2008) and although in their study they use 100%-partitioning, mass is another possibility for allocation. In the case of [P3] (rapeseed cold pressing), partitioning based on energy content and economic values of co-products could hold and the same partitioning factors as defined by Wardenaar et al. (2012) are used. Table 3 shows the partitioning factors per co-product for each of the partitioning methods and multi-functional processes described above.

The proposed method is tested by comparing two sets of LCA results. The first set corresponds to LCA results of the case study using a OAT sensitivity analysis to study the influence of different partitioning methods (i.e. without choice uncertainty) and process data uncertainty propagated with MC simulations. The second set corresponds to the LCA results for the case study using the method implemented in section 2.2.1 to propagate the uncertainty due to the choice of partitioning method while also accounting for process data uncertainty and both sources of uncertainty propagated with MC simulations. The former LCA results are referred to as "allocation scenarios" or simply as "scenarios" (i.e. excluding choice uncertainty) and the latter as the results of "this study" (i.e. including choice uncertainty).

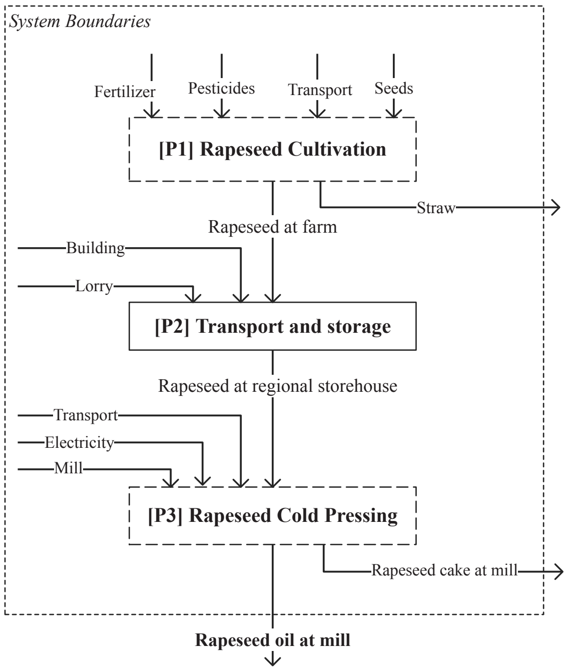


Figure 3. System for rapeseed oil production in Northern Europe. Boxes represent processes, dashed boxes are multi-functional processes.

Table 3. Allocation parameters definition as used in the case study.

				Methodological preference *p* (%)				
Multi-functional process	**Partitioning method / principle**	**Co-Product**	**Partitioning Factor**	**Scen1**	**Scen2**	**Scen3**	**Scen4**	**This study**
[P1] Rapeseed Cultivation	100%-partitioning	Straw	0	100	0	0	100	50
		Rapeseed	1					
	Mass-Partitioning	Straw	0.43	0	100	100	0	50
		Rapeseed	0.57					
[P3] Rapeseed cold pressing	Energy content-Partitioning	Rapeseed Oil	0.55	100	100	0	0	50
		Rapeseed Cake	0.45					
	Economic Value-Partitioning	Rapeseed Oil	0.7	0	0	100	100	50
		Rapeseed Cake	0.3					

Note: scenario in this study is a combination of the partitioning methods selected for process [P1] and process [P3].

The scenario results are calculated for four scenarios defined by the combinations of two multi-functional processes in the system with two applicable partitioning methods in each process. To include unit process data uncertainty, the method of Henriksson et al. (2013) was used to determine the unit process data distributions where possible despite that there are other methods available (van der Harst and Potting 2014; Hong et al. 2010; Imbeault-Tétreault et al. 2013; Heijungs and Lenzen 2014). Moreover, for propagation we used MC simulations with sample size of 1000 simulations for each of the four allocation scenarios. Further, as shown in Table 3, the methodological preference assigned to one partitioning method per multi-functional process in each scenario corresponds to 100, because as stated in section 2.2.1, choosing for one method corresponds to 100% preference of that method.

For the calculation of the LCA results of "this study" the unit process data uncertainty and the choice of partitioning are simultaneously propagated, using MC simulations based on unit process data distributions (same as in the allocation scenarios) and the methodological preference for the choice of partitioning method as defined in Table 3. A 50% methodological preference has been arbitrarily chosen for all applicable partitioning methods in both multi-functional processes in the case study, but although arbitrary, this preference allows an equal representation for all the methods enabling one to propagate uncertainty due to the choice of method. A total of 4000 MC simulations are run to create a representative sample to cover all possible partitioning scenarios. One would expect to be able to do with fewer simulations in order to have a computational gain compared to the 1000MC simulations for the four scenarios. However, as the aim of case study is to test the method, it was decided to have the same amount of runs in order to increase the chance of covering all partitioning combinations. Besides, for a more complex system (with more than 2 multi-functional processes) the computational gain becomes more evident as the chance of reproducing all partitioning scenarios is low, while the feasibility of capturing them with the method of "this study" is higher. These results are expected to cover the full range of the scenario results without choice uncertainty.

Finally, as an example of inventory results only the main greenhouse gases (GHG) i.e. carbon dioxide (CO_2), methane (CH_4) and di-nitrogen monoxide (N_2O) will be presented, as well as the LCIA results for global warming using the IPCC (2007) global warming potentials for a 100-years' time horizon.

2.3 Results

The median of the LCI results for the allocation scenarios varies for carbon dioxide emissions from around 0.7 to 1.2 kg CO_2 / kg of rapeseed oil, for methane emissions from around 1.0 to 1.7 g CH_4 / kg of rapeseed oil, and for di-nitrogen monoxide emissions from around 1.8 to 4.0 g N_2O / kg of rapeseed oil (Figure 4, left panels).

Thus, the differences between the median values of the scenarios only follow the choice of allocation methods for the two multi-functional processes in the case study.

Figure 4 shows the absolute GHG emissions per kg of rapeseed oil at mill for the 1000 MC simulations (left panels) for each allocation scenario separately including a statistical propagation of unit process data uncertainty. As expected, for those allocation scenarios with higher allocation factors for rapeseed and rapeseed oil (scenarios 1 and 4), the GHG emissions for the system studied are higher. The range that results for each of the allocation scenarios is smaller than the range resulting from all together. This indicates that scenario analysis can be misleading if all possible scenarios are not taken into account in the results.

Moreover, Figure 4 shows the absolute GHG emissions per kg of rapeseed oil at mill for the 4000MC simulations for the method introduced in "this study" (left panels column labelled 'This study'). The results, cover the full range of the four possible allocation scenarios but without separating between different scenarios as is seen in Figure 4 (left panels scenario 1, 2, 3 and 4 vs. "this study").

The histograms displayed in Figure 4 (right panels) show the distribution of the LCI results for the method of this chapter and the allocation scenarios.

For each allocation scenario there is a peak around the median of the LCI results and for the method of this chapter an overlapping distribution is observed. For instance, in the case of CO_2 emissions, there are three observable peaks (not four as the peak of scenario 1 and 3 overlap) which coincide with the medians of the allocation scenario. This outcome is also observable in the left panel graphs of Figure 4, in the form of more dense clouds of points around certain values of emissions, however, it is not always so clear in the whisker plots and this is the main reason for presenting the same results also in histograms.

Figure 5 (left panel) shows the global warming results for the same four scenarios and for the method developed in this chapter. The contribution of emissions to the global warming results varies depending on the allocation scenario between 49 and 55% for CO_2, around 2% for CH_4, and between 43 and 49% for N_2O emissions. Moreover, the scenario results now show less overlap, which is reflected by the histograms that more clearly show four discernible peaks around the medians of the allocation scenarios.

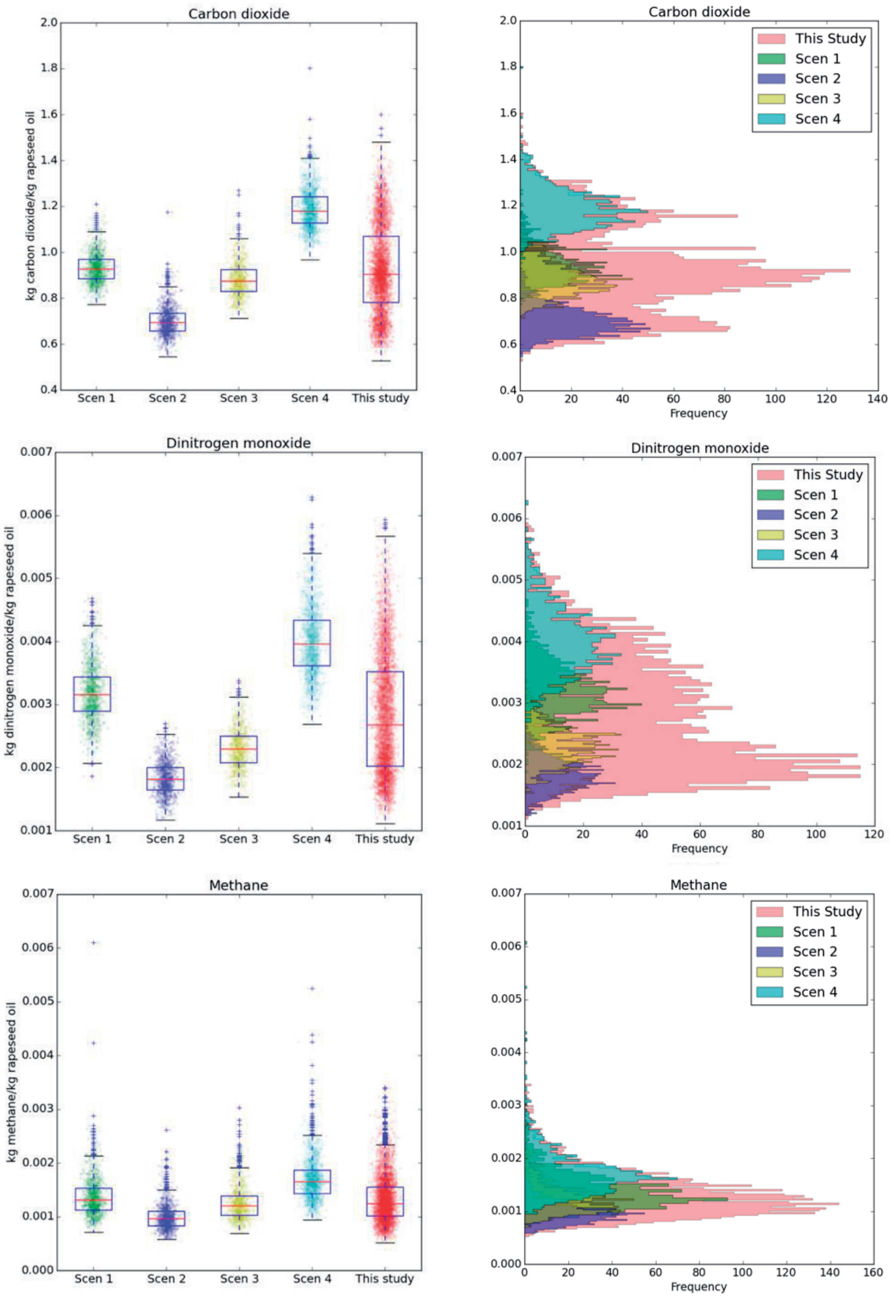


Figure 4. Left panels: LCI results for the main GHG emissions to air of 1000 MC simulations for the four allocation scenarios and 4000 MC simulations for the method introduced in "this study". The red line represents the median, the lower boundary of the blue box Q1, and the upper boundary Q3, so the height of the blue box is the interquartile range (IQR). The range of the whiskers (black horizontal lines) beyond the first and third quartiles is set to Q1(Q3) – (+) 1.5*IQR. The whiskers extend from the blue box to show the range of the data. The data points outside of this range, represent the outliers beyond the whiskers and are plotted as blue crosses. Right panels: histograms with a bin size of 100 based on the same MC simulations as in the left panels.

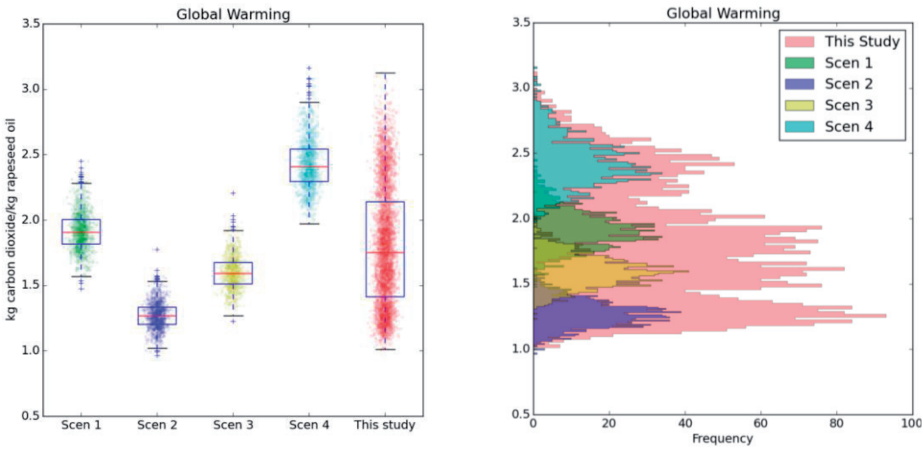


Figure 5. Left panel: Global warming in kg CO2 equivalents as an example of an impact category for the case study for 1000 MC simulations for the four allocation scenarios and 4000 MC simulations for the method introduced in "this study". See the caption of Figure 4 for an explanation of the blue boxes, red lines and crosses. Right panel: histograms with a bin size of 100 based on the same MC simulations as in the left panels.

2.4 Discussion

The method presented here to simultaneously propagate uncertainties in unit process data and due to the choice of partitioning methods is based on the introduction of the methodological preference of each applicable partitioning method for all multi-functional processes in a system.

In the case study presented, an equal methodological preference for all allocation methods applicable to the multi-functional processes in the systems was used. An equal methodological preference for all methods is of course an arbitrary choice, which can be made differently and in a more sophisticated way. One way to determine the methodological preferences of allocation methods could be to involve scientists, experts and stakeholders of specific sectors whose preference for the different allocation methods could be taken as basis for determining these values. Another way could be to determine patterns in the allocation choices already made by means of a meta-analysis (van der Voet et al. 2010) of existing case studies preferably specific for rapeseed oil.

Moreover, the methodological preference may influence the case study's results. We have investigated this influence by performing two distinct OAT sensitivity analyses. The two sensitivity analyses are variations of the two most extreme allocation scenarios i.e. scenario 2 and 4, arbitrarily changing the values of p as shown in Table 4 with the aim of exploring the effect of this parameter on the results.

Figure 6 illustrates the results of the sensitivity analyses compared to the equal methodological preference originally adopted for the case study.

The frequencies of the LCI results concentrate more around the median of a specific allocation scenario, as it is expected, once the methodological preference for one allocation method gets closer to 100%. Therefore, the values of *p* affect the distribution of the results for the approach of "this study". In Figure 6 (left panels), the range of results for the second sensitivity case reduces compared to the original range of our case study. But also, the amount of data points beyond the whiskers (outliers) increase. This could indicate that the LCI data distributions have long tails that show up in the results only for seldom MC runs. For the first sensitivity, the total range increases slightly and this is also an indication that the LCI data distributions are more sampled for values on the tails of the distributions.

Table 4. Allocation parameters definition as used in the sensitivity cases.

				Methodological preference *p* (%)		
Multi-functional process	**Partitioning method / principle**	**Co-Product**	**Partitioning Factor**	**This study**	**Sensitivity 1 (Variation of scenario 2)**	**Sensitivity 2 (Variation of scenario 4)**
[P1] Rapeseed Cultivation	100%-partitioning	Straw	0	50	80	20
		Rapeseed	1			
	Mass-Partitioning	Straw	0.43	50	20	80
		Rapeseed	0.57			
[P3] Rapeseed cold pressing	Energy content-Partitioning	Rapeseed Oil	0.55	50	80	20
		Rapeseed Cake	0.45			
	Economic Value-Partitioning	Rapeseed Oil	0.7	50	20	80
		Rapeseed Cake	0.3			

As mentioned before, to calculate the uncertainty due to the choice of allocation method in separate scenarios and not integrated with the MC based propagation of unit process data uncertainty, results have to be calculated for at least four scenarios for the simple case study (including only two multi-functional processes with two possible allocation methods each) and to run1000 MC simulations for each scenario in order to propagate LCI data uncertainty to the LCA results. This is a time consuming and a hardly ever performed work, and even less for more complex systems. In this context, the method proposed here, accounts in a pseudo-statistical manner for a representative sample of possible combinations and shows a representative range of possible results for a system with its likelihood (i.e. distribution) demanding less time from the practitioner than a normal setup of an OAT sensitivity analysis, but perhaps demanding more time for computation. The time spent in the case study for separate scenarios is the same as used by applying the method of this chapter, if the same number of MC simulations is adopted. However, we adopted more MC simulations for our method in order to ensure that all possible combinations of both data and allocation methods are sampled. For this reason, the time-demand of our method is higher.

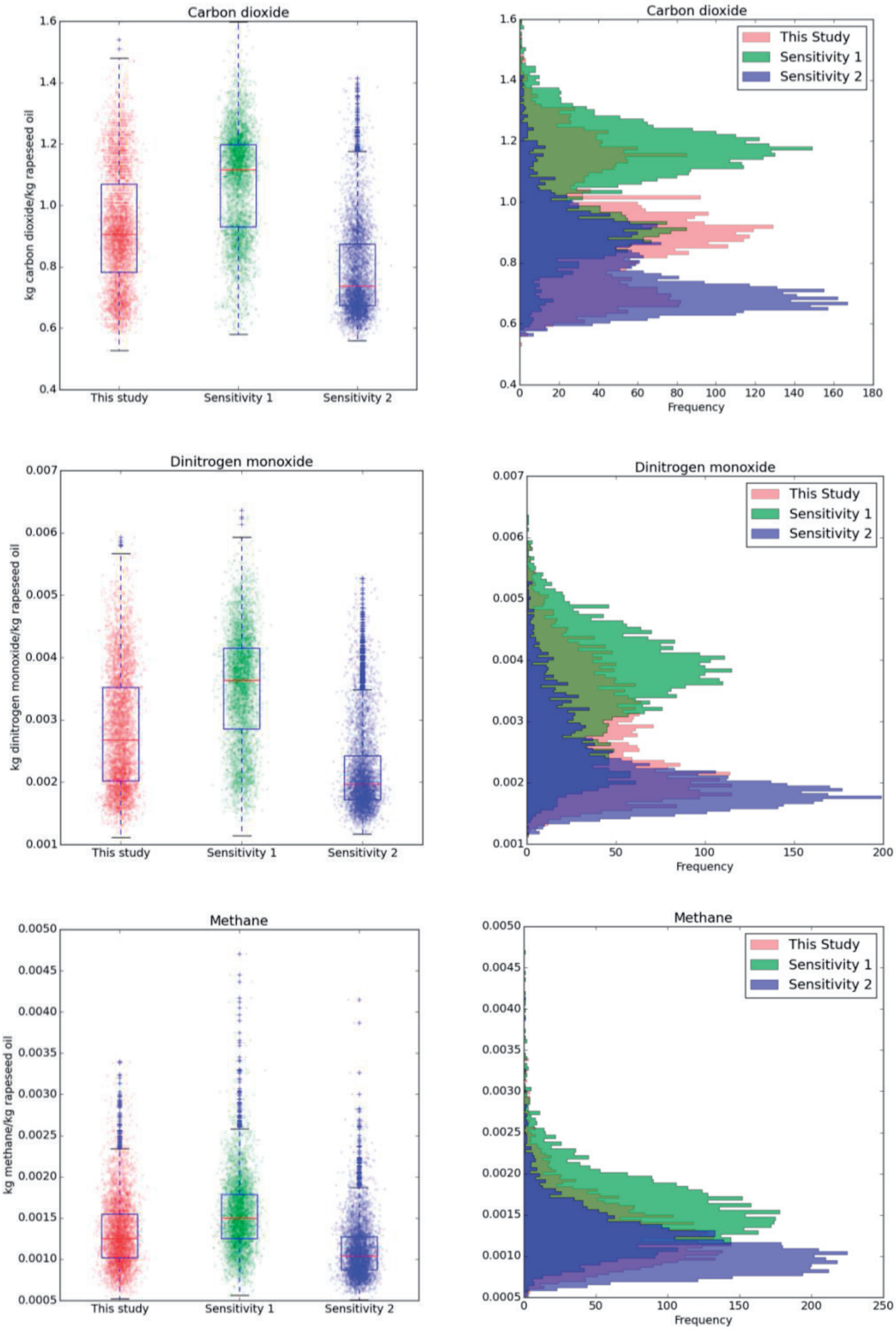


Figure 6. Left panels: LCI results for the main GHG emissions to air of 4000 MC simulations for the method introduced in this chapter using three different sets of methodological preferences for the allocation methods as defined in table 4. See the caption of Figure 4 for an explanation of the blue boxes, red lines and crosses. Right panels: histograms with a bin size of 100 based on the same MC simulations as in the left panels.

It can also be argued, that this method could be intensive in terms of computing capacity requirements as it uses MC simulations as a propagating method. Nevertheless, analytical methods do not yet exist for propagation of the choice of allocation methods, and we doubt if this is possible at all. Relying on increasing computational capacity, we consider the proposed method a good alternative to tackle two of the main sources of uncertainty in LCA in an integrated way. Possibilities for more efficient statistical propagation methods (e.g. Latin Hypercube sampling) also remain a topic for further research.

Another point for discussion, is the increased total uncertainties shown in the results of the method of this chapter, compared to those of the allocation scenarios. LCA studies are mostly relevant for comparing two or more alternative systems fulfilling the same functional unit. In the context of comparative LCA, relative uncertainties (Henriksson et al. 2015) play an important role for the application of this method. Therefore, the pseudo-statistical method becomes particularly relevant when comparing two or more alternative systems fulfilling the same functional unit.

Applying the method developed in this chapter for a comparison of 2 alternatives (A and B) fulfilling the same functional unit requires dependent MC sampling and comparison of the inventory and/or characterization results for each run, for example by subtracting the results from alternative B from the results of alternative A (A-B). In this way, each alternative builds upon the same sampled parameters for those parts of the systems that are shared (similar) for both A and B (Henriksson et al. 2015). Similarly, we here argue that the same allocation scenarios should be sampled for multi-functional processes that are shared between the two systems A and B. In fact, comparing two or more alternative systems providing the same function could be misguided if different allocation methods are chosen for each system. The method of this chapter can provide comparable relative results simultaneously accounting for the same or varying allocation choices and LCI data uncertainties where pertinent, which would be more meaningful information than the full absolute range of uncertainty as shown, for example, in the case study.

One could think that information about the influence of the allocation choice is disguised as the range of absolute uncertainty only increases. However, a Global Sensitivity Analysis (Figure 2e) could reveal back the influence of the choice in the results. The contribution of uncertainty of the input parameters to the total uncertainty of the outputs can be identified. Therefore, one could prioritize the main contributors to the total uncertainty and reduction of the overall uncertainty could be strived for, on the basis of which better data could be collected and/or consensus on allocation methods to be applied. This would never be possible with OAT sensitivity scenarios for allocation methods alone for a full scale LCA. Exercises such as a comparative LCA and a Global Sensitivity Analysis are, however, out of the scope of the present chapter and a topic for further research.

The method was presented for the example of dealing with the choice dilemma in solving multi-functionality by partitioning. The method could, however, also be applied to a higher level of choices for solving the multi-functionality problem. For instance, in the realm of consequential LCA, various scenarios of substitution or system expansion could also be assigned a methodological preference. In the realm of attributional LCA, as explored in the case study, various partitioning principles can be accounted for. As mentioned in other studies too, there is not one single way of solving multi-functionality in LCA (Guinée et al. 2004; Wardenaar et al. 2012), even when accepting that the solution should serve the purpose of the LCA (Pelletier et al. 2014).

The method could also be applied to other choices than only the one related to multi-functionality as long as the choice can be represented as a discrete choice. Then, a methodological preference can be assigned to each option and the uncertainty introduced by the choice can be propagated into LCA results. For example, in the case study the GWP_{100} was adopted to calculate the global warming results. We could also have adopted the GWP_{20} or GWP_{500}. Assigning a methodological preference to the GWP_{20}, GWP_{100} and GWP_{500} characterization factors and using the method developed in this chapter, would lead to inclusion of the influence of characterization factors simultaneously with the choice of allocation method and LCI data uncertainty, if desired. For this example, the calculation works correctly as long as the characterization factors for the different time horizons lead to the same type of LCA results, i.e. in kg of CO_2 -equivalents. On the other hand, if for example characterization factors for different methods lead to different type of results such as different type of units and scales, the method presented here could not be directly applied because the units could not be comparable among the different choices. In summary, the method developed in this chapter is valid for all discrete choices leading to comparable results.

Finally, we would like to discuss the terminology used throughout the chapter. As explained in the methods section, we believe this pseudo-statistical method is closer to the domain of uncertainty analysis, given that not only unit process data is propagated but also the methodological preference of allocation methods is propagated too by means of a statistical method (in this case Monte Carlo), to the LCA results. We are aware though, that for example, Andrianandraina et al. (2015), account for the propagation of the uncertainty due to methodological preference of allocation methods to the LCA results as a way of sensitivity analysis, therefore placing their method in the realm of sensitivity analysis. Independent of the type of analysis and admitting the debate around the semantics used to refer to our method, we consider more important the fact that robustness is added to the results by explicitly accounting for various sources of variability.

2.5 Conclusions

Methodological choices are unavoidable in all phases of LCA and are a source of uncertainty. Among these choices, practitioners typically choose between different methods to solve multi-functionality, and within partitioning methods different choices can be made again. Unresolved debates on these choices constitute a major source of uncertainty in LCA results. Ways to deal with this issue include standardization, OAT sensitivity analysis and analytical and statistical methods for uncertainty analysis. Standardization reduces uncertainty, while OAT sensitivity analysis serves to analyze the system using specific combinations of allocation methods, in order to show a range of possible results. The full range of results given all possible choices for allocation methods and combinations in a system with several multi-functional unit processes is only shown by means of statistical and analytical methods, however. Not showing all (or very many) possible combinations can be misleading when evaluating the environmental impacts of a production system and when comparing two or more systems even more. In addition, so far only one study showed all combinations of allocation methods, as well as accounting for unit process data uncertainty.

This chapter proposed, implemented and tested a pseudo-statistical method (not statistical in the strict sense of the word) to enable the use of Monte-Carlo simulations as a statistical approach to simultaneously propagate uncertainty in unit process data and uncertainty due to the choice of partitioning methods to LCA results. For this purpose, the methodological preference was introduced and assigned to each partitioning method for each multi-functional process in a system. The assignment of a methodological preference involves an arbitrary choice offering a possibility to more actively account for different views by involved scientists, experts and stakeholders or patterns from meta-analysis of existing case studies.

The distribution of LCA results was analyzed for a very simple case study, with and without the previous approach and in both cases including LCI data uncertainty. We conclude that the proposed method enables in a relatively simple way, i.e. with a few additional parameters and computational calculation capacity dependent on the system, the propagation of uncertainty due to the choice of partitioning methods to solve multi-functional problems and data uncertainty into LCA results while not requiring a detailed foreground model for the foreground system.

It is concluded that this method can be particularly useful when comparing relative uncertainties of several alternative systems, as increased absolute uncertainty in the LCA results does not necessarily lead to more meaningful conclusions. Moreover, information about the contribution of choice and data uncertainty to the total uncertainty could be further provided by for example, a global sensitivity analysis. However, these are topics for further research.

In addition, the results of the application of the method provides a more transparent and robust base for comparative LCAs than OAT sensitivity analyses or uncertainty analyses only accounting for uncertainty in unit process data or sub-sets of combinations between data and allocation methods. More sources of uncertainty are explicitly accounted in the results by making explicit the methodological preference of an allocation method per multi-functional process.

Moreover, exploring the implementation of the proposed method for higher levels of choices in LCA, such as methods to solve multi-functionality in a broader sense and other methodological choices in LCA is another topic for further research. We argue that the method will also be valid for these choices as long as they can be represented as discrete choices and lead to comparable results. Furthermore, implementation and testing of the method for more complex systems, i.e. higher numbers of multi-functional processes with various applicable allocation methods, is also required. We believe a trade-off between time spend by the practitioner in setting the analysis and calculation time could take place for more complex systems.

Acknowledgements

This research has been done as part of the IDREEM project (Increasing Industrial Resource Efficiency in European Mariculture, www.idreem.eu) and has received funding from the European Union's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° 308571. The authors would also like to acknowledge the invaluable contribution by Ruben Huele to the data visualizations of this chapter and to Valentina Prado for her insightful comments.

Supporting information

Supporting information of this chapter may be found in the online version of the original article: https://link.springer.com/article/10.1007%2Fs11367-015-0994-4

3.

Accounting for inventory data and methodological choice uncertainty in a comparative Life Cycle Assessment: The case of Integrated Multi–Trophic Aquaculture in an offshore Mediterranean enterprise

Angelica Mendoza Beltran
Mariachiara Chiantore
Danilo Pecorino
Richard A. Corner
Joao G. Ferreira
Roberto Cò
Luca Fanciulli
Jeroen B. Guinée

Re-print with minor changes from:

The International Journal of Life Cycle Assessment (2018) 23: 1063-1077.
doi/10.1007/s11367-017-1363-2

Abstract

Integrated Multi-Trophic Aquaculture (IMTA), growing different species in the same space, is a technology that may help manage the environmental impacts of coastal aquaculture. Nutrients discharges to seawater from monoculture aquaculture are conceptually minimized in IMTA, while expanding the farm economic base. In this chapter, we investigate the environmental trade-offs for a small to medium enterprise (SME) considering a shift from monoculture towards IMTA production of marine fish. A comparative Life Cycle Assessment (LCA), including uncertainty analysis, was implemented for an aquaculture SME in Italy. Quantification and simultaneous propagation of uncertainty of inventory data and uncertainty due to the choice of allocation method were combined with dependent sampling to account for relative uncertainties, and statistical testing and interpretation to understand the uncertainty analysis results. Monte Carlo simulations were used as a propagation method. The environmental impacts per kilo of fish produced in monoculture and in IMTA were compared. Twelve impact categories were considered. The comparison is first made excluding uncertainty (deterministic LCA) and then accounting for uncertainties. Deterministic LCA results evidence marginal differences between the impacts of IMTA and monoculture fish production. IMTA performs better on all impacts studied. However, statistical testing and interpretation of the uncertainty analysis results showed that only mean impacts for climate change are significantly different for both productive systems, favoring IMTA. For the case study, technical variables such as scales of production of the species from different trophic levels, their integration (space and time), and the choice of species determine the trade-offs. Also, LCA methodological choices such as that for an allocation method and the treatment of relative uncertainties were determinant in the comparison of environmental trade-offs. The case study showed that environmental trade-offs between monoculture and IMTA fish production depend on technical variables and methodological choices. The combination of statistical methods to quantify, propagate and interpret uncertainty was successfully tested. This approach supports more robust environmental trade-offs assessments between alternatives in LCAs with uncertainty analysis by adding information on the significance of results. It was difficult to establish whether IMTA does bring benefits given the scales of production in the case study. We recommend the methodology defined here is applied to fully industrialized IMTA systems or bay-scale environments, to provide more robust conclusions about the environmental benefits of this aquaculture type in Europe.

Keywords: Aquaculture, IMTA, offshore-mariculture, uncertainty, LCA, SME

3.1 Introduction

Marine aquaculture is not a zero waste activity and can be problematic, with increased organic nutrient loads around farms (Granada et al. 2015), in extremis potentially leading to eutrophication, algae blooms (Chopin et al. 2007) plus seabed impacts, for example. Marine culture of fish is an open production system and during fish growth, nutrients from excess and uneaten feed and metabolic products, such as faeces and urine, are released to the sea. To mitigate some of these issues, Integrated Multi-Trophic Aquaculture (IMTA) (Chopin et al. 2001; Reid et al. 2009; Price and Morris 2013) is a practice that could offset environmental impact and help with the management of coastal ocean aquaculture. In open water systems, IMTA typically involves production of a high-trophic level species of finfish around which lower-trophic level species of bivalves and/or seaweed are cultured (Buschmann et al. 2001; Troell et al. 2003). Other combinations of finfish or crustaceans with any filter-feeding organism are also possible (Klinger and Naylor 2012; Cubillo et al. 2016). IMTA offers the possibility of bioremediation for nutrients discharges while broadening the economic base of aquaculture farms by means of product diversification (Granada et al. 2015).

Research to understand the environmental benefits of IMTA has taken place (Abreu et al. 2009; Reid et al. 2009; Klinger and Naylor 2012) for ponds, tanks, land-based and marine-based setups (Buschmann et al. 2001; Troell et al. 2003), generally at experimental scales, or through mathematical modeling (Ferreira et al. 2012; Cubillo et al. 2016). Assessments focus on the productivity effects of co-culturing species at different trophic-levels, as well as the potential of nutrient uptake or waste discharge reduction by the different species mix. IMTA is potentially useful to eliminate waste and increase the productivity of the food production system (Troell et al. 2003), while increasing the economic and environmental performances of an industry or business (Neori et al. 2004; Hughes and Black 2016). IMTA can, therefore, be considered in terms of eco-intensification, where the productivity per unit input is increased (Amano and Ebihara 2005). What is lacking, however, is a better understanding of the environmental benefits of IMTA at industrial scales of production from a life cycle perspective.

LCA has been extensively applied to aquaculture and fisheries systems (Vázquez-Rowe et al. 2012; Henriksson et al. 2012; Ziegler et al. 2016). LCA of aquaculture typically compares different techniques for production of one species and/or assesses "hot spots" or main contributing activities to the total impact of production of one species (Henriksson et al. 2012; Ziegler et al. 2016). Identifying problem shifting, for instance the environmental impacts of the effect of feeding wild caught fish to the farmed fish or of using agricultural products to feed the fish (Pelletier and Tyedmers 2008), as well as identifying environmental trade-offs among alternatives (e.g. Henriksson et al. 2015b), are two of the strongest aspects of LCA applied to aquaculture systems.

Despite the usefulness of LCA to identify hot spots and trade-offs of aquaculture production technologies, there are various limitations to its application. One of the key challenges (see Ziegler et al. 2016 for more challenges) is the necessity to go beyond point-value estimates, and to incorporate uncertainty in the calculations to produce more robust outcomes. Uncertainty appears in many forms in LCA (Björklund 2002) and in aquaculture LCAs, for instance, it is present in inventory data, due to methodological choices, and in impact assessment methods (Ziegler et al. 2016). Two of these sources of uncertainty are expected to play a more determinant role in the impacts of IMTA namely: variability in the production data due to, for instance, unpredictable events such as storms or disease outbreaks and uncertainty due to the choice of allocation method because of the co-production of species in one site.

A critical question for IMTA is what are the environmental trade-offs for a small (or medium) enterprise (SME) considering in shifting its monoculture aquaculture practice towards IMTA? For this chapter there was a need to 1) understand what are the environmental trade-offs for a selected SME adopting IMTA and 2) to test a method for comparative LCAs with uncertainty analysis, dependent sampling and statistical testing, as proposed by Henriksson et al. (2015a), while integrating the method outlined in Chapter 2 (Mendoza Beltran et al. 2015) to propagate the uncertainty due to the choice of allocation method and inventory data simultaneously. Thus, this chapter has a double aim: to assess the environmental trade-offs for SMEs adopting IMTA, using an Italian SME who has a fish farm site and has been experimenting with fish/shellfish IMTA as a means to increase eco-efficiency and to assess a proposed method for comparative LCAs with uncertainty analysis. The application of LCA to aquaculture has been growing but to our knowledge it has been applied only once (Czyrnek-Delêtre et al. 2017) to IMTA systems for comparative purposes, but not while simultaneously dealing with two uncertainty sources (from here on referred to as uncertainties). Czyrnek-Delêtre et al. (2017) assess the implication of some modeling parameters via sensitivity scenarios but do not assess the effect of methodological choices such as allocation and in addition assess an IMTA setup with seaweed and salmon.

3.2 Method

3.2.1 LCA Goal and scope

The goal of this LCA is to quantify the life cycle environmental impacts of the monoculture production of Sea Bass (*Dicentrarchus labrax*) and Sea Bream (*Sparus aurata*) per kilo of whole boxed and gutted packed finfish and compare them to those of the production of the same fish in an IMTA setup. We study both productive systems for Aqua Soc. Agr. s.r.l. which is a small to medium enterprise (SME) with a fish production site located in the Ligurian Sea near Genoa, Italy who uses submersible cages to produce mixed cohorts of both fish species. In the analysis, the total number of fish, from both species, is considered as the total production by the farm, without distinguishing between species. The total production is further packed or processed onsite in two final products: the first is whole boxed fish and the second is gutted head-on packed sealed fish (from here on referred to as gutted packed fish). Both products are available at the farm gate. About 4% of total production per year is gutted on site, before being packed sealed for local distribution, the rest is packed whole with ice in polystyrene boxes, also for local distribution. In a recent demonstration pilot study, the company introduced Pacific Oyster (*Crassostrea gigas*) grown in lantern nets (see the glossary in the supporting information for some aquaculture terms) in proximity to the fish cages, under a concession of the site license, to assess whether this fish/shellfish IMTA system could be successful in reducing finfish impacts and enable the company to diversify product lines. LCA was used to compare the impacts between fish produced in monoculture and IMTA systems. The functional unit is the same for both systems: one kilo of whole boxed fish and gutted packed fish at farm gate. From this kilo 0.04 kg correspond to gutted packed fish and 0.96 kg to whole boxed fish. Any processes performed after the farm gate, including fish retail and human fish consumption, is equivalent in both systems.

Monoculture and IMTA systems

Produced fish are humanely killed at harvest, processed and packed as explained. Flows and system boundaries of the monoculture system were defined after consultation with the SME (Figure 7a) and consist of eight sub-systems: fry (juvenile fish) production and transport to farm (S1), infrastructure construction consisting of offshore and onshore infrastructure (S2), feed production (S3), feed transport to farm (S4), maintenance of the farm (S5), growth (S6), harvest (S7) and processing of the fish (S8). The farm feed conversion ratio (FCR) oscillates depending on the size of the fish and time of year but is a mean of 2.8, meaning 2.8 kg of feed is required to produce one kilo of fish.

There are almost no changes required to the fish monoculture site with the introduction of the oysters. Therefore, for the LCA of the IMTA system, the monoculture system is the same and the introduction of oysters was considered as an add-on called "IMTA sub-system" (Figure 7b). Various tests were carried out to define an appropriate layout at the site, but the selected design in the IMTA sub-system consisted of longlines attached to the existing fish cage mooring system to the north and south, in line with the water flows through the site, with lantern nets used to contain oysters while they underwent growth (See supporting information for farm layout).

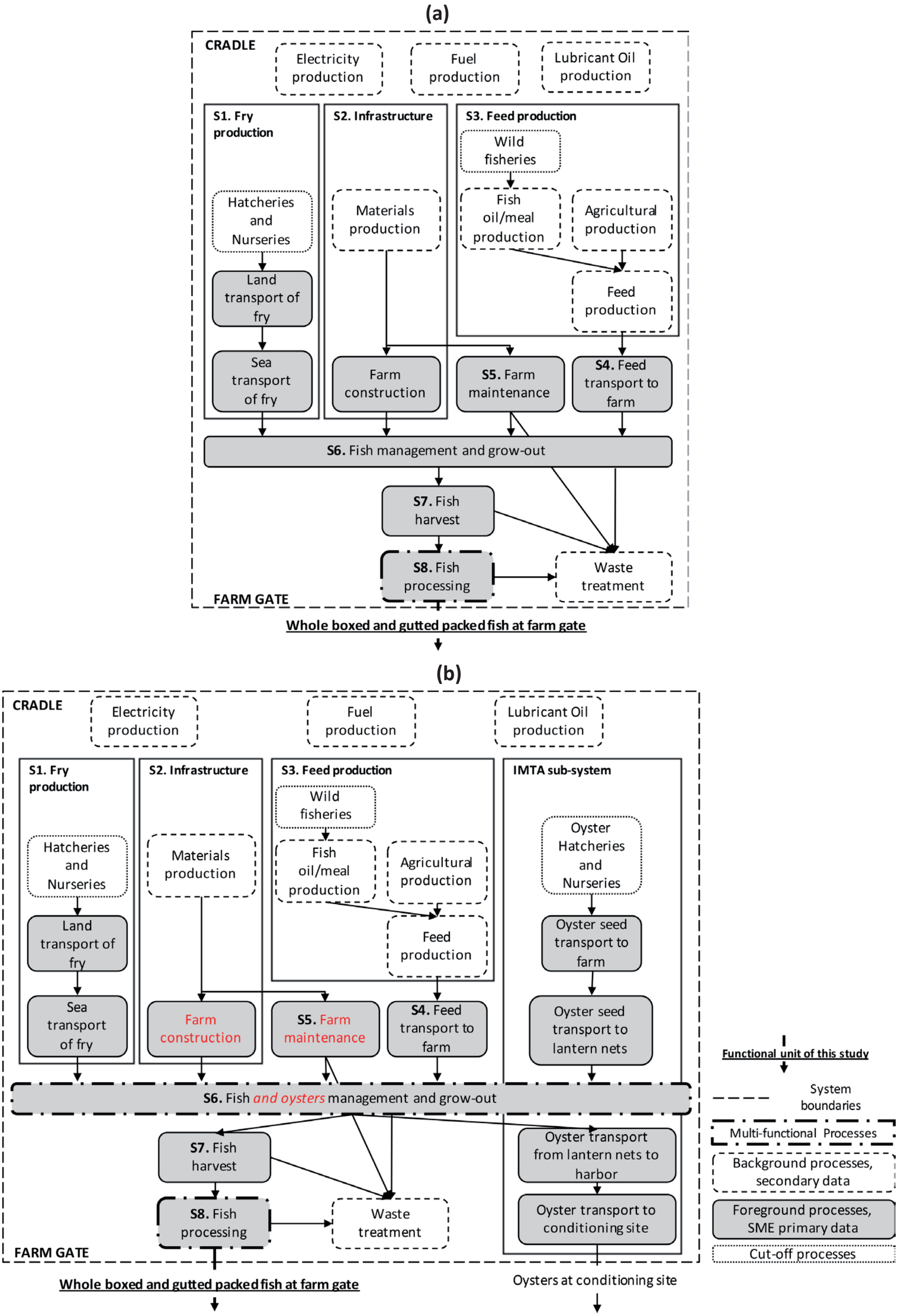


Figure 7. Flow diagrams of (a) the monoculture (Mono) system and (b) the Integrated Multi-Trophic Aquaculture (IMTA) system. Grey boxes represent the foreground processes for which primary data was collected and white boxes represent background processes for which secondary data was used. Processes highlighted in red are processes that changed in the IMTA system compared to the monoculture system due to introduction the oyster add-on.

The introduction of the IMTA sub-system resulted in additional processes, some of which were integrated within one or other of the eight monoculture sub-systems. These processes included: oyster seed production, oyster seed transport to farm, construction of the IMTA infrastructure (integrated in S2), seed transport to lantern nets, management and grow-out of oysters (integrated with S6), maintenance of the IMTA sub-system (integrated in S5). During the pilot, oysters were grown for 12 months on site to a degree in which they were ready for retail however, it is expected that in the industrial IMTA production transport of oysters to a different location for final fattening and conditioning could be required. Oysters fattening and conditioning are not included in this analysis. The farm gate for the LCA for the IMTA system was at the point where fish are ready for retail and oysters are ready for conditioning.

3.2.2 Inventory

The inventory description provided here for both systems focuses on stochastic inputs calculated via horizontal averaging of primary and secondary data (Henriksson et al. 2014). Details about other inventory data flows for foreground and background processes of both systems considered, their collection and implementation in the LCA software are provided in the supporting information. For all calculations, the CMLCA software version beta 5.2 was used. Full inventory tables for both systems are also provided in the supporting information. Data was collected over a full growth cycle for the fish component of the IMTA system, being 22 months, and encompassed two production cycles of 12-months for the oysters, after which all data was standardized to one year.

Foreground data

Foreground inventory data collection (see grey boxes in Figure 7) took place in two steps: 1) for the monoculture system and 2) for the IMTA sub-system which was subsequently integrated with the monoculture.

For the monoculture inventory, production data was collected over the period 2012 to 2014 (Table 5) and used as a basis for estimating the stochastic inputs for the inventory of fish management and grow-out, and fish processing. Following Henriksson et al. (2014), the data for the three years was horizontally averaged (Table 5) leading to weighted averages, lognormal distributions and an overall dispersion parameter Phi, used in the LCA software (Heijungs and Frischknecht 2004). Inherent uncertainties due to measurement or calculation imprecisions are estimated using basic uncertainties (Henriksson et al. 2014) for semi-finished products (Frischknecht et al. 2007), and data representativeness for the case study and spread due to variability in the yearly production were reflected from the three years production data and their representativeness for the case. Data for other foreground processes (including fuel use by boats, major onshore and offshore infrastructure including the production of component materials, chemicals use and so on), were collected for the 2012 fish production cycle and standardized to one year. Data were presented as point-values per year without uncertainty estimates. Therefore, for the deterministic LCA calculations (excluding uncertainties), point-values and the weighted averages for flows with stochastic estimates were used as the foreground inventory. For the uncertainty calculations, the stochastic inputs for fish growth and fish processing with point-values for the rest of the foreground inventory were used. For fish growth, an important flow that does not include uncertainty estimates is mortality of fish. Mortality is considered to be any reason for fish loss from the farm and includes losses from disease, which can be assessed, and escapees which cannot be assessed until after the harvest is completed and fish counted. Overall mortality was 30% of the fry seeded in 2012, due almost exclusively to escapees (Table 5). Fish loss is reported as an emission to marine water but it is not classified in any specific impact.

Under IMTA, it was assumed there were two sub-systems: the monoculture sub-system, for which data corresponded to that described above except for a few adaptations required (i.e. red processes in Figure 7b); and the IMTA sub-system for which IMTA pilot scale data were collected and further up-scaled. Foreground data was collected for oysters grown on site for one year (2014-2015) at an initial pilot scale of production. During the pilot, around 1400 individual oysters were delivered to site and cultivated in three lantern nets (with 10 layers and 45cm diameter) placed west of the farm, downstream relative to the main flow from the fish cages. Data for infrastructure, grow-out, maintenance, harvest and transport of the oysters were collected. In the pilot, oysters reached an average shell-on wet weight of 68 grams. Mortality was 20% of the oysters seeded. These pilot data from the IMTA sub-system were up-scaled to a more representative industrial level of production for the LCA assessment, based on a linear extrapolation with expert assessment. Experts confirmed the plausibility of these data as a good average representation of the oyster add-on despite of the different configuration between the pilot and the considered up-scaled IMTA system. It was assumed that the same oyster growth behavior, mortality and managing activities, developed under the pilot, apply to the industrial scale IMTA sub-system. Oyster seed input at the industrial scale was 77000 individuals based on the stocking density per lantern determined through the pilot study (around 480 individual oysters per lantern net) and the projected use of 160 lantern nets. Assuming growth of oysters under the pilot, the yearly production of oysters at the industrial scale IMTA system was calculated to be approximately 4.2 tonnes shell-on wet weight (Equation 1).

$$Oyster\ production_{Industrial\ scale} = individual\ oyster\ average\ weight\ at\ harvest_{pilot\ scale} * (number\ of\ oyster\ seed_{Industrial\ scale} - number\ of\ oyster\ mortality_{pilot\ scale}) \quad Eq.1$$

Table 5. Monoculture production data for 2012, 2013 and 2014 including both sea bream and sea bass for our case SME. The results of the horizontal averaging protocol from Henriksson et al. (2014) correspond to weighted means for the three years data, as well as lognormal distribution [L] and an overall dispersion parameter Phi (in parenthesis).

Unit process	Input / Output [NUSAP SCORES (Weidema and Wesnæs 1996)]	Unit	2012	2013	2014	Protocol Henriksson et al. (2014)
FISH GROWTH	**Inputs**					
	Fry, at cages [3,1,1,1,1,4]	fry/yr	850000	940000	1045000	945000 [L(0.134)]
	Fish feed, at farm [1,1,1,1,1,4]	kg/yr	589000	719050	841750	717000 [L(0.189)]
	Outputs					
	Grown life at farm[1] [3,1,1,1,1,4]	kg/yr	240000	223328	295776	253000 [L(0.172)]
	Mortality	Kg/yr	255000	n.c*	n.c*	255000
FISH PROCESSING	**Outputs**					
	Whole boxed fish at plant [1,1,1,1,1,4]	kg/yr	230400	214760	281700	242000 [L(0.16)]
	Gutted packed fish at plant [1,1,1,1,1,4]	kg/yr	8400	7450	12240	9360 [L(0.275)]
	Fish guts at plant[2] [3,1,1,1,1,4]	kg/yr	1200	1117.5	1836	1380 [L(0.291)]

[1] Calculated as the sum of whole boxed fish, gutted fish and guts
[2] Calculated as the 15% of the weight of gutted fish
n.c* = Not calculated, fish were still located in cages and mortality can only be measured after harvest

For the analysis, oyster growth was considered to be an integrated part of fish production (S6) and therefore the grow-out and management process in the monoculture systems (Figure 7a) becomes a multi-functional process growing both fish and oysters in the IMTA system (Figure 7b). Other data on foreground processes of the IMTA sub-system (including transport, additional maintenance and infrastructure) were collected for the pilot scale and up-scaled to the industrial production scale and integrated in the farm construction process (S2) and farm maintenance process (S5, see supporting information for details). These data correspond to point-values per year without uncertainty estimates as these were not available.

A key inventory flow for both systems is the net emission of particulate and dissolved nutrients to the sea during the cultivation period. Carbon emissions are not included as these mostly lead to carbon enrichment of the benthic layer. This is an impact rarely accounted for in aquaculture LCAs given the recent development of this impact within the LCA framework (Langlois et al., 2015). In this study, we focused on nitrogen and phosphorus emissions because of their potential to cause environmental damage in aquatic environments and their accountability in LCA impact categories such as eutrophication. In the monoculture system, fish were fed a pelleted feed and when ready they were harvested at the end of the production cycle, thus removing some added nutrients as harvestable product. Losses to the environment consisted of excretory products from fish metabolism (urine and faeces) and uneaten feed. Under the IMTA system emissions from the fish component were the same as those under monoculture, with no impact of co-cultivation on fish growth. Oysters remove phytoplankton and other detritus from the water column, convert this to tissue growth and emit both phosphorus and nitrogen in particulate waste, and through nitrogen excretion. There is no direct consideration of a coupling between fish waste being taken up by the oysters, simply the net change when both species are grown in the same space, although it is likely that at least a part of the detrital material ingested by the oysters will contain fish feed waste and faecal material (Reid et al. 2013).

Emissions were predicted using the FARM model (Ferreira et al. 2012; Cubillo et al. 2016) for the fish component (monoculture system) and for the fish and oyster component run simultaneously (IMTA system) to define the net emissions. Set-up of the FARM model is described in Cubillo et al. (2016) and model runs were completed using environmental driver data collected at the SME farm and based on the culture practices used (e.g. stocking density, seed, harvest weights and cultivation period). FARM models the outputs generated by species growth processes as nitrogen and phosphorus emissions to sea water, used as the inventory data for the monoculture system, being 62.4 tonnes N yr^{-1} and 2.4 tonnes P yr^{-1}. For the IMTA system the inventory data are the net nutrient emissions from fish growth minus the net nutrient uptake by oysters (0.1152 tonnes N yr^{-1} and 0.0091 tonnes P yr^{-1}), thus being 62.285 tonnes N yr^{-1} and 2.391 tonnes P yr^{-1}. The FARM model reports outputs in Kg yr^{-1}, converted to tonnes yr^{-1} to retain the same units throughout.

Background data

Background data for monoculture and IMTA fish production correspond to the sub-systems outlined in Figure 7. Each foreground flow is linked to background processes from the ecoinvent V2.2 database (Swiss Centre For Life Cycle Inventories 2007) for most inputs. The exception was the feed production sub-system where horizontal averaging (Henriksson et al. 2014) of various secondary sources for the feed mills (see supporting information) and data from the SEAT project (Henriksson et al. 2015b) for agricultural and capture fisheries were used. Ecoinvent v2.2. includes uncertainty estimates based on the NUSAP pedigree scores (Weidema and Wesnæs 1996) and despite this not being the most optimal quantification of uncertainty for background processes, it was the best available information.

Allocation

Multi-functionality takes place in two foreground processes of the IMTA system: 1) the fish and oyster management and grow-out; and 2) the fish processing (also part of the monoculture system). According to the International Organization for Standardization 14044 guidelines the allocation method choice involves a stepwise procedure (ISO 2006), being to (1a) avoid allocation by dividing multi-functional unit processes; (1b) avoid allocation by expanding the system; (2) divide the system (partitioning) using physical relations between products; (3) divide the system (partitioning) by other products relations. During the data collection for both systems it became evident that avoiding allocation for the grow-out process in the IMTA system was not possible, as this process will simultaneously grow fish and oysters, making it difficult to allocate inputs and outputs of this joint activity to individual processes for each species. System expansion was similar and no data were available for the monoculture system expansion to include the "monoculture" production of oysters in a similar location with a similar technology. Substitution was also not possible as the substituted products resulting from oyster production could not be determined. Therefore, allocation based on partitioning was applied in both processes. For the deterministic LCA results, mass-adjusted economic allocation (from here on referred as economic allocation) and mass partitioning were used in both processes. When uncertainty was included, we applied the pseudo-statistical method described in chapter 2 of this thesis (Mendoza Beltran et al. 2015). This method uses the so called "methodological preference" per partitioning method to propagate choice uncertainty simultaneously with inventory data uncertainty to the LCA results. Table 6 describes the principles, allocation factors used and the methodological preference applied to each partitioning method, which corresponds to equal preference. In both type of calculations i.e. the deterministic and the uncertainty LCA calculations, all environmental flows are allocated between the fish and the oysters. For background multi-functional processes, we use the allocation defined in ecoinvent 2.2 and mass-allocation for the processes derived from the SEAT project. The pseudo-statistical method to propagate uncertainty due to the choice of allocation method is therefore not applied to multi-functional processes in the background.

Table 6. Allocation factors used for the SME monoculture and IMTA systems.

Multi-functional Process	Partitioning principle	Co-Product	Partitioning factor	Mendoza Beltran et.al (2015) Methodological preference
Fish Processing**	Mass partitioning	Whole boxed fish	0.958	50
		Gutted fish	0.037	
		Guts	0.005	
	Mass-adjusted economic allocation	Whole boxed fish	0.95	50
		Gutted fish	0.05	
		Guts	0	
Fish and oysters management and grow-out***	Mass partitioning	Sea bass and sea bream at cages	0.98	50
		Oysters at lanterns	0.02	
	Mass-adjusted economic allocation	Sea bass and sea bream at cages	0.992	50
		Oysters at lanterns	0.008	
	Protein content*	Sea bass and sea bream at cages	0.99	-
		Oysters at lanterns	0.01	

* Protein content partitioning was not considered as a physical allocation principle as the allocation factors are very similar to those of economic allocation but it is shown here for indication
** Applied in both monoculture and IMTA systems
*** Applied in IMTA system only

3.2.3 Life Cycle Impact Assessment

Impacts were considered at the midpoint level. Characterization factors and impact categories were implemented according to the CML-IA database (CML - Department of Industrial Ecology 2016). The impact categories used were: abiotic resource depletion - elements, abiotic resource depletion - fossil fuels, global warming for a 100-year time horizon, (stratospheric) ozone depletion, human toxicity, photochemical oxidation, acidification (land and water) and eutrophication (land and water). Ecotoxicity for marine ecosystems has not been included as an impact category, following advice in the Declaration of Apeldoorn (UNEP/SETAC Life Cycle Initiative 2004). We also considered four additional categories from other sources: human toxicity, and freshwater ecotoxicity according to the USEtox model (Rosenbaum et al. 2008). For freshwater use the “blue water footprint” concept (Mekonnen and Hoekstra, 2011) was applied. Where freshwater is required to supply the functional unit throughout the supply chain use is accounted for, although no explicit reference to specific water sources is made. For land use, physical land occupation data (m^2) were added without specific characterization factors (or in other words was equal to one), for each process of the value chains analyzed. Finally, no normalization or weighting was undertaken.

3.2.4 Interpretation

Uncertainty analysis

Using the stochastic inventory data for the foreground and background processes of both systems, and the equal methodological preference for allocation methods in both systems, we simulated 1000 Monte Carlo (MC) runs to propagate these uncertainties to the characterized LCA results per impact category per alternative. Relative uncertainties between alternatives are captured by applying two techniques: first, dependent sampling and second, subtracting the characterization result between both systems for each MC run (Henriksson et al. 2015a). Dependent sampling implies that the characterized results for both systems is based upon the same parameter values randomly drawn in each MC run for the shared process on the background. Suppose that both the IMTA and the monoculture system share the same electricity production process in their backgrounds. As a result of dependent sampling, the characterized results per MC run for both alternatives, are based on the same parameter values for electricity production. In fact, the full technology matrix and the environmental extensions matrix are equal for both alternatives in each MC run. Subtracting the characterization result for IMTA from that of the monoculture system for each MC run serves to account for the comparative difference between the systems. Failing to look at the difference between systems, for instance by comparing the distribution of the 1000 MC runs per alternative, would be like comparing independent results for each alternative i.e. without accounting for the shared processes on the background. Therefore, for comparative LCAs, dependent sampling with subtraction of results between alternatives, is the only relevant option for the purpose of finding the statistical significance of the difference of performance of the alternatives; independent sampling disregards relative uncertainties in comparative LCA and therefore would be pointless for such purpose (Heijungs et al. 2017).

In order to test the significance of the difference of the impacts between both alternatives considered here, a null hypothesis was defined as the fish produced in IMTA and in monoculture systems have equal environmental impacts per kilo of fish. A paired t-test was used to determine statistical significance of the difference of environmental impacts between both systems. This method corresponds to the results of the null hypothesis significance testing (NHST) proposed in Henriksson et al. (2015a). The choice for this statistical test has two reasons: 1) the mean difference between the characterized results for IMTA and monoculture follow a normal distribution, according to normality test applied in SPSS v23 (i.e. Kolmogorov-Smirnov and Shapiro-Wilk) except for freshwater ecotoxicity, ozone depletion, human toxicity – USETox, photochemical oxidation and water use; and 2) the number of runs is large enough (1000 MC runs) to apply a parametric test, as the distribution of means of the difference between the characterized results for IMTA and monoculture will be approximately normally distributed (Agresti and Franklin 2007).

Other methods for uncertainty statistics of comparative LCAs

To further understand the environmental trade-offs between fish monoculture and the IMTA system, and to compare outcomes of different interpretation approaches, we also implemented three statistical methods, in addition to NHST, for advanced uncertainty results interpretation in the comparative LCA. They are: 1) the overlap area (Prado-Lopez et al. 2016) that shows the common area between the probability distribution of the alternatives results (i.e. IMTA and monoculture) per impact, where the closer to one the more equal the distributions are and the closer to zero the more separate the distributions are; 2) the discernibility analysis (Heijungs and Kleijn 2001) shows how often in percentage of total MC runs, one alternative has a higher result than the other. A 100% result means that for all MC runs one alternative scores higher than the other. The closer the result to 50% the more likely the two alternatives are to have the same result thus the less discernible they are for that impact; and 3) the modified NHST (Heijungs et al. 2016) shows the statistical significance of the null hypothesis in which the results of one alternative are "at least" a certain factor d_0 different from the results of the other alternative. Thus, d_0 is a dimensionless indicator for the acceptable threshold for the difference between the means of the two alternatives (so called "Cohen's d" as explained in Heijungs et al. 2016b).

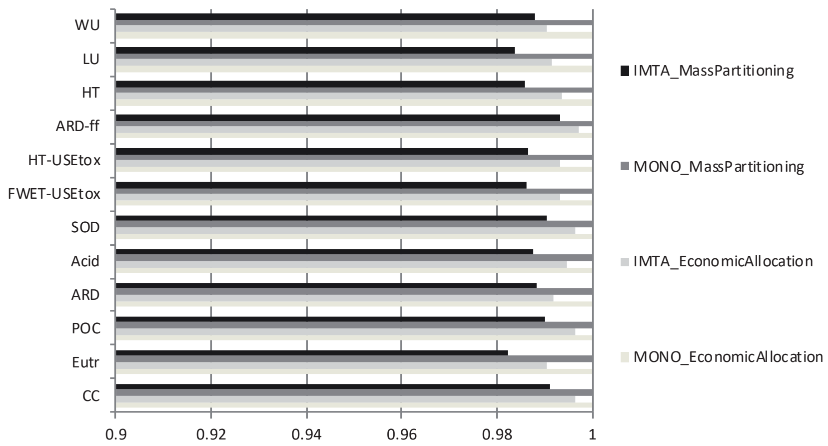
3.3 Results

Figure 8 shows the characterized LCA results for the deterministic calculations per impact category. According to these outcomes (Figure 8a) the IMTA system generally performs better than the monoculture system for all categories per kilo of fish produced for both allocation methods used. Eutrophication is the impact category showing the highest improvement although not more than about 2% in the case of mass partitioning allocation. Figure 8b shows each sub-system contribution to the total impacts of both alternatives. Almost no difference is observed between both alternatives. As expected, feed production had the highest impacts for all categories considered except for eutrophication impacts for which the on-site emissions to sea dominate. Also, infrastructure is responsible for about 60% of the impacts for abiotic resource depletion and plays an important role in human toxicity and freshwater ecotoxicity. These results hold for both types of partitioning considered.

Table 7 compares the deterministic LCA results in Figure 8a against the outcomes of other uncertainty statistics methods. From left to right, Table 7 first shows the deterministic results, based on point-values, in which IMTA impacts are lower for all impact categories considered per fish kilo. Also, the percentage of decrease of impacts in the IMTA system compared to monoculture are shown for the deterministic results. Second, the overlap area shows that the least overlapping categories are climate change and eutrophication and for the other impacts the overlap area is about one.

Discernibility shows that for almost all impacts, both IMTA and monoculture results are around 0.5. This indicates that both alternatives are likely to get the same result for all impacts. NHST shows that for all impact categories LCA results are not significantly different between the two alternatives except for climate change. This impact category is significantly different for fish produced in IMTA and in monoculture. Thus, fish produced in IMTA leads to lower emissions in CO_{2eq} per fish kilo than monoculture production. Finally, modified NHST results show that no impact, including climate change, is at least $d_0 = 0.2$ significantly different between these two systems. This indicates that despite that the means for climate change are significantly different (according to NHST) they are very close to each other i.e. less than the threshold of 0.2 units. The chance of finding statistical significance is increased for large sample datasets (such that from simulation models) and modified NHST was proposed as a way to deal with such limitation of significance tests (Heijungs et al. 2016).

a)



b)

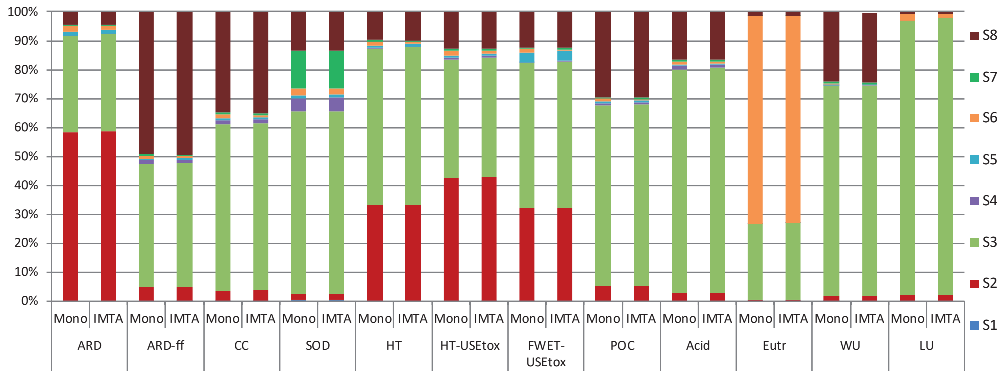


Figure 8. a) Deterministic LCA results for the IMTA and monoculture alternatives (scaled to the largest results per category) both calculated with economic allocation and mass partitioning for multi-functional processes in the foreground and b) contribution results for both alternatives and sub-systems as described in figure 1 and calculated with economic allocation (results are equal for mass partitioning). The impact categories are: climate change (CC), eutrophication (Eutr), photochemical oxidation (POC), abiotic resource depletion – elements (ARD), acidification (Acid), (stratospheric) ozone depletion (SOD), USEtox ecotoxicity – freshwater (FWET-USEtox), USEtox Human toxicity (HT-USEtox), abiotic resource depletion - fossil fuels (ARD-ff), human toxicity (HT), Land use (LU) and water use (WU). S1 – S8: as shown in Figure 7.

Impact Category	Deterministic LCA (point-values)			Overlap area	Discernibility		NHST	Modified NHST
Criteria Evaluated	Mono > IMTA (yes, no)	Percentage decrease (Mono-IMTA/Mono) Economic partitioning	Percentage decrease (Mono-IMTA/Mono) Mass Partitioning	Overlap of distributions (from 0 to 1)	Mono > IMTA (% of total MC runs)	IMTA > Mono (% of total MC runs)	H0: Mono = IMTA p < 0.05 = yes (significantly different) p > 0.05 = no (not significantly different)	H0: Mono - IMTA <= 0.2 p < 0.05 = yes (significantly different) p > 0.05 = no (not significantly different)
Climate Change	yes	0,4%	0,9%	0,96	47%	53%	yes	no
Eutrophication	yes	1,0%	1,8%	0,96	50%	50%	no	no
Photochemical Oxidation	yes	0,4%	1,0%	0,99	50%	50%	no	no
Abiotic Resource Depletion	yes	0,8%	1,2%	0,98	51%	49%	no	no
Acidification	yes	0,5%	1,3%	0,99	48%	52%	no	no
Ozone Depletion	yes	0,4%	1,0%	0,97	50%	50%	no	no
USETox Freshwater Ecotoxicity	yes	0,7%	1,4%	0,97	49%	51%	no	no
USETox Human Toxicity	yes	0,7%	1,4%	0,98	48%	52%	no	no
Abiotic Resource Depletion - Fossil Fuels	yes	0,3%	0,7%	1,00	51%	50%	no	no
Human Toxicity	yes	0,6%	1,4%	0,97	47%	53%	no	no
Land Use	yes	0,8%	1,6%	0,99	50%	50%	no	no
Freshwater Use	yes	1,0%	1,2%	0,99	51%	49%	no	no

Table 7. Results of deterministic LCA and four statistical methods to interpret the uncertainty analysis for the comparison between IMTA and monoculture (Mono) produced fish. Each method displays different results according to the evaluated criteria specified on the second row of the table.

3.4 Discussion

We discuss the results in the light of the two aims of this chapter: to assess the environmental trade-offs for SMEs adopting IMTA and to assess a proposed method for comparative LCAs with uncertainty analysis.

3.4.1 Case study

Monoculture fish production leads to nutrient emissions that are expected to be reduced in IMTA fish production. Deterministic results show that IMTA performs better than monoculture for all impacts per kilo of fish produced and eutrophication is the impact category with the largest improvement. On the other hand, uncertainty results and specifically NHST results showed that impacts are not significantly different for both technologies, except for climate change, which was found to be significantly lower under the IMTA system per kilo of fish produced. In addition, the overlap area between IMTA and monoculture distributions for all impact categories is very close to one, and discernibility results favor IMTA and monoculture each in around 50% of the cases for all impact categories as well. Therefore, deterministic results are oversimplified outcomes. To further understand the difference between deterministic and uncertainty results, Figure 9 illustratively presents the histograms for the MC runs for both alternatives for climate change and eutrophication. Deterministic results are based on the mean of the distributions, which is marginally lower for the IMTA system for both impact categories i.e. 0.4% for climate change and 1% for eutrophication. However, there is a larger difference between the means of both alternatives for climate change than for eutrophication (as confirmed by modified NHST results), while the dispersion of the difference between monoculture and IMTA is larger for eutrophication (the quartile coefficient of dispersion (Q3-Q1/Q3+Q1) of eutrophication is 2.1 times larger than for climate change). The bottom panels of Figure 9 show the difference between monoculture and IMTA per MC run for both impact categories. The top panels of Figure 9 show the results for each individual alternative while the bottom panels display the results accounting for relative uncertainties. Moreover, according to chapter 2 (Mendoza Beltran et al. 2015) the effect of the choice of allocation method, would be visible as peaks (separate peaks for each allocation method) of frequency of results in the top panels. Figure 9 shows only one peak per distribution for both impacts suggesting that inventory data uncertainty is responsible for most of the uncertainty. This finding is supported by the marginal difference in allocation factors for the allocation methods considered in this case study. To confirm which source of uncertainty in the inputs is responsible of uncertainty in the outcomes, global sensitivity analysis should accompany the method proposed here. This is however out of the scope of this research and a point for further research.

The lack of significance and differences between both systems can in part be explained by the scale of production of fish/shellfish species. Production of 4 tonnes of oysters annually is not small but remains insignificant in relation to the 240 tonnes of fish produced annually. Therefore, the result is a marginal intensification of the farm's production which in turn leads to approximately equal impacts of the two systems studied. What also must be factored in is the effect of additional environmental impacts originating from activities to construct and manage the IMTA sub-system. These are not visible in the results *per se* due to the effect of respective production scales. Moreover, as no uncertainty estimates were available for the IMTA sub-system, the effect of the dispersion of these data could not be included. Accounting for it on the oyster add-on would affect the results, as this sub-system corresponds to the differential part between the monoculture and IMTA system. This quantification remains a question for the future when industrial scale IMTA systems are established and data uncertainty for all components of the IMTA system become available.

Moreover, there is also an integration effect, which refers to the alignment of IMTA processes within the already existing monoculture production processes. These additional processes are essential to determine the magnitude of the impact increase

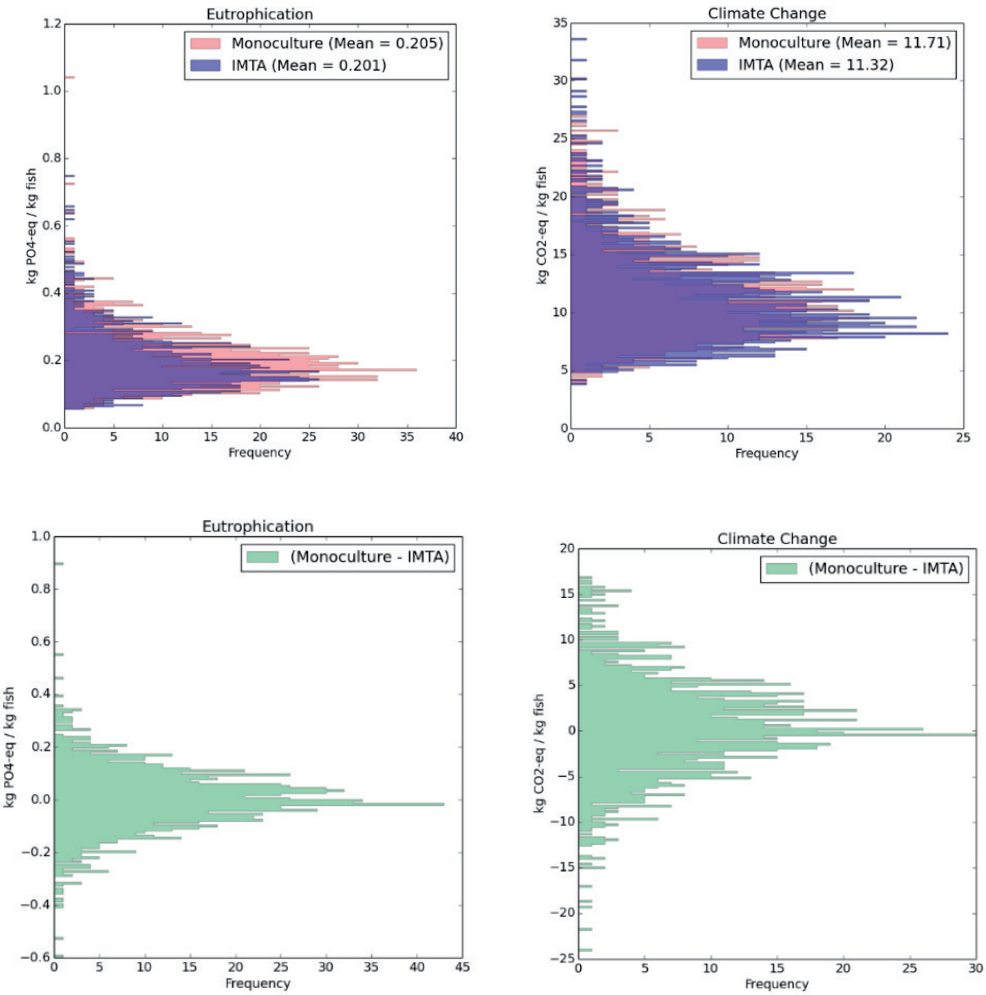


Figure 9. Top panels display the histogram for 1000 MC runs and 200 bins for eutrophication (top left panel) and climate change (top right panel) for the monoculture and IMTA systems. Bottom panels show the histograms for the difference between monoculture and IMTA per MC run for 1000 MC runs and 200 bins for eutrophication (bottom left panel) and climate change (bottom right panel).

of the IMTA system compared to the monoculture system. For instance, additional fuel use and its associated emissions will largely depend on the synchronization of boat use for maintenance, harvest and grow out activities of both fish and oysters, and the difference was not large under the current IMTA system. Moreover, the production, use and disposal of the add-on infrastructure required for the species added to the site cause additional environmental impacts, the magnitude of which depends on the way in which species integration physically occurs and on the species choice by the farm. In the case study, oyster growth, management and harvest demanded only a few additional

inputs due to the synchrony between tending to both stocks, which could be completed during the normal course of site management activity.
A big challenge for any IMTA system is spatial proximity and temporal synchronization of the species productive cycles. Cranford et al. (2013) has shown that shellfish ability to intercept waste particulates from fish cages diminish very quickly with distance from the fish site. Also, species considered for IMTA systems have specific growth periods that are not equal and may not overlap to any significant extent. In this study, however, there was a relatively high level of synchronicity. Shellfish were deployed within the existing fish mooring system; and fish were produced over approximately 22 months and oysters for 12 months; and because the oysters came from a hatchery the farm manager had power over when to deploy the oysters to sea. This is not always the case (Handå et al. 2012) if the IMTA system relies on natural settlement for seed collection (e.g. mussels). In the end the lack of difference in the impacts of the systems studied in the case study, mostly came from differences in production scales between the species. In general, variability between production scales of the species grown in the IMTA system, integration of production in time and space, and the choice of species determine, to a large extent, the trade-offs between implementing monoculture and IMTA systems.

There are some additional impacts that were not included in the current study despite indicators of such impacts being informative of the environmental performance of aquaculture farms. They do not currently correspond to developed LCA impact categories or lack characterization factors. For instance, disease treatment is one activity causing impacts measured by indicators such as the number of disease outbreaks. However, this indicator cannot yet be translated into impacts that are accountable throughout the life cycle of marine offshore aquaculture systems within the LCA methodology (see Rico et al. 2013 for other types of aquaculture), and this is an area where IMTA can have a positive impact (Ford et al. 2012). The presence of shellfish, filtering significant quantities of water to remove particulates, can have beneficial effects in potentially removing parasites, such as sea lice (Chopin et al. 2012) thus reducing infection potential. Moreover, for monoculture and IMTA there is often a lack of evidence of environmental improvement in the nutrients discharges because of difficulty in directly measuring changes in the environment (Pecorino et al. 2016). This is a major limitation for the proper assessment of the benefits of IMTA in LCA. Water quality around fish farms is intrinsically impacted by the presence of fish farms. However, it is often not measurable because of chemical transformations and mopping up of excess nutrients by other species, such as microalgae. Similarly, although particles are being removed from the water column by the addition of shellfish at the farm, they also produce particulate wastes, so have the potential to increase impacts (Troell and Norberg 1998), or at the very least have no positive change in sediment conditions.

In the case of life cycle impacts such as sea use and biotic resource use (Langlois et al. 2015), the study did not assess these impacts, as data gaps were encountered particularly in background processes such as wild fisheries. Recent work by Avadi et al. (2014) and by Fréon et al. (2014, 2017) on Peruvian *anchoveta* fishing and reduction, and by Samuel-Fitwi et al. (2013) and Parker and Tyedmers (2012) for other aquaculture feed ingredients such as Atlantic krill, should be coupled to the assessment of European aquaculture technologies to achieve a good representation of wild fisheries in the supply chain. However, as argued by Henriksson et al. (2015a) and by Heijungs et al. (2017) only relative uncertainties matter for comparative LCAs; and since the feed system remains the same, given that no additional feed is required for the oysters growth, these inventory gaps affect the absolute magnitude of the impact but not the comparison itself.

3.4.2 Comparative LCAs with uncertainty analysis

We implemented two methods to quantify, propagate and interpret results including uncertainties in comparative LCA. The first method relates to simultaneous propagation of inventory data uncertainty and the choice of allocation method as shown in chapter 2 (Mendoza Beltran et al. 2016). The second uses relative sampling and statistical testing to interpret the results of the uncertainty analysis (Henriksson et al. 2015a). Simultaneous implementation of these methods tackles two main sources of uncertainty in LCAs in a comparative context and helps interpret the results by means of statistical theory. Allocation methods were applied to foreground processes as they are fundamental in the comparison of monoculture and IMTA systems. We applied partitioning and allocation methods only. It is possible to use the pseudo-statistical propagation with substitution too if data were available (Mendoza Beltran et al. 2016). Combination of these methods increases the conclusions robustness as the uncertainty due to the allocation choice, together with the uncertainty of inventory data, can be treated from a statistical perspective instead of using one-at-a-time scenarios determined by the practitioner. The results showed that using economic allocation or mass partitioning, as in the deterministic LCA, one alternative (IMTA) performs better that the other (monoculture) for all impacts. However, taking into account the two sources of uncertainty and propagating them to the results together with relative sampling showed that there are no statistically significant differences between alternatives for all impacts, except for climate change. Deterministic results lead to oversimplified comparisons and exclude significance information. Therefore, uncertainty results based on the comparative methodology proposed in this chapter are more robust than deterministic results for comparative LCAs.

An important goal in uncertainty analysis of LCAs should be to treat background processes' multi-functionality, for instance from the ecoinvent database, in the same way as treating multi-functionality in the foreground processes by taking into account all the possible allocation methods for solving multi-functionality while accounting for inventory data uncertainty too. This chapter is a step forward in this goal as it shows how to apply a pseudo-statistical propagation method to foreground multi-functional processes of an LCA simultaneously with inventory data uncertainty. Applying the same method to multi-functional background processes would lead to much more robust LCA results because different configurations of the systems on the background would be accounted. For instance, in our case, agricultural processes and wild fisheries could be allocated with multiple methods. This is particularly important as many economies strive towards circularity, where LCA systems will encounter more often multi-functional processes (Mendoza Beltran et al. 2016). Despite some other studies treating uncertainty sources such as: methodological choices, modeling assumptions and inventory data uncertainty, by means of different approaches (Andrianandraina et al. 2015; Gregory et al. 2016), we are not aware of any study so far treating uncertainty due to the choice of allocation method for all multi-functional background processes.

Finally, an important limitation of the method proposed in this chapter is the management of correlations. We do not account for correlation between inputs and outputs in unit processes. For instance, in our LCA there is no correlation between fish produced and feed used. This means that the weighted averages and lognormal distributions determine, per MC simulation, how feed use and fish production correlate. This could lead to unrealistic FRCs for the farm under study. This point requires further development. Theories such as the one described by Groen and Heijungs (2017) may constitute a good basis for such further research in this area.

3.5 Conclusions

IMTA is a potentially innovative form of aquaculture in Europe, producing multiple species from different trophic levels within the same location, with lower trophic species utilizing the wastes from the higher trophic species, thus encouraging re-use of materials. In this sense, it is regarded as an environmentally beneficial form of aquaculture farming in comparison to traditional monoculture. This chapter implemented a comparative LCA with uncertainty analysis to understand the trade-offs between IMTA and monoculture fish production for a specific SME and concluded that the integration of fish and oyster culture led to marginal environmental benefits in comparison with the monoculture operation to produce fish. We found that the choice of allocation method had an influence on the magnitude of the benefits of IMTA production of fish. However, calculation of the same impacts including relative uncertainties due to inventory data and due to the choice of allocation method showed that there was no significant difference between the impacts of the systems, primarily due to the different scales of production between the two species. An increase in oyster seeding volume may well provide a more robust statistically provable benefit.

Moreover, statistical significance of the difference of the impacts between both systems could be determined because relative uncertainties were taken into account.

Thus, processes that were common to both systems were sampled using the same inventory data values and allocation method choice as well as the difference per MC run was calculated for the characterized results. Failing to use such an experimental setup would lead to LCA results that cannot be used as a base to establish statistical significance and should not be compared. Despite succeeding in the application of this comparative methodology including various uncertainties, what would be more useful is to apply it to a significantly larger, fully industrialized IMTA system, or at a bay-scale. Such scale, where the totality of production of different species is considered as a broad-scale IMTA system, thus individual farm integration is less relevant, and where uncertainty estimates are available for the IMTA sub-system inventory data, would provide more robust conclusions about the environmental benefits of this type of aquaculture in Europe and elsewhere. Moreover, to explain the outputs variability in terms of the inputs variability or to identify whether uncertainty due to methodological choices or inventory data uncertainty are responsible for uncertainty in the outcomes, the method applied here would have to be combined with global sensitivity analysis. Nonetheless, it was shown that for our case, most uncertainty in the results is probably due to inventory data dispersion and not due to the choice of allocation method, particularly given the small differences in the allocation factors for the allocation methods considered.

This case study provided a useful means to test a novel method of dealing with two major sources of uncertainty in LCA, namely inventory data and allocation choice. Both play a key role in determining the impacts of monoculture and IMTA fish production. When not accounting for uncertainties (deterministic LCA results), IMTA was the best performing option for all impacts considered here, and when accounting for uncertainties both options performed statistically equal for all impacts, except climate change. The comparative methodology including various uncertainties used here is a novel technique that can contribute to the robustness of conclusions as it adds information about the significance of results in a comparison between technologies, fish production in this case. Further research is required to extend this method to include other sources of uncertainty as well as other allocation choices, including for example substitution or system expansion. Further research is also required to more fully treat background multi-functional processes as was done with foreground multi-functional processes in this chapter and include correlations where relevant.

Acknowledgements
This research has been completed as part of the IDREEM project (Increasing Industrial Resource Efficiency in European Mariculture, (www.idreem.eu) and has received funding from the European Union's Seventh Framework Program (FP7/2007-2013) under grant agreement n° 308571. The authors would also like to thank the insightful comments of Professor Arnold Tukker as well as those of Glenn Aguilar Hernandez and three anonymous reviewers.

Supporting information

Supporting information of this chapter may be found in the online version of the original article: https://link.springer.com/article/10.1007%2Fs11367-017-1363-2

4.

When the background matters: Using scenarios from Integrated Assessment Models in Prospective LCA

Angelica Mendoza Beltran
Brian Cox
Chris Mutel
Detlef P. van Vuuren
David Font Vivanco
Sebastiaan Deetman
Oreane Y. Edelenbosch
Jeroen Guinée
Arnold Tukker

Submitted: *The Journal of Industrial Ecology (2018).*

Abstract

To support more robust future environmental assessments and decision-making prospective life cycle assessment (LCA) should deal with the large epistemological uncertainty about the future. This study proposes a novel approach to dealing with uncertainty by systematically changing the background processes in a prospective LCA based on scenarios of an Integrated Assessment Model (IAM), the IMAGE model. Consistent worldwide scenarios from IMAGE are evaluated in the life cycle inventory using ecoinvent v3.3. To test the approach, only the electricity sector was changed in a prospective LCA of an internal combustion engine vehicle (ICEV) and an electric vehicle (EV) using six baseline and mitigation climate scenarios until 2050. This case study shows that changes in the electricity background can be very important for the environmental impacts of EV. Also, this study approach demonstrates that the relative environmental performance of EV and ICEV over time is more complex and multifaceted than previously assumed. Uncertainty due to future developments manifests in different impacts depending on the product (EV or ICEV), the scenario and year considered. Expanding this approach to other economic sectors can lead to more robust prospective LCAs since a more systematic and structured composition of future inventory databases driven by IAM scenarios helps to acknowledge epistemological uncertainty and to understand exogenous system changes in prospective LCA.

Keywords: Prospective LCA, epistemological uncertainty, background changes, Integrated Assessment Models

4.1 Introduction

A robust assessment of the environmental impacts of product systems is the basis for assertive policy, business, and consumer decision-making (Hellweg and Canals 2014). Life cycle assessment (LCA) has developed into an environmental decision-support tool to assess product systems. Some LCAs, however, refer to product systems that either do not yet exist or are not commercially available. These forward-looking applications of LCA, or so-called prospective LCA (Pesonen et al. 2000; Arvidsson et al. 2017), are thought to help in anticipating unintended consequences of future product systems and to support environmentally assertive product design (Miller and Keoleian 2015). Prospective LCA has proven to be valuable in a range of cases, from assessing future public policies (Dandres et al. 2012, 2014) and emerging technologies (Frischknecht et al. 2009; Arvidsson et al. 2017) to the analysis of future production and consumption systems (Van der Voet et al. 2018). Nonetheless, in addition to dealing with the uncertainty related to any complex system (ontic uncertainty), prospective LCA needs to deal with the lack of knowledge about the future (epistemological uncertainty) (Björklund 2002). Addressing epistemological uncertainty is therefore a crucial challenge in the development of prospective LCA.

A common approach for dealing with epistemological uncertainty in prospective LCA is to integrate future scenarios (Pesonen et al. 2000; Spielmann et al. 2005). A scenario is understood as "*… a description of a possible future situation relevant for specific LCA applications, based on specific assumptions about the future, and (when relevant) also including the presentation of the development from the present to the future*" (Pesonen et al., 2000, p.21). Common approaches to integrating scenarios in prospective LCA draw from multiple databases exogenous to LCA to address future socio-technical changes or so-called exogenous system changes (Miller and Keoleian, 2015). For example, the New Energy Externalities Developments for Sustainability (NEEDS) project (NEEDS, 2009) modelled the future supply of metals, non-metallic minerals, electricity and transport using different scenarios at various levels of optimism regarding technological improvements, cost reductions, and market growth rates. NEEDS and other external databases, such as the IEA (International Energy Agency 2010), were used in the 'Technology Hybridized Environmental-Economic Model with Integrated Scenarios' (THEMIS) (Gibon et al. 2015) to integrate future changes in electricity production, industrial processes, and climate change mitigation policies into a hybrid input-output (IO) LCA model (Bergesen et al. 2014, 2016; Hertwich et al. 2015; Beucker et al. 2016). Another example is 'macro-LCA' (Dandres et al. 2012), which combined LCA with future changes in economic structure and energy production based on computable general and partial equilibrium models, respectively. Lastly, Van der Voet et al. (2018) identified important supply-related variables that are likely to change in the future of metal production (e.g. technologies' shares of production, resource grade, and efficiencies of technologies), and then adapted these using various assumptions and external data sources.

While the above examples are valuable for prospective LCA, they suffer from limitations. A first limitation is that the development of future scenarios is often inconsistent and lacks transparency. Scenario development involves two steps: scenario generation and scenario evaluation (Fukushima and Hirao 2002). Scenario generation refers to the formulation of assumptions about the future, while scenario evaluation refers to the assessment of such assumptions during the LCA phases, especially the Life Cycle Inventory (LCI) phase and the Life Cycle Impact Assessment (LCIA) phase (Fukushima and Hirao 2002). Because scenario generation and scenario evaluation are often mixed, it is difficult to establish which inventory parameters have been changed and, most importantly, to discern whether assumptions are consistent among each other. Part of this issue arises from the use of different datasets as sources of scenario information, a procedure that increases inherent uncertainties (Gibon et al. 2015) and makes the process of scenario generation possibly un-harmonized. Another limitation is that technology maturity (e.g. penetration and efficiency) is often not accounted for, thus misrepresenting future technology mixes (Dandres et al. 2012). Moreover, because technological development is intertwined with both economic development and predictions of product technology-supply mixes, such relationships should be appropriately reflected in a scenario covering all economic sectors worldwide. Finally, the reproducibility of some approaches can be hampered by the large amount of required data and the difficulty to trace the assumptions that were made during the scenario generation.

To overcome the above limitations for scenario development in prospective LCA, we first propose to explicitly differentiate between scenario generation and scenario evaluation. For scenario generation, we propose the use of system-wide Integrated Assessment Models (IAMs) as a platform for calculations of consistent, worldwide scenarios covering all economic sectors. IAM scenarios are possible socio-economic and technological pathways of future development (van Vuuren et al. 2014) that can help explore different futures in the context of fundamental future uncertainties (Riahi et al. 2017). Masanet et al. (2013), Plevin (2016), and Pauliuk et al. (2017) highlight the unrealized potential of IAM scenarios as consistent sources of information for prospective assessments.

For scenario evaluation, we introduce a novel approach that systematically integrates the scenario information of the technology-rich IAM "Integrated Model to Assess the Global Environment" (IMAGE) (Stehfest et al. 2014) with one of the most broadly used life cycle inventory databases in the LCA community, the ecoinvent database (Wernet et al. 2016). In contrast to the recent work of Arvesen et al. (2018) and Pehl et al. (2017), we concentrate on evaluating the usefulness of IAMs for prospective LCA rather than on informing the IAM with the prospective LCA results. Our approach can thus be understood as an alternative opportunity to further reconcile the knowledge from the IAM and the LCA communities (Creutzig et al. 2012) that now hold different views on how to perform future environmental impact assessments.

The research question of this study was as follows: "How can IAM scenarios be systematically linked with LCI parameters to account for future changes in prospective LCA?" We focused on a case study comparing the relative environmental impacts of electric vehicles (EV) and internal combustion engine vehicles (ICEV), given that future changes play a key role in these impacts. Drawing from previous research, we focused on changes in the electricity sector. Specifically, the relative carbon footprint of EVs is highly influenced by the electricity mix (Bauer et al. 2015; Cox and Mutel 2018), and extreme cases can lead to counterintuitive results; for instance, in Australia, the prevalence of coal power causes EV to underperform (Wolfram and Wiedmann 2017). Our approach can thus address a range of questions, such as "What will be the impacts of EVs in 2050?" and "Will a transition to EVs in the future bring environmental benefits?". Finally, we contribute to further integrate knowledge from the IAM and the LCA communities, with the aim to increase the robustness of prospective LCA assessments by bringing macro scenarios into the micro- or product-level LCA (Guinée et al. 2011).

4.2 Methods

We first introduce an overview of the proposed approach (section 4.2.1). Further, we provide detailed insights into how scenarios are generated using IAMs and particularly IMAGE (section 4.2.2). Next, we present a novel method for scenario evaluation using the 'Wurst' software (section 4.2.3). Finally, we describe the case study and products (section 4.2.4) and the scenarios used in this study (section 4.2.5).

4.2.1 Method overview

This study presents a novel approach to introduce consistent and systematic future changes in a prospective LCA application (see Figure 10 for an overview). Such changes refer to the LCA background system, namely those processes and emissions that are part of the supply chain of the studied product system, e.g. the electricity mix used to charge and produce EV batteries. This means that indirect emissions are accounted for. In addition and in line with a full life cycle approach, direct emissions are accounted for but are left unchanged in the foreground system, in particular those processes and emissions describing the product itself, e.g. vehicle energy requirements and fuel use (See Cox and Mutel 2018). Following Fukushima and Hirao (2002), we developed scenarios in two steps: 1) scenario generation and 2) scenario evaluation.

- Scenario generation: This step refers to the process of scenario formulation and calculation. The IAM model IMAGE (Stehfest et al. 2014) was selected as the modeling framework used to generate consistent scenarios. Section 4.2.2 contains a description of the IMAGE model and the type of scenarios develop by it. Section 4.2.5 describes the specific scenarios used in the case study.

- Scenario evaluation: This step refers to the assessment of the scenarios in all the phases of LCA. Yet, in this study, attention is particularly given to the evaluation of scenarios in the life cycle inventory phase. We identified three steps needed to accomplish this: first, analyzing the background system to identify the inventory parameters (i.e. input and output flows, as well as processes) that are affected by future changes; second, adapting these parameters using information from the IAM scenarios; third, using the adapted inventories to calculate the prospective LCA results of specific products.

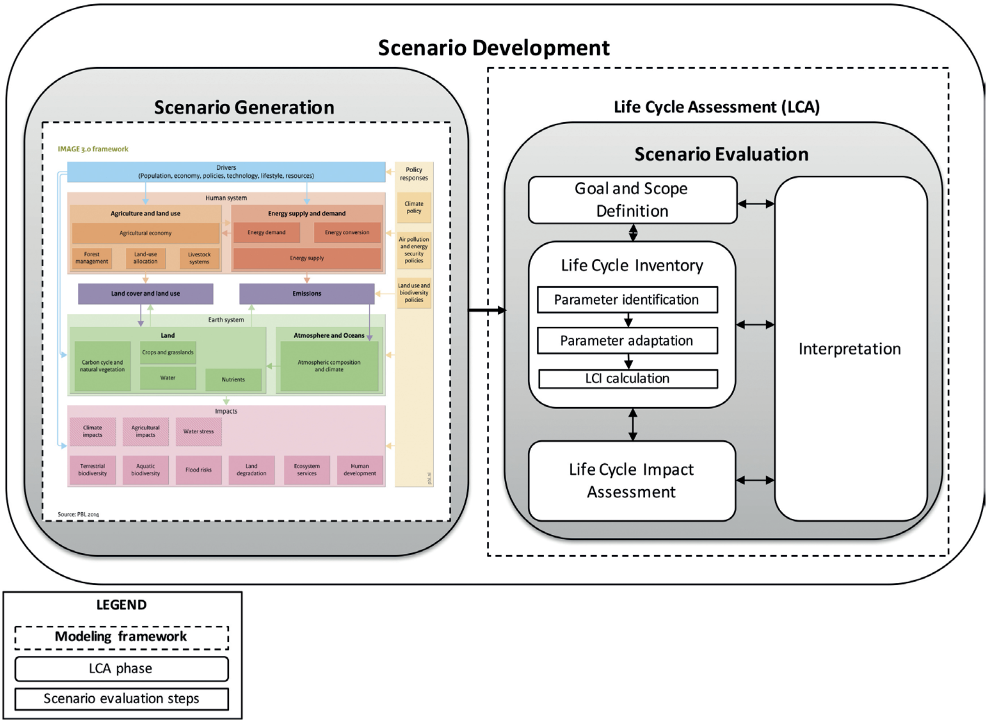


Figure 10. Overview of the proposed method for scenario development in prospective life cycle assessment (adapted from Fukushima and Hirao (2002)). Scenarios are generated using the IMAGE 3.0 framework and they are evaluated in the Life Cycle Assessment framework.

Relevant inventory parameters were adapted using so-called 'cornerstone' scenarios (Spielmann et al. 2005), as these scenarios refer to either unknown or new future situations. These scenarios have been chosen as they better inform long-term and strategic decision-making, which are fundamental characteristics of prospective LCA. The alternative is to use 'what-if' scenarios, which test changes in specific parameters to compare well-known alternatives in a sensitivity fashion (Pesonen et al. 2000). However, we did not choose this option as it is less structural than cornerstone scenarios because changes of only few parameters are captured. The approach of this study is distinct from other implementations of cornerstone scenarios (Spielmann et al. 2005) as we derived future changes of relevant parameters from the IAM-based scenarios instead of making separate assumptions for each parameter. We developed and applied the Wurst model (v0.1) in this study (https://wurst.readthedocs.io/index.html) for the parameter identification and adaption steps (see section 4.2.3). The LCA results of EV and ICEV were calculated with the Brightway2 (v2.1.1) software (Mutel 2017).

4.2.2 Scenario generation: Using IMAGE to develop scenarios

We used the IAM IMAGE 3.0 (from here on referred to as IMAGE) to generate scenarios (for a detailed model description, see Stehfest et al. 2014). In general, IAMs have been developed to describe the relationships between humans (the human systems) and the natural environment (the Earth system) and the impacts of these relationships that lead to global environmental problems, such as climate change and land use change. IAMs build on functional relationships between activities such as the provision of food, water, and energy and their associated impacts. The human system in IMAGE includes economic and physical models of the global agricultural and energy systems. The Earth system includes a relatively detailed description of the biophysical terrestrial, oceans and atmosphere processes.

Since this study focuses on the electricity sector, we will briefly describe the energy model of IMAGE, "The Image Energy Regional Model" (TIMER) (de Vries et al. 2001; van Vuuren 2007). TIMER consists of a technical description of the physical flows of energy from primary resources through conversion processes, transport systems and distribution networks to meeting specific demands for energy carriers or energy services. The model determines market shares for energy technologies based on the costs of competing technologies. It includes fossil fuels and renewable or alternative sources of energy in order to meet the demand, which depends on population size, efficiency developments, income levels, and assumptions on lifestyle. The model generates scenarios for future energy intensity and fuel costs, including competing non-fossil supply technologies. It models emission mitigation through the price signal of a carbon tax that induces additional investments in more efficient and non-fossil technologies, bioenergy, nuclear, and carbon capture and storage, thus changing market shares of different technologies. In this way, the model allows the generation of both baseline and mitigation scenarios in IMAGE, both of which are used to inform the background of the LCA in this study.

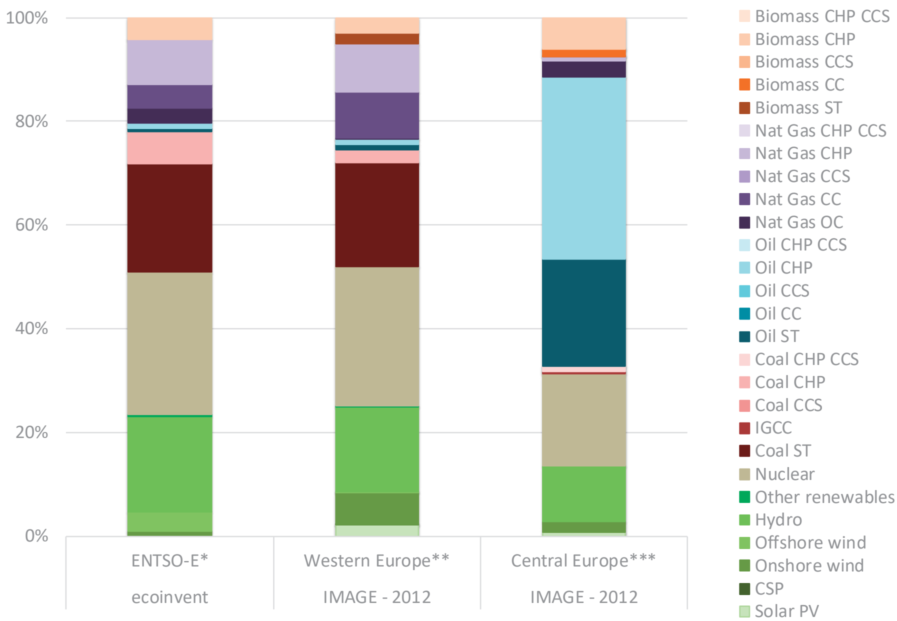
4.2.3 Scenario evaluation: The Wurst software

IMAGE scenarios serve as a source of information to adapt the LCI background data (Figure 10). Apart from being the most comprehensive and widespread LCI database, the ecoinvent database has also the advantage of distinguishing between two types of processes: transformation activities and markets (consumption mixes) (Wernet et al. 2016). This is an important feature because it simplifies identifying and changing parameters in ecoinvent when using IMAGE scenarios. To systematically approach the identification and changing of parameters in ecoinvent, we developed Wurst, a Python-based software that enables the systematic import, filtering, and modification of LCI databases. The current version of Wurst (available for download at: https://github.com/IndEcol/wurst) focuses on ecoinvent but includes other scenario data besides IMAGE. Other LCI and scenario databases are to be incorporated in the future. For this study, a specific functionality of the software was developed to link data formats of ecoinvent v3.3 (from here on referred to as ecoinvent) and IMAGE. The corresponding functions for import, filtering and modification of LCI databases are provided in the Supporting information (SI) in the format of Jupyter Notebooks. These notebooks call up functions in Wurst, for example those related to the regional match between databases, to generate ecoinvent LCI databases for different years into the future based on the IMAGE scenarios.

Data import

We first imported ecoinvent and IMAGE scenarios data into Wurst, for which we wrote specific importing and cleaning functions. In particular, the “cut-off system model” of the ecoinvent database was imported (see Weidema et al. 2013 for details of this model). This means that mono-functional processes were adapted using the IMAGE scenario data to generate modified (future) mono-functional processes. After importing the data, we mapped the available technologies for both datasets (Supporting information-SI, Annex I) as well as for all regions (SI, Annex II). For the technology mapping, technologies with greater detail in ecoinvent were grouped and assigned to an overarching IMAGE technology (SI, Annex I). Moreover, technologies that will be relevant in the future according to the IMAGE scenarios but that are missing in ecoinvent were added to the latter to create an *extended ecoinvent*. These technologies are concentrated solar power (CSP) and carbon capture and storage (CCS), which we included using datasets from ecoinvent v3.4 and from Volkart et al. (2013), respectively. For other technologies, such as natural gas combined heat and power generation with carbon capture and storage, which are missing in ecoinvent but less relevant in the future, we used proxy inventories from already existent technologies in ecoinvent (See SI, Annex I for all proxy technologies). Technologies were left unchanged if they were related to other sectors, such as fossil-fuel and biofuel production, transport and raw materials production.

For the regional mapping, a one-to-one correspondence was assigned between IMAGE and ecoinvent regions where possible (SI, Annex II). For regions in ecoinvent that involve more than one region from IMAGE, we used an average of IMAGE data. For smaller regions in ecoinvent, for instance provinces in a country, we used the data of the larger region from IMAGE. An example of region and technology mapping is shown in Figure 11, which illustrates that the electricity mix in ecoinvent has a closer match with that of IMAGE Western Europe, as electricity demand is dominated by Western European countries. In the interest of transparency, the complete region and technology mapping and the associated Python scripts are presented in the SI (Annexes I and II).



According to ISO 3166-1 2 letter country code:
*ENTSO-E countries are: AT, BE, CH, DE, FI, FR, GB, GR, IE, IS, IT, LU, LV, NL, NO, RS, SE, BA, BG, CZ, EE, HR, HU, LT, MK, PL, RO, SI, SK
**Western Europe countries are: AD, AT, BE, CH, DE, DK, ES, FI, FR, FO, GB, GI, GR, IE, IS, IT, LI, LU, MC, MT, NL, NO, PT, SE, SM, VA
***Central Europe countries are: AL, BA, BG, CS, CY, CZ, EE, HR, HU, LT, LV, MK, PL, RO, SI, SK

Figure 11. The 2012 electricity mix for Western and Central Europe regions in IMAGE and for the ecoinvent v3.3 process 'electricity, high voltage, production mix' for the European Network of Transmission Systems Operators for Electricity (ENTSO-E). Ecoinvent technologies are aggregated according to the map in the SI, Annex I and exclude the proxies for biomass steam turbine, oil combined cycle and biomass combined cycle to show original ecoinvent data without modifications.

Parameter identification (data filtering)

Parameters from ecoinvent that are to be modified were identified according to the process name and unit of the reference output flow. For instance, for electricity production technologies that use coal, the ecoinvent process names include the words 'hard coal' or 'lignite' and the unit of the reference output-flow is 'KWh'. For electricity markets, the same reference output-flow unit is used, but the names include 'market for electricity, high/medium/low voltage'. Such keys determine the processes that contain the parameters to be modified. These are technology-related parameters, i.e. economic and environmental flows (input and outputs) such as GHG emissions, for instance CO_2

emissions to air, or market-related parameters, i.e. electricity market mixes in ecoinvent, such as technology shares in high voltage electricity markets. The corresponding IMAGE parameters were filtered using the years, the sector (in this case electricity production), the overarching technology (e.g. coal steam turbine), the regions and the scenarios of interest. This procedure generates two sub-sets of data, one from ecoinvent and one from IMAGE, which are related to one another via the region and the technology, as was explained in the previous section.

Parameter changes

Starting with the ecoinvent and IMAGE sub-sets, we modified the ecoinvent parameters according to a number of rules (Figure 12). for GHG emissions available in both ecoinvent and IMAGE (i.e. CH_4, SO_2, CO, NO_x, N_2O emissions to air), we used the emission factors from the IMAGE scenarios as technology parameters, replacing those of ecoinvent for the different technologies. Emission factors in IMAGE were adapted by dividing them by the efficiency per technology in IMAGE because in IMAGE they are reported per MJ_{input} and not per $MJ_{electricity\text{-}output}$ as in ecoinvent. All other flows (economic and environmental), e.g. emissions other than greenhouse gases (GHG) emitted to air, were scaled using future technology efficiencies of the IMAGE scenarios. The final amounts of these flows, in their original ecoinvent units, was multiplied by a scaling factor (SF) calculated as shown in equation 2.

$$SF = \frac{efficiency_{ecoinvent}}{efficiency_{IMAGE}} \qquad \textit{Eq.2}$$

In ecoinvent, changes of market shares are applied to high voltage electricity markets (Treyer and Bauer 2016). We replaced the shares of electricity producing technologies defined in ecoinvent by the electricity mixes from the IMAGE scenarios. A different procedure was used for solar photovoltaics and small combined heat and power plants that supply electricity at the low or medium voltage level. We connected these technologies to the high voltage level and assumed that all electricity generation is supplied at the high voltage level. This procedure was chosen in favour of the systematic approach we propose, despite the error that this assumption might introduce, which we believe is small[1]. Moreover, as only electricity markets change, transmission grid markets and SF6 emissions generated during transmission were not adapted and were kept at the original ecoinvent levels. In the SI (excel files), we present per year tables, generated in the modification functions provided in the SI, with the changes made to technology and

1 The error is introduced because of the additional losses when converting from high to medium to low voltage, which technically does not take place if technologies supply the grid already at the low voltage level. Furthermore, imports and exports happen at the high voltage level, so technically technologies supplying at the medium or low voltage would not be in the import export mix. This is important for some countries with high losses (Treyer and Bauer 2016). For other countries the error introduced is smaller.

market parameters for one of the scenarios used in this study. The final output consists of future ecoinvent databases that are year- and scenario-dependent.

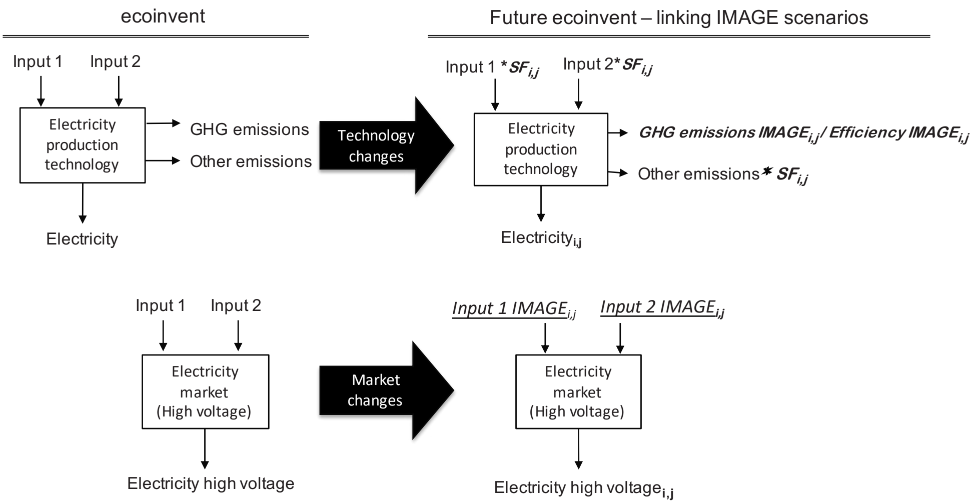


Figure 12. Schematic representation of technology and market parameters and their changes. Technology changes are presented in bold and market changes are represented with underlined font. Both are year- and scenario-dependent. The scaling factor (SF) is calculated as shown in equation 2.

LCI calculation

The final step of the scenario evaluation involves the calculation of the LCI results using the modelled future ecoinvent databases. Brightway2 (Mutel 2017) uses as input the future ecoinvent databases and calculates the inventory for the specified EV and ICEV (see section 4.2.4). The base year is 2012 because ecoinvent mostly represents the economy for this year. Selected future years are 2020, 2030, 2040 and 2050.

4.2.4 Case study

For the case study an EV is compared with its closest alternative, a small ICEV-EURO5 diesel vehicle. The foreground description corresponds to processes as defined in ecoinvent, and they remain unchanged in the future (See Cox et al. 2018 for foreground changes). The EV is based on the unit process 'transport, passenger car, electric' for the global average vehicle (Simons 2016), whereas the ICEV-EURO5 is based on the process 'transport, passenger car, small size, diesel, EURO 5' (Del Duce et al. 2016). These processes include the assembly, operation, maintenance and end of life of each vehicle. The functional unit is 1 kilometre driven by each vehicle, and so differences in use and further spending patterns are not considered (Font Vivanco et al. 2014, 2016). The effects of background changes on the LCIA results are studied separately for changes of technology and market parameters. The impact categories were chosen in line with those used in previous studies and relevant for the comparison (e.g. Bauer et al. 2015;

Nordelöf et al. 2014). The impact categories are climate change, particulate matter formation, fossil cumulative energy demand, human toxicity, metal depletion, and photochemical oxidant formation. The characterization factors are defined according to RECIPE 2008 (Goedkoop et al. 2013) hierarchist perspective at the mid-point level. For climate change, we use the global warming potentials (GWPs) of the IPCC Fifth Assessment Report, with a time horizon of 100 years (IPCC 2014), considering biogenic carbon (SI, Annex III for characterization factors).

4.2.5 Scenarios used in this chapter

The IMAGE scenarios we used are the Shared Socio-Economic Pathways (SSPs) (O'Neill et al. 2014). This family of climate scenarios consists of a set of five storylines on possible human development trajectories and global environmental change in the 21st century (van Vuuren et al. 2017a). Of the five storylines (Riahi et al. 2017), we used three that cover different challenges for mitigation and adaptation to climate change as well as a broad range of primary energy supply technologies from different sources (e.g. coal, oil + gas, renewables and nuclear) and different levels of final energy demand (Riahi et al. 2017; van Vuuren et al. 2017b). The storylines are SSP1 – Taking the green road, SSP2 – Middle of the Road and SSP3 – Regional Rivalry.

For each storyline, a baseline scenario was developed, assuming that such a pathway can unfold without specific additional policies and measures to limit climate change or to increase the adaptation capacity (Riahi et al. 2017). Each SSP baseline has been used as a starting point for exploring climate policy scenarios. The climate targets explored correspond to the radiative forcing levels of the Representative Concentration Pathways (RCPs) (van Vuuren et al. 2011). The RCPs were used in the International Panel for Climate Change Fifth Assessment Report (IPCC-AR5) as a set of scenarios exploring different long-term climate targets in 2100, i.e. 2.6, 4.5 and 6.0 W/m^2. The SSPs explored these and an additional target of 3.4 W/m^2, which is more policy-relevant. In this study, we used the data for the scenarios reaching a 2.6 W/m^2 target, which is consistent with a two-degree target (UNFCCC 2010). Also, a 3.4 W/m^2 target is used for the SSP3.

The results for both types of vehicles were compared for the following scenarios (see Table 8 for a summary): GreenRoad (SSP1), MidRoad (SSP2), RegRivalry (SSP3), GreenRoad-2.6 (SSP1-2.6), MidRoad-2.6 (SSP2-2.6) and RegRivalry-3.4 (SSP3-3.4). Also, we present a so called 0-scenario, in which no background changes are assumed, i.e. ecoinvent (original data) for 2012. For comparison, we also added the results for the 2012 IMAGE data, which are the same for all scenarios, as they correspond to historic data and not to forecast (scenario) data. The combination of the selected years, scenarios and products yields a total of 52 inventories that were calculated. Finally, for reference, the SI (Annex IV) shows the electricity mix for the IMAGE scenarios for Western and Central Europe regions.

Table 8. Scenarios, years, and databases used for the prospective life cycle assessment of a ICEV and a EV. ICEV: internal combustion engine vehicle; EV: electric vehicle; SSP: shared socio-economic pathway.

Vehicle	Database used for background	IMAGE scenario (SSP)	Year(s)	Label in this chapter
ICEV/EV	ecoinvent	n.a.	2012	ICEV/EV-ecoinvent
ICEV/EV	ecoinvent adapted with IMAGE scenario	n.a.	2012	ICEV/EV-IMAGE-2012
ICEV/EV	ecoinvent adapted with IMAGE scenario	Green Road (SSP1)	2020,2030,2040,2050	ICEV/EV-GreenRoad
ICEV/EV	ecoinvent adapted with IMAGE scenario	Green Road 2.6 (SSP1-2.6)	2020,2030,2040,2050	ICEV/EV-GreenRoad-2.6
ICEV/EV	ecoinvent adapted with IMAGE scenario	Middle of the Road (SSP2)	2020,2030,2040,2050	ICEV/EV-MidRoad
ICEV/EV	ecoinvent adapted with IMAGE scenario	Middle of the Road 2.6 (SSP2-2.6)	2020,2030,2040,2050	ICEV/EV-MidRoad-2.6
ICEV/EV	ecoinvent adapted with IMAGE scenario	Regional Rivalry (SSP3)	2020,2030,2040,2050	ICEV/EV-RegRivalry
ICEV/EV	ecoinvent adapted with IMAGE scenario	Regional Rivalry 3.4 (SSP3-3.4)	2020,2030,2040,2050	ICEV/EV-RegRivalry-3.4

4.3 Results

We present the prospective LCA results for EV and ICEV in section 4.3.1, and the disaggregated results according to market and technology changes in section 4.3.2.

4.3.1 Prospective LCA results for EV and ICEV

Our results show that the uncertainty about future developments in the electricity sector is overall large but manifests differently according to the studied product (EV or ICEV), the impact category, and the scenario and year considered (Figure 13). Regarding the product, uncertainty is larger for the EV, as is evident from the larger range of results, particularly in the long-term (see purple lines versus orange lines in 2050, Figure 13). As electricity production contributes more to the background impacts of the EV than to impacts of the ICEV, this result is expected. For the impact categories, we observe that for climate change, particulate matter formation, and fossil cumulative energy demand, the selected IMAGE scenario has a larger influence on the future impacts of the EV. These are impacts due to GHG emissions and use of fossil fuels. Thus, baseline scenarios which have a larger share of fossil-based technologies display a smaller reduction of these impacts than the original ecoinvent impacts for the EV. By contrast, ambitious mitigation scenarios that have larger shares of technologies emitting less GHG show large reductions of these impacts, particularly in the long-term. For impacts such as metal depletion, almost no effect of the scenario is observed for the EV and the ICEV.

This is mostly related to the fact that sectors that might contribute more to this impact, such as the raw materials production sector, were kept the same.

Considering the uncertainty about the future also makes it more complex to assess the relative environmental performance of EV over time (See SI, Annex V). There are impact categories such as particulate matter formation for which the results of the EV overlaps with those of the ICEV (see purple lines crossing orange lines, Figure 13). To understand these results, it is important to compare the ICEV and EV results within the same scenario. For climate change, for instance, the impacts of both types of vehicles overlap in 2050 for EV-RegRivalry and ICEV-RegRivalry-3.4. However, this comparison is not fair, as effectively these scenarios represent different futures. For particulate matter formation, on the other hand, EVs perform better than ICEVs in the MidRoad-2.6 and the GreenRoad-2.6 scenario after 2040, while the opposite is true for other years and scenarios. Thus, for ambitious mitigation scenarios, EV would lead to improvements in particulate matter formation while for non-ambitious scenarios, such as the baseline scenario, the ICEV would be preferred regarding this impact category.

Lastly, we observed striking differences in some cases between the original ecoinvent and the IMAGE-based adaptation of ecoinvent for 2012 (EV-ecoinvent and ICEV-ecoinvent, Figure 13). Such differences comprise reductions of up to 16%, 15,5% and 13,8% of the EV impacts in the categories climate change, photochemical oxidant formation and particulate matter formation, respectively. For the ICEV, the differences are smaller, with reductions ranging between 0.1 to 4.6% for all impact categories. In the case of climate change and photochemical oxidant formation, the relative environmental impacts of both vehicles were reversed in the scenario results for 2012 compared to those of the original ecoinvent. To better understand these results, a breakdown in market and technology changes is necessary.

4.3.2 Prospective LCA results for EV and ICEV by market and technology changes

Of the technology and market changes, the latter have the largest influence on the total change of impacts in general (see Figure 14 for climate change impacts as an illustration and SI, Annex VI for other impacts). Technology changes alone lead to the same impacts in both the baseline and the mitigation scenario, as technology efficiency is expected to improve in the future regardless of which electricity production technology has a larger penetration. Market changes are different for both scenarios given the higher penetration of technologies emitting less GHG in the ambitious mitigation scenarios. Together, both changes account for technology improvements but also for market penetration of electricity technologies. The impacts calculated with both changes are in line with those of market changes alone, particularly for the mitigation scenario (Figure 14).

Furthermore, market changes appear to interact with technology changes when both are taken into account (Table 9). Impacts calculated with technology or market

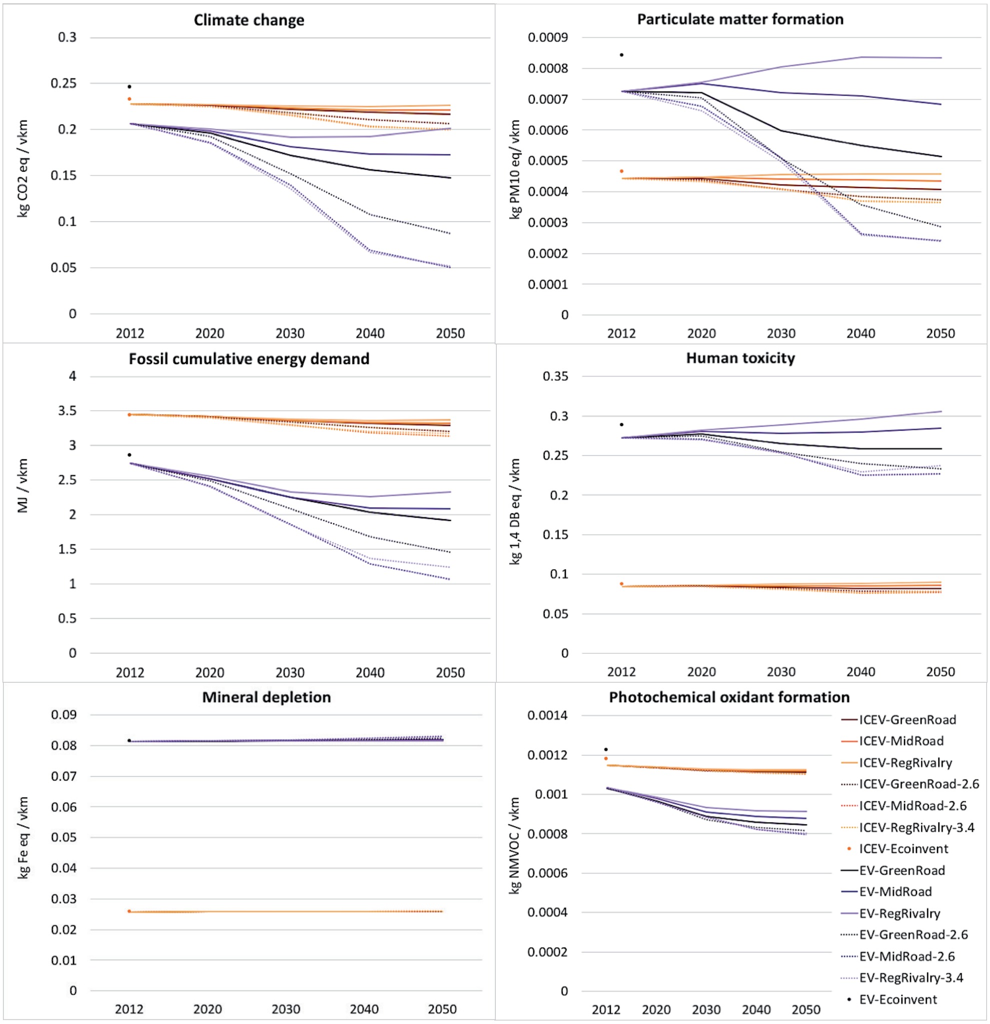


Figure 13. Prospective life cycle assessment results for an EV and an ICEV, for various impact categories, per vehicle-kilometer and considering background changes based on six IMAGE scenarios. ICEV: internal combustion engine vehicle; EV: electric vehicle.

changes alone do not capture joint effects of technology improvement and market penetration of different technologies. This becomes more evident in Table 9, where the changes in impacts for market and technology changes alone do not add up to the impacts calculated with both. To account for the actual individual contributions of each effect to the total impacts, one could use structural decomposition analysis (Hoekstra and Van Den Bergh 2002). However, this is beyond the scope of the present study.

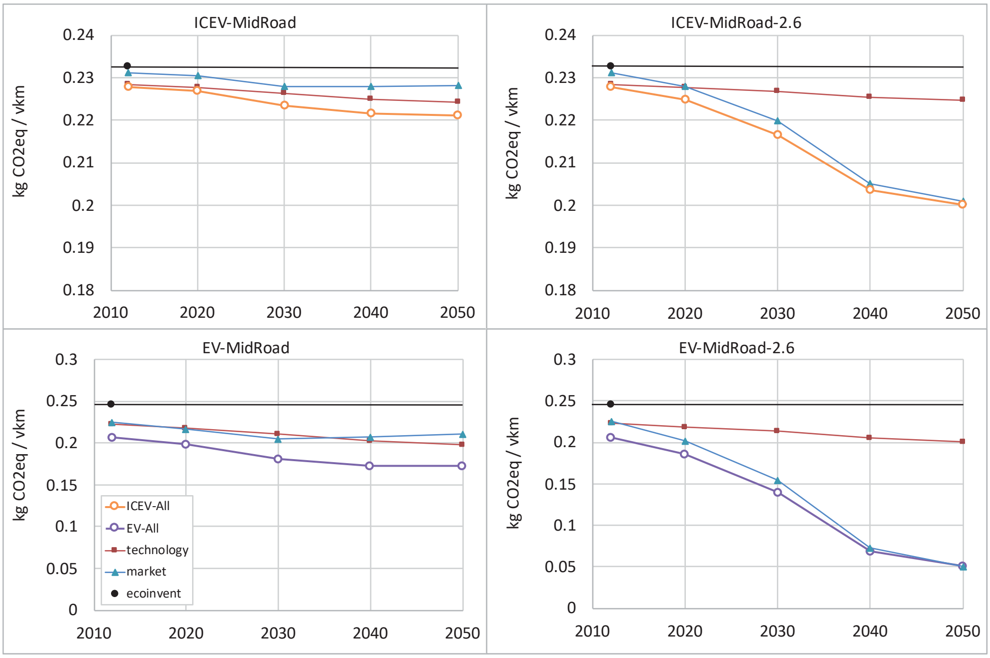


Figure 14. Prospective life cycle assessment results, for climate change impacts and per vehicle-kilometer (vkm), of an EV and an ICEV. The results correspond to the MidRoad and MidRoad-2.6 scenarios including background adaptions of technology parameters only (red squares), market parameters only (blue triangles) and including both changes (purple line for EV and orange line for ICEV, corresponding with the results shown in Figure 13. Impact using original ecoinvent background data is shown with a black dot and constant black line in time. ICEV: internal combustion engine vehicle; EV: electric vehicle.

Table 9. Change in the impacts per vehicle-kilometer (as % change from the original ecoinvent) for an EV and an ICEV using the MidRoad and MidRoad-2.6 scenarios, considering background adaptions of technology parameters only ('technology' rows), market parameters only ('market' rows) and both changes simultaneously ('all' rows). Shades of red represent an increase and shades of green represent a decrease of impacts compared to ecoinvent and hold for the range of outcomes for all impacts per scenario and type of vehicle. ICEV: internal combustion engine vehicle; EV: electric vehicle.

	year	Background adaptation	Fossil Cumulative Energy Demand	Climate Change	Human Toxicity	Mineral Depletion	Particulate Matter Formation	Photochemical Oxidant Formation		Fossil Cumulative Energy Demand	Climate Change	Human Toxicity	Mineral Depletion	Particulate Matter Formation	Photochemical Oxidant Formation
ICEV-MidRoad	2012	technology	1,1%	1,8%	1,7%	0,1%	6,4%	2,9%	EV-MidRoad	7,1%	9,4%	3,0%	0,1%	19,5%	15,0%
	2012	market	-1,4%	0,6%	2,2%	0,1%	-1,2%	0,7%		-2,6%	8,4%	2,4%	0,1%	-3,7%	5,6%
	2012	All	-0,5%	2,1%	3,9%	0,1%	4,6%	2,6%		3,9%	16,0%	5,3%	0,2%	13,8%	15,5%
	2020	technology	1,4%	2,1%	2,0%	0,1%	7,5%	3,5%		9,0%	11,2%	3,5%	0,1%	22,8%	18,4%
	2020	market	-0,5%	1,0%	-0,2%	0,0%	-2,8%	1,3%		5,0%	12,0%	-0,9%	0,0%	-8,8%	9,5%
	2020	All	0,5%	2,4%	1,8%	0,0%	3,7%	3,5%		11,6%	19,4%	2,6%	0,1%	11,0%	20,1%
	2030	technology	1,8%	2,7%	2,6%	0,1%	8,9%	4,3%		12,2%	14,1%	4,5%	0,2%	27,4%	22,6%
	2030	market	0,6%	2,0%	-0,4%	-0,2%	-3,2%	1,7%		11,9%	16,5%	-1,4%	-0,3%	-11,1%	11,7%
	2030	All	2,0%	3,9%	2,3%	-0,1%	5,1%	4,6%		20,9%	26,2%	3,3%	-0,2%	14,4%	25,6%
	2040	technology	2,3%	3,3%	3,4%	0,1%	10,1%	4,7%		15,9%	17,7%	5,9%	0,2%	31,1%	24,5%
	2040	market	1,0%	2,0%	-1,7%	-0,3%	-4,6%	1,8%		13,5%	15,8%	-3,9%	-0,5%	-16,4%	11,6%
	2040	All	3,1%	4,8%	2,1%	-0,2%	5,6%	5,0%		26,4%	29,5%	2,8%	-0,4%	15,7%	27,6%
	2050	technology	2,6%	3,6%	3,8%	0,1%	10,7%	4,9%		17,5%	19,3%	6,5%	0,2%	33,0%	25,8%
	2050	market	1,0%	1,9%	-3,1%	-0,4%	-4,1%	1,9%		12,3%	14,4%	-6,4%	-0,6%	-14,5%	12,3%
	2050	All	3,3%	4,9%	1,3%	-0,3%	6,5%	5,2%		26,7%	29,6%	1,3%	-0,5%	18,7%	28,2%
ICEV-MidRoad-2.6	2012	technology	1,1%	1,8%	1,7%	0,1%	6,4%	2,9%	EV-MidRoad-2.6	7,1%	9,4%	3,0%	0,1%	19,5%	15,0%
	2012	market	-1,4%	0,6%	2,2%	0,1%	-1,2%	0,7%		-2,6%	8,4%	2,4%	0,1%	-3,7%	5,6%
	2012	All	-0,5%	2,1%	3,9%	0,1%	4,6%	2,6%		3,9%	16,0%	5,3%	0,2%	13,8%	15,5%
	2020	technology	1,3%	2,1%	2,0%	0,1%	7,4%	3,5%		8,8%	10,9%	3,4%	0,1%	22,5%	18,3%
	2020	market	0,1%	2,0%	2,0%	0,0%	0,6%	1,9%		9,9%	17,8%	3,1%	0,0%	3,2%	12,8%
	2020	All	1,0%	3,3%	3,7%	0,0%	6,2%	3,8%		15,5%	24,2%	5,9%	0,0%	19,7%	21,5%
	2030	technology	1,7%	2,5%	2,4%	0,1%	8,7%	4,3%		11,4%	13,3%	4,1%	0,1%	26,5%	22,5%
	2030	market	2,9%	5,5%	5,4%	-0,2%	6,7%	3,0%		28,6%	37,1%	9,5%	-0,4%	25,8%	19,6%
	2030	All	4,0%	6,9%	6,8%	-0,2%	11,8%	4,9%		34,8%	43,1%	11,8%	-0,4%	39,6%	27,6%
	2040	technology	2,2%	3,1%	3,1%	0,1%	10,6%	5,1%		14,8%	16,4%	5,3%	0,2%	32,4%	26,6%
	2040	market	6,4%	11,8%	11,7%	-0,7%	18,0%	5,1%		50,7%	70,1%	21,2%	-1,1%	65,7%	31,2%
	2040	All	7,2%	12,5%	12,4%	-0,6%	20,3%	6,0%		54,6%	71,9%	21,9%	-1,1%	68,7%	32,8%
	2050	technology	2,4%	3,4%	3,4%	0,1%	11,2%	5,3%		16,6%	18,3%	5,9%	0,2%	34,3%	28,0%
	2050	market	8,1%	13,6%	11,3%	-1,1%	19,1%	5,6%		61,1%	79,6%	20,7%	-1,9%	69,7%	34,0%
	2050	All	8,6%	13,9%	11,9%	-1,1%	21,1%	6,4%		62,7%	79,3%	21,3%	-1,9%	71,4%	35,0%

4.4 Discussion

The aim of the present study was to demonstrate how IAM scenarios can be systematically linked with LCI parameters to account for future changes in prospective LCA. Integrating electricity scenarios from IMAGE with data from the ecoinvent database served to account for future background changes in the prospective LCAs of EVs and ICEVs. We showed that it is possible to use six IMAGE scenarios covering different socio-economic pathways of development to calculate the impacts of two types of vehicles because the integration proposed in this study follows a systematic procedure. For prospective LCA, this is an important modelling effort that helps to understand the effects of background changes independent of the product evolution, which is represented in the foreground (Miller and Keoleian 2015). As the results showed, background changes are important in the case of some key impacts for EV and can determine the relative environmental performance differences between EV and ICEV. For uncertainty analysis, this is also an important effort as epistemological uncertainty can be acknowledged by means of relevant and consistent scenarios representing possible futures, as was shown in the results. This type of uncertainty cannot be reduced given the fact that the nature of the system we studied is nonstationary, complex and based on human behavior (Plevin 2016). However, this study showed that exploring future pathways and related impacts rather than predicting them can help to outline and better inform directions for action by acknowledging the presence of this type of uncertainty and by making the assumptions and constraints as transparent as possible.

Our results show that future developments in the electricity sector will critically affect whether and by how much EV outperform ICEV for key impact categories such as climate change. These findings are to some extent consistent with the literature, although previous studies have mostly focused only on market changes related to increased diffusion of low-carbon power technologies. For example, Wolfram and Wiedmann (2017) estimated that the carbon footprint of EV in Australia in a business-as-usual scenario for the diffusion of renewable energies would decrease about 50% from 2009 to 2050. This magnitude is within the range of our results for MidRoad scenarios (which would be conceptually equivalent) and for climate change, which describe a decrease due to market changes alone of 14 to 80% between 2012 and 2050. Similarly, Messagie and Brussel (2017) described reductions of about 60% in the carbon footprint of EV when replacing the average EU electricity mix by that of countries where renewable and nuclear power prevail, such as Sweden or France.

Some important limitations of our study need to be discussed. First, some future emissions for electricity technologies were not adapted using specific emission factors but using best available data. Therefore, future emissions for these substances should be carefully assessed. For instance, in the case of PM emissions, changes were made according to future technology efficiency as IMAGE does not explicitly model different sizes of Particulate Matter (PM) emissions despite modelling Black Carbon emissions, which cover several PM sizes altogether. Hence, results for particulate matter formation do not account for developments such as end-of-pipe solutions, which would be better captured in specific emission factors for PMs. In this sense, there is room for improvement of the present approach, and it would make sense to invest in finding more suitable proxies, other than technology efficiency, modelled within the IAM model to change the LCI parameters wherever possible.

Secondly, we focused on the electricity sector, leaving all other sectors unchanged. By doing so we ignored other layer of complexity, realizing that additional changes are to be expected for other technologies in other sectors (e.g. the steel sector in the case of vehicles) and that these would affect the life cycle impacts of ICEVs and EVs found in this study. For instance, if we had coupled changes in the background for the main industry sectors (e.g. the steel sector), fossil-fuels production, transport and other sectors, such as the agricultural sector, this would have resulted in the possibility to evaluate the life cycle impacts of each product accounting for a fully consistent macro-level scenario. We did not pursue this full scope of all sectors yet, as this article mainly aimed to prove the concept. The availability of datasets for these other sectors in the IMAGE scenarios suggests that including them is the logical next step towards a more systematic construction of future LCI databases using IAM scenarios.

We still consider the results of this study to be representative for EVs, because the largest contribution to the EV impacts is electricity production to recharge the battery (Cox et al. 2018). Also, the technology and market changes that we did consider have roughly changed about 75% of the ecoinvent processes and have reduced their overall impact by 10% using the MidRoad-2.6 scenario for 2040 (Cox et al. 2018). For ICEVs, there could be changes in the production of oil due to changes in the resource accessibility and possibly due to new extraction technologies. Hence our results can be read as an exploration keeping the status quo for fossil-fuels production.

Lastly, we relied on inventories of technologies that are yet to be deployed, in particular CCS and CSP. While these inventories are crucial for achieving ambitious climate targets, there still are large parameter uncertainties for these inventories. The robustness of the assessment would be increased by addressing such parameter uncertainty jointly with other sources of uncertainty (see chapter 2 and 3 of this thesis) as well as acknowledging epistemological uncertainty. Cox et al. (2018) already made an effort in this direction for the case of EVs.

4.5 Conclusions

For dealing with the large epistemological uncertainty about the future in order to support more robust future environmental assessments and decision-making, we were able to demonstrate a new approach for systematically capturing background changes in prospective life cycle assessment (LCA). We evaluated scenarios from an Integrated Assessment Model (IAM), the IMAGE model, in the life cycle inventory phase of a prospective LCA using ecoinvent v3.3 as a background dataset. Our case study on the effects of future changes in the electricity sector on the prospective LCA of an electric vehicle (EV) and an internal combustion engine vehicle (ICEV) shows that the new approach is both feasible and valuable. Future changes include technology developments in terms of efficiency and emission factors as well as market changes, which were more extensively studied in previous literature, for electricity market mixes in the future.

Advantages of our approach include a systematic integration of data, based on consistent worldwide scenarios, with reproducible, transparent and traceable assumptions and results. Also, the approach meets demands to include macro scenarios into the micro or product level of LCA to help increase the robustness of the assessment. For prospective LCA, this method is a modelling effort helping to understand exogenous background changes. For uncertainty analysis, this is an effort that acknowledges, rather than reduces, epistemological uncertainty via the use of a broad spectrum of socio-economically driven scenarios, which lead to explorative instead of predictive results that can help outline and better inform directions for action in product design and policymaking.

The case study shows that background changes can be very important for future environmental impact assessment of EVs and ICEVs. Climate change impacts can be altered up to 80% by 2050 in an ambitious mitigation scenario compared to impacts calculated without accounting for background changes. The uncertainty about future developments in the electricity sector is overall large, but it manifests differently depending on the studied product (EV or ICEV), the impact category, and the scenario and year considered. Considering the uncertainty about the future also makes assessing the relative environmental performance of EV over time more complex and nuanced. Depending on the scenario, year and impact, EV can perform better or worse than ICEV. Electricity market changes have a larger influence than technology changes on the total impacts of both types of vehicles. For both types of vehicles, market changes can thus determine if the impacts are better or worse with respect to the impacts calculated with original ecoinvent background. Interactions between market changes and technology changes are observed when both are taken into account.

It is still possible to find more suitable data within the IAM model to account for technology changes. Also, it is important to improve further the inventories for relevant future technologies in line with the scenarios, such as carbon capture and storage (CCS) and concentrated solar power (CSP), or to account for their parameter uncertainty. Moreover, it is also possible to expand the present approach to other economic sectors as well as other products in search of a more systematic construction of future inventory databases using IAM scenarios for more robust prospective LCA. Then, LCA results can be further calculated for products delivering the same function but with a different technological profile, thus enabling the comparison of their future impacts in a wider context.

Acknowledgements
Authors would like to thank the PhD students and postdocs summer school on "System Models in LCA" (2016) organized by the Paul Scherrer Institut (PSI), ETH Zurich and ecoinvent, for creating the environment to shape ideas and to kick-off the collaboration that led to this study. We would also like to acknowledge David Gernaat for his assistance in gathering relevant IMAGE data. David Font Vivanco acknowledges funding from the European Commission (Marie Skłodowska-Curie Individual Fellowship [H2020-MSCA-IF-2015], grant agreement no. 702869).

Supporting information
If not provided below the material is available upon request.

ANNEX I

Table S. 1 Technologies map between IMAGE and ecoinvent v3.3.

Where proxies are indicated for ecoinvent processes, we copy the inventories of the proxy process indicated and assume that these correspond to the technology indicated by the IMAGE technology. Copied proxy processes are further renamed and modified according to the IMAGE scenario. For oil CCS and Oil CHP CCS the Carma project did not create datasets. Because the contribution of these technologies in the IMAGE scenarios is small, we use the best available data we have i.e. for coal and natural gas. We expect this over simplification to have no significant effect on the results.

IMAGE technology	Ecoinvent processes
Solar PV	'electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted' 'electricity production, photovoltaic, 3kWp slanted-roof installation, single-Si, panel, mounted' 'electricity production, photovoltaic, 570kWp open ground installation, multi-Si'
Concentrated Solar Power (CSP)	'Electricity production for a 50MW parabolic trough power plant' 'Electricity production at a 20MW solar tower power plant'
Wind onshore	'electricity production, wind, <1MW turbine, onshore' 'electricity production, wind, 1-3MW turbine, onshore' 'electricity production, wind, >3MW turbine, onshore'
Wind offshore	'electricity production, wind, 1-3MW turbine, offshore'
Hydro	'electricity production, hydro, reservoir, alpine region' 'electricity production, hydro, reservoir, non-alpine region' 'electricity production, hydro, reservoir, tropical region' 'electricity production, hydro, run-of-river'
Other renewables	'electricity production, deep geothermal'
Nuclear	'electricity production, nuclear, boiling water reactor' 'electricity production, nuclear, pressure water reactor, heavy water moderated' 'electricity production, nuclear, pressure water reactor'
Coal Steam Turbine (Coal ST)	'electricity production, hard coal' 'electricity production, lignite'
Coal Combined Heat and Power (Coal CHP)	'heat and power co-generation, hard coal' 'heat and power co-generation, lignite'
Integrated gasification combined cycle (IGCC)	'Electricity, at power plant/hard coal, IGCC, no CCS/2025' 'Electricity, at power plant/lignite, IGCC, no CCS/2025'
Oil Steam Turbine (Oil ST)	'electricity production, oil'
Oil Combined Heat and Power (Oil CHP)	'heat and power co-generation, oil'
Oil combined cycle (Oil CC)	**Proxy: Same processes as oil ST:** electricity production, oil
Natural gas open Cycle turbine (Natural gas OC)	'electricity production, natural gas, conventional power plant'

Natural gas combined cycle (Natural Gas CC)	'electricity production, natural gas, combined cycle power plant'
Natural gas Combined Heat and Power (Natural Gas CHP)	'heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical' 'heat and power co-generation, natural gas, conventional power plant, 100MW electrical'
Biomass Combined Heat and Power (Biomass CHP)	Heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014' 'heat and power co-generation, wood chips, 6667 kW' 'heat and power co-generation, biogas, gas engine'
Biomass combined cycle (Biomass CC)	**Proxy, Same processes as for biomass CHP** Heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014' 'heat and power co-generation, wood chips, 6667 kW' 'heat and power co-generation, biogas, gas engine'
Biomass Steam Turbine (Biomass ST)	**Proxy, Same processes as for biomass CHP:** Heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014' 'heat and power co-generation, wood chips, 6667 kW' 'heat and power co-generation, biogas, gas engine'
Coal Carbon Capture and Storage (Coal CCS)	'Electricity, at power plant/hard coal, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, oxy, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, oxy, pipeline 200km, storage 1000m/2025'
Coal Combined Heat and Power Carbon Capture and Storage (Coal CHP CCS)	**Proxy, Carma project didn't include Coal CHP CCS (Volkart et al. 2013)** 'Electricity, at power plant/hard coal, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, oxy, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, oxy, pipeline 200km, storage 1000m/2025'
Oil Capture and Storage (Oil CCS)	**Proxy, Carma project didn't include Coal CHP CCS (Volkart et al. 2013)** 'Electricity, at power plant/hard coal, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, oxy, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, oxy, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/natural gas, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/natural gas, post, pipeline 200km, storage 1000m/2025'
Oil Combined Heat and Power Carbon Capture and Storage (Oil CHP CCS)	**Proxy, Carma project didn't include Coal CHP CCS (Volkart et al. 2013)** 'Electricity, at power plant/hard coal, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, post, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/lignite, oxy, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/hard coal, oxy, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/natural gas, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/natural gas, post, pipeline 200km, storage 1000m/2025'
Natural gas Carbon Capture and Storage (Natural Gas CCS)	'Electricity, at power plant/natural gas, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/natural gas, post, pipeline 200km, storage 1000m/2025'
Natural Gas Combined Heat and Power Carbon Capture and Storage (Natural Gas CHP CCS)	**Proxy, same processes as natural gas CCS:** 'Electricity, at power plant/natural gas, pre, pipeline 200km, storage 1000m/2025' 'Electricity, at power plant/natural gas, post, pipeline 200km, storage 1000m/2025'

Biomass Carbon Capture and Storage (Biomass CCS)	'Electricity, from CC plant, 100% SNG, truck 25km, post, pipeline 200km, storage 1000m/2025' 'Electricity, at wood burning power plant 20 MW, truck 25km, post, pipeline 200km, storage 1000m/2025' 'Electricity, at BIGCC power plant 450MW, pre, pipeline 200km, storage 1000m/2025'
Biomass Combined Heat and Power Carbon Capture and Storage (Biomass CHP CCS)	**Proxy, same processes as biomass CCS:** 'Electricity, from CC plant, 100% SNG, truck 25km, post, pipeline 200km, storage 1000m/2025' 'Electricity, at wood burning power plant 20 MW, truck 25km, post, pipeline 200km, storage 1000m/2025' 'Electricity, at BIGCC power plant 450MW, pre, pipeline 200km, storage 1000m/2025'

ANNEX II

Table S. 2 Regional description for IMAGE used to match ecoinvent v3.3 processes.

IMAGE Regions	IMAGE countries in regions (ISO 3166-1 2 letter country code) See link for further reference: http://themasites.pbl.nl/tridion/en/themasites/_disabled_fair/definitions/datasets/index-2.html
Canada	CA
USA	US, PM
Mexico	MX
Central America	AI, AW, BB, BM, BZ, BS, CR, DM, DO, GD, GP, GT, HN, HT, JM, KY, MQ, MS, NI, AW, CW, SX, PA, PR, SV, KN, LC, VC, TT, TC, VG, VI
Brazil	BR
South America	AR, BO, CL, CO, EC, GF, GY, PE, PY, SR, UY, VE
Northern Africa	DZ, EG, EH, LY, MA, TN
Western Africa	BF, BJ, CF, CM, CV, CD, CG, CI, GA, GH, GN, GQ, GM, GW, LR, ML, MR, NE, NG, SL, SN, ST, SH, TD, TG
Eastern Africa	BI, DJ, ER, ET, KE, KM, MG, MU, RW, RE, SC, SD, SO, UG
South Africa	ZA
Western Europe	AD, AT, BE, CH, DE, DK, ES, FI, FR, FO, GB, GI, GR, IE, IS, IT, LI, LU, MC, MT, NL, NO, PT, SE, SM, VA
Central Europe	AL, BA, BG, CS, CY, CZ, EE, HR, HU, LT, LV, MK, PL, RO, SI, SK
Turkey	TR
Ukraine region	BY, MD, UA
Central Asia (Asia-Stans)	KZ, KG, TJ, TM, UZ
Russia	AM, AZ, GE, RU
Middle east	AE, BH, IL, IQ, IR, JO, KW, LB, OM, QA, SA, SY, YE
India	IN
Korea Region	KP, KR
China	CN, HK, MN, MO, TW
South Asia	BN, KH, LA, MM, MY, PH, SG, TH, VN
Indonesia Region	ID, PG, TL
Japan	JP
Oceania	AS, AU, CK, FJ, KI, MH, MP, FM, NC, NR, NU, NZ, PF, PW, SB, TK, TO, TV, VU, WS
Rest of South Asia	AF, BD, BT, LK, MV, NP, PK
Rest of Southern Africa	AO, BW, LS, MW, MZ, NA, SZ, TZ, ZM, ZW

Further details on the regional mapping in Wurst can be found in https://wurst.readthedocs.io/#spatial-relationships

ANNEX III

Global Warming Potentials (GWPs) from 2013 from the IPCC with a time horizon of 100 years as implemented by ecoinvent are used. All biogenic CO_2 flows are considered. The table below shows the GWPs used

Table S. 3 Global warming potential characterization factors used in the life cycle impact assessment.

Biosphere flow	kg CO_2 eq / kg	Biosphere flow	kg CO_2 eq / kg
Carbon dioxide, fossil	1	Ethane, pentafluoro-, HFC-125	3169.26
Carbon dioxide, from soil or biomass stock	1	Methane	29.7
Carbon dioxide, in air	-1	Methane, bromo-, Halon 1001	2.35
Carbon dioxide, to soil or biomass stock	-1	Methane, bromochlorodifluoro-, Halon 1211	1746.48
Carbon monoxide, fossil	4.06	Methane, bromotrifluoro-, Halon 1301	6291.63
Carbon monoxide, from soil or biomass stock	4.06	Methane, chlorodifluoro-, HCFC-22	1764.63
Carbon monoxide, non-fossil	2.49	Methane, chlorotrifluoro-, CFC-13	13893.35
Chloroform	16.4	Methane, dichloro-, HCC-30	8.92
Dinitrogen monoxide	264.8	Methane, dichlorodifluoro-, CFC-12	10239.23
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a	1301.27	Methane, dichlorofluoro-, HCFC-21	147.66
Ethane, 1,1,1-trichloro-, HCFC-140	160.1	Methane, difluoro-, HFC-32	676.81
Ethane, 1,1,1-trifluoro-, HFC-143a	4804.44	Methane, fossil	29.7
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	5823.73	Methane, from soil or biomass stock	29.7
Ethane, 1,1-dichloro-1-fluoro-, HCFC-141b	782.04	Methane, monochloro-, R-40	12.18
Ethane, 1,1-difluoro-, HFC-152a	137.56	Methane, non-fossil	28.5
Ethane, 1,2-dichloro-	0.9	Methane, tetrachloro-, R-10	1728.47
Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, CFC-114	8592.2	Methane, tetrafluoro-, R-14	6625.78
Ethane, 1-chloro-1,1-difluoro-, HCFC-142b	1982.04	Methane, trichlorofluoro-, CFC-11	4662.94
Ethane, 2,2-dichloro-1,1,1-trifluoro-, HCFC-123	79.37	Methane, trifluoro-, HFC-23	12397.6
Ethane, 2-chloro-1,1,1,2-tetrafluoro-, HCFC-124	526.55	Nitrogen fluoride	16070
Ethane, chloropentafluoro-, CFC-115	7665.36	Perfluoropentane	8546.7
Ethane, hexafluoro-, HFC-116	11123.49	Sulfur hexafluoride	23506.82

ANNEX IV

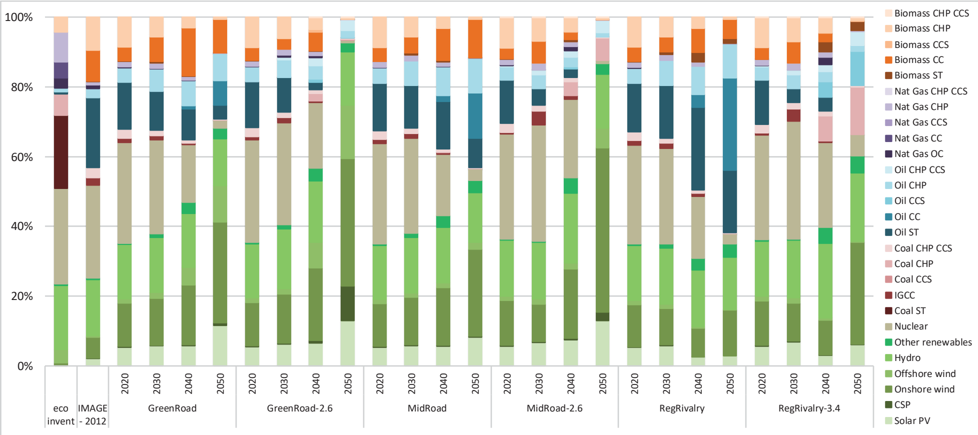


Figure S. 1 Energy mix for all scenarios and year for Western Europe in IMAGE.

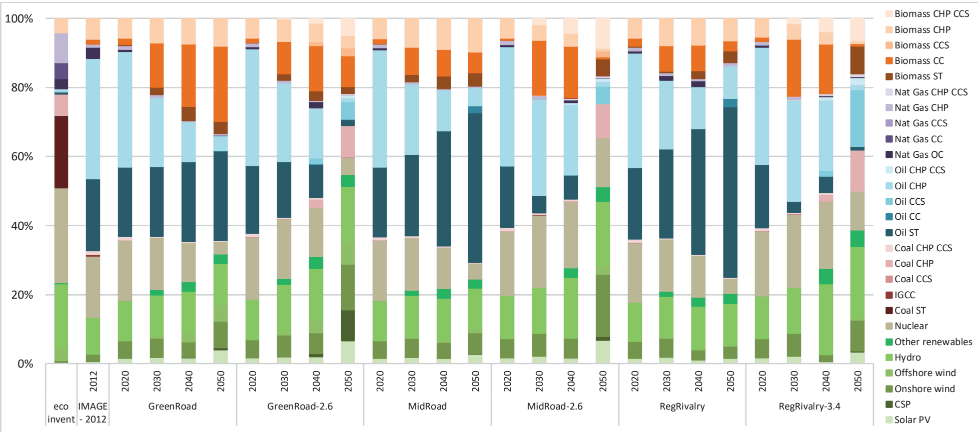


Figure S. 2 Energy mix for all scenarios and year for Central Europe in IMAGE.

ANNEX V

Relative impact category results of ICEV and EV. In the graphs below all data points above the diagonal represent years and scenarios for which EV performs better than the ICEV for each impact and points below the diagonal are years and scenarios for which EV performs worse than the ICEV.

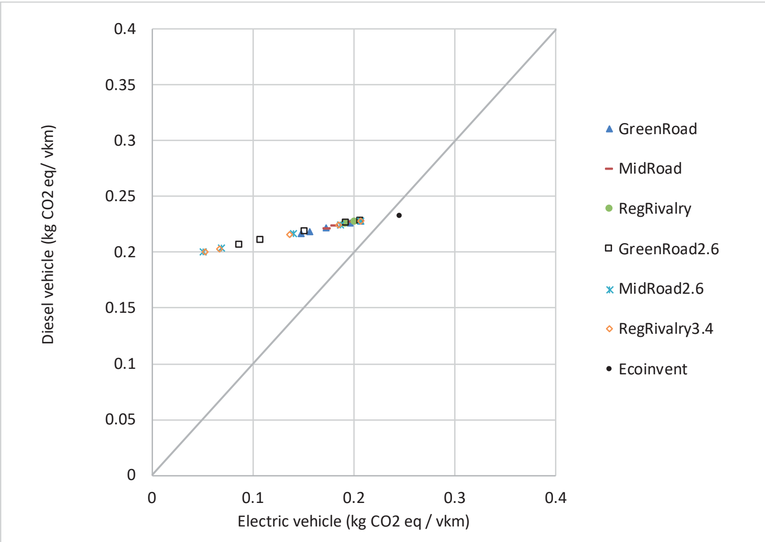


Figure S. 3. Climate change for ICEV and EV

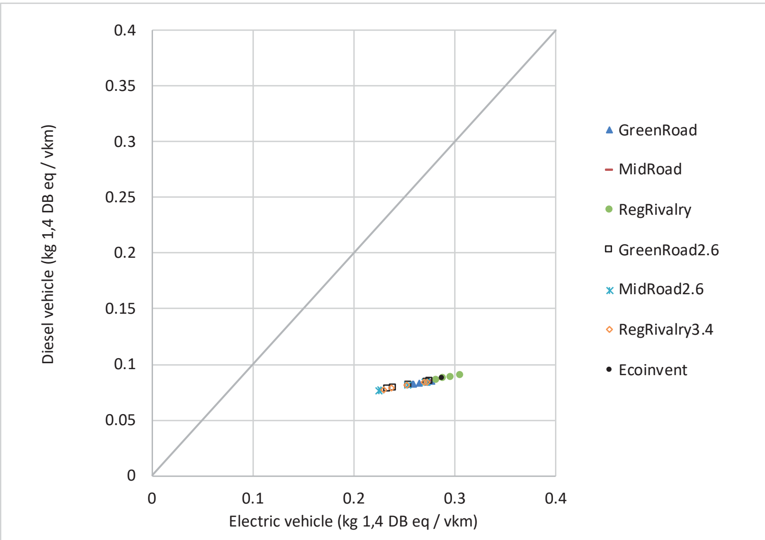


Figure S. 4 Human toxicity for ICEV and EV

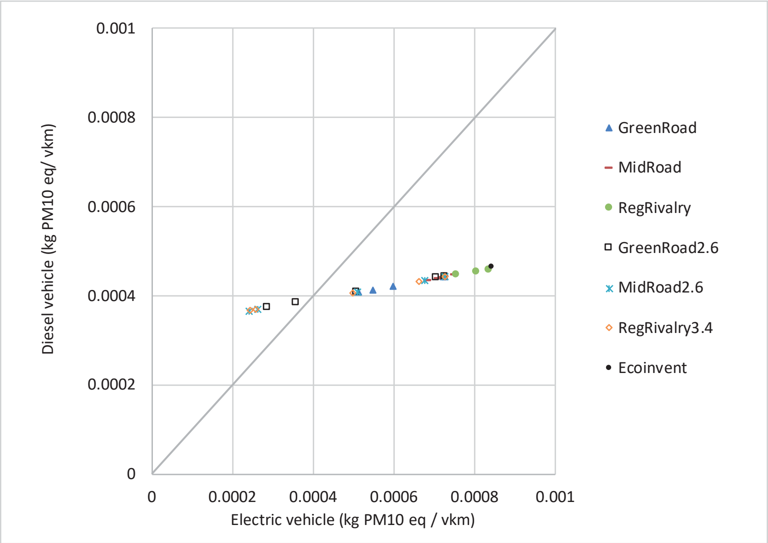


Figure S. 5 Particular matter formation for ICEV and EV

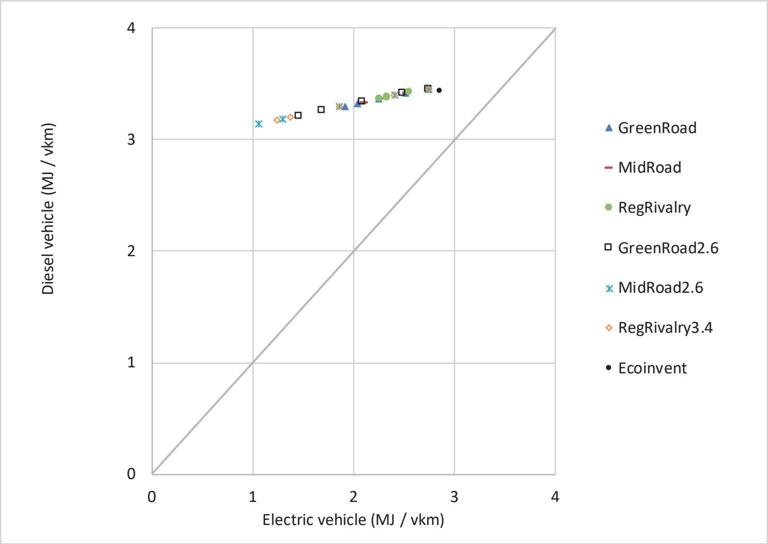


Figure S. 6 Fossil cumulative energy demand for ICEV and EV

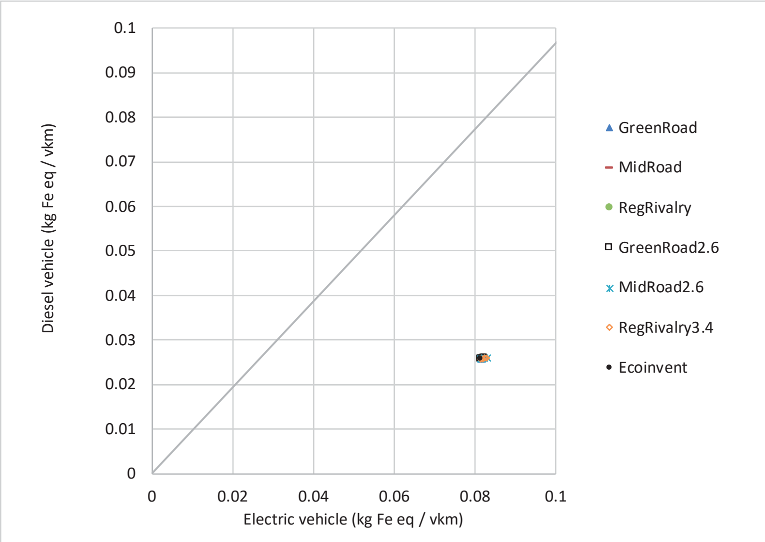


Figure S. 7 Mineral depletion for ICEV and EV

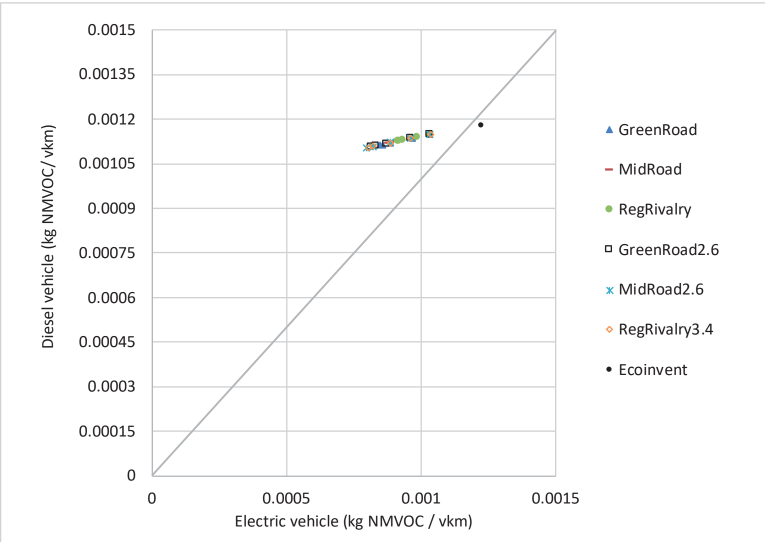


Figure S. 8 Photochemical oxidant formation for ICEV and EV

ANNEX VI

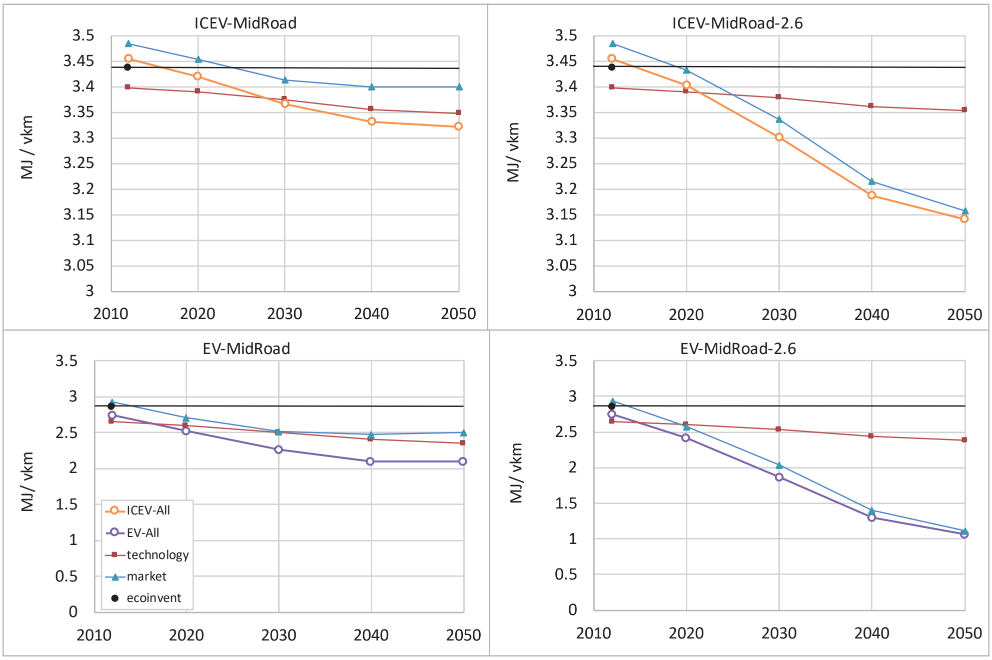


Figure S. 9 Technology (red squares), market (blue triangles) and both adaptations for the ICEV (orange line) and EV (purple line) for MidRoad and MidRoad-2.6 scenarios for Fossil cumulative energy demand.

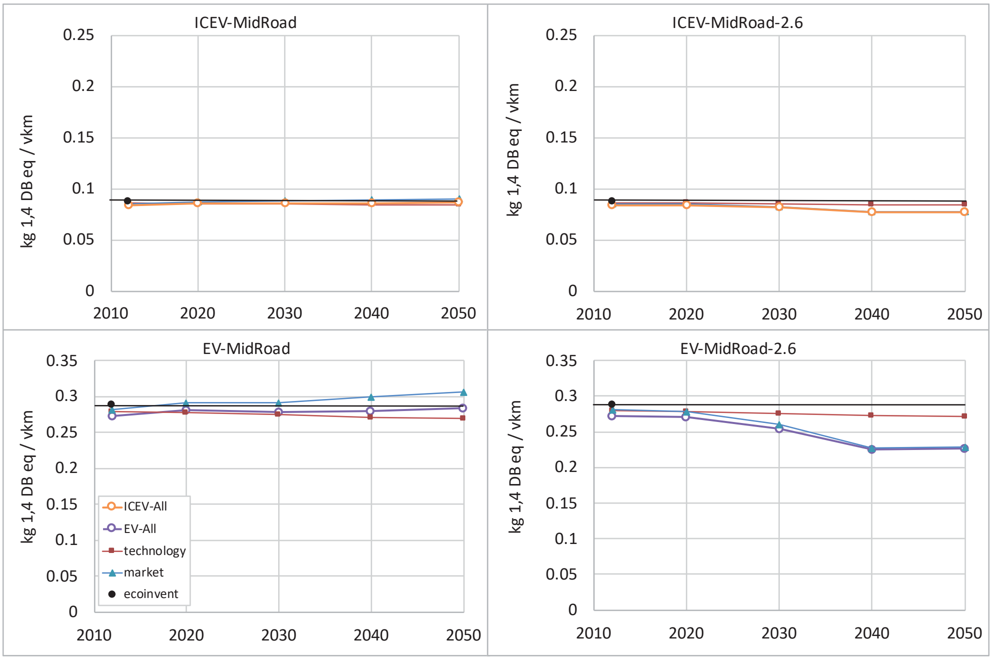


Figure S. 10 Technology (red squares), market (blue triangles) and both adaptations for the ICEV (orange line) and EV (purple line) for MidRoad and MidRoad-2.6 scenarios for Human toxicity.

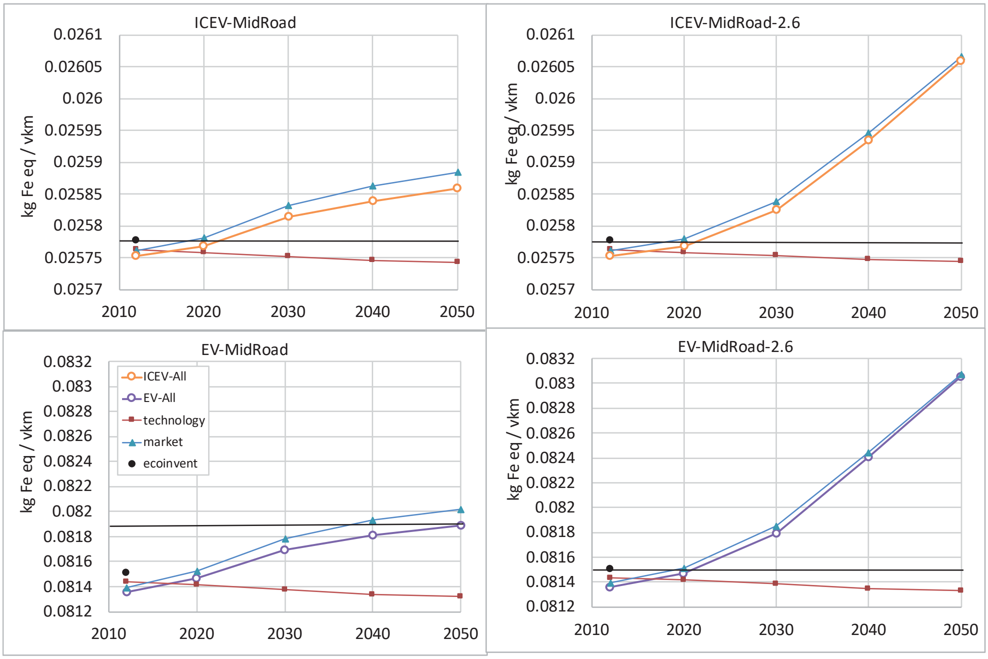


Figure S. 11 Technology (red squares), market (blue triangles) and both adaptations for the ICEV (orange line) and EV (purple line) for MidRoad and MidRoad-2.6 scenarios for Mineral depletion.

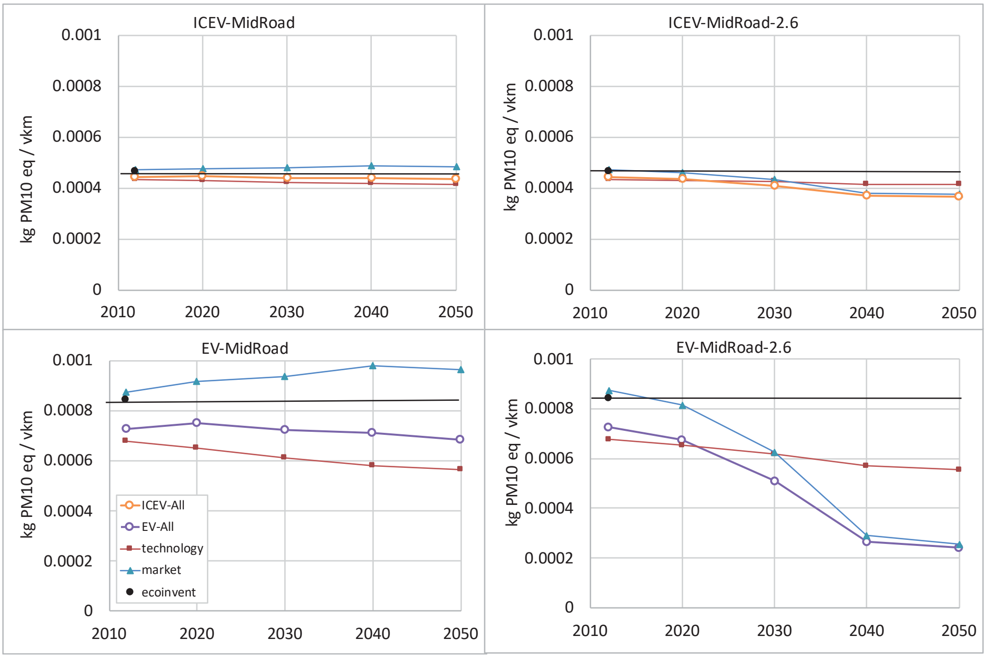


Figure S. 12 Technology (red squares), market (blue triangles) and both adaptations for the ICEV (orange line) and EV (purple line) for MidRoad and MidRoad-2.6 scenarios for Particular matter formation.

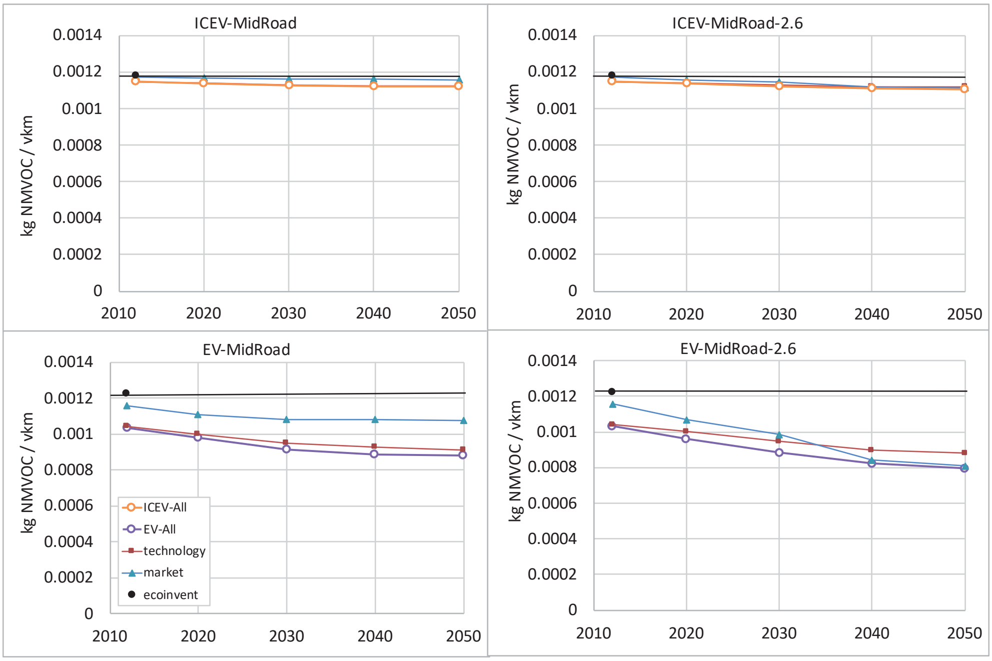


Figure S. 13 Technology (red squares), market (blue triangles) and both adaptations for the ICEV (orange line) and EV (purple line) for MidRoad and MidRoad-2.6 scenarios for Photochemical oxidant formation.

5.

Quantified Uncertainties in Comparative Life Cycle Assessment: What Can Be Concluded?

Angelica Mendoza Beltran
Valentina Prado
David Font Vivanco
Patrik J.G. Henriksson
Jeroen B. Guinée
Reinout Heijungs

Re-print with minor changes from:

Environmental Science & Technology (2018). 52(4): 2152–2161. doi/10.1021/acs.est.7b06365.

Abstract

Interpretation of comparative Life Cycle Assessment results (LCA) can be challenging in the presence of uncertainty. To aid in interpreting such results under the goal of any comparative LCA, we aim to provide guidance to practitioners by gaining insights into uncertainty-statistics methods (USMs). We review five USMs - discernibility analysis, impact category relevance, overlap area of probability distributions, null hypothesis significance testing (NHST), and modified NHST-, and provide a common notation, terminology, and calculation platform. We further cross-compare all USMs applying them to a case study on electric cars. USMs belong to a confirmatory or an exploratory statistics' branch, each serving different purposes to practitioners. Results highlight that common uncertainties and the magnitude of differences per impact are key in offering reliable insights. Common uncertainties are particularly important as disregarding them can lead to incorrect recommendations. Based on these considerations, we recommend the modified NHST as a confirmatory USM. Also, we recommend discernibility analysis as an exploratory USM along with recommendations for its improvement, as it disregards the magnitude of the differences. While further research is necessary to support our conclusions, results and supporting material provided can help LCA practitioners in delivering a more robust basis for decision-making.

Keywords: Comparative LCA, Uncertainty, Interpretation, Decision-making

5.1 Introduction

One of the main applications of life cycle assessment (LCA) is to support a comparative assertion regarding the relative environmental performance of one product with respect to other functionally equivalent alternatives (ISO 2006). In such a comparative LCA, claims can be tested by comparing the inventory and/or impact assessment results for any given set of alternative products (JRC-IES 2010). To date, practitioners usually calculate and compare point-value results, an approach described as deterministic LCA (Wei et al. 2016). This practice allows one to draw conclusions such as 'alternative B causes 45% larger impacts than alternative A' or 'alternatives B and C have strengths and weaknesses, but both outperform alternative D'. Typically, deterministic comparative LCAs find trade-offs between alternatives and across environmental impacts (from here on referred to as impacts). While uncertainty estimations can be useful in understanding trade-offs between alternatives, deterministic LCAs lack an assessment of uncertainties (Ross et al. 2002).

Uncertainty appears in all phases of an LCA (Björklund 2002; Huijbregts et al. 2003; Wiloso et al. 2014) and originates from multiple sources. Some of the more prevalent are: variability, imperfect measurements (inherent uncertainty (Henriksson et al. 2014)), gaps, unrepresentativeness of inventory data (also known as parameter uncertainty) (Björklund 2002), methodological choices made by practitioners throughout the LCA (also known as scenario uncertainty or uncertainty due to normative choices) (Björklund 2002) and mathematical relationships (also known as model uncertainty) (Björklund 2002). Using analytical and stochastic approaches, e.g. Monte Carlo (MC) simulations and first order Taylor series expansion (Groen et al. 2014), LCA practitioners have propagated these sources of uncertainty to LCA results (Lloyd and Ries 2008; Groen et al. 2014). Unlike deterministic LCA, the quantification of uncertainties related to LCA results allows for associating a level of likelihood to and confidence in the conclusions drawn. However, interpreting overlapping ranges of results is complex and therefore requires sophisticated interpretation methods (Lloyd and Ries 2008). To this end, various statistical methods have been applied within the field of LCA, including: discernibility analysis (Heijungs and Kleijn 2001; Gregory et al. 2016), impact category relevance (Prado-Lopez et al. 2014), overlap area of probability distributions (Prado-Lopez et al. 2016), null hypothesis significance testing (NHST) (Henriksson et al. 2015a, b), and modified NHST (Heijungs et al. 2016).

The application of statistical methods to uncertainty analysis results, hereafter referred to as 'uncertainty-statistic methods' (USMs), can aid practitioners in various ways. First, they help to establish a level of confidence behind the trade-offs between alternatives and across environmental impacts while considering various sources of uncertainty. Second, they go beyond the practice of one at the time scenario analysis by integrating series of otherwise independent sensitivity analyses into an overall uncertainty assessment of results (Ross et al. 2002). For instance, they enable the exploration of a broad range of possible combinations of all sorts of input data known as the scenario space (Gregory et al. 2016). Third, they allow for comparisons of alternatives in the context of common uncertainties, a crucial aspect in comparative LCAs (Henriksson et al. 2015a). Lastly, they help to identify the relative importance of different impacts for the comparison of alternatives (Hertwich and Hammitt 2001).

Choosing the most appropriate statistical method(s) to interpret the results of uncertainty analysis in the light of the goal and scope of individual LCA studies can be challenging. There is a lack of applications of these methods in real case studies, a lack of support in standard LCA software, incomprehensive and scattered documentation, and inconsistent terminology and mathematical notation. Moreover, literature is devoid of recommendations for LCA practitioners about which method(s) to use, under which LCA goal, to interpret the meaning of the uncertainty analysis results in comparative LCAs. Thus, our research question queries: "*Which statistical method(s) should LCA practitioners use to interpret the results of a comparative LCA, under the light of its goal and scope, when considering uncertainty?*" In this chapter, we answer this question by (1) critically reviewing the five above mentioned USMs, (2) comparing them for a single illustrative case study on passenger vehicles with a common calculation platform and terminology, and (3) by providing guidance to practitioners in the realm of application of these methods via a decision tree. It is the focus of this chapter to test the applicability and value of different USMs, including the visualization of results and the limitations encountered during their implementation. Testing and analyzing differences in methods to quantify and propagate uncertainties is out of the scope of this chapter, although we use some of them (e.g. Monte Carlo simulations as propagation method) for the uncertainty analysis.

5.2 Methods and case study

Statistical methods for interpretation of comparative LCA with uncertainty

In chronological order of publication, the methods we study are: discernibility analysis (Heijungs and Kleijn 2001; Gregory et al. 2016), impact category relevance (Prado-Lopez et al. 2014), overlap area of probability distributions (Prado-Lopez et al. 2016), null hypothesis significance testing (NHST) (Henriksson et al. 2015a, b), and modified NHST(Heijungs et al. 2016). The scope was narrowed to these statistical methods based on two criteria:

1) The method has been developed and published in peer reviewed journals and contains transparent and accessible algorithms. Consequently, the first-order reliability method (FORM) (Wei et al. 2016), could not be included due to incompletely documented optimization procedures.

2) The method is applied to interpret the results of uncertainty analysis of comparative LCAs with two or more alternatives and one or more emissions or impacts. This excludes studies addressing different impacts but not in a comparative way (Grant et al. 2016) and, studies focusing on methods for quantifying and/or propagating uncertainty sources through LCA. Studies developing and describing methods such as global sensitivity analysis (Groen et al. 2017) are also excluded as they are neither comparative and focus on just one emission or impact at a time. Finally, we have not revisited the enormous body of statistical literature, as the authors of the selected methods already have done this exercise.

To increase transparency in our comparison of methods and their features, we use a uniform terminology (Appendix I), and a common mathematical notation (Table 10). We interpret the state of the art for each method, and in some cases go beyond the original mathematical proposals by the authors. When this is the case, we indicate the differences.

We reviewed the methods according to the following aspects: the number of alternatives compared and approach to compare them, the inputs used by the method, the implementation, the purpose and the type of outputs. Table 11 summarizes the features of each method according to these aspects.

Some features that are consistent for all methods include: 1) they can be applied to dependently or independently sampled MC runs, meaning that the uncertainty analysis results are (dependently) or not (independently) calculated with the same technology and environmental matrices for all alternatives considered for each MC run; 2) they can be used to interpret LCA results at the inventory, characterization, and normalization level, although in our case study we only apply them at the characterization level as their use at other levels is trivial in the absence of additional uncertainties; 3) they all compare alternatives per pairs (pairwise analysis); and 4) they all originate from the idea of merging uncertainty and comparative analysis.

Discernibility

We refer to discernibility as the method described by Heijungs and Klein (2001) as the basis of comparative evaluation of Gregory et.al (2016) is the same as proposed by Heijungs and Klein (2001). Discernibility compares two or more alternatives, using a pairwise method as the comparison takes place by pair of alternatives, comparing the results of alternative j with alternative k per MC run. It assesses the stochastic outcomes on whether the results of one alternative are higher or lower than another alternative. The purpose of discernibility is to identify whether the results of one of the alternatives are higher than (irrespective of how much higher) the results of the other. This method disregards the distance between the mean scores (or other centrality parameters). For its operationalization, practitioners count how many realizations per pair of alternatives

Table 10. Mathematical notation for comparison of uncertainty-statistics methods (USMs)

Symbol	Description
j, k	Index of alternatives e.g. products, services, systems, etc ($j = 1 \ldots, n\, j = 1 \ldots, n, k = 1, \ldots, n\, k = 1, \ldots, n$)
i	Impact category (Climate change, eutrophication, acidification,…)
r	Index of Monte Carlo simulations (r=1, ,…, N)
X	Random variable
x	Realization
μ	Parameter of centrality (mean)
σ	Parameter of dispersion (standard deviation)
$\bar{X}$	Statistic of centrality (estimator of mean μ)
S	Statistic of dispersion (estimator of standard deviation σ)
$\bar{x}$	Obtained value of centrality (estimate of mean μ)
s	Obtained value of dispersion (estimate of standard deviation σ)
$f_{i,j,k}$	Fraction of runs with higher results on impact category i in alternative j compared to k
$\#(x)$	Count function, counts the number of runs fulfilling condition x
$\Upsilon_{i,j,k}$	Relevance parameter for the pair of alternatives j, k on impact category i
$A_{i,j,k}$	Overlap area of two probability distributions for the pair of alternatives j, k on impact category i

Table 11. Features of the different uncertainty-statistics methods (USMs) in comparative LCA

Methods	Alternatives compared (approach)	Type of input (From uncertainty analysis)	Implementation	Purpose (Type of question)	Type of output	Reference
Deterministic LCA (Comparison of point values)	As many as required (all together)	None	Overall (i.e based on one run or point-value)	Which alternative displays the lower results? (Exploratory)	Point-value	Abundant in literature. Included as standard result in LCA software packages
Discernibility	As many as required (pairwise analysis)	Monte Carlo runs (dependently or independently sampled)	Per run	How often is the impact i higher for j than for k, or vice versa? (Exploratory)	Counts meeting "sign test" condition (equation 3)	Heijungs and Klein (Heijungs and Kleijn 2001)
Impact category relevance	As many as required (pairwise analysis)	Estimates of statistical parameters (i.e. mean and standard deviation)	Overall (i.e. based on statistical parameters)	Which are the impacts playing a relatively more important role in the comparison of j and k? (Exploratory)	Measure of influence of impacts in the comparison (equation 4)	Prado-Lopez et al.(Prado-Lopez et al. 2014)
Overlap area of probability distributions	As many as required (pairwise analysis)	Moments of the fitted distribution (e.g. maximum likelihood estimates)	Overall (i.e. based on moments of the fitted distribution)	Which are the impacts playing a relatively more important role in the comparison of j and k? (Exploratory)	Overlap of probability distributions of j and k (equation 5)	Prado-Lopez et al.(Prado-Lopez et al. 2016)
Null hypothesis significance testing (NHST)	As many as required (pairwise analysis)	Monte Carlo runs (dependently or independently sampled)	Per run	Is the mean impact of j significantly different from the mean impact of k? (Confirmatory)	p-values Fail to reject (no) or reject (yes) the null hypothesis	Henriksson et al.(Henriksson et al. 2015a)
Modified NHST	As many as required (pairwise analysis)	Monte Carlo runs (dependently or independently sampled)	Per run	Is the difference between the mean impact of j and k at least as different as a threshold? (Confirmatory)	p-values Fail to reject (no) or reject (yes) the null hypothesis	Heijungs et al.(Heijungs et al. 2016)

Chapter 5

per impact i.e. $x_{i,j,r}$ and $x_{i,k,r}$ for $r = 1,\ldots,N$ meet the "sign test" condition. The counting function is indicated by the symbol $\#(\cdot)$, where the argument of the function specifies the "sign test" condition. We interpret these condition as the evaluation of whether the difference between the results per run for a pair of alternatives is bigger than zero. Equation 3 shows the calculations of the discernibility approach for each impact.

$$f_{i,j,k} = \frac{\#_{r=1}^{N}(x_{i,j,r} - x_{i,k,r} > 0)}{N}$$

Eq.3

The results of Equation 3 help assert that "Alternative j has a larger impact than alternative k in $100 \times f\ \%$ of runs".

Impact category relevance

This approach evaluates trade-offs using the relevance parameter ($\Upsilon_{i,j,k}$), as introduced in Prado-Lopez et al (2014) and it is not intended to calculate statistical significance. It stems from the idea that similar impacts among alternatives do not influence the comparison of alternatives as much as impacts for which alternatives perform very different. It uses the mean (statistics of centrality, $\bar{X}_{i,j}$, $\bar{X}_{i,k}$) and standard deviation (statistic of dispersion, $S_{i,j}$, $S_{i,k}$) calculated from the obtained values for each impact ($X_{i,j,r}$ and $X_{i,k,r}$), thus not per MC run. The value of $\Upsilon_{i,j,k}$, has no meaning on its own, rather its purpose is to help explore the comparison of two alternatives by means of sorting according to the extent of the differences per impact. This approach is therefore exclusive to analysis with more than one impact. When uncertainties increase (as indicated by larger standard deviations) or the difference between the means of two alternatives gets closer to zero (as indicated by nearly equal means), it becomes harder to distinguish between the performance of two alternatives for an environmental impact and hence this aspect is deemed to have a lower relevance in the comparison. A higher relevance parameter for a specific impact indicates that this impact is more important to the comparison than others. The relevance parameter works as a pairwise analysis, as shown in Equation 4.

$$\Upsilon_{i,j,k} = \frac{|\bar{x}_{i,j} - \bar{x}_{i,k}|}{\frac{1}{2}(s_{i,j} + s_{i,k})}$$

Eq.4

In this formula we interpret (in comparison to the original description of the method (Prado-Lopez et al. 2014)) μ as $\bar{x}$, because μ is unknown and only estimated by $\bar{x}$. Further, we interpreted the ambiguous SD in the original publication (Prado-Lopez et al. 2014), into s, which is an estimate of σ.

Overlap area of probability distributions

This method follows the same idea as the relevance parameter, but instead provides an indicator based on the overlap area of probability distribution functions (PDF). Similar to the relevance parameter, this method is not calculated per run and there is no significance threshold value in the overlap that defines statistical significance. The overlap area approach is exclusive to analysis with more than one impact (Prado-Lopez et al. 2016). It measures the common area between PDF of the stochastic impact results ($X_{i,j}$ *and* $X_{i,k}$) of two alternatives j and k, for a specific impact i. By doing this, the overlap area approach can technically apply to diverse types of distributions as opposed to assuming a normal distribution. The shared area between distributions ranges from one, when distributions are identical, to zero, when they are completely dissimilar. The smaller the overlap area, the more different two alternatives are in their performance for an impact. To compute the overlap area ($A_{i,j,k}$), two strategies can be followed. A conventional way is to assume a probability distribution for both $X_{i,j}$ and $X_{i,k}$ (for instance, a normal or lognormal distribution), to estimate the parameters ($\mu_{i,j}$, $\mu_{i,k}$, $\sigma_{i,j}$, $\sigma_{i,k}$) from the MC samples, and to find the overlap by integration. This is the approach followed by Prado-Lopez et al. (2016), using lognormal distributions. The second approach does not require an assumption on the distribution, but uses the information from the empirical histogram, using the Bhattacharyya coefficient (Kailath 1967). To our knowledge, the latter approach has not been used in the field of LCA. Here, we calculate the overlap area using the first approach. In our case, the statistic of centrality ($\bar{X}_{i,j}$, $\bar{X}_{i,k}$) and dispersion ($S_{i,j}$, $S_{i,k}$) of the assumed lognormally distributed stochastic impact results were calculated by means of the maximum likelihood estimation of parameters. The lower intercept (θ) and the upper intercept (ψ) of the two PDFs, are calculated using these parameters and used as a base to calculate the overlap area between two distributions (equation 5). Details on the calculation of θ and ψ, as well as the maximum likelihood estimation of parameters μ and σ, and the PDF Φ are described in the supporting information (SI, appendix II).

$$A_{i,j,k} = 1 - \left|\Phi(\theta; \mu_{i,j}, \sigma_{i,j}) - \Phi(\theta; \mu_{i,k}, \sigma_{i,k})\right| - \left|\Phi(\psi; \mu_{i,j}, \sigma_{i,j}) - \Phi(\psi; \mu_{i,k}, \sigma_{i,k})\right| \qquad \textit{Eq.5}$$

This method uses a pairwise analysis, yet when more than a pair of alternatives is compared, Prado-Lopez et al. (2016) proposed an averaging procedure for the overlap areas between all pairs. For reasons of comparability with the other methods, we did not pursue this extension and concentrate on the comparison per pair.

Null hypothesis significance testing (NHST)

This method is delineated in Henriksson et al.(2015a) and applied in Henriksson et al. (2015b). It largely relies upon established null hypothesis significance tests. In comparative LCAs, a generally implicit null hypothesis presumes that two alternatives perform environmentally equal: $H_0\colon \mu_{i,j} = \mu_{i,k}$. This method's purpose is to show whether the centrality parameter (mean or median) of the relative impacts of two alternatives are statistically significantly different from each other. It builds on the quantification and propagation of overall dispersions in inventory data (Henriksson et al. 2014) to stochastic LCA results ($X_{i,j}$ and $X_{i,k}$). From the stochastic results per impact, the difference per pair of alternatives per MC run is calculated ($x_{i,j,r} - x_{i,k,r}$). This distribution of differences can then be statistically tested using the most appropriate statistical test with regards to the nature of the data, as proposed by Henriksson et.al (2015a). For instance, for normally distributed data, a paired t-test is appropriate to determine whether the mean of the distribution significantly differs from zero (the hypothesized mean). For non-parameterized data, more robust statistical tests, such as Wilcoxon's rank test, can be used. When three or more alternatives are compared, a two-way ANOVA can be used for normally distributed data, while a Friedman test can be used in more general cases. In both of these cases a post-hoc analysis is also required to establish significantly superior products. The null hypothesis of equal means (or medians) may then be rejected or not, depending on the p-value and the predefined significance level (α), e.g., α = 0.05. For our case, we apply a paired t-test to the distribution of the difference per pair of alternatives and MC run, because the mean is expected to be normally distributed as the number of runs is relatively large (1000 MC runs) (Agresti and Franklin 2007). We also explored a Bonferroni correction of the significance value from $\alpha = 0.05$ to $\alpha_b = 0.05/30 = 0.0016$ as the chance of false positives is rather high when multiple hypothesis tests are performed (Mittelhammer et al. 2000). The factor 30 is explained by the ten impacts and the three pairs of alternatives.

Modified NHST

Heijungs et al. (2016b) proposed this method as a way to deal with one of the major limitations encountered while applying NHST to data from simulation models: significance tests will theoretically always reject the null hypothesis of equality of means since propagated sample sizes are theoretically infinite. It is a method that attempts to cover significance (precision) and effect of size (relevance). Thus, from the classic H_0 in NHST that assumes "no difference" between the parameters ($\mu_{i,j} = \mu_i, k$), this method includes a "at least as different as" in the null hypothesis, which is stated as $H_0\colon S_{i,j,k} \leq \delta_0$ where $S_{i,j,k}$ is the standardized difference of means (also known as Cohen's d (Cohen 1988)) and δ_0 is a threshold value, conventionally set at 0.2 (Heijungs et al. 2016). So far the method has not been applied in the context of comparative LCA outside of Heijungs et al. (Heijungs et al. 2016). For its operationalization, the authors proposed the following steps (Heijungs et al. 2016): 1) set a significance level (α); 2) set the difference threshold (δ_0); 3) define a test statistic D (see equation 6, which is a modification from the original proposal (Heijungs et al. 2016)); and 4) test the null hypothesis $H_0: \delta \leq \delta_0$ at the significance level α.

$$d_{i,j,k} = \frac{\bar{x}_{i,k} - \bar{x}_{i,j}}{s_{i,j,k}} \text{ that estimates } \delta_{i,j,k} = \frac{\mu_{i,k} - \mu_{i,j}}{\sigma_{i,j,k}}$$

$$s_{i,j,k} = \sqrt{\frac{1}{N-1}\sum_{r=1}^{N}\left(\left(x_{i,k} - x_{i,j}\right) - \left(\bar{x}_{i,k} - \bar{x}_{i,j}\right)\right)^2}$$

Eq.6

In equation 6, $s_{i,j,k}$ is the standard deviation of the difference between alternatives *j* and *k*. The t-value from the value of d as shown in equation 7. The t-value is a test statistic for t-tests that measures the difference between an observed sample statistic and its hypothesized population parameter in units of standard error.

$$t_{i,j,k} = \frac{d_{i,j,k} - \delta_0}{\sqrt{\frac{1}{N}}}$$

Eq.7

For our case, we consider the default values suggested by Heijungs et al. (2016b) where $\alpha = 0.05$ and $\delta_0 = 0.2$, and we calculate the test statistic D for the three pairs of alternatives (Equation 6 and 7). We also explored the significance with $\alpha_b = 0.0016$ as done for the NHST.

Case study for passenger vehicles

A case study for a comparative LCA that evaluates the *environmental performance of powertrain alternatives for passenger cars in Europe* is used to illustrate the USMs. Comparative assertions are common among LCAs that test the environmental superiority of electric powertrains over conventional internal combustion engines(Hawkins et al. 2012). Several LCA studies have comparatively evaluated the environmental performance of hybrid, plug-in hybrid(Samaras and Meisterling 2008; Nordelöf et al. 2014), full battery electric (Notter et al. 2010; Majeau-Bettez et al. 2011), and hydrogen fuel cell vehicles(Granovskii et al. 2006; Font Vivanco et al. 2014). Many of these studies describe multiple trade-offs between environmental impacts: while electric powertrains notably reduce tailpipe emissions from fuel combustion, various other impacts may increase (e.g. toxic emissions from metal mining related to electric batteries(Hawkins

Chapter 5

et al. 2013). Against this background, electric powertrains in passenger vehicles are an example of problem shifting and a sound case to test comparative methods in LCA.

Goal and Scope

The goal of this comparative LCA is to illustrate different USMs by applying these methods to the uncertainty analysis results for three powertrain alternatives for passenger cars in Europe: a full battery electric (FBE), a hydrogen fuel cell (HFC), and an internal combustion engine (ICE) passenger car. The functional unit for the three alternatives corresponds to a driving distance of 150,000 vehicle-kilometers (vkm). The scope includes production, operation, maintenance, and end of life. The flow diagram for the three alternatives can be found in the SI (Appendix III). The case has been implemented in version 5.2 of the CMLCA software (www.cmlca.eu), and the same software has been used to propagate uncertainty. The five USMs have been implemented in a Microsoft Excel (2010) workbook available in the SI.

Life Cycle Inventory

The foreground system was built using existing physical inventory data for a common glider as well as the FBE and ICE powertrains as described by Hawkins and colleagues (Hawkins et al. 2013), whereas the HFC power train data is based on Bartolozzi and colleagues (Bartolozzi et al. 2013). The background system contains process data from ecoinvent v2.2, following the concordances described by the original sources of data. A complete physical inventory is presented in the SI (Appendix IV). The uncertainty of the background inventory data corresponds to the pedigree matrix (Weidema and Wesnæs 1996) scores assigned in the ecoinvent v2.2 database. In addition, overall dispersions and probability distributions of the foreground inventory data have been estimated by means of the protocol for horizontal averaging of unit process data by Henriksson et al. (2014). Thus, the parameters are weighted averages with the inherent uncertainty, spread, and unrepresentativeness quantified. Specifically, unrepresentativeness was characterized in terms of reliability, completeness, temporal, geographical, technological correlation, and sample size (Frischknecht et al. 2007), to the extent possible based on the information provided in the original data sources. Further details of the implementation of parameter uncertainty are presented in the SI (appendix IV).

Life Cycle Impact Assessment (LCIA)

The environmental performance of the selected transport alternatives is assessed according to ten mid-point impact categories, namely: climate change, eutrophication, photochemical oxidation, depletion of abiotic resources, acidification, terrestrial ecotoxicity, ionizing radiation, freshwater ecotoxicity, stratospheric ozone depletion, and human toxicity. The characterization factors correspond to the CML-IA factors without long term effects (version 4.7) (CML - Department of Industrial Ecology 2016), and exclude uncertainty. No normalization or weighting was performed and the results are presented at the characterized level.

Uncertainty calculations

Uncertainty parameters of background and foreground inventory data were propagated to the LCA results using 1000 MC iterations. We provide a convergence test for the results at the characterized level for all impacts and alternatives considered to show that this amount of MC runs is appropriate for this case study (SI, Appendix VI). Although other sources of uncertainty could be incorporated by means of various methods (Andrianandraina et al. 2015; Mendoza Beltran et al. 2016), we did not account for uncertainty due to methodological choices (such as allocation and impact assessment methods) or modeling uncertainties, neither due to data gaps that disallow the application of such methods. Also, correlations between input parameters was not accounted for (Groen and Heijungs 2017). In our experimental setup, the same technology and environmental matrix was used to calculate the results for the three alternatives for each MC run. Thus, dependent sampling underlies the calculations of paired samples. This experimental setup is important because it accounts for *common uncertainties* between alternatives (de Koning et al. 2010; Henriksson et al. 2015a) that are particularly important in the context of comparative LCAs (Henriksson et al. 2015a; Heijungs et al. 2017). Although the five statistical methods under study could be applied to independent sampled datasets, it would lack meaning as common uncertainties would then be disregarded. Thus, only dependently sampled MC runs were explored for the purpose of the present research. These MC runs per impact are available in the Microsoft Excel (2010) workbook in the SI.

The five USMs are applied to the same 1000 MC runs dependently sampled for each of the three alternatives and for each impact. As all methods are pairwise, we apply them for three pairs of alternatives: ICE/HFC, ICE/FBE, and FBE/HFC.

5.3 Results

Figure 15 shows the results for our comparative LCA following the classic visualization of deterministic characterization, in which results are directly superposed for comparison. All impacts considered are lower for the HFC except for depletion of abiotic resources. Both the ICE and FBE show various environmental trade-offs: the ICE performs worse than both the FBE and HFC in five impacts, while the FBE performs worse than the ICE and HFC in six impacts. Overall, the HFC performs better than both the FBE and ICE on most impacts considered. However, these results bear no information on their significance or likelihood, as no uncertainties are included.

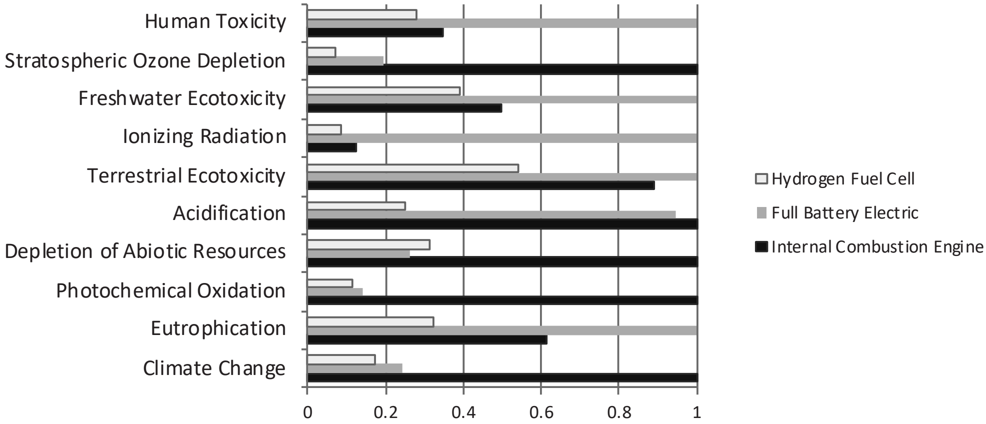


Figure 15. Deterministic results (scaled to the maximum results per impact) for comparative LCA of three alternatives of vehicles.

The complete set of results for the ten impacts considered and the five methods are found in the Microsoft Excel (2010) workbook in the SI. The *deterministic* LCA results shown in Table 12, correspond to those in Figure 15: HFC shows a better environmental performance than both the ICE and FBE for all impacts except for depletion of abiotic resources. In addition, Table 12 shows the results for the five statistical methods and for three selected impacts that display discrepant results.

For the *discernibility analysis,* and taking acidification as an example, the ICE and FBE vehicles have higher acidification results than HFC in 100% of the runs (Table 12, white cells under discernibility). Thus, the ICE and FBE are likely to be discernible alternatives from the HFC for acidification. For photochemical oxidation and acidification, there are pairs of alternatives that are not likely to be discernible as the percentage of runs in which one alternative is higher than the other is close to 50% (see Table 12 darker blue cells).

The *impact category relevance* results show the highest relevance parameter for acidification for the pairs ICE/HFC and FBE/HFC (Table 12, darker red cells). Thus, for the comparison between ICE, FBE and HFC vehicles, acidification is an impact that plays the most important role in the comparison. The lowest relevance parameter was obtained for the pair ICE/FBE for acidification as well as for the pair ICE/HFC for ionizing radiation these are impacts for which efforts to refine data would be most fruitful (Table 12, white cells under impact category relevance).

For the *overlap area,* the pair HFC/FBE has a large overlapping area for ionizing radiation and the pair FBE/ICE has a large overlap for acidification (Table 12, darker orange cells). Aspects contributing to the alternatives' performance in ionizing radiation and acidification would be areas to prioritize in data refinement. Other pairs have almost no overlapping area for instance HFC/ICE for photochemical oxidation and HFC/FBE for acidification (Table 12, white cells under overlap area). This means, that the choice of an alternative between pairs, HFC/ICE and HFC/FBE, represents a greater effect on photochemical oxidation and acidification respectively.

The results for the *NHST* consist of the p-values for the paired t-test performed and the decision to reject (yes) or to fail to reject (no) the null hypothesis. This latter outcome has been included in Table 12. The p-values for all impacts and pairs of alternatives are < 0.0001, and thus the null hypothesis was rejected in all cases (See worksheet 'NHST' in the Microsoft Excel (2010) workbook in the SI). Therefore, results for all pairs of alternatives were significantly different for all impact categories (Table 12, purple cells). With the corrected significance level (α_b) we re-evaluated the null hypothesis but still rejected the null hypothesis in all comparisons.

For the modified NHST the comparison between the ICE and FBE for the acidification impact, cannot reject (no) the modified null hypothesis. Yet in the case of the NHST method it is rejected. Table 12 does not correspond to a mirror matrix for this method because the direction of the comparison matters. For acidification, we see that the pair FBE/ICE is not significantly different as well as the pair ICE/FBE. Thus, in both comparisons the scores of the first alternative are not at least δ_0 significantly higher than the scores of the second alternative. Therefore, the distance between the means of both alternatives is less than δ_0 i.e. 0.2 standard error units. With the corrected significance level (α_b) we re-evaluated the null hypothesis but found no changes in the outcomes.

Cross comparison of methods

Exploring the results across methods for the same impact shows consistent results for most impacts i.e. seven out of ten. A higher relevance parameter coincides with a smaller overlap area between distributions, and this generally coincides with well-discernible alternatives. Likewise, pairs of alternatives are more likely to have significantly different mean results when discernible. Below we focus our comparison of methods on three impacts (Table 12) that show discrepancies or conflicting results for some of the five methods.

For photochemical oxidation, the results for the five methods seem to agree to a large extent. Deterministic results show that HFC has the lowest characterized results among the three alternatives. However, according to the discernibility results, HFC is lower than FBE, for 83% of the runs. This shows that point-value results can be misleading, because there is a 17% likelihood that a point value would have given an opposite result. The overlap area results show a 0.63 overlap between the HFC and FBE on photochemical oxidation, indicating a mild difference (given the range of 0 to 1) in their performance. NHST and modified significance are in agreement with results from other methods and show significant different means for the two alternatives.

For acidification, results for some methods are consistent (Table 12). Discernibility of almost 100% along with a high relevance parameter and a low overlap

Method >	Deterministic LCA (point values)				Discernibility			
Meaning of result >	Does *j* have a lower impact than *k* ?				% of total runs in which *j* has a lower impact than *k*			
		no	yes			0%	50%	100%
Impact								
Photochemical Oxidation	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		no	no	ICE		0%	0%
	FBE	yes		no	FBE	100%		17%
	HFC	yes	yes		HFC	100%	83%	
Acidification	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		no	no	ICE		45%	0%
	FBE	yes		no	FBE	54%		0%
	HFC	yes	yes		HFC	100%	100%	
Ionizing Radiation	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		yes	no	ICE		100%	0%
	FBE	no		no	FBE	0%		0%
	HFC	yes	yes		HFC	100%	100%	

Method >	Impact category relevance				Overlap area			
Meaning of result >	Which impact is important for the comparison of *j* and *k* ?				Overlap area between distribution of impact of *j* and *k*			
	least	0,24	6,68	most	no overlap	0,00	1,00	full overlap
Impact								
Photochemical Oxidation	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		2,37	2,53	ICE		0,01	0,00
	FBE	2,37		0,81	FBE	0,01		0,63
	HFC	2,53	0,81		HFC	0,00	0,63	
Acidification	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		0,24	5,44	ICE		0,88	0,00
	FBE	0,24		6,68	FBE	0,88		0,00
	HFC	5,44	6,68		HFC	0,00	0,00	
Ionizing Radiation	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		1,27	0,34	ICE		0,13	0,79
	FBE	1,27		1,36	FBE	0,13		0,08
	HFC	0,34	1,36		HFC	0,79	0,08	

Method >	NHST				Modified NHST			
Meaning of result >	Are the mean impacts of *j* and *k* significantly different?				Is the mean impact of *j* at least 0.2 standard deviation units significantly lower than that of *k* ?			
		no	yes			no	yes	
Impact								
Photochemical Oxidation	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		yes	yes	ICE		no	no
	FBE	yes		yes	FBE	yes		no
	HFC	yes	yes		HFC	yes	yes	
Acidification	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		yes	yes	ICE		no	no
	FBE	yes		yes	FBE	no		no
	HFC	yes	yes		HFC	yes	yes	
Ionizing Radiation	j↓ k→	ICE	FBE	HFC	j↓ k→	ICE	FBE	HFC
	ICE		yes	yes	ICE		yes	no
	FBE	yes		yes	FBE	no		no
	HFC	yes	yes		HFC	yes	yes	

Table 12. Results for selected impacts (those with discrepant outcomes between some methods) for the comparative LCA of full battery electric (FBE) vehicle, the hydrogen fuel cell (HFC) vehicle and the internal combustion engine (ICE) vehicle. Tables display different results for the comparison of alternatives j and k for the reviewed uncertainty-statistics methods (USMs). The meaning of results per method is shown in the second row of the table together with the color labels.

area are shown for two pairs of alternatives HFC/ICE and HFC/FBE. Nonetheless, for the pair FBE/ICE discernibility results show a close call (FBE scoring only higher than ICE on acidification results for 45% of the runs) suggesting similar performances in acidification for FBE and ICE. This outcome is confirmed by the results of the impact category relevance (0.24), the overlap area (0.88) and the modified NHST where the null hypothesis is accepted and therefore no statistical difference can be established. NHST results, however, show a rejection of the null hypothesis that FBE and ICE have significantly different means for acidification, confirming that this pair of alternatives has significantly different acidification impacts – thus opposing the outcome of the other methods. As the sample size is large (namely 1000 observations), so is the likelihood of significance in NHST (Heijungs et al. 2016). The extra feature of the modified NHST compared to NHST is that the null hypothesis in the modified NHST is evaluated with a minimum size of the difference ($\delta_0 = 0.2$). It then appears that the difference in mean acidification results is so small that the null hypothesis cannot be rejected and that the mean acidification results for the FBE/ICE pair are not significantly different. The modified NHST results show how a large number of observations can influence the outcome of results in a standard NHST. Thereby it is possible to change the conclusion of a study by sampling more MC runs. Given that LCA uncertainty data is simulated and does not represent actual samples, it is recommended to apply the modified NSHT.

Finally, for ionizing radiation we observe a discrepancy between the discernibility, NHST, and modified NHST results on the one hand, and the impact category relevance and overlap area results on the other hand. The HFC/ICE pair shows a low relevance parameter (0.34) with a high overlap area (0.79). However, the discernibility results show that ICE scores higher than HFC on ionizing radiation for 100% of the runs. NHST and modified NHST confirm these results and show that, despite the large overlap and a low relevance parameter, the alternatives are significantly different. Note that the results of the relevance parameter and the overall area is to be used relative to other impact categories for sorting purposes– it is not intended to provide a confirmation on the difference. Still, results for this impact show that such high overlap can correspond to significant differences. Opposing outcomes are due to the overall or per run set-up of the methods. The discernibility analysis, NHST and modified NHST perform the analysis on a per run basis (accounting for common uncertainties) and evaluate, per run, whether the performances fulfill a certain relationship. Alternatively, the overlap area and the relevance parameter look at the overall distribution of the two alternatives rather than the individual runs. They take into account the *extent* of the difference so that the output falls within a spectrum, e.g. from 0 to 1 for overlap area, as opposed to a binary type output, e.g. fail to reject or reject the null hypothesis for NHST and modified NHST. Figure 16 shows the histogram for the distribution of HFC and ICE outcomes as well as the discernibility in a scattered plot, for better understanding the contradicting results between overlap area and discernibility. Here we can see that while the histograms overlap a considerable amount, the performance between the alternatives can still be considered statistically different since all the runs fall within one side of the diagonal in the scattered plot, which disregards the distance of each point to the diagonal.

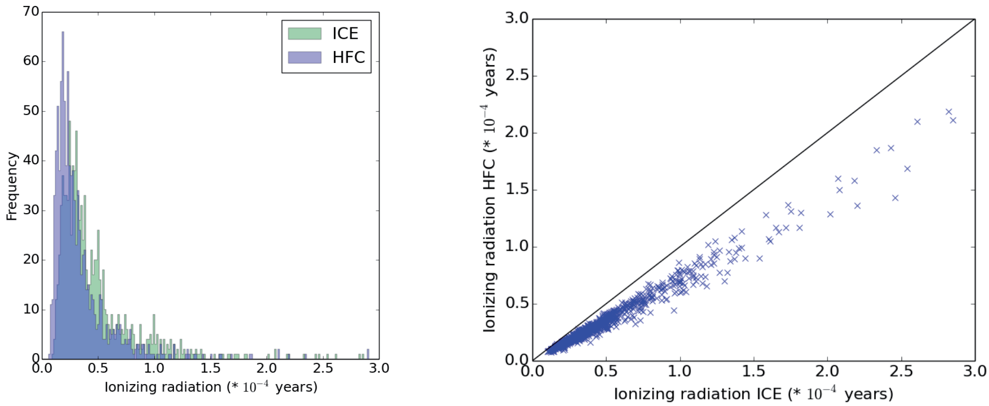


Figure 16. Histograms (left) and scatter plot (right) for 1000 MC runs for the hydrogen fuel cell (HFC) vehicle and the internal combustion engine (ICE) vehicle for ionizing radiation. The performances of ICE and HFC show great similarities in the histogram, and thus a large overlap area (i.e. 0.79). However, the scatter plot shows that for each MC run, the difference between HFC and ICE ≠ 0 (the diagonal line in the scattered plot represents equal values for both alternatives). Hence, alternatives are discernible in 100% of the runs.

5.4 Discussion and conclusions

We have reviewed, applied and compared different methods for uncertainty-statistics in comparative LCA. We showed how deterministic LCA can lead to oversimplified results that lack information on significance and likelihood, and that these results do not constitute a robust basis for decision-making. In addition, we found that, while in most instances (seven out of ten impacts), the five methods concur with each other, we identified instances where the methods produce conflicting results. Discrepancies are due to differences in the setup of the analysis (i.e. overall or per run) which accounts or not for common uncertainties and due to accounting or not for the magnitude of the differences in performances. We identify two groups of methods according to the type of analysis they entail: *exploratory* and *confirmatory* methods. This division corresponds with the statistical theories by Tukey (1973), in which data analysis initially requires an exploratory phase without probability theory, so without determining significance levels or confidence intervals, followed by a confirmatory phase determining the level of significance of the appearances identified in the exploratory phase. Exploratory statistics help delve into the results from uncertainty analysis and confirmatory methods evaluate hypotheses and identify environmental differences deemed statistically significant.

The NHST and modified NHST methods belong to the confirmatory group. Confirmatory methods are calculated per MC run, account for common uncertainties between alternatives and provide an absolute measure of statistical significance of the difference (Heijungs et al. 2017). These methods are appropriate for both single impact and multiple impact assessments and support statistical significance confirmation. NHST was shown to detect irrelevant differences of the means and to label them nevertheless as significant, while alternatives are considered to be indiscernible by modified NHST whenever the difference is small. The modified NHST approach is therefore recommended for confirmatory purposes and for all propagated LCA results, where the sample size in theory is indefinite and in practice is very large.

The impact category relevance and the overlap area methods belong to the exploratory group, as they help to identify some characteristics of uncertainty results among alternatives and impacts. These methods account for the magnitude of the difference per impact but do not consider common uncertainties or provide a measure of confidence or significance of the difference. These two methods are exclusively for exploring the uncertainty results in comparative LCAs with multiple impacts. Because the calculations are not per MC run, common uncertainties are disregarded and they do not serve confirmatory purposes. Disregarding common uncertainties can lead to instances where alternatives appear to be similar, while they actually perform different (like in ionizing radiation between ICE and HFC, Figure 16). Overcoming the fact that they do not account for common uncertainties would require generalization of the methods to "per run" calculations and could lead to a method similar to modified NHST accounting for the distance between means and common uncertainties.

Discernibility belongs to both groups. It accounts for common uncertainties, but it does not account for the magnitude of the difference per impact. It can be complimented with a *p*-value calculation, to develop its confirmatory potential, that would generate statistical significance based on the counts of the sign tests per pair. A proposal for such a procedure can be found in the SI (appendix V) and involves the use of the binomial distribution. As it stands now, we consider it to serve an exploratory purpose similar to the impact category relevance or the overlap area, but with a different mechanism.

Both exploratory and confirmatory methods are valuable and synergistic in data-driven research (Tukey 1980), yet the specific choice of method is not straightforward for LCA practitioners given the discrepancies and characteristics previously discussed. Figure 17 provides guidance on which statistical methods LCA practitioners should use to interpret the results of a comparative LCA in light of its goal and scope, and when considering uncertainty. Figure 17 is in line with the main findings of this chapter. That is, exploratory methods facilitate the decision-making process by identifying differences and trade-offs in impacts between alternatives as well as by pointing to places where data refinement could benefit the assessment. Moreover, confirmatory methods effectively aid in making complex decisions from comparative assessments but should be used with statistical significance. For instance, carbon footprints, product environmental declarations, and LCAs aiming for comparative assertions disclosed to the public, should use confirmatory methods supporting conclusions with statistical significance calculations and accounting for common uncertainties.

Moreover, modified NHST appears to be the most well-developed method for confirmatory purposes. For exploratory purposes, however, we do not find a method that considers both core aspects: accounting for common uncertainties and for the extent of the differences per impact. Between these two aspects, common uncertainties are the most crucial aspect to address in a comparative context. Therefore, we recommend discernibility as the most suitable method for exploratory purposes while recognizing areas for improvement. Namely, we recommend that discernibility is further developed by adding a threshold of acceptable difference (as done in modified NHST) that, despite of being arbitrary, can better inform the exploration of trade-offs. We also recommend practitioners to exercise caution when applying overlap area and impact category relevance, and we recommend further developments of both methods to account for common uncertainties. Lastly, we call for caution when applying NHST regarding the sample size as it has been conceived for real samples (Henriksson et al. 2015a) and not for propagating uncertainty estimates where the sample size is in theory indefinite.
We encourage practitioners to use the excel workbook provided in the SI with the calculations made for the five methods in this paper which can aid them in delivering a more robust basis for decision-making.

As the use of statistical methods is becoming more frequent and increasingly important in environmental decision support (Hellweg and Canals 2014), the definition of thresholds to determine the acceptable uncertainty demands attention. Arbitrarily set thresholds, such as p-value = 0.05, should be carefully used accounting for basic principles addressing misinterpretation and misuse of the p-value, as recently proposed by the American Statistical Association (Wassertein and Lazar 2016). In the field of LCA, we need practical guidelines to establish meaningful uncertainty thresholds for different applications. Methods like modified NHST and extended discernibility (see appendix V), require such threshold levels to calculate statistical significance. We depart from the premise that various sources of uncertainties of the inputs have been adequately quantified and propagated to uncertainty results. The effects of the quality of uncertainty quantification and propagation on the interpretation of uncertainty results in comparative LCAs requires further study (Mila i Canals et al. 2011). Any outcome of any test is only as good as the quality of the input data, which for all studied methods corresponds to the results of an uncertainty analysis.

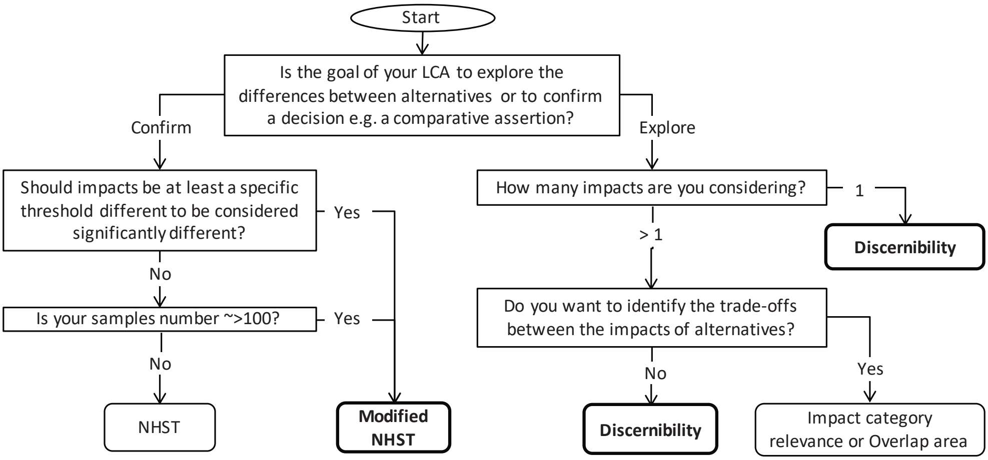


Figure 17. Decision tree to guide LCA practitioners on which uncertainty-statistics method (USM) to use for the interpretation of propagated LCA uncertainty outcomes in comparative LCAs. Thicker lines indicate recommended methods for confirmatory and exploratory purposes as per the considerations described in the main text. The type of information available from the uncertainty analysis results (in the following parenthesis) determines the choice between impact category relevance (statistical parameters of the distributions) or overlap area (MC runs).

Acknowledgements

Authors would like to acknowledge the ISIE Americas 2016 conference that took place in Bogota, Colombia, for providing the environment to shape the ideas further developed in this research. We also thank Sebastiaan Deetman and Sidney Niccolson for their insightful comments on visualizations.

Supporting information

Supporting information of this chapter may be found in the online version of the original article: https://pubs.acs.org/doi/abs/10.1021/acs.est.7b06365

6.

General Discussion and Conclusions

6.1 Introduction

LCA has become an important method to study environmental impacts of human activities. Still, there are several methodological issues in LCA that can adversely affect the reliability of results. Three of these issues relate to a) allocation, b) the representation of the time dimension and c) the interpretation of results in LCA. Uncertainties play a fundamental and underlying role for these issues. In the previous four chapters, this thesis unraveled some complexities of uncertainty analysis in LCA in relation to these three issues. This thesis aimed at deepening the uncertainty dimension of LCA i.e. provided a clearer understanding of the implications of different sources of uncertainty in LCA – and further developed methods to treat them. We departed, in the introduction chapter, from broad domains in which uncertainty has its roots. Then, the scope was narrowed down to some specific sources in the domains of risk and conventional uncertainty i.e. related to incomplete scientific knowledge and to potentially quantifiable uncertainties. The domains of ignorance and indeterminacies i.e. uncertainty related to bets on the completeness and validity of knowledge which also depends on its correspondence with the social world (Wynne 1992), were not further studied. This thesis focused on those sources of uncertainty which could be explicitly acknowledged in the results of an LCA. However, we recognized that not all sources of uncertainty can be quantified as well as not all can be known.

In particular, three sources of uncertainty related to some of the most pressing topics for the LCA community, were addressed: 1) allocation method choice (in combination with parameter uncertainty), 2) accounting for future socio-technical changes in prospective LCA and 3) interpretation of LCA results including uncertainty estimates. The choice for an allocation method introduces uncertainty in the results as different methods may lead to (significantly) different results. Also, future socio-technical changes may lead to large uncertainty of LCA results particularly for technologies or products expected to be industrially deployed in the future when socio-technical systems could look quite different compared to the present. Finally, interpretation of the results of uncertainty analysis in LCA can be done with different methods. Guidance on which method to use depending on the purpose of the LCA, was missing. These knowledge gaps have been translated into four research questions addressed in the previous chapters and which we discuss in the following sections.

6.2 Answers to research questions

Chapter 2 discussed two important sources of uncertainty in LCA: due to methodological choices and parameter uncertainty. The chapter presented and tested a method to simultaneously treat these two sources of uncertainty.

RQ1: How can parameter uncertainty and uncertainty due to methodological choices in a single alternative LCA be quantified and propagated to the results? (Answered in chapter 2)

Methodological choices are unavoidable in LCA and from all choices a practitioner has to face, the choice for allocation methods to solve multi-functionality is crucial. The allocation method selected for solving a multifunctional process can significantly change the LCA results. Parameter uncertainty is another typical issue that LCA practitioners should deal with. Parameter uncertainty can arise from different situations. For instance, when unit process datasets are not available (for the location and/or technology that the LCA study at stake deals with) and these data are then often estimated with data for other locations or technologies. Also, because unit process data can be inaccurate due to inherent measurement uncertainties. Likewise, and in many cases, because unit process data has natural variability. We proposed a pseudo-statistical protocol to simultaneously propagate parameter uncertainty and uncertainty due to the choice of partitioning methods to the LCA results. For example, in an agricultural process, uncertainty around N_2O emissions due to fertilizers application is stochastically combined with two options to allocate the emissions between the agricultural outputs with economic and mass allocation. In such way, these sources of uncertainty are propagated to the characterized results such as climate change in kg of CO_{2eq}. The protocol captures the large range of combinations resulting from sampling an allocation method per multi-functional process and a data value per process parameter in a product-system. While the choice of allocation method refers to a discrete choice described by the methodological preference of each allocation method, parameter uncertainty is better described with a probability distribution per parameter. Monte Carlo simulations were used to sample these methodological preferences and distributions, resulting in the pseudo-statistical propagation of uncertainty to the LCA results. Because the usual terms that are appropriate for data uncertainty (uncertainty, probability, statistical, etc.) are not entirely suitable for describing discrete choices, we added the qualifier "pseudo" to refer to the propagation and quantification of methodological choice uncertainty which is not, in a strict sense, statistical nor a probability applies to them as they are normative choices.

Application of the protocol to a single alternative LCA, proved that simultaneous propagation of both sources of uncertainty was possible. Yet, it also showed that absolute uncertainties only further increase in comparison to one at the time scenarios varying only the allocation method and including parameter uncertainty. This is because many (if not all) possible combinations of data and allocation methods are captured in the results (Chapter 2). Also, such results were expected because LCA integrates knowledge and uncertainty from many disciplines. However, because LCA is essentially comparative, increased absolute uncertainty of LCA results is not necessarily relevant. Thus, although the results showed an increased robustness for a single alternative LCA, the method is particularly useful for comparative LCAs in which relative uncertainties, i.e. uncertainties related to the differences between the compared product-systems, are more relevant.

Therefore, Chapter 3 expanded the application of the method developed in Chapter 2 to a comparative LCA context.

RQ2: What are the implications for uncertainty analysis in a comparative LCA context of quantifying and propagating parameter uncertainty and uncertainty due to methodological choices? (Answered in chapter 3)

Applying the pseudo-statistical protocol to propagate parameter uncertainty and uncertainty due to the choice of allocation methods in a comparative LCA context has implications primarily for the sampling procedure. Because it is vital to account for relative uncertainties between the pairs of product-systems compared, paired sampling should be the experimental setup (Chapter 3). In practice, this means that for unit processes and multi-functional processes that are common to both systems, the same parameter values and the same allocation method should be sampled and used to calculate the results per Monte Carlo simulation. The LCA results of a specific simulation should be directly compared to properly reflect the comparative, or relative uncertainty. If such a setup is used, statistical significance of the difference of the environmental impacts can be sensibly determined. The difference per Monte Carlo run, for instance for the characterized results, should be used as the basis to calculate significance. In deterministic point-value LCA outcomes, it is only possible to calculate the difference of the environmental impacts for the point-value results, which usually represent specific allocation choices and average assumptions and values. The pseudo-statistical method helps addressing parameter uncertainty and acknowledge large choice-related uncertainties (on top of parameter uncertainties). It further helps in asserting if under those uncertainties alternatives are significantly different. While it might appear that alternatives are different based on deterministic LCA results, they might not be statistically different when accounting for parameter and choice uncertainty and vice versa. The case study in chapter 3 compared two technologies to produce fish. In the first only fish is produced. In the second fish is co-produced with oysters. Thus, allocation plays an important role to make the systems comparable in addition to large parameter uncertainty due to seasonal changes in the production of fish, among others. While deterministic LCA results showed that co-produced fish performs better for all impacts evaluated, including uncertainty showed that the two systems did not perform significantly different except for climate change impacts. This additional information revealed that the specific technological setup evaluated for the co-production of fish, was not having the desired mitigating effect of impacts in comparison with the current production of fish. It was concluded that production of the farm was expanded due to the additional oyster production at no additional environmental cost and with reduction of climate change impacts.

In general, and as shown in the case of chapter 3, the pseudo-statistical protocol applied in a comparative LCA context is a novel technique that can contribute to the robustness of conclusions, adding information about the statistical significance of the difference of environmental impacts between the compared product-systems. This chapter also showed that there is a practical way to estimate uncertainty beyond one at the time scenario modeling for choice-related uncertainties. Moreover, it demonstrated that for comparative assertions it is necessary to account for relative parameter and choice-related uncertainties. To determine the statistical environmental superiority of products in a robust way these are mandatory conditions. Stochastic life cycle impacts of similar products calculated separately by different LCA practitioners, and thus using independent sampling, should not be compared. Such findings may have implications for LCA guidelines for policy applications, such as the Product Environmental Footprint (PEF) from the European Commission (See section 6.3.1 for a deeper discussion on this issue).

Chapter 4 aimed to address epistemological uncertainty in prospective LCAs. To address this type of uncertainty, a novel approach to systematically change the background processes in a prospective LCA was developed and illustrated with a case study.

RQ3: How can epistemological uncertainty for prospective LCA be systematically and consistently addressed? (Answered in chapter 4)

Prospective LCA refers to forward-looking applications of LCA. Usually, they help to anticipate unintended consequences of future product-systems and help to support environmentally conscious product design. Prospective LCA should deal with large epistemological uncertainty related to the fact that the future cannot be predicted and yet the environmental performance of products is evaluated in the future. For this, assumptions should be made systematically and consistently for all relevant parameters. For instance, if one looks at the performance of combustion engine versus electric vehicles (our case studies) consistent assumptions should be made for future changes in performances of these vehicles, but also in key input parameters such as the electricity mix and therefore to all LCA parameters that depend on the electricity mix. We proposed a novel approach based on a framework for scenario development in LCA to systematically and consistently address this issue. The approach deeply embeds – conceivable as hard linking – socio-technical scenarios from an Integrated Assessment Model (IAM) with background inventory data used in prospective LCA. The IAM used in the case study is the IMAGE model. For the background inventory, we use the ecoinvent database. Combining these allowed us to derive future background inventory data based on IMAGE scenarios. To operationalize this procedure, IMAGE output (covering all sectors and world regions) is systematically fed into the inventory of ecoinvent. Systematic implementation is facilitated by the fact that the same IMAGE variables are used for all scenarios and are linked to the same ecoinvent parameters, as shown in this thesis. Since the IMAGE data is harmonized in coherent scenarios, the risk of inconsistencies is minimized.

After this procedure has been implemented and the background has been made dynamic, one is confronted with epistemological uncertainty. Linking a variety of integrated assessment model scenarios with background inventory data helped acknowledge epistemological uncertainty and lead to more robust results that accounted for varied socio-technical future paths of development. The case study of chapter 4, illustrated the method for the prospective LCA of an internal combustion engine vehicle and an electric vehicle, as two future mobility alternatives. The electricity production sector was changed using various baseline and climate mitigation scenarios (several plausible futures). As a result of the scenario linkages, the relative environmental performance of EV and ICEV over time is more complex and multifaceted than previously assumed. Uncertainty due to future developments of the electricity sector manifests differently in the life cycle impacts (e.g. climate change, particulate matter formation, etc.) according to the product (EV or ICEV), the scenario (e.g. baseline or mitigation) and the year considered. Regarding the product, uncertainty is larger for the EV, as is evident from the larger range of results, particularly in the long-term i.e. towards 2050. Nonetheless, this is only because of the contribution of electricity production to the impacts of the EV in comparison to impacts of the ICEV. Linking the scenarios for other sectors could change this outcome. For the impact categories, we observe that for climate change, particulate matter formation, and fossil cumulative energy demand, the selected IMAGE scenario has a larger influence on the future impacts of the EV. These are impacts due to GHG emissions and use of fossil fuels. Thus, baseline scenarios which have a larger share of fossil-based electricity technologies display a smaller reduction of these impacts than the original ecoinvent impacts for the EV. By contrast, ambitious mitigation scenarios that have larger shares of technologies emitting less GHG show large reductions of these impacts, particularly in the long-term. For impacts such as metal depletion, almost no effect of the scenario is observed for the EV and the ICEV. This is mostly related to the fact that sectors that might contribute more to this impact, such as the raw materials production sector, were kept the same. For impacts like particulate matter formation, ambitious mitigation scenarios showed that EV would lead to improvements while for non-ambitious scenarios, such as the baseline scenario, the ICEV would be preferred. Exploring future pathways and related impacts, rather than predicting them as shown in chapter 4, can help outline and better inform directions for action in product-design and policy-making.

Finally, in chapter 5 a critical review of methods to interpret uncertainty analysis results was conducted. The implications of using these methods for interpretation of comparative LCA results was investigated, under the light of the goal and scope of the LCA study.

RQ4: Which statistical method(s) should LCA practitioners use to interpret the results of a comparative LCA, under the light of its goal and scope, when considering uncertainty? (Answered in chapter 5)

Comparative LCAs may support a comparative assertion regarding the relative environmental performance of one product with respect to other functionally equivalent alternatives (ISO 2006). We identified two types of goals for comparative LCAs, exploratory and confirmatory. Comparative LCAs with exploratory purposes are interested in facilitating the decision-making process by identifying differences and trade-offs in impacts between alternatives and by pointing to places in the life cycle where data refinement could benefit the assessment. For these LCAs exploratory methods to interpret uncertainty analysis results are recommended. Particularly, discernibility analysis is recommended as relative uncertainties are accounted for by this method if dependent sampling is used, while observing that trade-offs will not account for the magnitude of the difference. Comparative LCAs with confirmatory purposes are interested in evaluating hypotheses and in identifying if environmental differences are deemed statistically significant. For these LCAs confirmatory methods should be used. Particularly, modified NHST provides a better interpretation of the statistical significance of the difference in impacts between the alternatives considered. This is because this method accounts for relative uncertainties if dependent sampling is used as well as it accounts for the magnitude of the difference per impact, as part of the statistical test it is based on.

While it was evident from our critical review that for confirmatory purposes the modified NHST was the preferred method, for explorative purposes no method stood clearly out as each one had its benefits and limitations. The impact category relevance and the overlap area methods allow for the exploration of trade-offs between alternatives and account for the magnitude of the difference per impact. However, their calculation setup disregards relative uncertainties. Discernibility, which we identified as belonging to both exploratory and confirmatory types of methods, accounts for relative uncertainties but disregards the magnitude of the difference of the impacts between alternatives. Because we considered accounting for relative uncertainties more crucial in a comparative context (as shown in chapter 3 of this thesis) we suggested the use of discernibility as the preferred explorative method, with the caveat that it needs improvement to account for the magnitude of the difference of impacts between alternatives.

6.3 Further reflections

6.3.1 General implications for LCA

Acknowledging and dealing with different sources of uncertainty has implications for all phases of LCA and vice versa. Regarding the goal and scope, the goal of the LCA determines to a large extent the sources of uncertainty, which may play a crucial role in the assessment. Single-alternative LCA, comparative LCA or prospective LCA can intrinsically be affected by different sources of uncertainty given their different natures. For example, epistemological uncertainty is more important for prospective LCAs than it is for an assessment in the present, and the choice of allocation can be more important in a comparative LCA with several multifunctional processes on the foreground than it is for a single alternative LCA without multifunctional processes on the foreground. A clear notion of the goal and scope can be a good departure point for practitioners to determine which sources of uncertainty they should be addressing.

Further, some sources of uncertainty such as parameter uncertainty and methodological choices prevail in phases such as the inventory and life cycle impact assessment phases of LCA, independently of the type of assessment. Dealing with these requires specific methods applicable to LCA in a broader sense and preferably pertinent to all LCA calculation platforms to facilitate their adoption by the community. This thesis contributed to this topic and provided methods applicable to different platforms (e.g. pseudo-statistical approach) as well as supporting information that practitioners can further adopt in their assessments (e.g. prospective LCA implementation of IMAGE scenarios code in python and implementation of uncertainty-statistic methods in excel).

We showed that dealing with parameter uncertainty and uncertainty due to methodological choices can have further implications for the experimental setup used in the calculation of the LCA results. Particularly for comparative LCAs, where relative uncertainties are of outmost importance, independent sampling should not be used for comparative LCA as more recently also acknowledged by Lesage et al. (2018). These findings may be of particular importance for LCA guidelines for policy applications, such as the Product Environmental Footprint (PEF) from the European Commission. We dedicate a word to this particular aspect here.

According to the European Commission, the PEF project aimed to develop a harmonized environmental footprinting methodology that can accommodate a broader suite of relevant environmental performance criteria and to assess environmental impacts of product, through their life-cycle, in order to support the assessment and labelling of products (European Commision 2016). For this purpose, ongoing pilots in different sectors were stablished to test and develop further the product environmental footprints category rules (PEFCR). PEFCRs, still under development, mostly consist of deterministic LCAs that follow the legal approach, i.e. standardization of much of the methodological choices and data that are pre-defined in order to reduce uncertainty and increase comparability among studies of similar products in one sector. This thesis showed that embracing uncertainty, where quantifiable (as we also recognized that not all sources of uncertainty can be quantified), could be an alternative way to increase comparability of the environmental impacts between products. It provides additional information about the outcomes benefiting decision-making and it supports a statistic approach to compare similar products. For instance, the impacts of a product including many sources of uncertainty, could belong to the x% of worse, average or better performing products in a category for a specific impact. Despite that we do not develop further ideas on how to adopt some of the methods developed in this thesis in a context such as that of the PEFCR, some concrete ideas based on this thesis to progress PEFCRs towards an approach acknowledging the comparative character of uncertainty analysis, may include: using as a technique to treat choice-related uncertainties, a stochastic approach capturing many possible combinations instead of a specific-standardized choice with sensitivity scenarios (Chapter 2-3); using inventory data with underlying dependent sampling (see Lesage et al., 2018 for implications for aggregated datasets, Chapter 3); and possibly using information of the likelihood of the results to help communicate the preferred product choice (Chapter 5).

Finally, although other sources of uncertainty like ignorance and indeterminacies were not explicitly treated in this thesis, we believe they can gain particular relevance in the interpretation phase, not to say they do not appear in other phases, as they underlie the construction of scientific knowledge in general (Wynne 1992). The knowledge gained from an LCA may result in the emergence of additional uncertainties once it is used to support commitments, decision and policy making. For instance, using uncertainty analysis results to inform consumers may not necessarily be used in the expected way by consumers and quantifying such uncertainty could possibly be very difficult if possible at all. In other words, knowledge from an LCA may or may not result in additional uncertainties if expected to be valid under different social interpretations and different situations under which it was developed. Although, there is simply no way to know whether the knowledge from an LCA will influence decisions and choices leading to a sustainable future this thesis showed that the knowledge gained from acknowledging uncertainty where possible, can provide valuable and additional information about the LCA result, increasing the chances that decision and choices are indeed in the right direction. Chapter 5 showed that dealing with epistemological uncertainty enters a nonstationary, complex domain based on human behavior (Plevin 2016) which makes it difficult to predict environmental impacts, reason why the approach of this chapter is rather explorative than predictive.

6.3.2 The need to increasing replicability, transparency and robustness of LCA

There is a growing need for deepening the uncertainty dimension of LCA to increase transparency and robustness of LCA. This pressing need calls for the LCA community to further develop the science of LCA to address new societal questions and deal with issues that remain unsolved obstacles. For example, prospective LCA is one of the most prominent sub-disciplines in which a shared foundation in terms of methods, data, best practice and software solutions are lacking (Vandepaer and Gibon 2018). The UNEP-SETAC Life Cycle Initiative's Flagship Activity on Data, Methods, and Product Sustainability Information is an initiative aiming to bring technical advances to LCA and improve replicability of LCA results (Kuczenski et al. 2018). This community and initiative have declared that better model documentation is fundamental in increasing transparency and robustness in LCA. Despite of the efforts undertaken, the LCA community has still to become increasingly aware of the benefits of uncertainty analysis. This thesis showed that transparency and robustness come when explicitly acknowledging, in the case of this thesis by quantifying as much as possible, the levels of unknowns. This thesis also made an effort to provide supporting material for practitioners to further replicate the methods and case results of this thesis. Yet, acknowledging and dealing with other sources of uncertainty in LCA (where possible), for instance sources of actual ignorance and indeterminacies, has still to be pursued and simply more broadly recognized. Issues like the uncertainty of the uncertainty estimations used in this thesis e.g. the use of data quality indicators, or the applicability of these methods to different situations from the ones used in this thesis (e.g. new product-systems and new uses of the LCA results), deserve future attention.

Nowadays, uncertainty analysis is still a sub-discipline within LCA. However, uncertainty analysis has the capacity to account for many issues (e.g. data quality, allocation choice, unknown future) that diminish the scientific quality of the more widely applied deterministic point-value LCA practice. The future of LCA is in incorporating, as part of its standard practice, reproducible and transparent methods to increase the robustness of results and to explicitly acknowledge as much as possible, sources of unknowns. Although this inclusion might come at the price of more complex models, higher demands for data and data quality indicators, as well as bigger datasets, the efforts can be profitable and may even change deterministic conclusions. This thesis showed some concrete examples of ways towards more reproducible and transparent LCAs with more robust results while keeping the balance between model complexity and data demands. Documentation and relying in the probabilistic language were two fundamental aspects in achieving such a purpose and in preserving transparency.

6.4 Recommendations for future research

This thesis aimed at deepening the uncertainty dimension of environmental LCA. We addressed four questions around how to deal with three specific sources of uncertainty in different LCA applications. Yet, some issues remain to be further developed. Below, we summarize our main further research recommendations in relation to each of the chapters that addressed one research question each.

Chapter 2 and 3. On addressing choice-related and parameter uncertainty in different LCA contexts, extending and exploring other applications of the pseudo-statistical method is recommended. This and other recommendations in relation to chapter 2 and 3 are:

- Exploring the application of the pseudo-statistical method to higher level of choices for solving multi-functionality e.g. using substitution and system expansion as possible choices.
- Expanding the application of the pseudo-statistical method to propagate other discrete methodological choices in LCA e.g. different characterization methods for the same impact category.
- Applying a global sensitivity analysis to results of the pseudo-statistical method to understand how allocation choice and parameter uncertainty contribute to the total uncertainty and gain better understanding of the influence of sources of unknowns in the outcomes.
- Expanding the pseudo-statistical method to multi-functional processes in the background.
- Develop methods to map and determine which allocation methods and their methodological preference should be used in the pseudo-statistical protocol. For instance, participatory approaches actively accounting for different views by involved scientists, experts and stakeholders and patterns from meta-analysis of existing case studies.
- Standardizing the semantics around uncertainty and sensitivity analysis in LCA to facilitate the dissemination of novel methods in the two domains. Some methods like the one presented in Chapter 2, do not entirely fall in one or another type of analysis which made it difficult to communicate what it entailed.

Chapter 4. On addressing epistemological uncertainty in prospective LCA, to further improve the linkages between the ecoinvent database and IAM output is recommended. This and other recommendations in relation to chapter 4 are:

- Further data mining of the IMAGE scenarios to include as much as possible improvements of efficiency of renewable technologies and other emissions e.g. from electricity transmission.
- Expanding the use of IMAGE scenarios for prospective LCA to other economic sectors beyond the electricity sector e.g. steel, transport, agriculture, etc.
- Apply the prospective LCA approach using IMAGE scenarios to other case studies and combine it with foreground related sources of uncertainty e.g. parameter and choice uncertainty

- To improve further the inventories for relevant future technologies in line with the scenarios, such as carbon capture and storage (CCS) and concentrated solar power (CSP), and to account for their parameter uncertainty.

Chapter 5. On the interpretation of LCA results with uncertainty estimates, we recommend to further understand new issues arising from the critical review of interpretation methods as well as with incorporating this knowledge into assessing several impacts. This and other recommendations in relation to chapter 5 are:

- Investigate the effects of different techniques to quantify and propagate uncertainty on the interpretation of uncertainty analysis results in comparative LCA.
- To expand and test the discernibility method to include the magnitude of the impacts as well as the overlap area and the impact category relevance methods, to include relative uncertainties.
- Provide practical guidance to establish thresholds for acceptable uncertainty levels for different LCA applications.
- Develop understanding of the implications of acknowledging uncertainty for decision-making and communication of results to broader audiences e.g. consumers particularly in the context of product claims and consumer choices.
- Develop further understanding of the implications of dependent sampling for calculations of standardized Product Environmental Footprints (PEF) and Product Environmental Footprint Category Rules (PEFCR).

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Summary

Introduction

LCA has become an important method to study environmental impacts of human activities. Still, there are several methodological issues in LCA that can adversely affect the reliability of results. Three of these issues relate to a) allocation, b) the representation of the time dimension and c) the interpretation of results in LCA. Uncertainties play a fundamental and underlying role for these issues. The choice for an allocation method can have a large influence on the outcomes of LCA. Therefore, addressing the sensitivities related to the choice becomes important. Regarding time, some LCAs aim to be relevant for future decisions, which means that relevant parameters for the LCA might change in ways that are fundamentally unknown to us. Addressing epistemological uncertainties becomes crucial. Finally, selecting a method to interpret LCA results with uncertainty estimates affects the interpretation of results as different methods might lead to different conclusions. Thus, addressing uncertainty introduced due to the choice of interpretation method is also important.

It is widely-agreed that correctly dealing with these different sources of uncertainty is a vital step towards increasing the usefulness and reliability of LCA results. Practical ways to deal with uncertainty are needed. Most recent efforts have been in the direction of recognizing and increasing the community's understanding of the different sources of uncertainty as well as of their implications for different LCA applications. The aim of this thesis is to deepen the understanding of the uncertainty dimension of current LCA. By means of addressing different sources of uncertainty not yet addressed, with new methods, a clearer picture of the implications of different sources of uncertainty in LCA is provided. Although this thesis departed from broad domains of uncertainty including risk, uncertainty as conventionally described, ignorance and indeterminacies, the selected sources of uncertainty were narrowed down to the domains of risk and conventional uncertainty i.e. those due to incomplete scientific knowledge and that are to some extent quantifiable. We emphasize that this does not mean that all can be known or quantified and we make visible that ignorance and indeterminacies exist.

The issues addressed in this thesis and their related sources of uncertainty in LCA are:

1) allocation method choice in combination with parameter uncertainty,
2) accounting for future socio-technical changes in prospective LCA (epistemological uncertainty) and
3) choice of the interpretation method of uncertainty analysis results.

Each of these topics introduces uncertainty in the LCA results and to treat them this thesis uses different approaches, already existent in literature: the statistical, the scientific and the legal approaches. Within each approach, new methods are proposed

and developed such that these sources of uncertainty in LCA could be accounted for and explicitly acknowledged in the LCA results. This thesis consists of one introductory chapter (Chapter 1), four content chapters (Chapter 2 to 5) each treating one of the sources of uncertainty for a specific LCA application, and one overall discussion chapter (Chapter 6).

Research questions

On the basis of the identified sources of uncertainty and the knowledge gaps identified for each of them, the following research questions were addressed in this thesis:

RQ1: How can parameter uncertainty and uncertainty due to methodological choices in a single alternative LCA be quantified and propagated to the results? (Chapter 2)

RQ2: What are the implications for uncertainty analysis in a comparative LCA context of quantifying and propagating parameter uncertainty and uncertainty due to methodological choices? (Chapter 3)

RQ3: How can epistemological uncertainty for prospective LCA be systematically and consistently addressed? (Chapter 4)

RQ4: Which statistical method(s) should LCA practitioners use to interpret the results of a comparative LCA, under the light of its goal and scope, when considering uncertainty? (Chapter 5)

Answers to research questions

How can parameter uncertainty and uncertainty due to methodological choices be addressed? (RQ1, Chapter 2)

One way to treat parameter uncertainty and methodological choice uncertainty due to the choice of allocation methods is by means of the pseudo-statistical method proposed in chapter 2. This approach is based on Monte Carlo simulations for uncertainty propagation of quantified parameter uncertainties and of methodological preferences of allocation methods for solving multi-functional unit processes. This method enables accounting for the sensitivities of the choice of allocation method simultaneously with parameter uncertainty covering many possible combinations of these two and explicitly showing the results of such combinations without the need for one at the time scenarios. The application of this approach to a case study of a single alternative LCA showed that stochastically accounting for parameter uncertainty and for the choice of allocation methods leads to a wider range of results. These results, better cover the full uncertainty range but only further increase absolute uncertainties in single alternative LCA results. The illustrative case study showed that for scenarios varying one at the time the allocation method the climate change impacts vary from 1.5 to 2.3, from 1 to 1.5, from 1.2 to 1.9 and from 2 to 3 kg CO_{2eq} per kg of rapeseed oil, respectively per scenario. Results for the pseudo-statistical method proposed in this chapter range from 1 to 3 kg CO_{2eq} per kg of rapeseed oil with peaks of frequency of outcomes around the medians of the one at the time allocation scenarios. The range of results of the one at the time scenarios is fully covered by the proposed method, but as mentioned this only further increases absolute uncertainties which is not per se more useful. This approach appears to be more powerful in a comparative LCA context where relative uncertainties play a role. By extending it with a global sensitivity analysis, the contribution of uncertainty due to the choice of allocation method and of parameter uncertainty to the total uncertainty of the outcomes can be determined.

What are the implications of addressing parameter uncertainty and uncertainty due to methodological choices in a comparative LCA context? (RQ2, Chapter 3)

Applying the pseudo-statistical method to propagate parameter and uncertainty due to the choice of allocation methods in a comparative LCA context has implications primarily for the sampling procedure. Because it is vital to account for relative uncertainties between the pairs of product-systems under comparison, applying paired sampling of all parameters under consideration, is the most suitable experimental setup for uncertainty analysis in comparative LCA. Failing to use such setup will not enable a sensible comparison reflecting the comparative, or relative, uncertainty. If such a setup is used, statistical significance of the difference of the environmental impacts can be sensibly determined. The comparison of two aquaculture technologies to produce finfish showed that while deterministic LCA results can portrait one alternative as "better performing" for all impacts studied, no significant differences were observed when accounting for relative parameter and choice uncertainties with a pseudo-statistical approach. Deterministic results do not provide information on the likelihood of the outcome which portraits integrated production of fish as superior. The pseudo-statistic method results showed that monoculture production of fish leads to very similar environmental impacts as integrated multi-trophic production of the same fish, but the latter includes an additional production of oysters that could expand the economic base of the fish farm. Thus, a marginally bigger produce can be made with very similar environmental impacts. Having such information gave a more realistic assessment of the impact caused by the change in productive technology in this specific fish farm.

How can epistemological uncertainty for prospective LCA be systematically and consistently addressed? (RQ3, Chapter 4)

Scenario development in LCA is the most broadly used tool to deal with epistemological uncertainty in prospective LCA. However, to develop scenarios in LCA, it is really hard to replace all input data consistently across the LCA study in order to account for changes according to the scenarios. This is even more so, because a consistent method would not only require replacement of the foreground assumptions (i.e. parameters related directly to the activity looked at) but also all background assumptions (i.e. parameters related with supply chains of the activity looked at). For instance, in the case study discussed in Chapter 4, we discuss the choice between combustion versus electric engine vehicles. Here, not only consistent assumptions need to be made on the future performance of these vehicles, but also how changes in the future electricity mix (e.g. more renewables) would change all input parameters in the LCA. For this, we propose to link coherent integrated assessment model scenarios (a set of varied plausible futures) with background inventory data (i.e. LCI databases) to make scenario development in LCA more systematic and consistent. Because the future is unknown, one is confronted with epistemological uncertainty. To acknowledge epistemological uncertainty, we use several integrated assessment model scenarios covering different storylines that address the fact that we don't know how the future will unfold. Such approach leads to more robust results that account for varied socio-technical future paths of development and that serve to explore environmental impacts of products in the future. We showed how combustion and electric vehicles' impacts depend on the scenario and year. For some impacts, there appears to be a clearer difference in the future performance of the two vehicles, e.g. for human toxicity the scenario makes no difference as EV always performs worse. For other impacts, e.g. particulate matter formation and climate change, it is harder to distinguish which technology will perform better in the future.

Which statistical method(s) should LCA practitioners use to interpret the results of a comparative LCA, under the light of its goal and scope, when considering uncertainty? (RQ4, Chapter 5)

After quantifying different sources of uncertainty and propagating them to LCA results the last phase is the interpretation of the uncertainty analysis outcomes. Methods to interpret LCA uncertainty analysis results can 1) help in identifying differences and trade-offs in environmental impacts between alternatives and point to places where data refinement could benefit the assessment (exploratory methods) and 2) establish statistical significance of the difference (confirmatory methods). Depending on the goal and scope of the LCA, exploratory or confirmatory methods should be used. The two most important features of interpretation methods include: 1) accounting for common uncertainties and 2) accounting for the magnitude of the difference per impact. In chapter 5 we reviewed five interpretation methods and illustrated with a case on combustion, hybrid and electric vehicles that disregarding relative uncertainties leads to incorrect recommendations. Therefore, we considered this feature as a crucial one to be accounted for in interpretation methods. Also, we provided guidance on which method to choose according to the goal and scope of the LCA. It became evident that for exploratory purposes, no method is sufficiently developed yet as they do not cover both key features. For confirmatory purposes, one method was superior and helps establish statistical significance of the difference in environmental performance of two alternatives compared.

Main conclusions

This thesis contributed in deepening the understanding of uncertainty analysis in LCA. Three approaches to deal with uncertainty sources were used: the statistical, the scientific and the legal approaches. Each one leads to the development of guidance or a method useful to deal with different sources of uncertainty for different LCA applications. Overall, one of the most important conclusions of this thesis is that explicitly acknowledging different uncertainty sources in LCA results can provide additional information of important value. For instance, the likelihood of the results becomes known by explicitly dealing with uncertainty in comparison to deterministic LCA where the likelihood of the outcome is not known and it is usually associated with an average. Such information is important to understand the robustness of the results and thus can be valuable in decision and policy-making. Moreover, in a rapidly changing world with more unknows than knowns and where a transition towards sustainable technologies, products and systems has never been so urgent, this information and the capability to deal with different sources of uncertainty in LCA are of outmost importance to generate reliable assessments.

Outlook

Much has yet to be done and this thesis is another step toward increasing the capacity of the LCA community to deal with uncertainty. A detailed future research agenda derived from this thesis was outlined in section 6.4. In general, any efforts in the direction of better understanding how to deal with different sources of uncertainty, their implications for different LCA types and different applications, can contribute to enlarge the knowledge and the available toolbox for LCA practitioners. An important gap yet to be filled is the ability of the LCA community to communicate in transparent and accessible ways results of uncertainty analysis to society and relevant stakeholders. Unfortunately, the value of uncertainty analysis in LCA is not so recognized perhaps because it has been depicted as a complex type of analysis which might not yield valuable information. As shown in this thesis, to answer questions regarding the environmental sustainability of product-systems, in the present and in the future, requires more than ever embracing and recognizing as much as possible, what is unknown.

Samenvatting

Introductie

LCA is een belangrijke methode geworden om de effecten van menselijke activiteiten op het milieu te bestuderen. Echter zijn er nog verschillende methodologische zaken in LCA die de betrouwbaarheid van de resultaten negatief kunnen beïnvloeden. Drie van deze zaken zijn gerelateerd aan a) allocatie, b) de representatie van tijd en dimensie en c) de interpretatie van resultaten in LCA. Bij al deze zaken spelen onzekerheden een fundamentele onderliggende rol. De keuze voor een bepaalde allocatiemethode kan grote invloed hebben op de uitkomst van een LCA. Daarom is het belangrijk om de gevoeligheden gerelateerd aan de keuzes te toetsen. Met betrekking tot tijd, sommige LCA's hebben als doel om relevant te zijn voor toekomstige keuzes, wat betekent dat de relevante parameters voor de LCA zouden kunnen veranderen op een manier die tot zo ver onbekend voor ons is. Het aanpakken van epistemologische onzekerheden wordt cruciaal. Ten slotte beïnvloedt de selectie van een methode voor het interpreteren van LCA-resultaten met onzekerheidsinschattingen de interpretatie van de resultaten, omdat verschillende methoden tot verschillende conclusies kunnen leiden. Het aanpakken van onzekerheid die is geïntroduceerd als gevolg van de keuze van de interpretatiemethode, is dus ook belangrijk.

Men is het er algemeen over eens dat een juiste aanpak van deze verschillende bronnen van onzekerheid een essentiële stap is naar het vergroten van de bruikbaarheid en betrouwbaarheid van LCA-resultaten. Praktische manieren om met onzekerheid om te gaan zijn nodig. De meest recente inspanningen zijn gericht op het erkennen en vergroten van het begrip van de gemeenschap van de verschillende bronnen van onzekerheid, alsmede van hun implicaties voor verschillende LCA-toepassingen. Het doel van dit proefschrift is om de onzekerheidsdimensie van de huidige LCA te verdiepen. Door het meenemen van nog niet eerder aangepakte bronnen van onzekerheid met nieuwe methoden, wordt een duidelijker inzicht in de gevolgen van verschillende bronnen van onzekerheid in LCA verkregen. Hoewel dit proefschrift start vanuit de brede domeinen van onzekerheid, waaronder risico, conventioneel beschreven onzekerheid, onwetendheid en onbepaaldheid, zijn de geselecteerde bronnen van onzekerheid daarna beperkt tot de domeinen risico en conventionele onzekerheid, zoals onzekerheid door onvolledige wetenschappelijke kennis die alleen tot op zekere hoogte kwantificeerbaar zijn. We benadrukken dat dit niet betekent dat alles gekend of gekwantificeerd kan worden en we maken zichtbaar dat onwetendheid en onbepaaldheid bestaan.

De problemen die in dit proefschrift worden behandeld en de bijbehorende bronnen van onzekerheid in LCA zijn:

1) de keuze van allocatiemethode (in combinatie met parameter onzekerheid),

2) meenemen van toekomstige socio-technische veranderingen in toekomstgerichte LCA (epistemologische onzekerheid), en
3) keuze van de methode voor de interpretatie van onzekerheidsanalyseresultaten.

Elk van deze onderwerpen introduceert onzekerheid in de LCA-resultaten en om ze te behandelen maakt dit proefschrift gebruik van verschillende benaderingen, die al bestaan in de literatuur: de statistische, de wetenschappelijke en de juridische benaderingen. Binnen elke benadering worden nieuwe methoden voorgesteld en ontwikkeld, zodat deze bronnen van onzekerheid in LCA kunnen worden meegenomen en expliciet erkend in de LCA-resultaten. Dit proefschrift bestaat uit een inleidend hoofdstuk (hoofdstuk 1), vier inhoudelijke hoofdstukken (hoofdstuk 2 tot 5) die elk een van de bronnen van onzekerheid behandelen voor een specifieke LCA-toepassing, en een algemeen discussiehoofdstuk (hoofdstuk 6).

Onderzoeksvragen

Op basis van de geïdentificeerde bronnen van onzekerheid en de kennislacunes die voor elk van deze zijn geïdentificeerd, zijn de volgende onderzoeksvragen in dit proefschrift behandeld:

OV1: Hoe kunnen parameteronzekerheid en onzekerheid als gevolg van methodologische keuzes in een LCA met één alternatief worden gekwantificeerd en doorgerekend naar resultaten? (Hoofdstuk 2)

OV2: Wat zijn de implicaties voor onzekerheidsanalyse in een vergelijkende LCA-context van het kwantificeren en doorrekenen van parameteronzekerheid en onzekerheid als gevolg van methodologische keuzes? (Hoofdstuk 3)

OV3: Hoe kan epistemologische onzekerheid voor toekomstgerichte LCA systematisch en consequent worden aangepakt? (Hoofdstuk 4)

OV4: Welke statistische methode(s) moeten gebruikers van LCA gebruiken om de resultaten van een vergelijkende LCA te interpreteren, in het licht van het doel en de reikwijdte, bij het beschouwen van onzekerheid? (Hoofdstuk 5)

Antwoorden op de onderzoeksvragen

Hoe kunnen parameteronzekerheid en onzekerheid als gevolg van methodologische keuzes worden geadresseerd? (OV1, Hoofdstuk 2)

Een manier om parameteronzekerheid en onzekerheid als gevolg van de keuze van allocatie methoden te behandelen is door middel van de pseudo-statistische methode die wordt voorgesteld in hoofdstuk 2. Deze methode is gebaseerd op de Monte Carlo steekproefmethode als basis voor het doorrekenen van gekwantificeerde parameteronzekerheden en van methodologische voorkeuren van allocatiemethoden voor multifunctionele processen. Met deze methode kan er tegelijkertijd rekening worden gehouden met de gevoeligheden van de keuze voor allocatiemethode en parameteronzekerheid en de vele mogelijke combinaties van deze twee, en kunnen deze combinaties expliciet meegenomen worden in de resultaten. De toepassing van deze methode in een casus van een LCA met één alternatief toonde aan dat het stochastisch gelijktijdig meenemen van parameteronzekerheid en de keuze van allocatiemethoden leidt tot een grotere spreiding van de resultaten. Deze resultaten omvatten beter het volledige bereik van de onzekerheid, maar vergroten verder alleen de absolute onzekerheden in LCA-resultaten van één alternatief. De voorbeeldcasus toonde aan dat voor scenario's die een-voor-een de allocatiemethode variëren, de effecten van de klimaatverandering variëren van 1.5 tot 2.3, van 1 tot 1.5, van 1.2 tot 1.9 en van 2 tot 3 kg CO2eq per kg koolzaadolie, respectievelijk per scenario. De resultaten voor de pseudo-statistische methode die in dit hoofdstuk wordt voorgesteld, variëren van 1 tot 3 kg CO2eq per kg koolzaadolie met frequentie pieken van uitkomsten rond de medianen van de een-voor-een allocatiescenario's. Het bereik van de resultaten van de een-voor-een scenario's wordt volledig omvat door de voorgestelde methode, maar zoals eerder gesteld, verhoogt dit alleen de absolute onzekerheden wat op zichzelf niet veel zegt. Deze benadering lijkt krachtiger te zijn in een vergelijkende LCA-context waarin relatieve onzekerheden een rol spelen. Door deze uit te breiden met een globale sensitiviteitanalyse kan vervolgens ook de bijdrage van onzekerheid als gevolg van de keuze van de allocatiemethode en van parameteronzekerheid aan de totale onzekerheid van de uitkomsten bepaald worden.

Wat zijn de implicaties van het adresseren van parameteronzekerheid en onzekerheid als gevolg van methodologische keuzes in een vergelijkende LCA-context? (OV2, Hoofdstuk 3)

Het toepassen van de pseudo-statistische methode om parameteronzekerheid en onzekerheid als gevolg van de keuze van allocatiemethoden door te rekenen naar LCA-resultaten in een vergelijkende LCA-context heeft voornamelijk gevolgen voor de steekproefprocedure. Omdat het essentieel is om rekening te houden met relatieve onzekerheden tussen de paren van productsystemen die worden vergeleken, is het toepassen van gepaarde steekproeftrekking van alle beschouwde parameters de meest geschikte experimentele opstelling voor onzekerheidsanalyse in vergelijkende LCA. Het niet gebruiken van een dergelijke opstelling zal geen zinnige vergelijking mogelijk maken die de vergelijkende of relatieve onzekerheid weergeeft. Als een dergelijke opstelling wordt gebruikt, kan de statistische significantie van het verschil in milieueffecten op zinnige wijze worden bepaald. De vergelijking van twee aquacultuurtechnologieën om vinvis te produceren toonde aan dat deterministische LCA-resultaten één alternatief laten zien als "beter presterend" voor alle beschouwde milieueffecten, terwijl als we rekening houden met relatieve parameter- en keuzeonzekerheden met een pseudo-statistische benadering, er geen significant verschil tussen de twee technologieën blijkt te zijn. Deterministische resultaten geven geen informatie over de waarschijnlijkheid van de uitkomst dat de geïntegreerde productie van vis beter is. De resultaten van de pseudo-statistische methode toonden aan dat de monocultuurproductie van vis tot zeer vergelijkbare milieueffecten leidt als de geïntegreerde multi-trofische productie van dezelfde vis, maar de laatstgenoemde methode omvat extra productie van oesters die de economische basis van de viskwekerij zouden kunnen uitbreiden. Een marginaal grotere opbrengst kan dus bereikt worden met bijna gelijke milieueffecten. Met dergelijke informatie kon een meer realistische beoordeling gemaakt worden van de milieueffecten van de verandering in productietechnologie in deze specifieke viskwekerij.

Hoe kan epistemologische onzekerheid voor toekomstgerichte LCA systematisch en consequent worden aangepakt? (OV3, hoofdstuk 4)

Scenario-ontwikkeling in LCA is de meest gebruikte tool om epistemologische onzekerheid in toekomstgerichte LCA aan te pakken. Bij het implementeren scenario's in LCA is het echter heel lastig om alle invoergegevens die naar aanleiding van de scenario's zouden moeten wijzigen op een consistente manier te vervangen door de gehele LCA-studie heen. Dit is met name het geval, omdat een consistente werkwijze niet alleen vervanging van de voorgrondaannames vereist (dat wil zeggen parameters die direct verband houden met de activiteit waarnaar wordt gekeken), maar ook van alle achtergrondaannames (dat wil zeggen parameters die verband houden met toeleveringsketens van de bestudeerde activiteit). In de casestudy die we in hoofdstuk 4 hebben besproken, bespreken we bijvoorbeeld de keuze tussen voertuigen met verbrandingsmotoren en elektrische motoren. Hier moeten niet alleen consistente veronderstellingen worden gemaakt over de toekomstige prestaties van deze voertuigen, maar ook hoe veranderingen in de toekomstige elektriciteitsmix (bijvoorbeeld meer hernieuwbare energie) alle invoerparameters in de LCA zouden veranderen. Daarom stellen we voor om coherente scenario's van geïntegreerde beoordelingsmodellen (een reeks gevarieerde plausibele toekomsten) te verbinden met achtergrondinventarisatiegegevens (i.e. LCI-gegevens) om de scenario-ontwikkeling in LCA meer systematisch en consistent te maken. Omdat het toekomst onbekend is, wordt men ook geconfronteerd met epistemologische onzekerheid. Om recht te doen aan epistemologische onzekerheid, hebben we verschillende scenario's uit "integrated assessment" modellen gebruikt, die verschillende verhaallijnen beschrijven over hoe de toekomst zich zou kunnen ontvouwen. Een dergelijke aanpak leidt tot robuustere resultaten die rekening houden met verschillende sociaal-technische toekomstige ontwikkelingspaden en die dienen om de milieueffecten van producten in de toekomst onderzoeken. We hebben laten zien hoe de milieueffecten van auto's met verbrandings- en elektrische motoren afhangen van het scenario en het jaar. Voor sommige effecten lijkt er een duidelijker verschil te zijn in de toekomstige prestaties van de twee voertuigen; voor humane toxiciteit maakt het scenario bijvoorbeeld geen verschil, want de EV presteert altijd slechter. Voor andere milieueffecten is het moeilijker om te onderscheiden welke technologie beter zal presteren en zijn de effecten zeer afhankelijk van scenario's, bijvoorbeeld fijnstofvorming en klimaatverandering.

Welke statistische methode(s) moeten gebruikers van LCA gebruiken om de resultaten van een vergelijkende LCA te interpreteren, in het licht van het doel en de reikwijdte, bij het beschouwen van onzekerheid? (OV4, Hoofdstuk 5)

Na het kwantificeren van onzekerheden en doorrekening naar de LCA-resultaten, is de laatste fase de interpretatie van de onzekerheidsanalyseresultaten. Methoden voor het interpreteren van LCA-onzekerheidsanalyseresultaten kunnen 1) helpen bij het identificeren van verschillen in en afwentelingen tussen milieueffecten tussen alternatieven en verwijzen naar plaatsen waar dataverfijning de beoordeling ten goede zou kunnen komen (verkennende methoden) en 2) statistische significantie van het verschil vaststellen (bevestigingsmethoden). Afhankelijk van het doel en de reikwijdte van de LCA, moeten verkennende of bevestigende methoden worden gebruikt. De twee belangrijkste kenmerken van interpretatiemethoden zijn: 1) rekening houden met veelvoorkomende onzekerheden en 2) rekening houden met de omvang van het verschil per impact. In hoofdstuk 5 hebben we vijf interpretatiemethoden besproken en hebben we voor een casus over auto's met verbrandings-, hybride, of elektrische motoren laten zien dat het negeren van relatieve onzekerheden leidt tot onjuiste aanbevelingen. Daarom beschouwden we deze functie als een cruciale om rekening mee te houden bij interpretatiemethoden. We hebben ook richtlijnen gegeven over welke methode te kiezen op basis van het doel en de reikwijdte van de LCA. Het werd duidelijk dat voor verkennende doeleinden geen enkele methode nog voldoende ontwikkeld is omdat ze de beide hoofdkenmerken niet omvatten. Voor bevestigingsdoeleinden was één methode superieur en helpt deze de statistische significantie vast te stellen van het verschil in de prestaties van twee vergeleken alternatieven.

Belangrijkste conclusies

Dit proefschrift heeft een bijdrage geleverd aan het verdiepen van het begrip van onzekerheidsanalyse in het kader van LCA. Drie benaderingen voor de aanpak van bronnen van onzekerheid zijn toegepast: de statistische, de wetenschappelijke en de juridische. Elk van deze drie leidt tot de ontwikkeling van richtlijnen of van een methode voor de aanpak van verschillende bronnen van onzekerheid voor verschillende toepassingen van LCA. Eén van de belangrijkste algemene conclusies van dit proefschrift is dat het expliciet erkennen van verschillende bronnen van onzekerheid in LCA belangrijke toegevoegde informatie kan opleveren. Door het expliciet behandelen van onzekerheden verkrijgt men bijvoorbeeld een beeld van de waarschijnlijkheid van de resultaten, iets wat in deterministische LCA onbekend is en gewoonlijk gekoppeld is aan een gemiddelde. Zulke informatie is belangrijk voor een beter begrip van de robuustheid van de resultaten en kan zo waardevol zijn voor besluit- en beleidsvorming. Bovendien zijn zulke informatie en bekwaamheid om met verschillende bronnen van onzekerheden in LCA om te gaan, in een snel veranderende wereld met meer onbekendheden dan bekendheden en waarin een transitie naar duurzame technologieën, producten en systemen nog nooit zo urgent is geweest, van buitengewoon belang om betrouwbare beoordelingen te kunnen maken.

Vooruitblik

Ondanks dat er nog heel veel te doen overblijft, is in dit proefschrift weer een stap gezet in de richting van het vergroten van de kennis voor de LCA-gemeenschap over hoe om te gaan met onzekerheden. In sectie 6.4 is op basis van dit proefschrift een agenda voor toekomstig onderzoek geschetst. In het algemeen kunnen alle inspanningen om een beter inzicht te krijgen hoe met verschillende bronnen van onzekerheid om te gaan en de gevolgen daarvan voor verschillende typen LCA en toepassingen, bijdragen aan het vergroten van de kennis en de beschikbare gereedschapskist voor LCA-beoefenaars. Een belangrijk hiaat in kennis dat overbrugd zou moeten worden is vermogen van de LCA-gemeenschap om onzekerheidsresultaten op en transparante en toegankelijke wijze over te brengen naar de samenleving en belangrijke stakeholders. Helaas wordt het nut van onzekerheidsanalyses in LCA nog niet zo onderkend omdat het vaak neergezet wordt als een complexe analyse die niet zulke waardevolle informatie zou genereren. Zoals dit proefschrift laat zien vereist het beantwoorden van vragen betreffende de milieuduurzaamheid van productsystemen nu en in de toekomst, meer dan ooit tevoren het zo veel mogelijk omvatten en erkennen van dat wat onbekend is.

Acknowledgements

Four years researching the topic of uncertainty have taught me that it is hard to be sure about anything, but a sure fact is that these past years would have not been possible without the unconditional support and presence of many people to whom I here dedicate some deserved words.

I would like to start by thanking four scientist whose endless commitment to science inspired me throughout these years. Jeroen, without your guidance and dedication this achievement could have not been possible. Thanks for bringing the light back in the dark moments and for teaching me that the answer is hardly ever "42". Arnold, thanks for masterly running the stage from behind the scenes and for making me aware of "the other sides of uncertainty". I believe they deserve more than a word and I wish I could have dedicated more space to them. Detlef, more than a promotor you are a mentor. Thanks for about 10 years of lessons and for the infinite scientific inspiration. Although I am sure we will meet again, "so long and thanks for all the fish". Reinout, it was a true honour having you as a probability teacher. Thanks for making the complex and abstract, so tangible and simple. I really enjoyed our discussion about how god is a mathematician.

My stay in CML started earlier during my master's degree. Back then, I had the pleasure of studying with teachers who not only inspired me during this degree but who also inspired my career further. Ruben, without you this PhD probably would had never happened. Thanks for helping me figure out that this was the path to pursue and for encouraging me to always think outside of the box. Ester, Rene, Arjan, Lauran, I cannot be grateful enough with you for being part of the minds consolidating the field of Industrial Ecology. Thanks for your relentless persistence and for planting the seed of curiosity in me.

At CML I also had the pleasure of working together with talented researchers who inspired every day at work. Patrik, you deserve special thanks for IDREEM and for teaching me the meaning of "fingerling" among other concepts. Benjamin, Coen, Laura B., Jeroen A., Guanchao, Mingming, Valentina, Alexandra, Stefano and Krijn, no words can express how many memories I take with me but most of all I thank you all for sharing your passion for science with me. Sebastiaan, my roomie, my friend. No words can express the admiration I have for you and for your work. Thanks for many years of friendship and for always motivating me to go beyond. In my last years at CML many "young pros" came to CML and despite it being a relatively short time that I shared with some of them, I take lots of memories shared with them too: Bernhard, Nabeel, Bertram, Cherry, Leon, Anne, Yingjii, Georgios, Carlos S., Glenn, Amy, Efje, Yujia, Mili, Ellen, Daniel, Henrik, Carlos B., Chimere, Franco, Rita, Yelitza, Alexander, Elizabeth, Giovanni M., Subodh, Marinda, Giulia and Laura S, thanks for the good times. Life in the Netherlands was much better thanks to the support and unconditional friendly smile of four wonderful ladies, Suus, Esther, Joyce and Jori. Thanks so much for making the harsh Dutch weather easier to bare. To other CML academic and administrative staff among which Jan, Martina, Peter, Maarten, Rianne, Els, Jasper, Paul and the many more that I might be forgetting, thanks for a wonderful time and for being part of a great place to be.

I would also like to dedicate some words to the members of the IDREEM project with whom I shared four years and endless memories in the strive to implement integrated multi-trophic aquaculture in Europe. Specially Chiara, Danilo, Richard, Joao, Dror, Dafna, Oded, Johan, Celine, Demetris, Alexis and Adam, thanks for IDREEM and for teaching me so much about fish. Shreya, I did not forget you. Thanks for your support with data gathering in IDREEM and for flying all the way from the US for this experience.

This chapter would not be complete without thanking all the people that are indirectly part of this achievement. To my "PBL family" Jasper, Andries, Marc, Rineke, Oreane and Maarten: Ik hoop dat het leven zal ons nog een keer samen brengen. Ik probert nog steeds met mijn Nederlands… het is nooit te laat. Bedankt voor het deelen van mijn eerste stapjes in onderzoek en heel veel meer.

I also want to thank my Unilever colleagues, specially Sarah and Henry, for their patience and emotional support during the last phase of this thesis.

To my family abroad Carmen E., Bas, Carina, Nic, Pili, Paul, Lia, Juliette, Fanny, Jamal, Sophia, Jorge, Julia, Maurice, Jeanette, Andrea, Justin, Elena, Aya, Kath, Dalia, Rafa, Lara, Elias, Tjerk, around 12 years of friendship with you are also part of this thesis. To my recently "officially acquired" family Ana, Miquel, Sergi, Isa and Nora, thank you for the good times and emotional support. Mona and Mafe, thanks for a life together and for pushing me to finish. To many other family members in Colombia, whose names I cannot list here as it would take many pages, thanks for always being there.

This thesis is dedicated to the two women of my life, my mother Clemencia and my grandmother Isabel. Mami, you are the personification of determination, courage, perseverance and infinite love. Without your example I would have never pursued a science career. Abue, you are the example of ceaseless action and will to learn. Thanks for showing me that there is always something to learn and that "If you search you will find". Beyond the two women of my life I want to dedicate this thesis to women in science. Their endeavour to make science accessible to women, made it possible for girls, like me, to pursue a career in science. Hopefully we will be more in the future.

Finally, the universe would not be complete without the three men of my life. To my dad Cesar, I am infinitely thankful for sparking the love for nature. In the end I kind of followed your example, I am an accountant!... of the environment. To my brother Cesar, I am grateful to life for making you my big brother. I want to thank you for your nihilist, anarchist views because they are a source of inspiration to me (you did not see that one coming). What would be of a scientist without the capacity of being critical? Last but not least, David. You literally made the last point of this thesis possible, so I want to finish it with your name. I think we have become poetry together, like that of Bécquer: “What is poetry? you ask, while fixing your blue pupil on mine. What is poetry! And you are asking me? Poetry...is you”. I can’t wait for the new adventures to begin! Simply thank you for all, David.

Curriculum Vitae

María Angélica Mendoza Beltrán was born the 26th July 1983 in Bogotá D.C., Colombia. She completed her high school studies at Gimnasio Iragua in Bogota where she also earned the degree of International Baccalaureate in Chemistry, Biology and English in 2000. Between 2001 and 2006 she finalized her studies in Environmental Engineering at University of Los Andes in Bogota. Afterwards she travelled to the Netherlands and earned an MSc degree in Industrial Ecology at Leiden University in 2008. She then worked at the PBL - Netherlands Environmental Assessment Agency, as a junior policy researcher between 2008 and 2012. She worked in topics like reductions of emissions from deforestation and forest degradation (REDD+), international climate policy, climate change scenarios and production-consumption systems analysis. She participated in international modeling exercises such as the Energy Modeling Forum (EMF) and the Representative Concentration Pathways (RCPs) part of the climate scenarios of the Intergovernmental Panel on Climate Change (IPCC) fifth Assessment Report (AR5). In 2013, she became affiliated to the Institute of Environmental Sciences (CML) of Leiden University in The Netherlands, as a leading researcher of the work package on environmental sustainability in the EU FP7 project Increasing Industrial Resource Efficiency in European Mariculture (IDREEM). She worked in collaboration with aquaculture SMEs and research institutes. Between 2014 and 2018 she wrote her PhD thesis on uncertainty in Life Cycle Assessment at CML in Leiden University. Since the end of 2017 and up to present, she has been working at Unilever in the United Kingdom as a sustainability scientist.

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