Analyse et propagation de l'incertitude dans l'analyse de cycle de vie en agriculture

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N° ordre : 2014-19

N° Série : D-74

THESE / AGROCAMPUS OUEST

Sous le label de l'Université Européenne de Bretagne

pour obtenir le diplôme de :

DOCTEUR DE L'INSTITUT SUPERIEUR DES SCIENCES AGRONOMIQUES, AGRO-ALIMENTAIRES, HORTICOLES ET DU PAYSAGE

Spécialité : « Biologie et Agronomie »

Ecole Doctorale : « Sciences de la Matière»

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soutenue le 31 octobre 2014 devant la commission d'Examen

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“I can live with doubt and uncertainty and not knowing. I think it is much more interesting to live not knowing than to have answers that might be wrong. If we will only allow that, as we progress, we remain unsure, we will leave opportunities for alternatives. We will not become enthusiastic for the fact, the knowledge, the absolute truth of the day, but remain always uncertain … In order to make progress, one must leave the door to the unknown ajar.”

— Richard P. Feynman

Acknowledgements

I would like to express my deep gratitude to my research supervisor, Patrick Durand, for his patient guidance, enthusiastic encouragement and useful critiques of this research work. Your great patience and complete confidence have been very much appreciated, in particular when I tried to explain the Dempster-Shafer theory.

I am truly grateful to my co-supervisor, Michael Corson, who always generously gave his time to help me do this thesis. You always gave me valuable suggestions ("nit-picking", you said), which taught me how to perform rigorous scientific research. I thank you for encouraging and helping me to try out every new idea I had for this research work. I also appreciate your explicit explanations for improving my English skill.

I would like to express my gratitude to the members of my thesis committee: Hervé Monod (INRA, MIA-Jouy), Laurent Lardon (INRA, LBE), Hayo van der Werf (INRA, UMR SAS), and Joël Aubin (INRA, UMR SAS), for their constructive advice. I really appreciate the critiques given by Laurent and Hervé during my mid-term defense, which allowed me to realign the conceptual problem of my research work.

I want to send my great thanks to David Makowski (AgroParisTech), Christian Bockstaller (INRA Colmar), Lucile Montagne (Agrocampus Ouest), and Claudine Basset-Mens (CIRAD) for accepting to be jury members for my oral defense.

I would like to thank all colleagues of UMR SAS for their warm hospitality. I really enjoyed the nice ambiance with you during work and coffee breaks. I give many thanks to my colleagues in the ASAE research team for sharing their knowledge and passions, not only about research, but also about personal activities. Thank you for knocking the door and calling me for lunch. I am particularly grateful for the advice and encouragement given by Joël Aubin, Hayo van der Werf, Aurélie Wilfart, and Nouraya Akkal, who helped me blend into the team.

There are many more people who helped me a lot during my Ph.D. study, to whom I want to express my gratitude:

I want to thank Thibault Salou for helping me to understand the Agri-BALYSE system; also, it was pleasure to work with you to create the "Young Researcher Wall" at LCA Food 2012. I also want to thank Olivier Godinot for his help importing data into Excel.

I would like to thank Emmanuel Tete for his friendship. Thanks for sharing your experiences and knowledge during the past three years. And it was my honor to play football with you in the Cap Malo tournament.

I am thankful to Elisabeth Samson and Joël Aubin for giving me complete trust in writing the paper on “bootstrapping the samples of trout”. I very much appreciated your willingness to give your time for discussions.

I would like to thank Monique Delabuis, who helped me to use Endnote. Without your help, my bibliography would have been a mess.

I would like to thank my officemate Christophe Fléchard and “daily passenger” Yannick Fauvel for their curiosity about Chinese culture (saying “hello” in Chinese every morning). I especially appreciate your showing me your work in the forest, which helped me understand how emissions are measured in the field and where the data that feed my research come from.

I want to send my gratitude to Christophe Cudennec. I really had fun talking to you and appreciate your inspiring ideas.

I would like to express my gratitude to all the secretaries of UMR SAS: Tiphaine Labbé, Karine Derrien, Maryvonne Pertue, and Françoise Prigent of Agrocampus Ouest. With your help, I never worried about administrative issues.

I would like to thank our “Chinese community” members at INRA: Hongtao (红涛), Wenjie (文杰), Lina (李娜), and Ruixuan (老曹) for sharing their working experiences and personal stories with me. I especially want to express my sincere appreciation to Hongtao (红涛). You always voluntarily shared your experiences, even detailed things I never realized. When I have questions about my research or my personal life, you always give me pertinent advice. The most important thing is that you taught me how to say “no” in some embarrassing situations. I also want to thank your family, who treats me like a family member (with delicious dumplings).

I would like to thank my former boss Sandrine Blanchemanche and my former colleagues Eve and Akos for supporting me to continue my Ph.D. study. I also want to thank Isabelle Albert, who visited me in Rennes every year.

I would like to thank my former professor Meng Qinxiang for his suggestions and encouragement for my Ph.D. study. I really appreciate your trust in letting me work on the translation of the “French Red Table”.

I send many thanks to my friends for being my family in France: Louise, Lucile, and Alice, and their families, who helped me start my new life in France.

I would like to thank all my friends for taking loneliness away from me and bringing happiness to me. I thank my dear friend Haoyu (妤雨) for bringing me positive energy, which made me keep fighting in the last year of my thesis. I want you to know that I did not complain too much, but kept doing my best for my research work. I want to give my best thanks to my brother-like friends

Xuguang (光哥), Min (敏娃), Hongding (鼎娃), and Xiaolei (小雷). I really have good memories with all of you in Aberdeen, Amsterdam, Barcelona, Beijing, and Paris. Also, I want to express my great thanks to my football teammates for suffering my bad temper on the playground during these past three years. I am so glad to be friends with you and really had fun with you guys in Lyon.

Last but not least, I am enormously thankful to my beloved parents for being healthy and happy during these years when I am away from home. Thank you for your endless love, and I love you so much.

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Table d'abréviations et d'acronymes

BCa bootstrap	Bias-Corrected and Accelerated Bootstrap
Bel	Belief Function
bpa	Basic Probability Assignment
CC	Climate Change
CDF	Cumulative Distribution Function
CI	Confidence Interval
CTV	Contribution to the Variance
CV	Coefficient of Variation
DQI	Data Quality Indicator
DST	Dempster-Shafer Theory
EDEN	Évaluation de la Durabilité des ExploitatioNs
EF	Emission Factor
FAO	Food and Agriculture Organization of the United Nations
FCR	Feed Conversion Ratio
FPCM	Fat- and Protein-Corrected Milk
FU	Functional Unit
GHG	Greenhouse Gas
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LHS	Latin Hypercube Sampling
MCS	Monte-Carlo Simulation
MND	Multivariate Normal Distributions
NPPU	Net Primary Production Use
PC	Principal Component
PCA	Principal Component Analysis
PDF	Probability Distribution Function
Pl	Plausibility Function
RIW	Relative Interval Width
SD	Standard Deviation
SEM	Standard Error of the Mean
SETAC	Society of Environmental Toxicology and Chemistry
UAA	Usable Agricultural Area
UNEP	United Nations Environment Programme
WHO	World Health Organization

Abstract

Life Cycle Assessment (LCA) is a methodological framework for assessing environmental impacts of a product, a service or a system throughout its life cycle: from extraction of raw materials, through production and use, to recycling and waste treatment (i.e., “cradle to grave”). Its wide applicability to agricultural systems provides useful information for decision makers to estimate environmental impacts of products, compare environmental impacts of different systems, and make suggestions to improve systems. However, the LCA’s need for large amounts of data and high-quality models yields several sources of uncertainty that influence the feasibility of LCA of agricultural systems and the credibility of its results. For example, it is difficult to obtain measurements of nitrate emissions due to fertilizer or manure applications, but estimating emissions using emission factors may not represent all conditions, especially in regions with specific farming practices (conventional *vs.* organic). Therefore, the scientific objectives of this thesis are to identify sources of uncertainty in agricultural LCAs and help practitioners use appropriate methods to represent different types of uncertainty in agricultural systems and analyze their influence on total uncertainty in environmental impacts through LCA.

Uncertainty in LCA can be divided into two types according to its nature: epistemic uncertainty (lack of knowledge) and variability (inherent difference). Both types of uncertainty have fundamentally different definitions, and distinguishing them helps practitioners reduce epistemic uncertainty (e.g., by improving measurements) and better understand variability in the system (e.g., by seeking more representative information). To be more explicit, each type of uncertainty can be divided into three sub-categories depending on its source: parameter, model, or scenario uncertainty and spatial, temporal, or natural variability. The type of uncertainty determines the method(s) used to represent and propagate it; their characteristics and limits depend on both the context of the agricultural site studied and that of the study itself. Therefore, to better address uncertainty in LCA studies, the decision tree developed in this thesis can help LCA practitioners choose which method(s) to use. Application of the methods, however, should be performed on a case-by-case basis, because particular situations may occur in real case studies that cannot be covered by a general guideline. Sometimes other factors, such as computational cost and acceptable confidence level, should also be considered when performing uncertainty analysis in LCA.

The probabilistic approach is commonly used to quantify both natural variability and parameter uncertainty, while intervals (“fuzzy” or “crisp”) may be more appropriate for representing parameter uncertainty. In agricultural systems, both types of uncertainty often occur together. Therefore, the two methods were applied to represent natural variability in farm characteristics and parameter uncertainty in emission factors, respectively, to estimate environmental impacts of dairy farms in Brittany, France. These uncertainties in input variables were propagated using Monte-Carlo simulation to the

uncertainty in estimated impacts, which was represented using Dempster-Shafer theory (DST). In parallel, correlations among farm-characteristic input variables were maintained using multivariate probability distributions, which yield more realistic estimates than random independent distributions. Representing uncertainty in impacts using DST distinguished variability in potential impacts from epistemic uncertainty in their mean values. Hence, interpretation of the uncertainty analysis should carefully explain the differences between them. The attitude of decision makers to risk (i.e., confidence index) can be integrated into this DST-based form of representation to create a single weighted distribution of impact, which seems easier to interpret than an impact whose range is bounded by two separate distributions. However, there are some limits to applying DST in uncertainty analysis, and studies should be performed in the future to focus on maintaining correlations between variables that are represented imprecisely, using *ad hoc* optimization algorithms to increase propagation efficiency, and integrating other types of uncertainty in the same LCA framework. In addition, there is a need to apply the DST in more case studies to validate its use.

In conclusion, uncertainty analysis, as an important component of LCA, should provide reasonable and realistic assessment of studied systems in the face of many sources of uncertainty. The existence of uncertainty, which is unavoidable, should not restrict research and decision making, but rather help LCA practitioners to improve their understanding of studied systems by identifying the key information needed. The existence of a variety of methods for uncertainty analysis provides LCA practitioners with an array of methods to choose from, depending upon the context of the agricultural system and that of the LCA study. Moreover, using an appropriate method provides credible estimates of impacts, which reflect the real state of knowledge and may encourage scientists to seek more information.

Keywords: life cycle assessment; agricultural system; environmental impacts; epistemic uncertainty and variability; probability theory; fuzzy intervals; Dempster-Shafer theory; Monte-Carlo simulation

Résumé

L’Analyse du Cycle de Vie (ACV) est un cadre méthodologique pour évaluer les impacts environnementaux d'un produit, d’un service ou d’un système tout au long de son cycle de vie: depuis l'extraction des matières premières, jusqu'au recyclage ou à la mise en déchet (« du berceau au tombeau ») en passant par les processus de production et d’utilisation. Ses larges applications dans l'agriculture offrent des informations utiles pour les décideurs pour évaluer des impacts environnementaux des produits, comparer des impacts environnementaux entre les systèmes différents, et améliorer un système de production. Cependant, l'exigence en données et en modèles de bonne qualité utilisés en ACV entraîne différentes sources d'incertitude qui influent sur la faisabilité de l'ACV des systèmes agricoles et la crédibilité de ses résultats. Par exemple, il est difficile d'obtenir des mesures des émissions de nitrate après l'application d'engrais ou de fumier au sol, et l'estimation des émissions avec des facteurs d'émission ne peut pas représenter toutes les conditions, surtout dans une région où les pratiques agricoles sont particulières (gestion conventionnelle versus biologique). En conséquence, les objectifs scientifiques de cette thèse sont d'identifier les sources d'incertitude en ACV agricole et d'aider les analystes à choisir les méthodes appropriées pour représenter différents types d'incertitude dans le système agricole et pour analyser leurs influences sur l'incertitude totale des impacts environnementaux.

L'incertitude en ACV peut être divisée en deux types selon sa nature: incertitude épistémique (manque de connaissances) et variabilité (différence intrinsèque). Les deux types d'incertitude ont les définitions fondamentalement différentes, et la distinction entre eux aide les analystes ACV à réduire incertitude épistémique (ex., en améliorant des mesures) et à mieux comprendre la variabilité du système étudié (ex., en recherchant des informations plus représentatives). Pour être plus explicite, chaque type d'incertitude peut être divisé en trois sous-catégories selon la source : l’incertitude paramétrique, de modèle, ou de scénario et la variabilité spatiale, temporelle, ou naturelle. Le type d'incertitude détermine la méthode utilisée pour le représenter et propager, dont chacune a ses propres caractéristiques et limites en fonction du contexte du système agricole étudié et de l’étude elle-même. Donc, afin de mieux aborder l’incertitude dans les études ACV, l’arbre de décision proposé dans cette thèse permet les analystes ACV d'avoir plusieurs choix de méthodes face à différents types d'incertitude. Cependant, l'application de méthodes différentes doit être réalisée au cas par cas, parce que des situations particulières peuvent se produire dans une étude de cas réelle qui ne peuvent pas être traité dans une guide générale. Parfois d’autres facteurs, comme le coût de calcul et le niveau de confiance acceptable, doit aussi être considéré lors de l'analyse de l'incertitude en ACV.

L'approche probabiliste est en général utilisée pour quantifier la variabilité naturelle et l'incertitude paramétrique, tandis que les intervalles (flous ou précis) peuvent être plus appropriés pour représenter l'incertitude paramétrique. Dans les systèmes agricoles, les deux types d'incertitude se

produisent souvent ensemble. En conséquence, les deux méthodes ont été appliquées pour représenter la variabilité naturelle sur les caractéristiques des fermes agricoles et l'incertitude paramétrique sur les facteurs d'émission, respectivement, pour estimer des impacts environnementaux des exploitations laitières en Bretagne (France). Ces incertitudes des données d'entrée ont été propagées par la simulation de Monte Carlo vers l'incertitude finale des impacts potentiels, représentés avec la théorie de Dempster-Shafer (DST). En parallèle, les corrélations entre les variables d'entrée de caractéristiques des exploitations ont été contrôlées en utilisant des distributions de probabilité multidimensionnelles. Cette démarche permet d'avoir une estimation plus réaliste que d'utiliser des distributions aléatoires indépendantes. La représentation de l'incertitude totale avec la DST a distingué la variabilité sur les impacts potentiels de l'incertitude épistémique sur ses valeurs moyennes. Ainsi, l'interprétation de l'analyse d'incertitude devrait expliquer soigneusement les différences entre eux. Les attitudes des décideurs en face du risque (i.e., l'indice de confiance) peuvent être intégrées dans la représentation DST sous la forme d'une seule distribution pondérée d'impact, qui semble plus facile à interpréter qu'un impact dont son étendue des valeurs est limitée par deux distributions séparées. Cependant, il y a des limites sur l'application de la DST à l'analyse de l'incertitude, et d'autres études devraient être réalisées à l'avenir sur les corrélations entre les variables qui sont représentées de manière imprécise, les algorithmes d'optimisation *ad hoc* pour améliorer l'efficacité de la propagation et l'intégration d'autres types d'incertitude dans le même cadre de l'ACV. En outre, il est nécessaire d'appliquer la DST dans plusieurs études de cas pour la valider.

En conclusion, l'analyse de l'incertitude, comme un composant important de l'ACV, devrait offrir une évaluation raisonnable et réaliste des systèmes étudiés face à diverses sources d'incertitude. L'existence d'incertitude, qui est inévitable, ne devrait pas restreindre la recherche et la prise de décision, mais au contraire devrait aider les analystes ACV à compléter leurs connaissances par rapport au système étudié, en identifiant les informations clés nécessaires. L'existence de plusieurs méthodes d'analyse de l'incertitude donne aux analystes ACV des choix flexibles dans les différents contextes de système agricole ou d'étude ACV. De plus, utiliser une méthode appropriée fournit des estimations crédibles des impacts, qui reflètent l'état réel des connaissances et peut encourager les scientifiques à chercher plus d'informations.

Mots-clés: analyse du cycle de vie ; système agricole ; impacts environnementaux ; incertitude épistémique et variabilité ; théorie de probabilité ; intervalles flous ; théorie de Dempster-Shafer ; simulation de Monte Carlo

Chapitre 1.
Introduction générale

1.1 Contexte : l'agriculture et l'environnement

Les principales formes d'agriculture ont été pratiquées par l'humanité depuis le néolithique, pour atteindre un objectif initial : l'autosuffisance alimentaire (Mazoyer and Roudart 1997). Beaucoup plus récemment, le développement de l'agriculture fait face à un grand challenge à cause de l'augmentation de la population mondiale, ce qui provoque des exigences d'économie supplémentaires (économie financière et économie des ressources naturelles) et de préservation de l'environnement (Espagnol and Leterme 2010). De nombreuses études ont mis en évidence le lien entre l'activité agricole et l'environnement. L'environnement contrôle la production forestière et agricole. Par exemple, une hausse des températures (de 1 à 3 °C) locales pourrait augmenter le potentiel de production alimentaire (Pachauri and Reisinger 2007) ; les événements climatiques extrêmes peuvent endommager des prairies, des cultures et des forêts (Vert et al. 2013). A l'inverse, les pratiques agricoles affectent l'environnement. Par exemple, l'utilisation des fertilisants dans l'agriculture est responsable de l'accroissement des quantités d'azote et de phosphore dans la biosphère (Bennett et al. 2001; EMEP-CORINAIR 2002). En 2011, les surfaces agricoles et forestières émettent plus de dix milliards tonnes de gaz à effet de serre (GES), parmi lesquelles, les cultures et les élevages représentent environ 5,3 milliards tonnes, une augmentation de 14 % par rapport à 2001 (FAO 2014). Les sources d'émissions agricoles viennent principalement de la fermentation entérique (40 %), puis des émissions au pâturage (16 %) et des engrais synthétiques (13 %). En particulier, les secteurs d'élevage (environ 80 % des émissions agricoles) engendrent des impacts directs et indirects sur le changement climatique, la pollution du sol et de l'eau, la dégradation des services écosystémiques, les ressources naturelles et la biodiversité (Steinfeld et al. 2006). De ce fait, les progrès des sciences de l'agriculture ne visent plus seulement à satisfaire l'autosuffisance alimentaire pour l'humanité, mais aussi à prendre en compte ses influences sur les autres aspects (ex., environnement, économie et société).

Plusieurs méthodes multicritères ont été développées pour estimer et évaluer les impacts environnementaux de l'agriculture, ainsi que pour identifier des pistes d'amélioration du système agricole (van der Werf and Petit 2002). L'Analyse du Cycle de Vie (ACV) est l'une des méthodes d'évaluation environnementale largement utilisées actuellement. La structure d'ACV, dont l'idée initiale a été proposé depuis les années 1970 pour l'industrie, a pour la première fois été standardisée par la Société de Toxicologie et de Chimie Environnementales (SETAC) en 1993 (SETAC 1993). La SETAC fournit une plateforme d'échange scientifique qui se consacre à traiter les sujets importants (ex, évaluation des impacts, qualité des données) sur l'implémentation de l'ACV par les groupes de travail (Klöpffer 2006). À partir de 2000, l'Organisation Internationale de Normalisation (ISO) a publiée une série de normes ISO 14 000 sur le système de management environnemental. Parmi les normes, la série ISO 14 040 (2006) concerne la pratique de l'ACV, qui est détaillée par les normes

complémentaires (ISO 14 041, ISO 14 042, ISO 14 043), et puis intégrées dans la norme ISO 14 044 (2006). Plusieurs pays adoptent ces normes ISO comme une base de référence pour le management environnemental dans leurs réglementations. Une troisième organisation internationale engagée dans le développement de l'ACV est le Programme des Nations Unies pour l'Environnement (UNEP). L'UNEP, en collaboration avec la SETAC depuis 2002 (lancement de *l'Initiative pour le Cycle de Vie*), a pour objectif de développer et diffuser l'ACV au niveau mondial. En parallèle, des méthodes et des données spécifiques ont été développées au sein de l'ACV, telles que, les guides opérationnels de l'ACV (Guinée et al. 2002; Heijungs et al. 1992) et la base de données d'inventaire *ecoinvent* (Frischknecht et al. 2005). La méthode d'ACV sera détaillée dans la prochaine section.

1.2 Analyse du Cycle de Vie

1.2.1. La définition de l'ACV

Selon la norme standard ISO 14 040 (2006), l'ACV est un cadre méthodologique pour évaluer des impacts environnementaux d'un produit, d'un service ou d'un système en considérant l'ensemble de son cycle de vie, depuis l'extraction de la matière première (« berceau ») jusqu'à son recyclage ou sa mise en déchet (« tombeau »). L'ACV estime les charges environnementales du produit, du service ou du système « du berceau au tombeau » en agrégeant ses émissions et utilisations de ressources, exprimées dans un inventaire des flux de matière ou d'énergie (ex., émissions de nitrate, méthane, dioxyde de soufre, consommation d'électricité), dans quelques indicateurs d'impact. Ces indicateurs peuvent refléter des flux vers l'air (ex., changement climatique provoqué par des GES), vers l'eau (ex., eutrophisation provoquée par les nitrates) et vers le sol (ex., toxicité terrestre provoquée par des métaux lourds). Elle fournit des informations pouvant être utilisées par plusieurs secteurs (ex., gouvernement, entreprise, consommateurs) lors de la prise de décision (Jolliet et al. 2010). Les applications principales de l'ACV sont (1) d'analyser les charges environnementales d'un produit, d'un service ou d'un système particulier, (2) d'identifier les actions prioritaires pour améliorer les processus du système en respectant l'environnement et (3) de comparer les charges environnementales entre les produits, les services ou les systèmes différents (Guinée et al. 2002). La méthodologie de l'ACV est divisée en quatre étapes (Boeglin and Veuillet 2005; ISO 14040 2006; JRC 2010): définition des objectifs et du champ de l'étude, analyse de l'inventaire, évaluation de l'impact et interprétation (Fig. 1). Ces quatre étapes sont interdépendantes tout au long de l'étude, ce qui rend une ACV itérative.

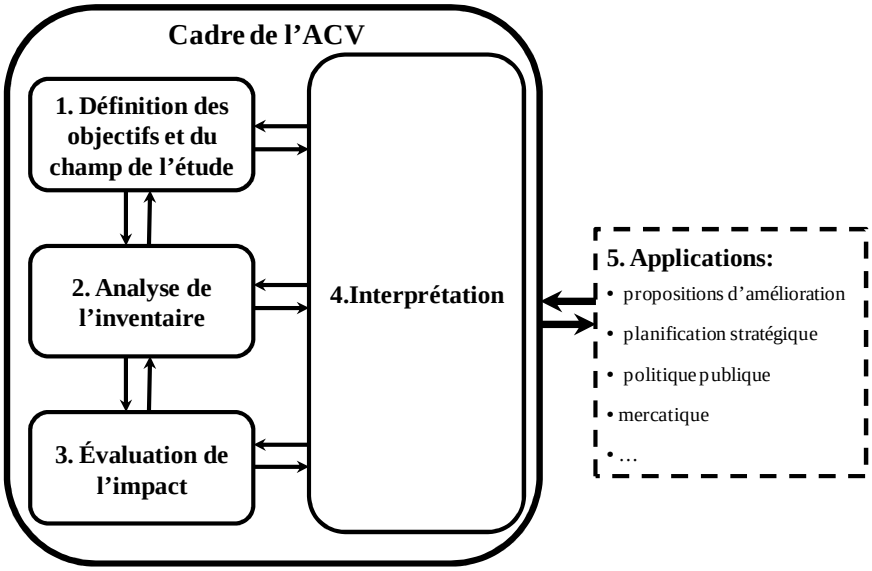

Figure 1. Les quatre étapes du cadre de l'analyse du cycle de vie (ACV) reprise de Boeglin & Veuillet (2005). Les applications de l'ACV ne font pas partie du cadre.

- ***La définition des objectifs et du champ de l'étude*** permet de définir les objectifs de l'étude en vue de ses applications, et de déterminer le champ de l'étude, y compris la frontière du système, les choix méthodologiques, la fonction du produit ou du système, l'unité fonctionnelle (UF), et les exigences de qualité des données (ISO 14044 2006). Ces éléments essentiels doivent être décrits clairement pour l'exécution des étapes suivantes afin de répondre aux objectifs définis. Par exemple, la frontière du système détermine les processus du système inclut dans l'ACV. Dans des systèmes agricoles, la frontière est souvent délimitée jusqu'à la sortie de l'exploitation (Aubin et al. 2009; van der Werf et al. 2009). Mais certain études (Cederberg et al. 2013; FAO 2010) ont inclus des processus après l'exploitation (ex., la transformation alimentaire et le transport vers les distributeurs). Les choix méthodologiques concernent le choix des valeurs et des méthodes utilisées pour les calculs (Steen 2006). La fonction définit les caractères de performance du produit ou du système, et l'UF quantifie cette fonction, dans laquelle les flux de matières, d'énergies et d'émissions sont effectués. Lors d'une étude comparative, les produits ou systèmes doivent être basés sur une fonction commune, et l'UF offre une référence de comparaison en normalisant les flux entrants et sortants (les « flux de référence ») des systèmes. Le choix de l'UF est crucial pour répondre aux objectifs de l'étude. L'UF est généralement basée sur la masse de produit (ex., par kg de produit) (Basset-Mens et al. 2009; Nguyen et al. 2012), mais plusieurs UFs peuvent être utilisées pour considérer, par exemple, la fonction d'occupation de surface ou du service écologique (par ha de surface agricole) ou la fonction économique (par euro de chiffre d'affaires) (van der Werf et al. 2009).

  Ainsi, les données choisies dépendent des objectifs et du champ de l'étude. En réalité, les données récoltées sont un mélange de sources de données différentes (ex., empirique, observée, calculée,

estimée). Donc, la qualité des données doit être vérifiée spécifiquement dans cette première phase, en ce qui concerne la précision, la complétude, la représentativité, la cohérence, la couverture temporelle, géographique et technologique, et l'incertitude (Weidema and Wesnaes 1996). Comme cette première phase se précise de manière itérative, le champ de l'étude peut être modifié tout au long de l'étude lorsque les informations supplémentaires sont obtenues.

- ***L'analyse de l'inventaire*** : une fois que le champ de l'étude est défini, la deuxième phase de l'ACV est de quantifier des ressources extraites ou occupées (ex., matières premières, surfaces de terre), des consommations d'énergie (renouvelable et non-renouvelable) et des émissions des substances polluantes vers l'air, l'eau et le sol au cours du cycle de vie du produit, du service ou du système étudié. La réalisation de calcul exige une recherche de données d'inventaire soit à partir d'expérimentations *ad hoc*, soit dans la littérature (Jolliet et al. 2010). Plusieurs bases de données sont disponibles pour fournir des données d'inventaire au niveau local ou global, et la base de données *ecoinvent* intègre plusieurs sources de données pour avoir une base de données générique incluant la fonction d'évaluation de la qualité de données (Frischknecht et al. 2005). Par ailleurs, certains processus d'un système génèrent plus qu'un produit (un produit principal et des « co-produits » ; ex., lait et viande d'une l'exploitation laitière). Par conséquent, les charges environnementales d'un processus sont attribuées (« allouées ») à chaque co-produit. Pour quantifier la contribution aux charges uniquement du produit principal, des méthodes d'allocation différentes s'effectuent au sein de l'analyse de l'inventaire (Ardente and Cellura 2012; De Vries and De Boer 2010; Wardenaar et al. 2012).

- ***L'évaluation de l'impact*** permet d'évaluer des impacts environnementaux reliés avec les émissions des substances différentes, les extractions des ressources et les consommations d'énergies du système. Le choix des indicateurs d'impact intermédiaires (ex., changement climatique, eutrophisation, acidification, utilisation de ressources naturelles, toxicité), ainsi que des indicateurs de dommage (ex., sur la santé humaine, sur l'environnement naturel biotique/abiotique), est réalisé dans la première étape de l'ACV. Par exemple, à travers l'outil EDEN (Évaluation de la Durabilité des ExploitatioNs), un inventaire de l'utilisation de ressources et les émissions était établi pour évaluer des impacts environnementaux des exploitations laitières en Bretagne en France (van der Werf et al. 2009) (Fig. 2). Donc, cette phase classifie les émissions et les extractions de ressources selon leurs effets sur les indicateurs d'impact. La quantification des impacts se fait par la multiplication des émissions avec les facteurs de caractérisation correspondants (ex., Eco-indicator 99 (Goedkoop and Spriensma 1999), Impact 2002+ (Jolliet et al. 2003)). D'ailleurs, comme les différentes catégories d'impact ont des unités différentes, ceci peut être difficile de juger l'impact le plus critique ou de comparer les résultats entre les différents systèmes. Pour cette raison, trois étapes optionnelles sont comprises au sein de cette phase. Le

choix des facteurs et les bonnes pratiques associées à ces trois étapes ont été décrits en détail par Finnveden (2002).

- la normalisation (rapport de la contribution d'impact du produit ou du système par rapport à l'effet total au niveau global ou local) permet d'exprimer les différentes catégories d'impacts avec la même unité.
- le regroupement attribue (semi-)qualitativement des rangs d'importance aux indicateurs d'impact.
- la pondération permet d'agréger les résultats normalisés par un facteur de pondération (un score à valeur unique) afin d'exprimer l'impact environnemental global du produit ou du système.

- ***L'interprétation*** permet d'interpréter les résultats obtenus par les phases précédentes à plusieurs niveaux (ex., au niveau des émissions, des impacts intermédiaires et des impacts de dommage). Dans cette phase, on identifie les points clés (avec plus d'impact) au sein des processus du système et propose des options pour réduire les impacts environnementaux du produit, du service ou du système. On évalue également la qualité des données, les points sensibles et les incertitudes au travers du cycle de vie. De plus, on tire une conclusion sur la limite du système ACV et propose les recommandations pour la recherche future. Cette phase doit apporter des informations transparentes et compréhensibles pour l'aide à la décision.

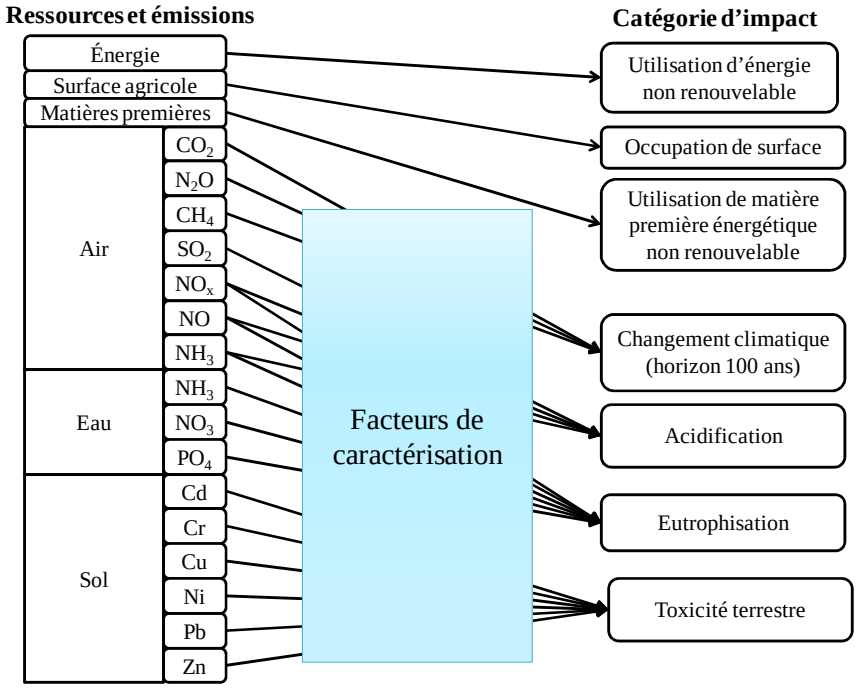

Figure 2. Les ressources et les émissions agrégés (après multiplication par des facteurs de caractérisation, pour la plupart) par l'outil EDEN (van der Werf et al. 2009) pour estimer des impacts environnementaux des exploitations laitières.

Les premières trois étapes offrent une meilleure communication de la prédiction des impacts potentiels, qui est interprétée dans la dernière étape pour fournir des informations transparentes à la prise de décision. Cependant, plusieurs sources d'incertitude associées avec la qualité des données, la différence individuelle et le choix des méthodes, ..., affectent les prédictions de l'ACV.

1.2.2. Une limitation de la mise en œuvre de l'ACV

Bien que l'ACV soit bien définie et largement appliquée pour l'évaluation des impacts environnementaux en agriculture, il existe certaines limites (sources d'incertitude) sur la mise en œuvre de l'ACV (Guinée et al. 2002). Par exemple, la réalisation de l'ACV implique un certain nombre d'hypothèses sur les choix des valeurs, des modèles de calcul et des méthodes d'allocation, … Les hypothèses arbitraires peuvent être une source d'incertitude en ACV (De Schryver et al. 2013; Hertwich et al. 2000). La méthodologie ACV ignore souvent les informations temporelles et spatiales qui ont des influences sur l'évaluation des impacts (Potting and Hauschild 1997; Reap et al. 2008). Par exemple, les facteurs de caractérisation pour les GES montrent de grande différence en fonction du temps et de la localisation (Huijbregts 1998; Röös and Josefine 2013).

Basset-Mens et al. (2009) ont considéré l'incertitude issue du choix des horizons temporels d'impact en utilisant les facteurs de caractérisations pour 20, 100 et 500 ans dans une analyse ACV de la production laitière en Nouvelle-Zélande. Une autre source d'incertitude principale est issue des données utilisées en ACV. La variabilité des données des exploitations (Henriksson et al. 2011), le manque des données pour cause de limites de mesure ou sources inaccessibles (Crosson et al. 2011) et les données de mauvaise qualité (Weidema and Wesnaes 1996) peuvent intervenir sur la qualité de la réalisation de l'ACV. Par exemple, IPCC (2006a) fournit des méthodes (de simple à complexe) pour calculer les émissions des GES dans des systèmes d'élevage. Le choix de méthodes dépend de la disponibilité des données qui sont variées en fonction de la variabilité des données de l'exploitation et de l'incertitude sur les facteurs d'émission. Dans ce cas, le manque de données spécifiques limite le choix des méthodes et influe les résultats estimés de l'ACV. De plus, une ACV agricole est plus compliquée que celle en industrie. Par exemple, un système agricole n'est pas un « pur » utilisateur des ressources naturelles, mais certaines ressources agricoles (ex., fertilité des sols, graines et bétails) sont autoproduites au sein du système (Haas et al. 2000). Donc la balance des ressources doit être considérée proprement à l'intérieur du système. Par ailleurs, les systèmes agricoles sont souvent interconnectés, et un changement dans un système (ex., système de la culture pour produire les aliments animaux) peut influer un autre (ex. système d'élevage) (Harris and Narayanaswamy 2009). De ce fait, la maîtrise de ces limites (incertitudes) peut améliorer la faisabilité et la crédibilité de la méthodologie ACV.

1.3 Définition du problème

Ignorée depuis longtemps, la prise en compte de l'incertitude dans les résultats de l'ACV est devenue un sujet de préoccupation, et des articles focalisent sur cette question (Benetto 2005; Geisler et al. 2005; Maurice et al. 2000). Bien que l'analyse des incertitudes soit bien définie et recommandée au sein de l'ACV (IPCC 2006b; ISO 14040 2006), l'intégration des incertitudes dans l'ACV est encore limitée (Reap et al. 2008), mais augmente avec le temps (Ciroth 2004). L'approche probabiliste, dans laquelle un jeu de données d'entrée est caractérisé par des distributions probabilistes, permet d'estimer leurs influences sur les résultats à travers de la simulation de Monte Carlo (MCS). Cette approche est la plus utilisée dans l'ACV pour analyser l'incertitude (Baker and Lepech 2009; Lloyd and Ries 2007). Par exemple, Payraudeau et al. (2007) l'ont utilisée pour estimer l'incertitude sur les pertes d'azote dans une ACV des exploitations en Bretagne.

Actuellement, des logiciels de l'ACV (ex., SimaPro, Gabi, CMLCA) offrent la possibilité de faire de l'analyse probabiliste à partir de données présentant statistiquement des incertitudes (ex., écart type), qui se trouvent de plus en plus dans des bases de données ACV (ex., *ecoinvent*). Cette approche, cependant, considère les paramètres comme indépendants, alors qu'ils ne le sont pas dans certains cas réels. De plus, la forme de distribution (ex. normale) et les paramètres nécessaires (ex., moyen, écart type) pour pouvoir faire varier les variables sont souvent inconnus, voire estimés de façon imprécise. D'autres approches plus complexes (ex., intervalle flou (Tan 2008), propagation d'erreur par des expansions des séries de Taylor (Ciroth et al. 2004)) commencent à apparaître aussi, mais leur complexité rend leur utilisation marginale. Les différentes méthodes utilisées en ACV pour décrire et propager l'incertitude ont pour le moment très peu cherché à différencier les types d'incertitude mais au contraire à les agréger. Plus de recherche est donc nécessaire pour faire sauter les verrous de l'analyse d'incertitude en ACV: identification, estimation et hiérarchisation des sources d'incertitude; développement de méthodes pour visualiser les sources différentes et leurs impacts relatifs sur l'incertitude globale; et démarche pour prendre en compte des incertitudes lors de la prise de décision.

1.4 Objectifs et structure de la thèse

Les objectifs de la thèse porte sur (1) l'identification et la classification des incertitudes dans des systèmes agricoles, notamment le système d'élevage (car le plus complexe et présentant le plus de processus interdépendants), (2) l'analyse de la représentation de ces incertitudes et (3) l'analyse de leurs influences sur l'incertitude globale des indicateurs d'impact évalués par l'ACV. Ce travail a été réalisé en utilisant un jeu de données récolté pour et généré par l'outil d'analyse EDEN, qui est un outil ACV permettant d'évaluer des impacts environnementaux des exploitations laitières (van der Werf et al. 2009). Cette thèse comporte six chapitres (Fig. 3): le chapitre 1 (celui-ci) présente le contexte général et la problématique agro-environnementale, l'ACV agricole, et les objectifs de la

thèse. Le chapitre 2 est une recherche bibliographique sur les définitions des incertitudes différentes et les méthodes pour représenter et propager ces types d'incertitude ; ce chapitre a pour objectif de guider les analystes ACV à choisir les méthodes appropriées pour l'analyse des incertitudes. Une fois les sources d'incertitude classifiées, les chapitres d'après se focalisent sur l'analyse de l'incertitude paramétrique et la variabilité en suivant cet arbre de décision. Dans le chapitre 3, la MCS classique est appliquée pour estimer des impacts environnementaux potentiels des exploitations laitières dans une étude ACV en considérant l'incertitude paramétrique et la variabilité. De plus, la distinction entre l'incertitude paramétrique et la variabilité ainsi que la limitation de la méthode MCS sont discutées. D'une part, cette démarche souligne la différence entre l'incertitude paramétrique et la variabilité, qui peut provoquer la recherche pour un alternatif à l'approche probabiliste pour représenter l'incertitude paramétrique. De l'autre part, elle révèle une des limites de l'application de la MCS classique (c.-à-d., la prise en compte de la corrélation). Donc, le chapitre 4 se focalise sur le contrôle des corrélations entre des variables d'entrée afin d'améliorer la précision de la méthode MCS. Le chapitre 5 intègre des méthodes différentes, pour analyser l'incertitude paramétrique et la variabilité (intervalle flou et distribution probabiliste, respectivement), basé sur la recherche du chapitre 2. Les impacts potentiels sont représentés sous forme de structure de Dempster-Shafer. Enfin, le chapitre 6 synthétise le travail de la thèse et discute ses limites et les perspectives pour la recherche future.

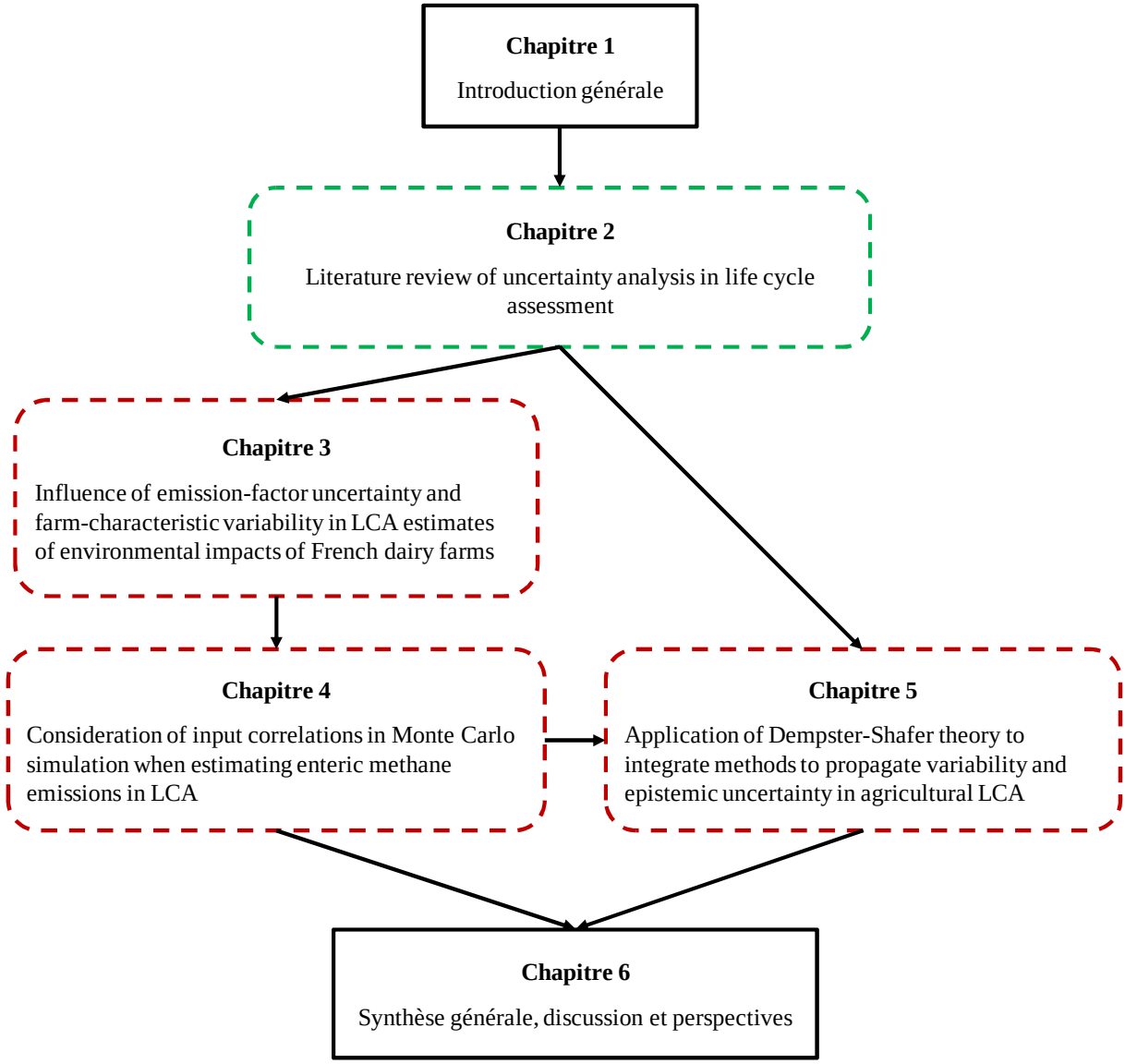

Figure 3. Schéma de la structure de la thèse

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Chapitre 2.
Literature review of uncertainty analysis in life cycle assessment

In general, LCA, as a systematic tool for assessing the environmental impacts of product system during its life cycle, is used to support decisions. The assessment process integrates multiple mathematical models to estimate resource consumption and pollution emissions. Hence, the confidence in LCA results relies on having selected appropriate models and data. However, these requirements may not be attained due to the existence of uncertainty.

Uncertainty is a phenomenon that describes a lack of knowledge about a studied system. This state of knowledge contains inherent characteristics of the specific individual or system (variability) and measurements of these characteristics (epistemic uncertainty). Uncertainty analysis attempts to capture uncertainty in LCA to support decision-making with an acceptable confidence level. The objective of this study is to review classifications of uncertainty and various methods to represent and propagate uncertainties in previous studies, and to propose a guideline for choosing appropriate methods of uncertainty analysis in LCA studies.

2.1 Terminology of uncertainty

Uncertainty can be conceptualized as a state of having limited scientific knowledge. Many authors have addressed the classification and terminology of uncertainty (Baker and Lepech 2009; Benetto 2005; De Rocquigny et al. 2008; Huijbregts 1998a; Merz and Thieken 2005; Morgan and Henrion 1992; US EPA 1992, 1996; Vose 2008; Walker et al. 2003). Although they defined uncertainty in a variety of ways, most concurred that uncertainty can be divided into two types according to its nature: variability and epistemic uncertainty.

Variability refers to the inherent property of individuals in the real world. It is due to natural heterogeneity in physical phenomena, and it is not reducible. It has also been called “aleatory”, “stochastic”, “objective” or “irreducible” uncertainty.

Epistemic uncertainty results from incomplete knowledge about the system studied. It is defined as the lack of knowledge, imprecision, ignorance and human errors. Thus, it is reducible by acquiring new knowledge or expert opinions or improving measurement accuracy. It has also been called “subjective” or “reducible” uncertainty.

Some authors defined epistemic uncertainty only as lack of knowledge, excluding imprecision and ignorance of information. For example, Benetto (2005) considered imprecision due to measurement errors (bias) as an independent source of uncertainty apart from uncertainty and variability. Indeed, imprecision and ignorance may influence estimate of variability and thereby influence results.

The importance of distinguishing variability from epistemic uncertainty is commonly emphasized in uncertainty analysis. Morgan and Henrion (1992) argued that it is important to

distinguish types and sources of uncertainty, whose variety may generate confusion. Thompson (2002) stated that the distinction between uncertainty and variability was important in risk management and communication, because knowing variability leads to better understanding the distribution of risk, and knowing uncertainty helps decision makers seek appropriate information and improve systems.

Although variability and epistemic uncertainty are clearly distinguished by their definitions, application of approaches for uncertainty analysis is still limited in practice at this level of classification. Taking both variability and epistemic uncertainty into account with a single probability distribution may result in a loss of information about the proportion of the distribution in results due to randomness and the proportion due to ignorance about system (Vose 2008). Therefore, more detailed identification and prioritization of sources of uncertainty is helpful for choosing the most relevant methodologies to quantify different types of uncertainty (Baker and Lepech 2009; De Rocquigny et al. 2008).

2.2 Sources of uncertainty

Uncertainty can be classified according to the sources of uncertainty. Heijungs and Huijbregts (2004) compared classifications of uncertainty, and stated that a classification is useful if it distinguishes between sources and types of uncertainty. The principal sources of epistemic uncertainty in LCA come from three sub-categories: parameter, model and scenario (Walker et al. 2003; WHO 2008). As for variability in LCA, Huijbregts (1998a) classified three sub-categories: spatial, temporal and "sources and objects" (due to the use of different technologies).

Parameter uncertainty is associated with data and methods to calibrate parameters in LCA models (Walker et al. 2003). It reflects incomplete knowledge about the true values of parameters. Inaccuracy, unrepresentativeness and lack of data are common raisons of parameter uncertainty (Huijbregts 1998a). In LCA, parameter uncertainty is considered as the main source uncertainty in most studies, including uncertainty in inventory data or, in impact assessment, uncertainty in characterization factors (Lloyd and Ries 2007). For example, inventory analysis is affected by poor data quality (inaccuracy), while the use of data from a different context may cause uncertainty (unrepresentativeness) (Bjorklund 2002; Reap et al. 2008). In addition, certain impacts such as biodiversity and human toxicity are difficult to estimate due to lack of data (Finnveden 2000). Moreover, uncertainty in parameter distributions (Heijungs and Frischknecht 2005) and a lack of information about correlations between input parameters remains a challenge in most LCA studies (Heijungs and Huijbregts 2004; Payraudeau et al. 2007).

Model uncertainty is defined as lack of knowledge about mechanisms of the system studied. It is due to simplification of models without considering parameters or ignorance of dependency among model parameters (WHO 2008). In LCA, model uncertainty results from the loss of

temporal and spatial characteristics in the model, assumptions of linear relations in impact assessment and calculation of characterization factors with simple models (Huijbregts 1998a). For example, LCA models that represent specific properties of substances can estimate environmental impacts more realistically than models based on general properties of the substances, but such detailed models are only available for a few substances. Hence, the lack of precise information about the substance-specific models may increase model uncertainty (Wegener Sleeswijk and Heijungs 1996). Moreover, univariate and multivariate models usually provide more realistic results than linear regression (Moreau et al. 2012).

Scenario uncertainty (uncertainty due to choice) is associated with the information used to define scenarios. It indicates that choices made in the scenario may reflect the reality of the system studied. Scenario uncertainty arises when defining objectives of the LCA and choosing data and models to attain them. It also involves allocation methods used in the inventory analysis, waste-handling approaches, and differences in characterization factors in time or space (Huijbregts et al. 2003). These scenario choices can have considerable impacts on the outcomes of LCA studies (Wardenaar et al. 2012). Scenario analysis and the theory of combination of evidence are used to assess this type of uncertainty (Morgan and Henrion 1992; Sentz and Ferson 2002). Standardization of processes (Guinée et al. 2002; ISO 14040 2006; Lindfors 1995) and expert judgment help reduce scenario uncertainty in LCA (Huijbregts 1998a).

Spatial variability is associated with the variation introduced by geographic differences in the system studied. In most LCA studies, environmental interventions are aggregated in impact assessment without spatial differentiation (a “site-generic” approach), which may introduce uncertainty in impacts of certain impact categories due to lack of site-specific data (Ross et al. 2002). For these impact categories, the absence of spatial differentiation may decrease the credibility of LCA. On the other hand, a site-specific approach can lead to unnecessary complex, or even biased, evaluation of impacts at a global scale. Potting and Hauschild (1997) argued that a site-dependent approach using spatial modeling (i.e., incorporating spatial factors in models) can avoid the limits of two approaches (site-generic and site-specific). Thus, spatial differentiation factors need to be developed in LCA (Hauschild 2006).

Temporal variability is associated with variation introduced by temporal changes in the system studied. This variation can be due to a difference over time in factors modeled. For example, large variability in emission factors was observed over time in Swedish paper plants (Hanssen and Asbjørnsen 1996). In addition, temporal variability in characterization factors, caused by the lifetime of a reference substance, can be assessed by choosing different time horizons (Huijbregts 1998a). This source of temporal variability can be avoided by choosing appropriate

characterization factors for short-term or long-term impact assessment (scenario uncertainty). Also, inventory data are commonly collected annually, thus considering data over years may create another source of temporal variability. In such a case, the means and variances of these data can be estimated to represent the variability during the time period.

Variability between sources and objects is associated with inherent variation among different technologies used to produce the same material or with differences between objects that determine the environmental impacts (Bjorklund 2002). Inherent differences in input variables may influence potential impacts. For example, large variation in the carbon footprint of milk resulted from a large variation in milk yields, feed dry-matter intake and nitrogen excretion of dairy farms in Sweden (Henriksson et al. 2011). Indeed, since variability between sources and objects represents the natural heterogeneity of individuals (e.g., farms, factories, humans, animals), it can be called natural variability and modeled using a probabilistic approach.

Apart from the above six types of epistemic uncertainty and variability, some have identified uncertainty in linguistic imprecision, ambiguity and disagreement (Bedford and Cooke 2001; Benetto 2005; Morgan and Henrion 1992). In LCA, these types of uncertainty are often dealt with arbitrarily using expert judgment (Krueger et al. 2012; Reap et al. 2008). Bjorklund (2002) included poor data quality (e.g., data inaccuracy or gaps, unrepresentative data), epistemological uncertainty, mistakes and estimation of uncertainty itself in the classification of uncertainty of Huijbregts (1998a). By definition, all of these types of uncertainty can be included as main sources of epistemic uncertainty. Indeed, the classification of uncertainty of Huijbregts (1998a) is commonly applied in most uncertainty analysis in LCA studies (Leroy and Lasvaux 2013; Lloyd and Ries 2007). Huijbregts (1998a) also showed examples of types of uncertainty in the phases of LCA (Table 1), indicating that inventory analysis, characterization and weighting process are the most important sources of all types of uncertainty. A variety of approaches has been developed to analyze uncertainty given available information (Benetto 2005; Bjorklund 2002; Ciroth et al. 2004; Huijbregts 1998a, b; Huijbregts et al. 2003; Imbeault-Tetreault et al. 2013; Lloyd and Ries 2007; Morgan and Henrion 1992; Tan 2008; Vose 2008; Weidema and Wesnaes 1996).

Table 1. Examples of types of variability and epistemic uncertainty in the phases of LCA (Huijbregts 1998a)

	Phase					
Uncertainty	Goal and scope	Inventory	Choice of impact categories	Classification	Characterization	Weighting
Parameter uncertainty		Inaccurate emission measurements			Uncertainty in life times of substances	Inaccurate normalization data
Model uncertainty		Linear instead of non-linear modeling	Unknown impact categories	Unknown contribution to impact category	Characterization factors are not known	Weighting criteria are not operational
Uncertainty due to choices	Functional unit	Use of several allocation methods	Leaving out known impact categories		Using several characterization methods within one category	Using several weighting methods
Temporal variability		Differences in yearly emission inventories			Change in temperature over time	Change of social preferences over time
Spatial variability		Regional differences in emission inventories			Regional differences in environmental sensitivity	Regional differences in distance to targets
Variability between objects/sources		Differences in emissions between factories that produce same product			Differences in human characteristics	Differences in individual preferences, when using panel method

2.3 Approaches for uncertainty analysis

Uncertainty analysis is defined as a procedure to quantity the uncertainty in the results of LCA due to input-variable uncertainties and their influences on reliability of the results (ISO 14044 2006). As mentioned in the previous section, different approaches to uncertainty analysis exist. Morgan and Henrion (1992) introduced a terminology of uncertainties and existing approaches to deal with uncertainties. Huijbregts (1998a, b) reviewed available approaches to deal with types of variability and epistemic uncertainty in LCA. Probabilistic approaches are widely used to analyze parameter uncertainty and variability in LCA (Baker and Lepech 2009), while other approaches, such as fuzzy-interval analysis (Dubois and Prade 1991), analytical arithmetic (Heijungs 1996), Bayesian approaches (Hoff 2009) and Dempster-Shafer theory (Dempster 1966) can also be considered, depending upon the goal of the study, the availability of information or the suitability of the uncertainty analysis approach. In addition, uncertainty due to choice can be analyzed by scenario modeling, standardization and expert judgment. Model uncertainty and spatial/temporal variability can be addressed by modeling

approaches (e.g., linear/non-linear regression, multi-media modeling) (Huijbregts 1998a). This section describes and discusses approaches for uncertainty analysis.

2.3.1 Probabilistic approach

Probability theory is a mathematical theory concerned with the analysis of random phenomena (Felleb 1957). There are two basic views of probability. The *frequentist* view considers probability as the frequency that a random event occurs, while the *subjective* view considers it as a person's degree of belief that an event will occur based on his/her experiences and opinions (Morgan and Henrion 1992). The ISO standard (Bipm et al. 1995) distinguished these two views of evaluation of uncertainty in measurement as Type A (based on statistical analysis of observations) or Type B (based on the degree of belief). These distinct interpretations allow variability and parameter uncertainty to be distinguished.

Based on the frequentist view, the probability distribution assigns a probability of any possible event in a random experiment. Suppose that random variable *X*, which is an element of all real numbers ($\mathcal{R}$), has a probability *Pr*(*x*) of having value *x*. In the discrete case (the number of random variables is countable), there exists a discrete probability distribution function (PDF):

$$Pr(x) = \sum_{x \in X} d(x), with \sum_{x \in \mathcal{R}} d(x) = 1 \quad \text{Eq. 1}$$

where *d(x)* is the frequency of observations of *x*, i.e. the number of observations of *x* divided by the number of trials.

The discrete distributions characterize the countable random variables. For example, throwing a die to have an equal probability of each of six values (from 1 to 6) is a discrete case. Common discrete distributions are Bernoulli, Binomial and Poisson distributions. However, the number of observations is sometimes uncountable due to infinite numbers or measurement limits. In such cases, the continuous PDF can be used to calculate the probability of random variable *x* falling into a given interval [a, b]:

$$Pr[a \leq x \leq b] = \int_a^b f(x) * dx, with \int_{-\infty}^{\infty} f(x) * dx = 1 \quad \text{Eq. 2}$$

where *f(x)* is the PDF of observing *x*, and $\mathcal{R}\ is\ [-\infty, \infty]$.

The continuous PDF can be described by its cumulative distribution function (CDF):

$$F(x) = Pr(X \leq x) = \int_{-\infty}^{x} f(x) * dx, for\ all\ X \in \mathcal{R} \quad \text{Eq. 3}$$

which represents the probability that random variable *X* takes on a value less than or equal to *x*.

In LCA, the most frequently assumed distributions are uniform, triangular, normal (Gaussian) and lognormal (Heijungs and Frischknecht 2005; Lloyd and Ries 2007) (Fig. 1). The properties of these distribution forms are given by Morgan and Henrion (1992):

- **Uniform distribution**: it is one of the simplest continuous distributions, defined only by minimum and maximum values. It is generally used when the shape of distribution is unknown; thus, it assumes that any value in the minimum-maximum range has equal probability, as stated in Laplace's analytic theory of probabilities (de Laplace 1820).

- **Triangular distribution**: it can be used when one value occurs more often than others within the minimum-maximum range. A trapezoidal probability distribution is a special case of the triangular distribution in which the mode is expressed as an interval. It can be symmetric or asymmetric depending on the location of the most likely value(s). When uncertainty is high, triangular distribution can be transformed to log-triangular distribution (Morgan and Henrion 1992).

- **Normal (Gaussian) distribution**: it is a commonly used continuous distribution based on the mean and variance of a population. It is widely useful because of the central limit theorem (given a well-defined mean and variance, the arithmetic mean (or the sum) of a large number of independent random variables from the same population is approximately normally distributed). Thus, the normal distribution can be used to model natural variability when the mean and variance of population are known (Smith 2002). However, it may be not appropriate for representing some strictly positive variables if three times the standard deviation is larger than the mean (i.e., there are negative values according to empirical rules[1]). In this case, a truncated normal distribution can be applied to avoid negative values (De Rocquigny et al. 2008). The symmetry of the normal distribution also limits its application when the variable has an asymmetric distribution.

- **Lognormal distribution**: it is applied to represent the probability of random variable whose logarithm is normally distributed. It provides good representation of physical quantities that are only positive and non-zero. Due to its long tail, the lognormal distribution represents extreme events better than the normal distribution. It yields values with a skewed distribution, which is more appropriate for many LCA input variables (Frischknecht et al. 2005; Geisler et al. 2005; Huijbregts et al. 2003).

The more common use of normal and lognormal distributions in LCA is to quantify the data quality associated with Data Quality Indicators (DQIs), developed by Weidema and Wesnaes (1996).

Apart from the probability distributions mentioned above, there exist other useful but little-developed distributions (Lloyd and Ries 2007). For example, the beta distribution is a family of continuous distributions of variables limited to the interval [0, 1] (transformable to any closed interval)

[1] Empirical rule: when a standard normal model is used in statistics, about 68% of values fall within one standard deviation from the mean, about 95% of values fall within two standard deviations from the mean, and almost all the values (about 99.7%) fall within three standard deviations from the mean. It is also called the "68-95-99.7 rule".

and characterized by two positive shape parameters, α and β (Bedford and Cooke 2001). It is useful for representing uncertainty in variables whose distributions and associated parameters are not available but whose shape parameters and range endpoints can be specified; thus, it can be applied to model inventory data in LCA (Canter et al. 2002; Kennedy et al. 1996). In addition, the beta distribution is used as a prior distribution in Bayesian theory to determine the posterior distribution (Hoff 2009). Otherwise, t-distributions (Bjorklund 2002) and PERT distributions (Maurice et al. 2000) are more appropriate for representing small sample sizes than normal distributions and triangular distributions, respectively. Finally, the Poisson distribution predicts the number of discrete events that occur in a time period; thus, it can be used to represent temporal variability in a time series (Morgan and Henrion 1992).

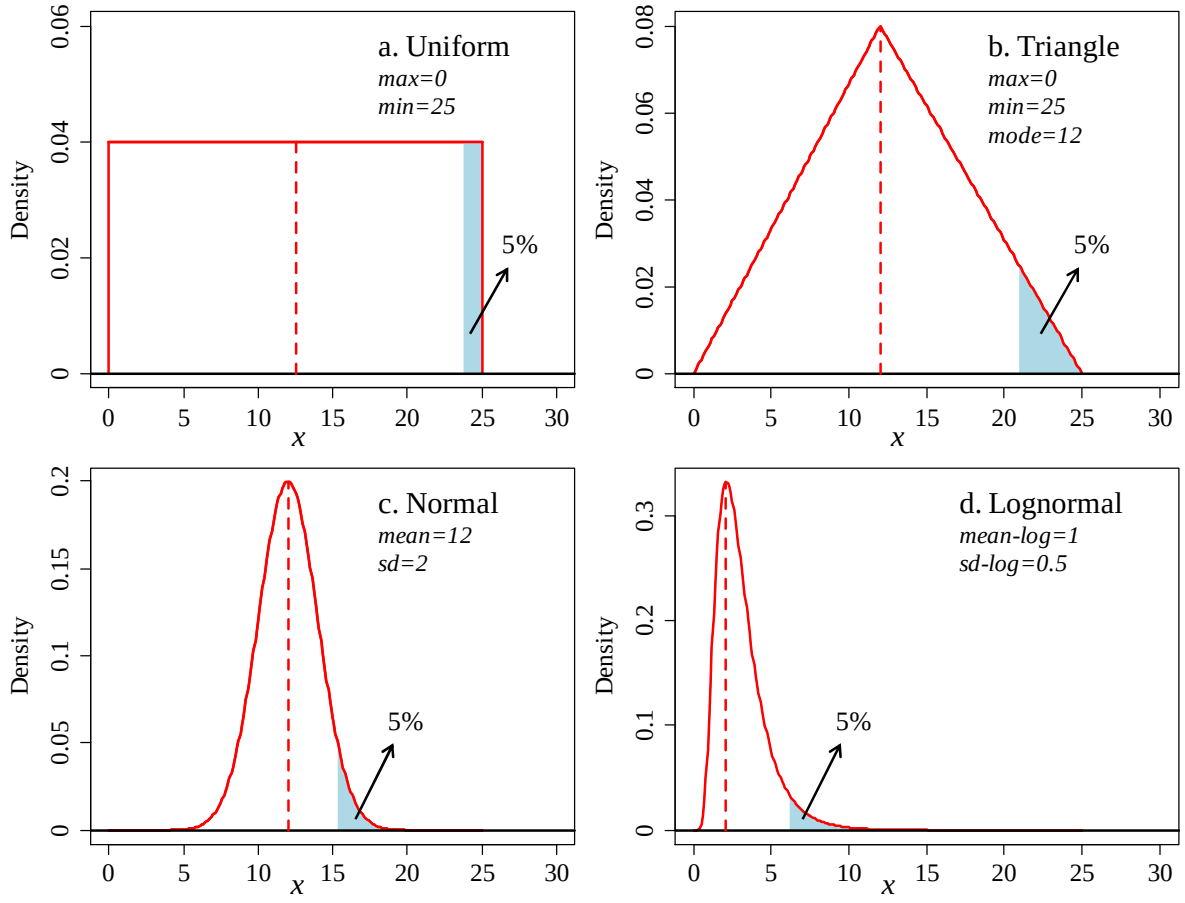

Figure 1. Four principal continuous probability density distribution used in LCA: a. uniform, b. triangular, c. normal, d. lognormal. Parameters necessary to characterize each distribution are given (sd: standard deviation; mean-log: mean of logarithm of variable x; sd-log: standard deviation of logarithm of variable x). Blue zones indicate the probability that the value of a random variable x exceeds that limit. Dashed lines indicate the most likely value of each distribution, except for the uniform distribution, in which the dashed line indicates the median.

Parameterization of probability distributions is a delicate issue that depends on what data are available (Slob 1994; Venkatesh et al. 2011). Weidema et al. (2013), however, argued that the choice of distribution has limited influence on the overall uncertainty of a product system due to the aggregation of a large number of independent variables, which results in a normally distributed result according to the central limit theorem (Vose 2008). Thus, when the specific shape of distribution of individual parameters in LCA is unknown, some authors suggest using the same distribution for all of them to avoid bias among them (Geisler et al. 2005). Doing so, however, is questionable, because choosing different shapes of distribution may result in different outcomes, and statistically based parameterization is more appropriate for approximating the distribution of individuals (Cooper et al. 2012). Bjorklund (2002) and Benetto (2005) explained that parameterization of uncertainty distributions should be determined from a large sample of data points. Specific distributions of individual parameters can be estimated by goodness-of-fit tests or maximum likelihood estimation (Firestone et al. 1997; IPCC 2000; Sankararaman and Mahadevan 2011; Sonnemann et al. 2003). Measurements are frequently unavailable in LCA, however; so, literature information and expert judgment can be incorporated to determine shapes of distributions and their associated parameters (Albert et al. 2012). For example, Weidema et al. (2013) recommended using the lognormal distribution to represent inventory data with uncertainty, in which data quality is considered as additional uncertainty and transformed into a quantitative indicator (pedigree matrix) based on expert opinions. Slob (1994) developed an arbitrary dispersion factor to characterize the parameters of a lognormal distribution and considered it a useful factor when data were scarce. Hence, the introduction of expert judgment is based on the subjective view of probability.

Based on the subjective view, the occurrence of an event (e.g., value of a variable) is not seen as random, but as the probability of what the true value of a variable might be. According to this interpretation, the PDF or CDF can be used to describe epistemic uncertainty in model parameters and in the model itself. However, Huijbregts (1998b) argued that uncertainty factors and distribution shapes may not represent a “real-life” case if they are entirely arbitrary. Therefore, combining expert opinions in uncertainty modeling should be treated carefully (Krueger et al. 2012). Sometimes both empirical and subjective information about a physical system exists, and it is desirable to use both sources of information to make decisions. For example, when relevant data are not available to determine the shape of distribution, a Bayesian approach (Hoff 2009) can be used to combine the empirical data with expert opinion to adjust the distribution.

Many authors (Basset-Mens et al. 2009; Geisler et al. 2005; Henriksson et al. 2011; Maurice et al. 2000; Payraudeau et al. 2007; Steen 1997) have applied probability theory to turn deterministic models into stochastic models in LCA-based studies, which can capture epistemic uncertainty and variability. Some of them also distinguished both types of uncertainty in the analysis. For example,

Basset-Mens et al. (2009) represented variability and epistemic uncertainty of an average New Zealand dairy farm using its standard deviation (SD) and standard error of mean (SEM), respectively. Geisler et al. (2005) highlighted the difference between variability and parameter uncertainty and argued that both types of uncertainty can be propagated into LCA results well using probabilistic simulation (Monte-Carlo simulation). However, it is sometimes not appropriate to use probability distributions when little information is available to determine them. Although the assumed distribution could be applied with little information, it seems too arbitrary, even with Bayes's rule, which is currently not used much in LCA (Lo et al. 2005).

Bayes's theorem (Bayes 1763) is a mathematical interpretation of probability with subjective evidence. Based on it, expert opinions (defined as prior distribution) can be combined with the distribution of empirical data (likelihood function) to determine a probability distribution (posterior distribution) of an event by following Bayes's rule (Hoff 2009). Therefore, approach updates available information with the belief of experts.

Given a numerical value of $\theta \in \Theta$, there is a prior distribution $p(\theta)$ to describe the belief that θ represents the true value of population. Assuming θ is true, the empirical sample (y) can be modelled as a conditional probability distribution $p(y|\theta)$. Thus the posterior distribution $p(\theta|y)$, which describes the belief that θ is true given the empirical sample y, is obtained according to Bayes's rule:

$$p(\theta|y) = \frac{p(y|\theta) * p(\theta)}{p(y)}$$

2.3.2 Imprecise probability

When the value of a parameter is expressed as a set of possible values with unknown distribution, the state of knowledge about this parameter is called "imprecise". In this situation, making an arbitrary assumption may not represent the "real" world accurately. To overcome this limit, "imprecise probability" was developed as a generalization of classic probability (Walley 1991). It assigns an interval of probability to describe uncertainty in an imprecise manner. For an uncertain variable X ($X \in \mathcal{R}$), the PDF assigns a probability to each x ($0 \leq Pr(x) \leq 1$). When *Pr(x)* is not precisely known and can only be expressed as an interval of lower and upper probabilities, such as $\left[\underline{Pr}(x), \overline{Pr}(x)\right]$, there is imprecision about the probability of variable *X*, and the true probability falls into this interval:

$$\underline{Pr}(x) \leq Pr\ (x) \leq \overline{Pr}(x), x \in \mathcal{R} \qquad \text{Eq. 4}$$

Likewise, the CDF of *X* with imprecise probability is expressed as:

$$\underline{F}(x) \leq F(x) \leq \overline{F}(x), x \in \mathcal{R} \qquad \text{Eq. 5}$$

Risk analysts debate the use of imprecise probability in uncertainty analysis. Some believe that imprecise probability might confuse people due to its interpretation of imprecise results. For example, Lindley (2000, 2013) argued that imprecise probability leads to unnecessarily complicated statistical

procedures. Moreover, the subjective (or Bayesian) approach makes it easier for a decision maker to rank different sources of opinion with a single estimate of the probability (Soundappan et al. 2004). Others, however, state that making decisions in risk analysis based on imprecise results should not follow the subjective (or Bayesian) view of probability if expert judgment cannot provide more precise expression, because the subjective approach ignores imprecision (Aven and Zio 2011; Caselton and Luo 1992; Ferson and Tucker 2006; Hall 2006; Rinderknecht et al. 2012). Their debate raises questions about how to choose between methods requiring more empirical information vs. those requiring less, but more imprecise, information, according to the interests of practitioners and the confidence level accepted by decision makers. When both precise and imprecise information appear in the same study, combining both methods may provide a useful and practical interpretation of results. For example, information about variability is best conveyed by a single probability distribution, while information about imprecision is best conveyed using families of probability distributions (Walley 1991). Ferson et al. (2002) used imprecise CDF (Eq. 5) to demonstrate a graphical box, called a "probability box" or *p-box*, in which the true distribution of an uncertain variable is located but unknown due to imprecision. The *p-box* constructs an interval probability distribution in which $\underline{F}(x)$ is the lower bound and $\overline{F}(x)$ is the upper bound. It is able to distinguish natural variability from epistemic uncertainty due to imprecision (Ferson and Ginzburg 1996). Moreover, different expressions of imprecision can be integrated in an imprecise probability distribution, such as fuzzy intervals (see section 2.3.4). For example, the parameters (i.e. mean, SD) of a probability distribution can be modeled by fuzzy membership functions (Arunraj et al. 2013). Therefore, imprecise probability is more flexible than classic probability without requiring precise knowledge about the distribution (e.g., exact estimates of parameters) in situations when imprecision cannot be ignored. Indeed, both of these approaches are based on probability theory, but other approaches to express uncertain quantities exist. In the following sections, we introduce two non-probabilistic methods: Dempster-Shafer theory and the fuzzy-interval approach.

2.3.3 Dempster-Shafer theory

Dempster-Shafer theory (DST) is a "mathematical theory of evidence" introduced by Dempster (1967) and further developed by Shafer (1976) to represent the state of knowledge, based on all available evidence. As a generalization of Bayesian probability (Dempster 1968), DST evaluates the degree of belief about the probability of a related claim based on two basic functions: the belief function (Bel) and the plausibility function (Pl), which are defined from the basic probability assignment (*bpa*), also called "mass". The properties of the *bpa* are:

$m: 2^{\Omega} \rightarrow [0, 1]$ Eq. 6

$m(\emptyset) = 0$ Eq. 7

$\sum_{A \in 2^{\Omega}} m(A) = 1$ Eq. 8

where 2^{Ω} is the power set that comprises all possible subsets, including the empty set $\emptyset$. *A* is a given set (called a "focal element") of the power set. Given a set *A*, its *bpa* (denoted *m(A)*) expresses the proportion of the available evidence which supports the belief that a particular element belongs to the set *A* only. Any additional evidence that supports the belief that a particular element belongs to a subset of *A* will change the degree of belief about the *bpa* of this subset. Hence, the *bpa* is measure of belief closely tied with the available evidence.

The belief function of *A* is defined as the sum of the *bpa* of all subsets (*B*) of *A* ($B \subseteq A$):

$$Bel(A) = \sum_{B \subseteq A} m(B), B \text{ is all of the subsets of } A, \text{and } B \neq \emptyset \quad \text{Eq. 9}$$

The plausibility function of *A* is defined as the sum of the *bpa* of any subset (*C*) of a power set, with the condition that the intersection of *C* and *A is a non-empty set* ($C \cap A \neq \emptyset$):

$$Pl(A) = \sum_{C \cap A \neq \emptyset} m(C), C \in 2^{\Omega}, \text{and } C \neq \emptyset \quad \text{Eq. 10}$$

In the probability distributions, each focal element of the uncertain parameter *X* can be expressed as an interval[2] ($[a_i, b_i]$) with m_i (where $a_i \leq b_i$ for all *i*). The set of all the intervals with their corresponding m_i can be expressed as:

$$\{([a_1, b_1], m_1), ([a_2, b_2], m_2), \ldots ([a_n, b_n], m_n)\}, where \sum_{a_i \leq b_i}^{n} m_i([a_i, b_i]) = 1, i = 1,2, \ldots, n \quad \text{Eq. 11}$$

For a discrete distribution, the belief and plausibility functions of uncertain parameter $X \in \mathcal{R}$ ($\mathcal{R}$ *is a real number*) can be obtained according to Eq. 3 as:

$$Bel(X \in \mathcal{R}) = \sum_{[a_i, b_i] \subseteq x} m([a_i, b_i]) \quad \text{Eq. 12}$$

$$Pl(X \in \mathcal{R}) = \sum_{[a_i, b_i] \cap x \neq \emptyset} m([a_i, b_i]) \quad \text{Eq. 13}$$

For a continuous distribution, the CDF of *X* can be expressed as $F(X \in]-\infty, x]), x \in \mathcal{R}$. Thus, the belief and plausibility functions of $X \in]-\infty, x]$ can be obtained as:

$$Bel(X \in]-\infty, x]) = \sum_{[a_i, b_i] \subseteq]-\infty, x]} m([a_i, b_i]) \quad \text{Eq. 14}$$

$$Pl(X \in]-\infty, x]) = \sum_{[a_i, b_i] \cap]-\infty, x] \neq \emptyset} m([a_i, b_i]) \quad \text{Eq. 15}$$

Next, Eq. 14 and 15 can be written as:

$$Bel(X \in]-\infty, x]) = \sum_{b_i \leq x} m([a_i, b_i]) \quad \text{Eq. 16}$$

$$Pl(X \in]-\infty, x]) = \sum_{a_i \leq x} m([a_i, b_i]) \quad \text{Eq. 17}$$

Properties of the belief and plausibility functions were given by Yager (1987):

$$Bel(A) \leq Pr(A) \leq Pl(A) \quad \text{Eq. 18}$$

$$Bel(A) = 1 - Pl(A^c) \quad \text{Eq. 19}$$

$$Pl(A) = 1 - Bel(A^c) \quad \text{Eq. 20}$$

$$Bel(A) + Bel(A^c) \leq 1 \quad \text{Eq. 21}$$

[2] The continuous probability distribution can be considered as the accumulation of many intervals by using a discretization technique. In statistics, "discretization technique" refers to the process of converting continuous intervals (e.g., *p-box*) to a set of discrete values or intervals with a corresponding *bpa*.

$$Pl(A) + Pl(A^c) \geq 1 \quad \text{Eq. 22}$$

where A^c is a complement set of *A*. According to their definitions and properties, the belief function measures the degree of belief that an event (or a claim about the "true" event) must occur, while the plausibility function measures the degree of possibility that an event (or a claim about the "true" event) could occur. With two functions, experts can conclude that the probability that an event occurs is at least *Bel(A)* and possibly as large as *Pl(A)*. The difference between *Bel(A)* and *Pl(A)* is defined as ignorance, which indicates the imprecision of evidence. When *Bel(A)=Pl(A)* (ignorance = 0), the evidence is perfect, and uncertainty is expressed by classic probability as *Pr(A)*. Given the relation between belief and plausibility functions (Eq. 19 and 20), one function can be calculated from the other.

Unlike classic probability (Bayesian) theory, which sometimes requires additional assumptions (e.g., the shape of prior distribution) beyond those already available in order to obtain a precise single-value probability, DST can represent the state of knowledge with imprecise information without such assumptions (Soundappan et al. 2004). For example, the belief and plausibility functions constitute a DST structure, which is similar to a *p-box*. Thus, the DST structure is often illustrated as being bounded by two CDFs (Fig. 2). In this way, Ferson et al. (2002) compared DST structure with the upper and lower bounds of imprecise probability. They demonstrated how DST functions can be converted given the two bounds of imprecise probability using a discretization technique (Kotsiantis and Kanellopoulos 2006), and concluded that any characterization and aggregation method can be used with both objects.

Besides using DST to express imprecise information, another important use of DST is to combine different independent and equally credible sources of evidence (i.e., information about the object gathered from multiple sources) (Dempster 1967; Moral and Del Sagrado 1998; Nau 2002; Sentz and Ferson 2002; Yager 1987). For example, models or scenarios coming from different sources of evidence are sometimes combined into a single expression when it is unknown which model or scenario is true. This single expression considers the uncertainty due to the choice of model or scenario. Ferson et al. (2002) compared methods to aggregate different sources of evidence, expressing their quantities as a DST structure or *p-box*. In this section, we describe four main operations: intersection, envelope, mixing, and Dempster's rule (and its modifications).

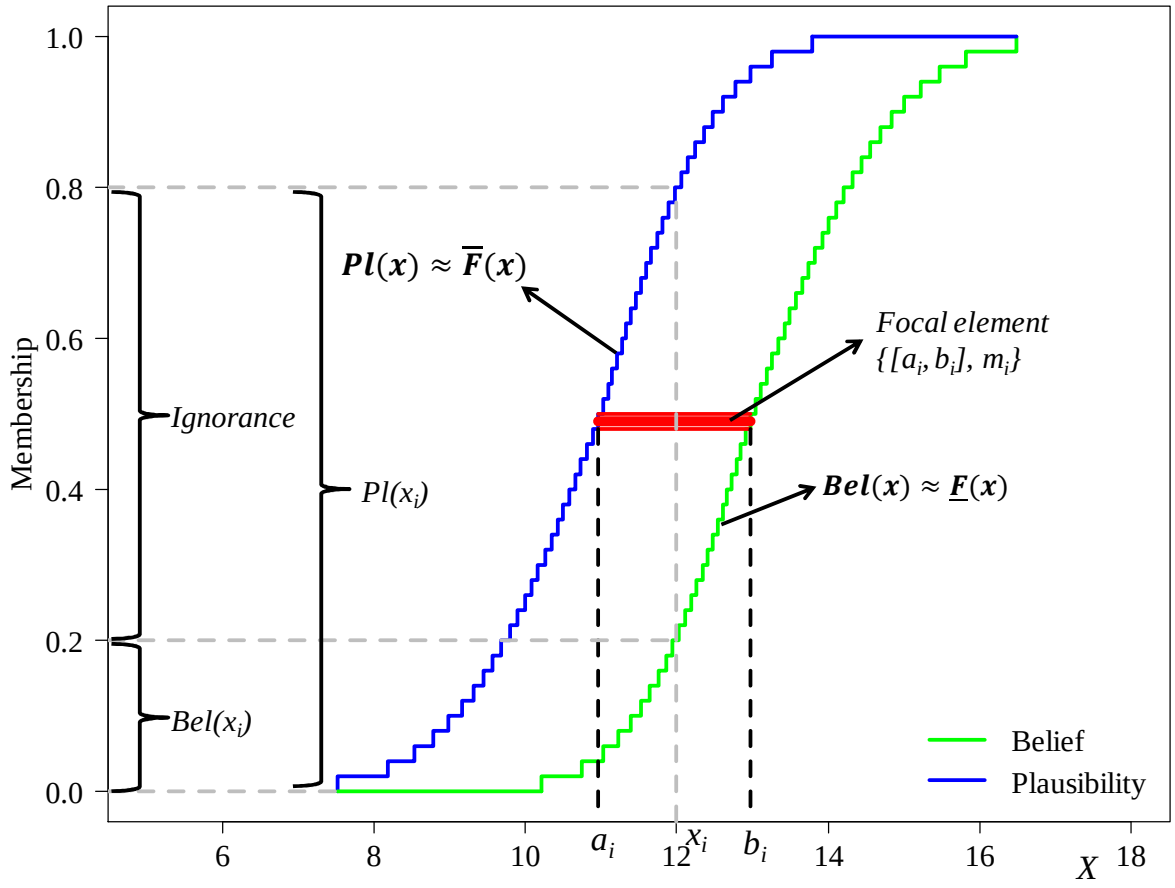

Figure 2. Dempster-Shafer structure of an uncertain variable *x*. The green and blue lines indicate the belief and plausibility functions, respectively. The red area indicates a focal element [a_i, b_i] associated with a basic probability assignment (m_i).

- **Intersection**

When each source of evidence comes with a strong claim that the quantity is sure to fall within given limits (e.g., interval, DST structure, imprecise probability, possibility distribution), intersection can be an appropriate operation. It defines overall uncertainty around the quantity as the smallest region in which all estimates agree. Suppose that there are *n* sources of evidence expressed as *p-boxes* (approximation of a DST structure): $F_1 = \left[\overline{F_1}, \underline{F_1}\right], F_2 = \left[\overline{F_2}, \underline{F_2}\right], \ \ldots, F_n = \left[\overline{F_n}, \underline{F_n}\right]$. Thus, the DST structure base on the intersection is defined as:

$$Bel(x) \approx \underline{F}^*(x) = max\ (\underline{F_1}(x), \underline{F_2}(x), \ldots, \underline{F_n}(x) \qquad \text{Eq. 23}$$

$$Pl(x) \approx \overline{F}^*(x) = min\ (\overline{F_1}(x), \overline{F_2}(x), \ldots, \overline{F_n}(x) \qquad \text{Eq. 24}$$

Since this method assumes that all sources of evidence are completely reliable (i.e., that they do not completely disagree), the intersection of all sources of evidence cannot be an empty set. Therefore, it is not appropriate to apply this operation when this assumption is not satisfied (i.e., there is complete

disagreement among the sources of evidence). If there are, the true value of the quantity could belong to any of the sources of evidence; thus, another operation (envelope) may be more appropriate.

- **Envelope**

When we know that at least one source of evidence contains the true distribution of the quantity, but do not know which one it is, the envelope operation should be used to combine estimates. It defines overall uncertainty around the quantity as the largest region in which any estimate is possible. Hence, given *n p-boxes*, $F_1 = \left[\overline{F_1}, \underline{F_1}\right]$, $F_2 = \left[\overline{F_2}, \underline{F_2}\right]$, …,$F_n = \left[\overline{F_n}, \underline{F_n}\right]$, the DST structure based on the envelope is defined as:

$$Bel(x) \approx \underline{F}^*(x) = min\ (\underline{F_1}(x), \underline{F_2}(x), \ldots, \underline{F_n}(x) = Bel(x) \quad \text{Eq. 25}$$

$$Pl(x) \approx \overline{F}^*(x) = \max\ (\overline{F}_1(x), \overline{F}_2(x), \ldots, \overline{F}_n(x) \quad \text{Eq. 26}$$

This operation is commonly used when the reliability of individual estimates is uncertain. Thus, any source of evidence could be the "truth". It provides a conservative estimate of the quantity since the DST structure based on the envelope maximizes the range of probability of the quantity. However, its broad estimate of uncertainty in the quantity might be useless or misleading for decision makers, because a few estimates with large intervals may dominate and bias the result.

- **Mixing**

When different sources of evidence have variability due to different times, places or situations, the mixing operation is appropriate. The simplest mixture uses the arithmetic mean. For *n p-boxes*, $F_1 = \left[\overline{F_1}, \underline{F_1}\right]$, $F_2 = \left[\overline{F_2}, \underline{F_2}\right]$, …,$F_n = \left[\overline{F_n}, \underline{F_n}\right]$, mixture is defined as:

$$Bel(x) \approx \underline{F}^*(x) = \left(\underline{F_1}(x), + \underline{F_2}(x) + \cdots + \underline{F_n}(x)\right)/n \quad \text{Eq. 27}$$

$$Pl(x) \approx \overline{F}^*(x) = \left(\overline{F}_1(x) + \overline{F}_2(x) + \cdots + \overline{F}_n(x)\right)/n \quad \text{Eq. 28}$$

Unlike an intersection operation, mixing can capture the differences in all conflicting sources of evidence believed to be reasonable. Like an envelope operation, mixing can combine two estimates whose intersection is empty, but it provides a narrower estimate because it averages sources of evidence (assuming equal weights) instead of maximizing them. It is also possible to combine estimates using different weights (i.e., unequally credible sources). Given *n p-boxes*, $F_1 = \left[\overline{F_1}, \underline{F_1}\right]$, $F_2 = \left[\overline{F_2}, \underline{F_2}\right]$, …,$F_n = \left[\overline{F_n}, \underline{F_n}\right]$, with weights w_1, w_2, ..., w_n, respectively, the weighted mixture is defined as:

$$Bel(x) \approx \underline{F}^*(x) = \left(w_1\underline{F_1}(x), + w_2\underline{F_2}(x) + \cdots + w_n\underline{F_n}(x)\right)/\sum w_i \quad \text{Eq. 29}$$

$$Pl(x) \approx \overline{F}^*(x) = \left(w_1\overline{F}_1(x) + w_2\,\overline{F}_2(x) + \cdots + w_n\overline{F}_n(x)\right)/\sum w_i \quad \text{Eq. 30}$$

The weighted mixture can overcome the influence of large but infrequent biases from some sources of evidence on the mixed estimate. Hence, the weight of each source is often determined according to its frequency, which depends on experimental samples or the degree of expert belief (Moral and Del Sagrado 1998; Nau 2002).

- **Dempster's rule**

Dempster's rule, the theoretical center of DST, is commonly applied in risk analysis and decision-making studies (Caselton and Luo 1992; Dubois and Guyonnet 2011; Sentz and Ferson 2002). Given two independent sources of evidence expressed by DST structures (focal elements of sources *B* and *C* with their own mass functions: m_i and m_j, respectively) for the same universal set *X*, the combination of *B* and *C* is:

$$m(A) = \frac{\sum_{B\cap C=A} m_i(B)m_j(C)}{1-K}, where\ K = \sum_{B\cap C=\emptyset} m_i(B)m_j(C)\ \ and\ \ i,j = 1,2,\dots,n \qquad \text{Eq. 31}$$

where *K* is called the degree of conflict, and *1-K* is a normalization factor used to exclude all conflicts ($B \cap C = \emptyset$) in the sources of evidence. The following example illustrates application of Dempster's rule to combine two imprecise discrete probabilities *B* and *C* (Table 2). With results from the intersection between two sources of evidence, we construct a DST structure of their combination according to Eq. 31 (Fig. 3). Using the same example, we also illustrate DST structures combined by the other three operations (Fig. 3). The envelope operation shows a wider bound of estimates, while the unweighted mixture averages estimates of both sources. Intersection and Dempster's-rule operations have the narrowest bounds because they consider only the agreement among sources.

Indeed, Dempster's rule allocates conflicts (i.e., empty sets resulting from intersection among the sources) to each focal element by normalizing the degree of conflict (Sentz and Ferson 2002). It is appropriate to use when there are relatively small conflicts among sources of estimates; however, its use is criticized when large conflicts exist. For example, if two sources of information conflict completely, the normalization factor 1-K equals 0, and Dempster's rule cannot be used. Zadeh (1986) showed that combining highly conflicting estimates with Dempster's rule might lead to counterintuitive results. Consequently, extensions of Dempster's rule have been developed to overcome this limit of application, such as Yager's modified Dempster's rule (Yager 1987), Inagaki's rule (Inagaki 1991), Zhang's center combination rule (Zhang 1994) and a disjunctive consensus rule proposed by Dubois and Prade (1992a). Even though the choice of combination rules depends on the sources of evidence and the application context, Sentz and Ferson (2002) compared them and concluded that Dempster's rule might be appropriate when there are small or irrelevant conflicts and all sources of evidence are highly reliable, while Yager's rule is better when high conflict cannot be ignored, because it does not use the normalization factor as a denominator (like Dempster's rule), but

attributes conflicts to the universal set *X*. More details can be found in their report (Sentz and Ferson 2002).

Table 2. Intersection of two sources of evidence *B* and *C* by Dempster's rule. Basic probability assignments (m_i and m_j) were calculated for each focal element (expressed as an interval with corresponding m_i and m_j) from the intersection of B and C.

	Source *B* (m_i)	$\boldsymbol{m_1}$	$\boldsymbol{m_2}$	$\boldsymbol{m_3}$
		[1, 5]	[2, 6]	[3, 7]
Source *C* (m_j)		0.2	0.4	0.4
$\boldsymbol{m_1}$	[2, 7]	[2, 5]	[2, 6]	[3, 7]
	0.3	0.06	0.12	0.12
$\boldsymbol{m_2}$	[5, 9]	[5 ,5]	[5, 6]	[5, 7]
	0.3	0.06	0.12	0.12
$\boldsymbol{m_3}$	[7, 12]	⌀*	⌀*	[7, 7]
	0.4	0.08	0.16	0.16

* *empty set due to the intersection of two intervals*

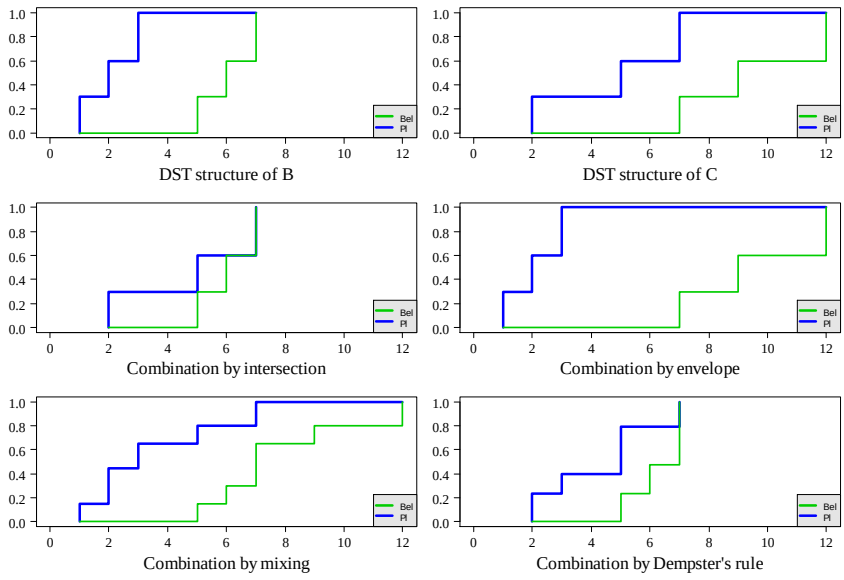

Figure 3. Dempster-Shafer structure (*A*) combining two sources of evidence *B* and *C* using four main operations: intersection, envelope, mixing and Dempster's rule.

2.3.4 Fuzzy-interval approach

Fuzzy-set theory, the basis of possibility theory, was proposed by Zadeh (1965; 1978) as a way to represent imprecise, incomplete or vague information (Bosc and Prade 1997; Dubois and Prade 1985). According to Dubois and Prade (1998), fuzzy-set theory is applied to three classes of applications: classification and data analysis, reasoning under uncertainty, and decision-making

problems. Fuzzy sets are an extension of so-called "crisp" sets (for which membership of elements is binary: yes or no) in which a gradual membership function (range = [0, 1]) is used to attribute a degree of possibility to each element of the set (Klir and Yuan 1995). Given a universal set *X*, there is a value of *A(x)* ($A(x) \in [0,1]$) which represents the degree of possibility that element *x* belongs to *X*. Therefore, the assignment of values *A(x)* to the elements *x* of the universal set *X* is called a membership function of the fuzzy set (Ayyub and Klir 2010). The membership function of a real value ($x \in \mathcal{R}$) can be described as:

$$A(x) = \begin{Bmatrix} f(x) & for\ x \in [a,b] \\ 1 & for\ x \in [b,c] \\ g(x) & for\ x \in [c,d] \\ 0 & otherwise \end{Bmatrix}, where\ a \le b \le c \le d\ \in \mathcal{R} \quad \text{Eq. 32}$$

in which *f(x)* is an increasing part of the membership function and *g(x)* is a decreasing part. The values *a* and *b* indicate the lowest and highest values of *x*, respectively, Like probability distributions, membership functions are constructed from expert judgment and empirical data. The following examples show two commonly-used membership functions: triangular and trapezoid, denoted as $A(a_L, a_M, a_R)\ and\ A(a_L, a_{LM}, a_{RM}, a_R)$, respectively (Eq. 33 and 34), where a_L and a_R are the left (lowest) and right (highest) bounds of *x*, respectively, a_M is the mode of the triangular membership function, and $[a_{LM}, a_{RM}]$ is the range of the mode of the trapezoidal membership function (Fig. 4).

$$A(a_L, a_M, a_R) = \begin{Bmatrix} \frac{x-a_L}{a_M-a_L} & for\ a_L \le x \le a_M \\ \frac{a_R-x}{a_R-a_M} & for\ a_M \le x \le a_R \\ 0 & otherwise \end{Bmatrix} \quad \text{Eq. 33}$$

$$A(a_L, a_{LM}, a_{RM}, a_R) = \begin{Bmatrix} \frac{x-a_{LM}}{a_{LM}-a_L} & for\ a_L \le x \le a_{LM} \\ 1 & for\ a_{LM} \le x \le a_{RM} \\ \frac{a_R-x}{a_R-a_{RM}} & for\ a_{RM} \le x \le a_R \\ 0 & otherwise \end{Bmatrix} \quad \text{Eq. 34}$$

Several concepts describe membership functions, the essential elements for representing fuzzy sets of an uncertain value *x*. The interval between the lowest and highest limits of all possible values of *x* is called the "support", while the most likely value of *x* is called the "core". The core is the mode for a triangular membership function or the interval of modes for a trapezoidal membership function. Any interval between the support and the core is called an "α-cut interval", associated with a degree of possibility, α. Indeed, the support and core can be considered as specific α-cut intervals in which α is zero and one, respectively. The set of all α-cut intervals, associated with their degrees of possibility, constitutes fuzzy intervals, $\pi(\alpha_i)$:

$$\pi(\alpha = 1) \subseteq \pi(\alpha_i \in [0,1]) \subseteq \pi(\alpha = 0), \text{where } \alpha \in [0,1] \quad \text{Eq. 35}$$

According to this definition, fuzzy intervals can be considered as a subjective evaluation of expert belief. Unlike the subjective view of probability, fuzzy intervals do not need to have the shapes

of distributions specified. It models an uncertain quantity based only on limited knowledge about the possibility of compatibility rather than the probability of occurrence. Hence, it is based on the notion that not all uncertainties can be appropriately described in terms of a frequency of occurrence (i.e., an unknown quantity is not randomly distributed). In this case, it is appropriate to model this type of uncertainty with a subjective degree of possibility to represent a degree of belief, as an alternative to subjective probability distributions (Dubois and Prade 1985; Tan 2008). This expression of uncertainty considers incomplete/imprecise information about the uncertain variable, such as an unknown distribution. It indicates that any possible probability distribution is likely to be "true" within the bound of limits. Thus, fuzzy intervals can be considered a family of all possible distributions, and their membership functions can be transformed into *p-boxes*, like those of imprecise probability (Dubois and Prade 1992b). Dubois and Prade (1993) addressed the relation between probability theory and fuzzy-set theory. They argued that possibility measures can be viewed as an upper probability (plausibility function) and discussed transformation between the two types of expressions. As mentioned, if the plausibility function is known, the belief function can be obtained (Eq. 19). Thus, a DST structure can be constructed from its fuzzy-interval membership function (Fig. 4). From their review of joint application of fuzzy sets and probability, Dubois and Prade (1993) concluded that building a bridge between the two theories is better than considering them as conflicting issues to strengthen the modeling of uncertainty and vagueness (imprecision)

Fuzzy intervals have been used to represent uncertainty due to imprecise information in models for environmental assessment (e.g., Mertens and Huwe (2002), Assaghir (2010)) and also in several LCA studies (e.g., Weckenmann and Schwan (2001), Tan et al. (2008; 2002), Andre and Lopes (2012)). Among them, Tan et al. (2002) used fuzzy intervals to represent uncertainty in LCA, especially that of data imprecision. They concluded that this approach provided more accurate representation of non-random uncertain variables in LCA and more flexibility for datasets whose probability distributions were difficult to determine. Moreover, the propagation of uncertainty by this approach was more computationally efficient than probabilistic simulations. In contrast, Andre and Lopes (2012) concluded that although fuzzy intervals were computationally efficient and provided results comparable to those of a probability approach, they offered poor information about uncertainty in output (i.e., a rough confidence interval), which could be less useful for LCA purposes. Thus, interpreting fuzzy-set-based results for decision making appears to be a challenge (Frey 2007). Moreover, its practical application is still limited due to the complexity of the model studied. For example, Heijungs and Tan (2010) illustrated the feasibility of fuzzy propagation in matrix-based life cycle inventory (LCI) but observed that it had low efficiency when the model was not monotonic.

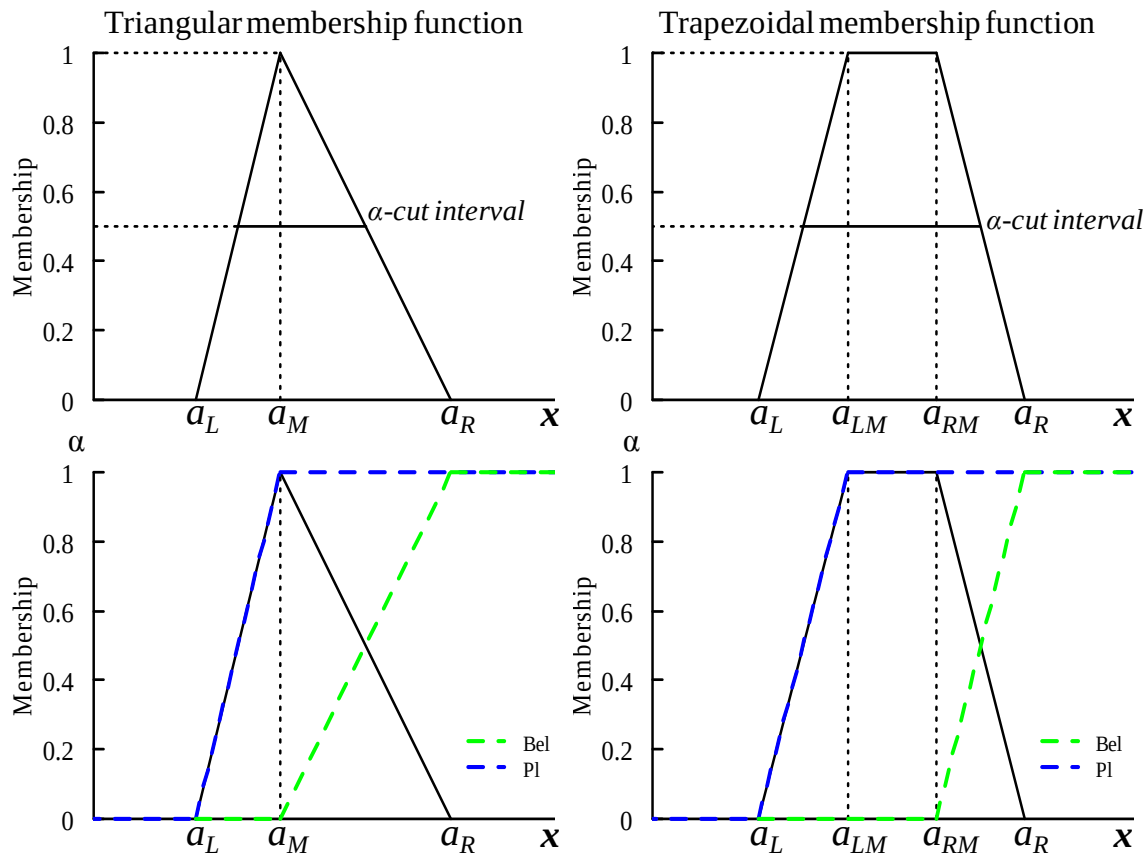

Figure 4. Top: Triangular (left) and trapezoidal (right) fuzzy-interval membership functions of an uncertain variable x denoted by $A(a_L, a_M, a_R)$ and $A(a_L, a_{LM}, a_{RM}, a_R)$, respectively. Bottom: DST structures of x. Green and blue dashed lines indicate belief and plausibility functions, respectively.

2.3.5 Qualitative and semi-qualitative approaches

Data/model quality is a crucial issue for the reliability of LCA results (De Smet and Stalmans 1996). Although LCA practitioners try to ensure the accuracy of input data and models, it is sometimes necessary to use reference data (e.g., a global estimate of emissions instead of a site-specific value) or a simple but less precise model, which may induce additional uncertainty due to the lack of specific information. The uncertainty in data/model quality is associated with the data collected, data sources and the choice of models or measurements in all LCA phases. When quantitative approaches (e.g., probabilistic, possibilistic) are infeasible, qualitative and semi-qualitative approaches are useful for representing data and model uncertainty. They linguistically describe the quality (e.g. “poor”, “good”) of data and models used in the system. Several standards and guidelines (Basket et al. 1995; ISO 14040 2006; Lindfors 1995; Weidema et al. 2004) offer methods to improve data quality and deal with its associated uncertainty, such as including independent critical review to validate the data used, creating databases to be used in LCA for data-quality assessment and increasing the transparency of data. For example, a SETAC workshop (Fava 1992) provided guidelines for assessing data quality as a systematic method to identify and measure the suitability of

LCI data. A conceptual framework for LCA data-quality assessment was developed using data quality indicators (DQIs), which assess data quality in several qualitative and quantitative categories (e.g., consistency, representativeness, precision, completeness). However, some aspects of DQIs, such as the inclusion of other types of uncertainty and variability, make them less focused on data validity or model quality and more on basic uncertainties, such as statistical error or variability within a population. Later, Weidema and Wesneas (1996) developed a "pedigree matrix" of five DQIs to evaluate data quality that focus on reliability, completeness, temporal correlation, geographical correlation and further technological correlation. This method transforms DQI scores into uncertainty factors (i.e., variance) of input variables, combines them with the variables' basic uncertainty, and propagates both using stochastic simulation (see section 2.4) (Maurice et al. 2000). Van den Berg et al. (1999) reviewed the literature on quality assessment in LCA and argued that most studies related to data quality assessment only concern the quality of input data (e.g., inventory data), ignoring model quality. Consequently, they developed a framework to extend quality assessment to models. Their DQIs cover four aspects related to the validity and reliability of input data and models through all phases of LCA. However, the final scores of each DQI are subjectively selected by practitioners, which may not account for disagreement in scores among experts. Pedigree matrices can be adapted to specific fields (e.g., industry *vs.* agriculture) or objectives of study (Kennedy et al. 1996; May and Brennan 2003; Rousseaux et al. 2001); consequently, the DQIs used and their arbitrary uncertainty factors may differ among studies.

2.4 Approaches to propagating uncertainty

Propagating uncertainty is one way to estimate uncertainty in final results due to uncertainty in related input variables, scenarios, model parameters and models themselves. Given an LCA framework (f) which contains input variables $X=(x_1, x_2,\ldots, x_i)$ with means defined as $\overline{X} = (\overline{x}_1, \overline{x}_2, \ldots, \overline{x}_i)$, output can be obtained as follows:

$$y = f(x_1, x_2, \ldots, x_i) \quad \text{Eq. 36}$$

with mean output corresponding to:

$$\overline{y} = f(\overline{x}_1, \overline{x}_2, \ldots, \overline{x}_i) \quad \text{Eq. 37}$$

Denoting uncertainty in the input variables with $u_1, u_2,\ldots, u_i$ and uncertainty in the framework with u_f, the uncertainty in output can be expressed as:

$$u_y = U(u_f, u_1, u_2, \ldots, u_i) \quad \text{Eq. 38}$$

where U represents the approach of uncertainty propagation. The u_i can be expressed as SD, variance or coefficient of variation, etc.; here we define it as SD. The uncertainty on the framework itself (u_f) includes parameter uncertainty in models, model uncertainty and scenario uncertainty; the expression of u_f differs depending on the type(s) of uncertainty. The approach to apply to propagate

input uncertainties through the framework to LCA results depends on how uncertainty is represented (described in the previous section). Of the several well-understood approaches used in LCA (Heijungs and Huijbregts 2004; Lloyd and Ries 2007), we discuss five in this section: an analytical method, interval arithmetic, stochastic simulation, scenario analysis and combined methods.

2.4.1 Analytical method

This analytical method to propagate uncertainty is a well-defined estimate of output variance based on a first-order Taylor series approximation (Bipm et al. 1995; Morgan and Henrion 1992). Given a mathematical function (*f(x)*), Taylor series are defined as a function with an infinite order of derivatives of a constant real number *a* (means of input variables):

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots \quad \text{Eq. 39}$$

The application of a Taylor series keeps only the first-order of Eq. 39 to estimate output variance when the model is linear (Bipm et al. 1995). Thus, given a multivariate model defined by Eq. 36, the deviation from the mean of output equals:

$$y - \overline{y} = f(X) - f(\overline{X}) \approx f'(\overline{X})(X - \overline{X}) - f'(\overline{X})(\overline{X} - \overline{X}) = f'(\overline{X})(X - \overline{X}) \quad \text{Eq. 40}$$

where $f'(\overline{X})$ is a partial derivative $\left|\frac{\partial y}{\partial X}\right|$. Thus, Eq. 40 is transformed into:

$$y - \overline{y} \approx \sum_{i=1}^{n}(x_i - \overline{x_i}) \left|\frac{\partial y}{\partial x_i}\right| \quad \text{Eq. 41}$$

Thus, the variance of *y* is obtained as:

$$Var(y) = \mathbb{E}(y - \overline{y})^2 \quad \text{(Expected value of the squared deviation from the mean)}$$

$$\approx \mathbb{E}\left[\left(\sum_{i=1}^{n}(x_i - \overline{x_i}) \left|\frac{\partial y}{\partial x_i}\right|\right)^2\right]$$

$$= \mathbb{E}\left[\sum_{i=1}^{n}\sum_{j=1}^{n}(x_i - \overline{x_i})\,(x_j - \overline{x_j}) \left|\frac{\partial y}{\partial x_i}\right| \left|\frac{\partial y}{\partial x_j}\right|\right]$$

$$= \sum_{i=1}^{n}\mathbb{E}[(x_i - \overline{x}_i)^2] \left|\frac{\partial y}{\partial x_i}\right|^2 + 2\sum_{i=1}^{n}\sum_{i>j}^{n}\mathbb{E}[(x_i - \overline{x_i})\,(x_j - \overline{x_j})] \left|\frac{\partial y}{\partial x_i}\right| \left|\frac{\partial y}{\partial x_j}\right|$$

$$= \sum_{i=1}^{n} Var(x_i) \left|\frac{\partial y}{\partial x_i}\right|^2 + 2\sum_{i=1}^{n}\sum_{i>j}^{n} Covar(x_i, x_j) \left|\frac{\partial y}{\partial x_i}\right| \left|\frac{\partial y}{\partial x_j}\right| \quad \text{Eq. 42}$$

Assuming that the input variables are independent, the covariance between input variables is zero. Finally:

$$Var(y) \approx \sum_{i=1}^{n} Var(x_i) \left|\frac{\partial y}{\partial x_i}\right|^2 \quad \text{Eq. 43}$$

This analytical method works well for low uncertainties with relatively less complex functions (Baker and Cornell 2003) because it is more computationally efficient than Monte-Carlo simulation with many iterations. Heijungs (1996) applied the analytical method to a simple matrix-based LCA study to propagate uncertainty. He stated that it could identify the influence of input variables (so-

called “key issues”) on outputs but pointed out that it may estimate uncertainty roughly due to a lack of knowledge about data uncertainty. More recently, Imbeault-Tetreault et al. (2013) confirmed the feasibility of the analytical method to propagate input uncertainties (expressed as geometric SDs) in a LCA case study. The sensitivity of input variables provided by this method was also useful in uncertainty analysis.

The method’s formula (Eq. 43) is first based on the assumption that the input variables are independent, which may be not always true in LCA. Hence, it is likely to under- or over-estimate uncertainty in output if strong correlation among input data exists (Ciroth et al. 2004). To address this problem, Hong et al. (2010) applied a second-order approximate method that considered correlations among input variables to two scenarios in a comparative LCA study. They concluded that their analytical method generated results similar to those obtained by Monte-Carlo simulation (MCS, described next), but much more computationally efficient. Including correlations implies using a higher-order analytical formula that may improve the accuracy of results but also increases the complexity of calculations (Heijungs and Suh 2002). Despite its computational advantage, this analytical method is rarely used in LCA (Heijungs and Huijbregts 2004), perhaps because of its mathematical complexity (e.g., the feasibility of calculating partial derivatives for all input variables) and because its requirements for more precise input variances are not easily satisfied due to lack of data. Moreover, when the function is significantly nonlinear, Eq. 40 will not be acceptable, and higher-order terms will be needed in a Taylor-series expansion. Doing so can also increase its mathematical complexity.

2.4.2 Stochastic simulation

When uncertain input variables are expressed by probability distributions, stochastic (random) simulation, such as MCS, can propagate their uncertainties into the uncertainty in output (Firestone et al. 1997). MCS involves 4 steps:

1. Generate a value for each input variable based on a random value [0, 1] and the inverse function of its PDF.
2. Repeat step 1 to obtain a set of input variables $(x_1', x_2', \dots, x_i')$.
3. Calculate the output $y' = f(x_1', x_2', \dots, x_i')$.
4. Repeat the previous steps many times (e.g., B=5 000) to obtain a mean and SD of y, which represent its predicted value and uncertainty, respectively.

In general, a classic MCS merges uncertainty in more than one input variable (expressed by probability distributions) into a single CDF output. However, to better understand input variables and their parameter uncertainty and variability, two-dimensional Monte-Carlo simulation (2D-MCS) is one advanced modeling approach (Kentel and Aral 2005). The 2D-MCS uses two loops of simulation

(inner and outer) to characterize parameter uncertainty and variability, respectively, when both are represented by probability distributions. The result of 2D-MCS is an imprecise probability distribution that covers a family of single probability distributions. Since this approach has two iteration steps, its computational time greatly exceeds that of classic MCS. Application of 2D-MCS in risk analysis was discussed explicitly by Kentel and Aral (2005), who introduced a 2D fuzzy MCS to integrate fuzzy-set theory into a probabilistic approach in risk assessment studies. Details of this method are described in a following section (2.4.4).

Since random MCS (using a random sampling technique), often used in LCA, assumes independence among input variables, all possible values of input variables can appear in a random set. This assumption, however, ignores any correlations between input variables, which may under- or over-estimate uncertainty in output if strong correlations exist (Bjorklund 2002). Correlations among variables (if known) can be considered in MCS using a covariance matrix. For example, Bojaca and Schrevens (2010) used multivariate normal distributions (based on a covariance matrix) in MCS in an LCA case study of potato production. This method yielded less uncertainty in impacts than a univariate normal distribution without correlations. Based on the same theory, we applied a modified MND method considering correlations in MCS using different probability distributions in a case study to estimate enteric methane emissions of cattle in French dairy farms (see Chapter 4). Besides correlations among input variables, correlation among systems implies that different systems of a comparative study use common input variables. Huijbregts et al. (2003) used an indicator to compare impacts of two production systems using MCS when input variables occur in both systems. In this way, the distribution of comparison indicator can be used to judge the significance between both product systems.

Generally, MCS uses 1000 to 10,000 iterations to explore a wide range of possible values. In theory, increasing the number of iterations increases the precision of estimated distributions of input variables but in practice decreases computational efficiency due to the considerable time required for calculation (Vose 2008). Therefore, using more efficient sampling techniques, such as Latin Hypercube sampling (LHS) (Helton and Davis 2003; Wyss and Jorgensen 1998), modified LHS (Wang et al. 2004) or importance sampling (Smith et al. 1997), can reduce the number of iterations necessary for comparative predictions. Since application of sampling techniques in MCS was not an objective of this thesis, more details can be found in the references cited.

MCS is widely used in uncertainty propagation in LCA (e.g., Röös and Josefine (2013), Henriksson et al. (2011), Gerber et al. (2010), Basset-Mens et al. (2009), Payraudeau et al. (2007), Sonnemann et al. (2003)) because of its flexibility and simple implementation via software packages (e.g., R, MATLAB®, Crystal Ball). This makes it feasible to use MCS for complex models (e.g., those with multiple sub-models or correlated input variables) (Hammonds et al. 1994). Moreover,

correlations between input variables can be controlled more easily in MCS than in analytical methods. However, MCS has some limitations (Ferson 1996). First, MCS requires a large amount of information, mainly from empirical data, to determine distributions of input variables. The lack of such information may limit the use of MCS, while arbitrarily assumed distributions may introduce additional uncertainty in input variables (see section 2.3.1). Second, based on probability theory, classic MCS can deal with stochastic uncertainty (i.e., natural variability), but is not appropriate for propagating non-statistical uncertainty due to imprecision or ignorance, nor can it handle model or scenario uncertainty. Finally, a high number of iterations requires considerable computational efforts, sometimes yielding calculation times too long to be achieved in practice.

Bootstrap sampling (Efron 1979) is an alternative to MCS for estimating sample error of a specific statistic (e.g., median, coefficient of correlation, eigenvalue) when empirical data are available but sample sizes are small. Unlike MCS, bootstrap sampling can estimate a statistic's confidence interval (CI) without needing distributions of input parameters. For example, an LCA case study using bootstrapped Principal Component Analysis to estimate the CIs of impacts of trout farming is illustrated (Appendix 1).

2.4.3 Interval arithmetic

Interval arithmetic is applied when input variables are expressed as intervals in the model. Its rules, developed by Moore (1966), calculate the smallest and the largest values of output under the following operations. Given real numbers *a*, *b*, *c*, *d* ($a \leq b, c \leq d$):

$$[a,b] + [c,d] = [a + c, b + d] \quad \text{Eq. 44}$$

$$[a,b] - [c,d] = [a - d, b - c] \quad \text{Eq. 45}$$

$$[a,b] * [c,d] = [min(ac, bc, ad, bd), max(ac, bc, ad, bd)] \quad \text{Eq. 46}$$

$$[a,b]/[c,d] = [min(a/d\,, b/c\,, a/c\,, b/d), max(a/d\,, b/c\,, a/c\,, b/d)], with\ c \neq 0, d \neq 0 \quad \text{Eq. 47}$$

The straightforward use of interval arithmetic to propagate uncertainty can yield robust results with best-case and worst-case estimates. It is an alternative propagation method when the computational burden of MCS appears too great. Although a single interval of output cannot take into account the level of belief, interval arithmetic can be used to propagate uncertainty of fuzzy intervals (Klir and Yuan 1995; Mauris et al. 2001). Given the output $y = f(x_1, x_2, \ldots, x_i)$, where input variables x_i (i = 1, 2… *n; n is the number of input variables*) are expressed by fuzzy intervals as $\pi(\alpha)_i$, the operational steps of propagation are:

1. Set the degree of possibility α=0 and calculate the minimum and maximum of output *y* with all possible combinations (2^n) of input variables x_i through the model: $y_{\alpha=0} = [min(f(\pi(\alpha)_i), max(f(\pi(\alpha)_i)]_{\alpha=0}$.

2. Set $\alpha = \alpha + \Delta\alpha$ $(e.g., \Delta\alpha = 0.01)$ and repeat step 1 to obtain $y_{\alpha=\alpha+\Delta\alpha} = [min(f(\pi(\alpha)_i), max(f(\pi(\alpha)_i)]_{\alpha=\alpha+\Delta\alpha}$.
3. Repeat step 2 until α=1, giving $N = 1 + 1/\Delta\alpha$ (e.g., N=1+1/0.01=101) fuzzy intervals y_α with their corresponding α.

Note that all combinations of input variables must be calculated to find the minimum and maximum of the output. Thus, increasing the number of intervals exponentially increases the number of combinations (2^n). Indeed, Heijungs (1996) discussed shortcomings of this approach when looking for the minimum and maximum of combinations of all input variables in LCI; in particular, when recycling loops occur (i.e., non-monotonic functions), the minimum and maximum may not be predicted intuitively[3]. In such cases, it may be impossible to calculate results with a large number of LCI input variables (e.g., combinations = $2^{10\ 000}$). Despite this limitation, several authors (Benetto 2005; Mauris et al. 2001; Tan 2008) have used fuzzy-interval propagation in LCA case studies. For example, Tan (2008) showed its computational efficiency with a small number of iterations (e.g., N = 101) in matrix-based LCI, when the smallest and largest emissions in inventory results can be determined without having to consider all combinations. Later, Heijungs and Tan (2010) validated this method for monotonic matrix-based LCI models.

If the propagation assumes strong interdependence between the sources of input variables, the same degree of belief is used for all input variables in each iteration (Baudrit et al. 2006). This refers to a subjective dependence between input variables related to their degrees of belief; for example, all input variables should be the most possible at the same time. It should be noted that this subjective dependence differs from objective dependence (i.e., correlations) between input variables. The latter indicates a functional relation between input variables, which is rarely considered in fuzzy-interval propagation modeling in LCA.

2.4.4 Combined methods

The choice of propagation methods depends on how uncertainty is represented (Lloyd and Ries 2007). Huijbregts et al. (2003) outlined different methods to account for different types of uncertainty simultaneously in a LCA case study for a Dutch one-family dwelling. They argued that simultaneous assessment can estimate combined effects of different types of uncertainty in LCA results. Helton et al. (2004) compared methods for representing uncertainty and discussed ways to aggregate their influence on model predictions. They translated different ways to represent input uncertainty into probabilistic structures (CDF or imprecise CDF) and propagated them through models with MCS. This propagation is similar to that of classic MCS, except that the sampling process generates a random

[3] The minimum and maximum of simple addition (Eq. 44) or subtraction (Eq. 45) can be estimated intuitively, while those of multiplication (Eq. 46) and division (Eq. 47) are more complicated because they require minimizing and maximizing all four combinations of the two intervals [a, b] and [c, d].

interval instead of a single random value. Then, each iteration is calculated with interval arithmetic. For example, given a model $y = f(x_1, x_2, \dots, x_i)$, in which input variables x_i (i = *1, 2… n; n is the number of input variables*) are expressed as imprecise CDFs, the steps of propagation are as follows:

1. Select a random value [0, 1] for an input variable and then generate an interval for it with minimum and maximum values $[\underline{x_i'}, \overline{x_i'}]$ according to its inverse function of imprecise PDF.
2. Repeat step 1 for each input variable to obtain a set of random intervals $([\underline{x_1'}, \overline{x_1'}], [\underline{x_2'}, \overline{x_2'}] \dots, [\underline{x_i'}, \overline{x_i'}])$.
3. Calculate the output interval using interval arithmetic $[\underline{y'}, \overline{y'}] = [min(f([\underline{x_1'}, \overline{x_1'}], [\underline{x_2'}, \overline{x_2'}] \dots, [\underline{x_i'}, \overline{x_i'}])), max(f([\underline{x_1'}, \overline{x_1'}], [\underline{x_2'}, \overline{x_2'}] \dots, [\underline{x_i'}, \overline{x_i'}]))]$.
4. Repeat the previous steps many times (e.g., B=5000) to construct an interval PDF of y.

Combining MCS and interval arithmetic allows stochastic uncertainty and imprecise information to be considered simultaneously in the model when both types exist. This propagation method can also be developed to combine probability distributions and fuzzy intervals. For example, Clavreul et al. (2013) modeled inventory data using both trapezoidal probability distributions and fuzzy intervals (according to the type of uncertainty) to estimate potential impacts in an LCA study. Results were presented as a bounded probability distribution that distinguished the uncertainty due to randomness from that due to incomplete information. Others, such as Arunraj et al. (2013), Baraldi and Zio (2008), Baudrit et al. (2006; 2005) and Guyonnet et al. (2003) have developed hybrid approaches for joint propagation of probability distributions and fuzzy intervals in risk assessment. These studies considered the combined method an alternative propagation approach when information is scarce (e.g., parameter uncertainty is described by fuzzy intervals). Application of this method is limited, however, due to the computational intensity of both MCS and interval arithmetic. Otherwise, the interdependence between random and imprecise variables (or lack thereof) remains to be explored (Ferson et al. 2004).

2.4.5 Scenario propagation

Pesonen et al. (2000) defined an LCA scenario 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.*" "Assumptions" refers to uncertainty in predicting the future, and this uncertainty can be addressed by scenario analysis, the comparison of different possible futures of a system. Approaches for assessing scenario uncertainty depend on the purpose of the research. There are two basic approaches in LCA (Pesonen et al. 2000): "what-if" scenarios and cornerstone scenarios. The what-if scenario approach is widely used to compare systems under different assumptions (e.g., alternative processes, different products, and different models). For example, Basset-Mens and van der Werf (2005) compared the

environmental performance of current and alternative systems of pig production. Potential impacts of "favorable" and "unfavorable" scenarios indicated an overall uncertainty range. Compared to the one-by-one analysis of what-if scenario approach, the cornerstone scenario approach combines multiple possible scenarios with long-term horizons to serve as basic guidelines for future prediction of the studied field. If considered as independent cases, all possible scenarios can be considered as probabilistic events and propagated via stochastic simulation (e.g., MCS or bootstrap sampling). Huijbregts et al. (2003) assigned a probability (i.e., a degree of belief) to each normative choice of LCA practitioners and quantified potential impacts as a probability distribution reflecting the uncertainty due to different normative choices. Hence, a probabilistic approach can integrate scenario uncertainty with parameter uncertainty in the same framework.

It should be noted that the previous example referred to a case when probability assignments came from a single source of information (i.e., evidence). If there is more than one source of information (e.g., different experts or observations), evidence theory (e.g., DST) can express the degree of belief of each scenario by combing the sources. For example, Chowdhury (2013) assessed a water treatment plant using certain factors as risk indicators. They classified factors into five linguistic levels (i.e., "very poor" to "very good") provided by multiple experts and used Dempster's rule (see 2.3.3) to obtain the factors' *bpa*. When multiple sources of information are available, DST-based combination rules represent the status of a studied system better than a single arbitrary assignment of probability. As mentioned, the *bpa* is used in DST to define belief and plausibility functions, which are identical to lower and upper probabilities, respectively. Thus, scenario uncertainty can be expressed in probabilistic form (*p-box*) and propagated via MCS.

2.5 Choice of uncertainty analysis in LCA

Although the consideration of uncertainty in LCA is mentioned in its ISO standards (ISO 14044 2006), it provides little guidance about how to perform uncertainty analysis in LCA, and a lack of consensus about this issue remains (Bjorklund 2002). LCA practitioners have applied various methods to deal with uncertainty (Lloyd and Ries 2007), but decisions about methods raise concerns because results can vary depending on which method is chosen (Reap et al. 2008). Therefore, LCA practitioners should explicitly identify in the first step of LCA (goal and scope) the types of uncertainty in their studies and the uncertainty analysis methods they chose. Huijbregts (1998a) reviewed tools for addressing epistemic uncertainty and variability in LCA, including ways to represent and propagate uncertainty (e.g., stochastic simulation), reduce epistemic uncertainty and better represent variability (e.g., additional measurements, standardization). Based on his work, we mainly reviewed approaches that focus on representing epistemic uncertainty and variability (Table 3).

Probabilistic approaches include both classic (precise) and imprecise probability distributions. Bayes's theorem can be considered as a subjective probabilistic approach to estimate the posterior distribution of an uncertain variable using both expert opinions (prior distribution) and observed data (likelihood function). Non-probabilistic approaches (e.g., interval, fuzzy intervals, DST) assign a level of belief to express the state of knowledge. DST combination rules (e.g., Dempster's rule) can combine multiple sources of information; thus, they can be used to integrate different choices (sources of evidence) into the same framework. In addition, we considered expert judgment and peer review (e.g., rule of thumb) only as an assessment of data quality; thus, these two subjective assessments are replaced by the qualitative approach when evaluating data/model quality. Scenario analysis includes ways to treat uncertainty due to choice (see section 2.4.5). Among them, "what-if" scenario analysis can be applied to address spatial or temporal variability (e.g., using specific or generic data). It should be noted that scenario analysis also refers to propagation of scenario uncertainty, since the results of scenario analysis contain information about different scenarios. We classified modeling approaches (non-linear/multi-media modeling) as ways to account for model uncertainty using multiple complex models, if they exist. Moreover, modeling approaches can incorporate spatial and temporal information that make models more complete; however, complex models may introduce other sources of uncertainty (e.g., parameter uncertainty) related to spatial and temporal factors or the fact that they require more parameters, for some of which information may be scarce. For example, the IPCC (2006) provides three tiers to estimate CO_2 emissions from mineral fertilization. The model-based method (Tier 3) can be applied when detailed activity data is available; if not, uncertainty in these activity data may influence predictions significantly or even make model use infeasible. In such a case, the IPCC recommends using a simpler equation (Tier 2 or Tier 1) for a generic rather than site-specific estimate, but less complex methods may predict emissions less precisely. Finally, statistical correlation and regression analysis can be integrated into other approaches (e.g., correlation control using multivariate distributions) if the information is available.

Since a given type of uncertainty can be expressed by more than one approach (Table 3), there is a need to help LCA practitioners choose appropriate approaches. Considering the properties of each approach for representing uncertainty, we propose a guide for choosing appropriate approaches to represent different types of uncertainty (Fig. 5). The guidelines start by identifying the types of uncertainty according to their natures and sources. Then, depending on their objectives and the information available, LCA practitioners can follow its specific questions to find approaches appropriate for representing a given type of uncertainty. For example, natural variability can be represented with a classic probability distribution (red arrows). In the same way, parameter uncertainty (green arrows) can be represented with probability distribution when the parameter is (or is assumed to be) randomly distributed (see chapters 3 and 4). If not, (fuzzy) interval analysis (blue arrows) can be applied (see chapter 5). However, it should be noted that addressing one type of uncertainty may

induce another source of uncertainty. For example, a spatial or temporal model can be used to consider spatial or temporal variability, respectively, but that model may have uncertainty in its associated parameters. Hence, this decision tree can be used iteratively when new sources of uncertainty are identified.

Table 3. Overview of approaches for representing uncertainty in LCA and their suitability for different types of uncertainty (based on *Huijbregts, 1998a*)

	Type					
Approach	Parameter uncertainty	Model uncertainty	Uncertainty due to choices	Spatial variability	Temporal variability	Natural variability
Probabilistic approach (classic and imprecise probability distribution, Bayes's theorem)	+		+			+
Non-probabilistic approach (interval, fuzzy intervals, Dempster-Shafer theory)	+					+
Combination rules (e.g., Dempster's rule)			+			
Qualitative/semi-qualitative method	+	+				+
Scenario analysis (bootstrap sampling, "what-if" scenario analysis, cornerstone analysis)			+	+	+	
Non-linear/multi-media modeling		+		+	+	

Ultimately, the choice of propagation methods depends on how uncertainty is represented. MCS is widely used when probability distributions (both precise and imprecise) are applied. Interval arithmetic can provide a rough estimate of output intervals (minimum-maximum), especially to propagate parameter uncertainty represented by classic intervals or fuzzy intervals. The combined methods based on DST makes it feasible to integrate both of the above methods. The analytical method is useful for dealing with parameter uncertainty and variability when models and variances of uncertain variables are well-known. However, as previously mentioned, application of the analytical method is limited due to its mathematical complexity and data requirements. Finally, bootstrap sampling can estimate overall impacts of several scenarios if they are judged to be equally probable. In addition, bootstrap sampling can also be applied to propagate sampling errors (e.g., SEM) from input variables onto impacts when observed samples are given (Annexe).

2.6 Discussion and Conclusions

Despite the existence of many terminologies of uncertainty, we follow the classification of uncertainty applied by Huijbregts (1998a), which explicitly separates states of knowledge according to their natures and sources. First, this classification allows LCA assessors to better understand inherent

differences (e.g., variability) in the system and readily assess the potential to improve the system by reducing epistemic uncertainty. Second, sub-classes of variability and epistemic uncertainty focus on the sources of uncertainty, which provide detailed understanding about the key points where uncertainty appears. Finally, this classification and the definitions of uncertainties have been accepted in most LCA studies that provided good examples of representing and propagating uncertainty.

In general, the classic probabilistic approach is the mainstream way to treat parameter uncertainty and natural variability in LCA. It is commonly applied by most LCA practitioners, because (1) its basic theory is well developed in many fields (e.g., risk analysis, environmental assessment) and easy to understand, (2) its application is practical with the aid of statistical software (e.g., Microsoft Excel®, R, MATLAB®) and LCA software (e.g., SimaPro®, OpenLCA) that can perform MCS to propagate uncertainty through LCA models, and (3) results are easy to interpret using single values for the common statistical terms (e.g., mean, variance). However, this classification of uncertainty suggests that (1) natural variability and parameter uncertainty are different by definition, so it is better to interpret them separately, and (2) other types of uncertainty (e.g., scenario uncertainty, spatial variability) also occur in LCA that most likely will influence estimates of environmental impacts. The probabilistic approach is less feasible when available information is scarce, since too many assumptions about variable distributions may result in arbitrary estimates. Consequently, alternative methods are necessary to address different types of uncertainty. These methods enable LCA practitioners to have more flexible choices depending on the information they have available. For example, imprecise assessment (e.g., imprecise probability, interval analysis) can provide conservative estimates and require less information or sometimes computational time than a classic probability distribution when a high confidence level is not absolutely necessary. On the other hand, other types of uncertainty (e.g., scenario uncertainty) can be integrated into uncertainty analysis, though the ability to address them is still limited in LCA. For example, DST combination rules can merge information about models or scenarios from different sources of evidence into the same LCA framework. In addition, although interpretation of DST-based results seems complex and harder to understand than a single probabilistic distribution, which Lindley (2013) argued simplified representation of uncertainty, DST structures (p-box) have the advantage of considering imprecision and ignorance for uncertainty analysis and providing more realistic estimates.

This chapter illustrated several methods adapted for LCA to represent and then propagate different types of uncertainty. Many factors determine the choice of methods, such as type of uncertainty, the information available, study objectives, and acceptable confidence levels. Based on these factors, we developed a decision tree for choosing appropriate methods to represent different types of uncertainty (Fig. 5). It offers initial guidelines for LCA practitioners to analyze uncertainties using different methods. The method selected may influence how impact assessment is modeled. For

example, dynamic models are used with probabilistic methods, while static models are used with deterministic input variables. Hence, construction of LCA models should consider how to integrate uncertainty during the assessment process. However, application of uncertainty-analysis methods should be performed on a case-by-case basis, since this general guideline cannot cover all circumstances. Sometimes, computational costs or practitioner preferences also play an important role in the choice of method. Therefore, uncertainty analysis should be described explicitly in a separate section of an LCA study when a confidence level about potential impacts is required.

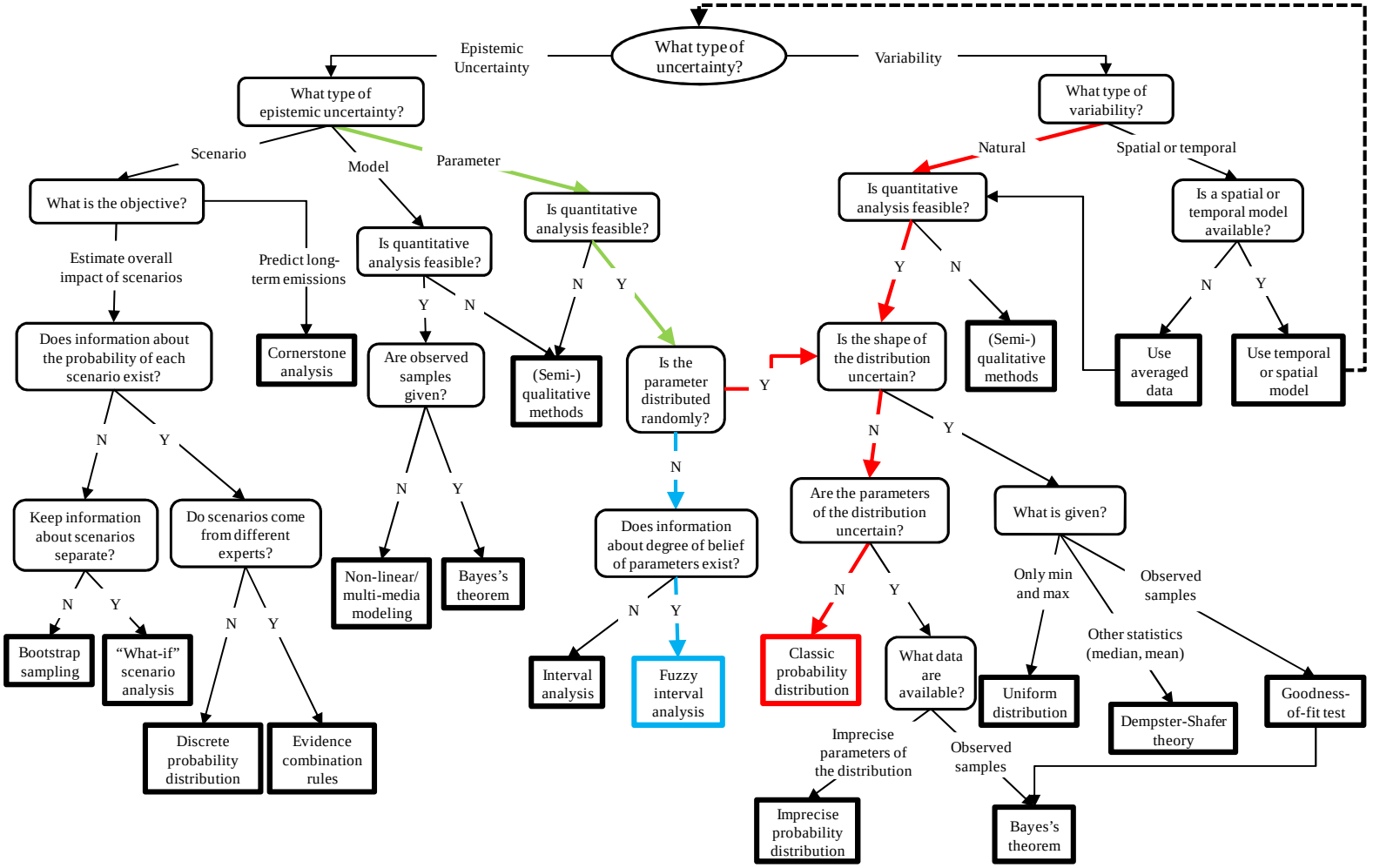

Figure 5. Decision tree of the choice of methods to represent different types of uncertainty. For example, red arrows indicate representation of natural variability with probability distributions (chapters 4 and 5). Green arrows indicate representation of uncertainty in randomly distributed parameters, either with probability distributions (red arrows, chapter 3) or fuzzy interval analysis (blue arrows, chapter 5). The dashed arrow indicates iterative use of the decision tree when new sources of uncertainty are identified in temporal or spatial models.

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Chapitre 3.
Influence of emission-factor uncertainty and farm-characteristic variability in LCA estimates of environmental impacts of French dairy farms

Journal of Cleaner Production, (2014), 81:150-157

Influence of emission-factor uncertainty and farm-characteristic variability in LCA estimates of environmental impacts of French dairy farms

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Abstract

Life Cycle Assessment (LCA) is a useful framework for environmental assessment; however, the reliability of LCA results suffers from many sources of uncertainty and variability. Now that systematic uncertainty analysis in LCA is recommended, it can be useful to revisit past LCA studies to see whether inclusion of uncertainty (or additional types of it) changes interpretation of their results. In this study, we added uncertainty in 67 emission factors (EFs) to the variability in farm characteristics of 47 French dairy farms analyzed in a previous LCA study (van der Werf et al., 2009). We propagated uncertainty in EFs with Monte-Carlo simulation to estimate contributions of uncertainty and variability to uncertainty in potential climate change, acidification, and eutrophication impacts. For individual farms, uncertainty in emission factors added uncertainty to the farm's formerly deterministic impacts (coefficients of variation of 2-7% for climate change, 4-11% for acidification, and 2-46% for eutrophication). By farm type (conventional vs. organic), the addition of uncertainty in EFs increased uncertainty in impacts. Although uncertainty in emission factors contributed less to impact uncertainty than variability in farm characteristics did, it did add enough to potentially change decisions about whether differences in certain impacts between farm types were significant, depending upon the significance level and functional unit chosen. Variance-based sensitivity analysis identified emission source categories whose uncertainty contributed most to the uncertainty in impacts: manure deposited in pasture for climate change, cattle housing and manure storage for acidification, and leachate for eutrophication. Although larger uncertainties in potential impacts decrease apparent differences between the systems or scenarios studied, considering more than one type of uncertainty provides decision makers with a more complete and realistic assessment of the state of knowledge. Based on the degree of uncertainty in impacts, they can decide which location on impact intervals (e.g., mean, lower limit, upper limit) is best suited for decisions in a given system. Future studies should explore additional methods to combine multiple sources of uncertainty in LCA and express their relative influences on potential impacts.

Keywords: life cycle assessment; emission factor; uncertainty; variability; Monte-Carlo simulation

1. Introduction

Environmental impacts of agricultural systems have become an increasingly important issue in the past several years. As a framework for environmental assessment, Life Cycle Assessment (LCA) can estimate potential environmental impacts and resource use of entire farming systems (van der Werf and Petit 2002). LCA results can help decision makers assess environmental impacts of a given production system or compare different systems to identify those with lower impacts (International Organization for Standardization (ISO) 2006). Application of LCA, however, requires many simplifying assumptions, methodological choices, and input data. Unfortunately, the influence of uncertainty in these assumptions, choices, and data on potential impacts is not systematically assessed (though its frequency is increasing), which may lead to inaccurate or overly confident interpretations of potential impacts or their differences between systems. Thus, uncertainty analysis in LCA can illustrate how uncertainties affect the reliability of its results, providing more useful information for decision making (International Organization for Standardization (ISO) 2006; Weidema and Wesnaes 1996).

The broadly defined concept of uncertainty includes two types with different natures: uncertainty and variability (Huijbregts 1998a; Thompson 2002). Uncertainty (sometimes called "epistemic uncertainty" (Clavreul et al. 2013; Helton and Oberkampf 2004) for clarity), defined as incomplete or imprecise knowledge, can be further subdivided into parameter, model, and scenario uncertainties (Huijbregts 1998a; WHO 2008), which can arise from uncertainty in data about the system, choice of models used to calculate emissions, and choice of scenarios to define system boundaries, respectively (Röös and Josefine 2013). These types of uncertainty can be reduced by increasing measurement accuracy, increasing model accuracy, and collecting data that better represent systems of interest, respectively. Unlike epistemic uncertainty, variability, defined as inherent differences over time, space, or within a group, cannot be reduced, but it can be represented more precisely if more information about the group is available (Morgan and Henrion 1992).

Most LCA studies considering uncertainty use probability distributions to represent both types of uncertainty in inventory data (Heijungs and Huijbregts 2004; Huijbregts 1998b) and Monte-Carlo simulation (MCS) to propagate them through LCA models to estimate uncertainty in potential impacts (Lloyd and Ries 2007). MCS generates hundreds or thousands of sample sets of input data, each containing a combination of input variables taken randomly from their distributions (Firestone et al. 1997). For complex models, such as those in LCA, it is more feasible and efficient to apply MCS than analytical methods (Hammonds et al. 1994; Leinonen et al. 2012). With MCS, predicted impacts can be expressed as probability ranges instead of single values, which provides more complete information for decision makers about the magnitude of uncertainty in predictions (Sonnemann et al. 2003).

Now that assessment of uncertainty in LCA predictions is strongly recommended (Lazarevic et al. 2012; Williams et al. 2009), it can be useful to revisit past LCA studies to see whether inclusion of uncertainty (or additional types or sources of uncertainty) changes interpretation of their results. We did so for a previous study (van der Werf et al., 2009), whose authors had performed LCA for each of 47 dairy farms in Brittany, France, with a custom-built tool, EDEN-E (Evaluation de la Durabilité des ExploitatioNs). Because (1) that study had already estimated uncertainty in impacts due to variability in farm characteristics and (2) the configuration of EDEN-E precluded including some key farm characteristics in MCS (described later), we focused our study on estimating how the addition of uncertainty in emission factors (EFs) influenced uncertainty in impacts of the dairy farms. This approach had the advantage of separating the two sources of uncertainty (EFs and farm characteristics), allowing us to assess each one's influence on impacts, which may affect how decision makers interpret them.

2. Material and methods

2.1. EDEN-E tool and inventory data

We used data previously collected and calculated with the EDEN-E tool, developed (in Microsoft Excel®) to estimate LCA-based environmental impacts of individual dairy farms (van der Werf et al. 2009). Tables in EDEN-E contain an inventory of farm inputs and characteristics, such as energy carriers, mineral fertilizers, animal feeds, and machinery, which are used in built-in emission models or multiplied by per-unit environmental burdens to calculate emissions and resource use. Other factors such as animal production (e.g., meat, milk), number of animals by age and sex, and usable agricultural area (UAA) are also used to estimate emissions from farm activities (Fig. 1). Consequently, EDEN-E can distinguish "direct" environmental interventions (occurring on the farm's UAA) from "indirect" interventions (associated with upstream inputs, emissions, and UAA to produce materials imported to the farm) when predicting impacts. Thus, direct impacts consider only on-farm activities and hectares, while total impacts (i.e., direct + indirect) also include estimates of off-farm activities and hectares. It should be noted that intensive dairy farms importing feedstuff from lower-impact crop farms may have direct impacts per ha (on-farm) that exceed total impacts per ha (on- and off-farm). Data collected with EDEN-E in the previous study represented one year of operation of 47 dairy farms of two production modes (41 conventional, 6 organic) in Brittany, France, during the period 2003-2005.

2.2. System boundary, functional units, and impact categories

We used the same two system boundaries as the previous study (van der Werf et al. 2009) to calculate impacts (direct and total) according to two functional units, respectively (Fig. 1). Per ha of on-farm UAA, the boundary included all interventions, while per 1000 kg of fat-and-protein-corrected

milk (FPCM) sold, the boundary excluded all inputs, output and UAA of cash crops (i.e., produced but not auto-consumed) to leave only the milk-production subsystem (thereby avoiding allocation between crop and animal products). To facilitate interpretation of results, we predicted impacts only for those impact categories regrouping emissions that would vary due to uncertainty in the EFs ultimately selected for analysis: climate change (from nitrous oxide (N_2O), methane (CH_4), and nitrogen oxides (NO_x)), acidification (from ammonia (NH_3)), and eutrophication (from nitrate (NO_3) and phosphate (PO_4)).

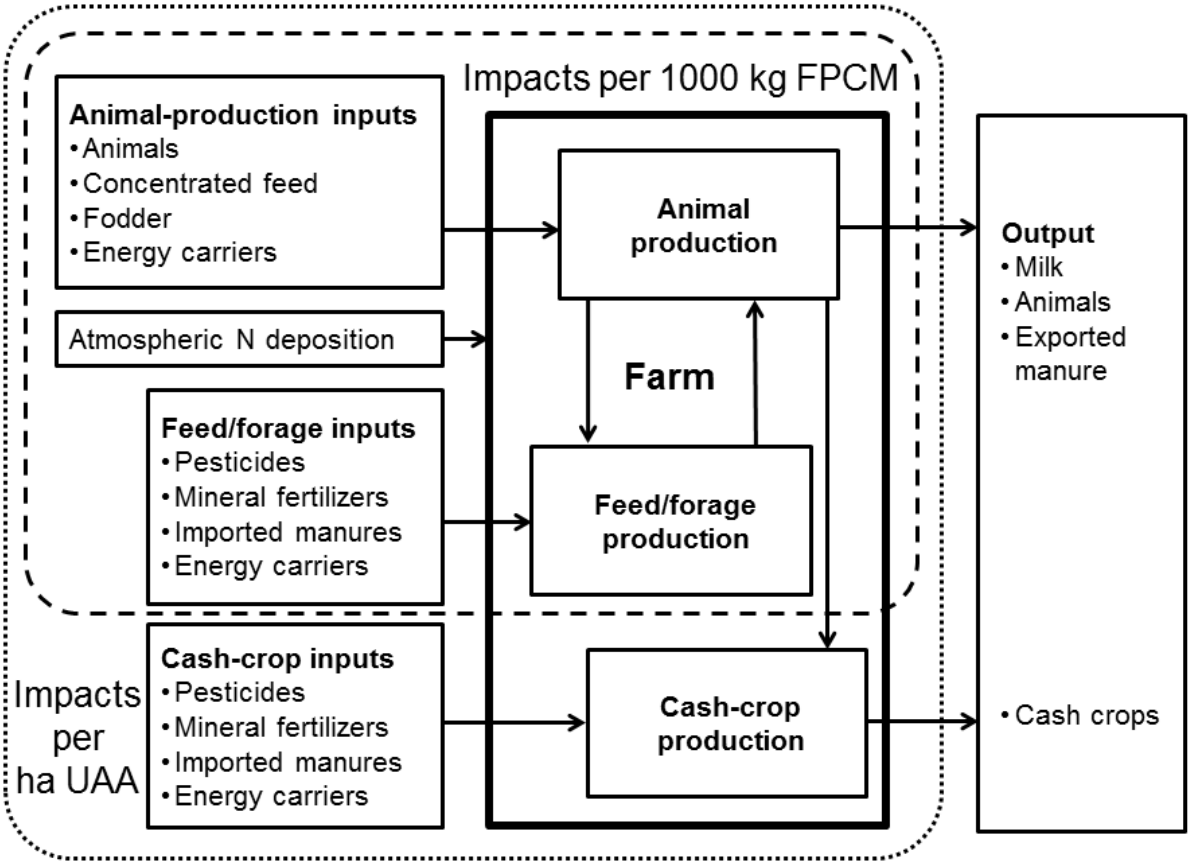

Figure 1. Flow diagram of dairy farms and system boundaries used to calculate impacts per ha of usable agricultural area (UAA) (dotted line) and per 1000 kg of fat-and-protein-corrected milk (FPCM).

2.3. Variability in farm characteristics and uncertainty in emission factors

Since certain key farm characteristics, such as feed rations and manure management, are stored as codes in EDEN-E, they could not be assigned probability distributions for inclusion in MCS. Reconstructing EDEN-E's dairy-farm LCA model in another form (e.g., SimaPro) to allow propagation of variability in all farm characteristics, besides being a study unto itself, would have changed LCA predictions, at odds with our objective of adding uncertainty to results of a pre-existing study. We thus focused on exploring the influence of uncertainty (epistemic uncertainty and variability

combined) in EFs with MCS. As in the previous study, variability in impacts due to variability in farm characteristics within the sample of each farm type (conventional and organic) was considered.

We used the same default EFs as in the previous study, despite the advanced ages of some of them (1997-2007), since our objective was to compare results between studies (Table 1). Most of the EFs selected convert quantities of manure or fertilizer into emissions of nitrogenous gases (i.e., NH_3, N_2O, NO_x). As in van der Werf et al. (2009), NO_3 emissions were set equal to the farm-gate N balance minus these gaseous N emissions. EFs for manure varied as a function of its type (e.g., species, water content), season, and site of excretion (e.g., on pasture or in buildings). EFs for CH_4 emissions from enteric fermentation and manure management were estimated with the Tier 2 method of the IPCC (2006a). The EF for PO_4 emissions from manure application came from Rossier and Charles (1998). Uncertainty shapes and ranges (usually 95% confidence intervals (IPCC 2006c)) for EFs for CH_4 were taken from IPCC (2006a), those of N_2O were taken from IPCC (2006b), and those of other nitrogenous compounds were taken from Payraudeau et al. (2007) (Table 1). We assumed an uncertainty range for the EF for PO_4 of ±50% due to lack of data. Although the references we used described differences between uncertainty (i.e., epistemic) and variability, they did not separate them when estimating uncertainty ranges for EFs. Hence, the uncertainty ranges we used included both epistemic uncertainty (e.g., due to measurement error) and variability (e.g., due to site-specific characteristics, such as temperature and humidity).

2.4. Monte-Carlo simulations and comparison with deterministic results

We propagated uncertainty in EFs into predictions of environmental impacts of each of the 47 farms using MCS (1000 iterations per farm in Excel®). Two EFs were excluded from MCS because they could be calculated from other EFs or input variables and thus were not independent: the EF for dinitrogen ($N\text{-}N_2$) was three times that for $N\text{-}N_2O$ (Webb 2001), while dairy-cow enteric CH_4 emissions were a function of milk production per cow. We assumed that the remaining 67 EFs in the MCS were independent. After the 1000 iterations, we calculated mean impacts for each farm and their coefficients of variation (CVs) due to uncertainty in EFs. For each of the 1000 MCS iterations, we calculated mean impacts and their CVs for each farm type (conventional and organic) to express variability in farm characteristics. Then, we expressed mean impacts, their variabilities, and p-values of differences in means over the 1000 iterations as 95% confidence intervals (2.5^{th}-97.5^{th} percentiles) due to uncertainty in EFs. We also recalculated the results of the previous study (van der Werf et al., 2009) using default values of EFs. We used R software (R Development Core Team 2012) to perform all statistical tests and, to remain consistent with the previous study, inferred significant differences at the significance level α=0.05.

2.5. Sensitivity analysis

We performed a simple sensitivity analysis to identify which emission sources contributed most to variances predicted in direct impacts only, since the indirect portion of total impacts did not change when EFs varied. We grouped direct emissions into seven source categories: mineral fertilization, cattle housing and manure storage, manure deposited in pasture (N_2O, NH_3, NO_x, and CH_4 for all three), manure spreading (N_2O, NH_3, NO_x, and PO_4), leachate (NO_3), N_2O emissions due to both atmospheric NH_3 deposition and NO_3 in leachate, and "other" (e.g., direct fuel and plastic use). Then we estimated contributions to the variance ($CTV_{i,j}$) in direct impacts from variation in the source categories using an equation of Geisler et al. (2005):

$$CTV_{i,j} = r_{i,j}^2 / (\sum_i^n r_{i,j}^2) \quad \text{Eq. 1}$$

where $r_{i,j}$ is the Spearman's rank-order correlation coefficient (which represents non-linear correlation more robustly than the Pearson correlation) between impacts from source category *i* for impact category *j*, and *n* is the number of source categories. The combined effect of sample size and variability in farm characteristics on CTVs was represented with 95% confidence intervals of mean CTVs for each farm type.

Table 1. Default values, uncertainty ranges, and distributions (normal (N) or log-normal (L)) of emission factors and their sources. Ranges in percentages indicate 95% confidence intervals.

Emission factor		Value	Unit	Range	Dist.
Cattle housing and manure storage	NH_3-N emitted in housing	0.12[a]	kg NH_3-N/kg N excreted	±60%[e]	N
	NH_3-N emitted during storage	0.06[a]	kg NH_3-N/kg N stored	±60%[e]	N
	N_2O-N from solid manure	0.01[c]	kg N_2O-N/kg N excreted	0.005-0.02[c]	L
	N_2O-N from liquid manure	0.005[c]	kg N_2O-N/kg N excreted	0.0025-0.01[c]	L
Pasture	NH_3-N emitted in pasture	0.08[a]	kg NH_3-N/kg N excreted	±30%[e]	N
	N_2O-N emitted in pasture	0.02[d]	kg N_2O-N/kg N excreted	0.007-0.06[d]	L
NH_3 from manure spreading in winter	Solid cattle or pig manure	0.57[b]	kg NH_3-N/kg TAN[k]	±60%[e]	N
	Liquid cattle manure	0.20[h]	kg NH_3-N/kg TAN	±60%[e]	N
	Liquid pig manure	0.15[h]	kg NH_3-N/kg TAN	±60%[e]	N
	Solid poultry manure	0.338[b]	kg NH_3-N/kg TAN	±60%[e]	N
	Liquid poultry manure	0.15[g]	kg NH_3-N/kg TAN	±60%[e]	N
NH_3 from manure spreading in spring, summer, autumn	Solid cattle or pig manure	0.76[b]	kg NH_3-N/kg TAN	±60%[e]	N
	Liquid cattle manure	0.25[h]	kg NH_3-N/kg TAN	±60%[e]	N
	Liquid pig manure	0.20[h]	kg NH_3-N/kg TAN	±60%[e]	N
	Solid poultry manure	0.45[b]	kg NH_3-N/kg TAN	±60%[e]	N
	Liquid poultry manure	0.20[g]	kg NH_3-N/kg TAN	±60%[e]	N
Mineral fertilizer application	NH_4NO_3, $(NH_4)_2SO_4$, $Ca(NO_3)_2$, $CaCN_2$, KNO_3	0.02[a]	kg NH_3-N/kg N	±20%[e]	N
	$CO(NH_2)_2$	0.15[a]	kg NH_3-N/kg N	±20%[e]	N
	NH_3	0.04[a]	kg NH_3-N/kg N	±20%[e]	N
	$(NH_4)_2HPO_4$	0.05[a]	kg NH_3-N/kg N	±20%[e]	N
	Other NPK compounds	0.02[a]	kg NH_3-N/kg N	±20%[e]	N
	NO-N from applications	0.003[i]	kg NO-N/kg N applied	±60%[j]	N
N_2O-N from manure or fertilizer application or crop residues		0.01[d]	kg N_2O-N/kg N applied or in residues	0.003-0.03[d]	L
Atmospheric deposition of NH_3-N		15.00[g]	kg NH_3-N/year/ha	10.00-20.00[e]	N
N_2O-N from NO_3 leaching		0.008[d]	kg N_2O-N/kg N leached	0.0005-0.025[d]	L
N_2O-N from atmospheric deposition		0.01[d]	kg N_2O-N/kg NH_3-N + NO_x-N volatilized	0.002-0.05[d]	L
PO_4 from manure or fertilizer application		0.01[f]	kg PO_4/kg PO_4 applied	±50%[j]	N
CH_4 from enteric fermentation	Heifers or males 0-1 year	37.20[c]	kg CH_4/head/year	±20%[c]	N
	Heifers or males 1-2 years	84.60[c]	kg CH_4/head/year	±20%[c]	N
	Heifers 2+ years or bulls	90.30[c]	kg CH_4/head/year	±20%[c]	N
CH_4 from manure: emission of VS[m]	Cows	5.10[c]	kg dry matter/head/day	±20%[c]	N
	Other 3 animal classes above	2.60[c]	kg dry matter/head/day	±35%[c]	N
CH_4 from manure: potential CH_4 production (B_o)	Cows	0.24[c]	m^3 CH_4/kg VS	±15%[c]	N
	Other 3 animal classes above	0.18[c]	m^3 CH_4/kg VS	±15%[c]	N

[a]EMEP-CORINAIR(2002), [b]EMEP-CORINAIR(2001), [c]IPCC(2006a), [d]IPCC(2006b), [e]Payraudeau *et al.* (2007), [f]Rossier and Charles (1998), [g]Expert judgment (INRA UMR SAS, Rennes, France), [h]Morvan and Leterme (2001), [i]Skiba *et al.* (1997), [j]Assumption, [k]TAN: total ammoniacal nitrogen, [m]VS: volatile solids

3. Results

3.1 Impacts of individual farms

For individual conventional farms, uncertainty (expressed as a CV) in acidification (8-14%) was higher than that in climate change (3-6%) or in eutrophication (2-8%) for both functional units (Fig. 2). For organic farms, however, half (three) had higher uncertainty in eutrophication, especially per ha of UAA (CVs of 15%, 19% and 46%).

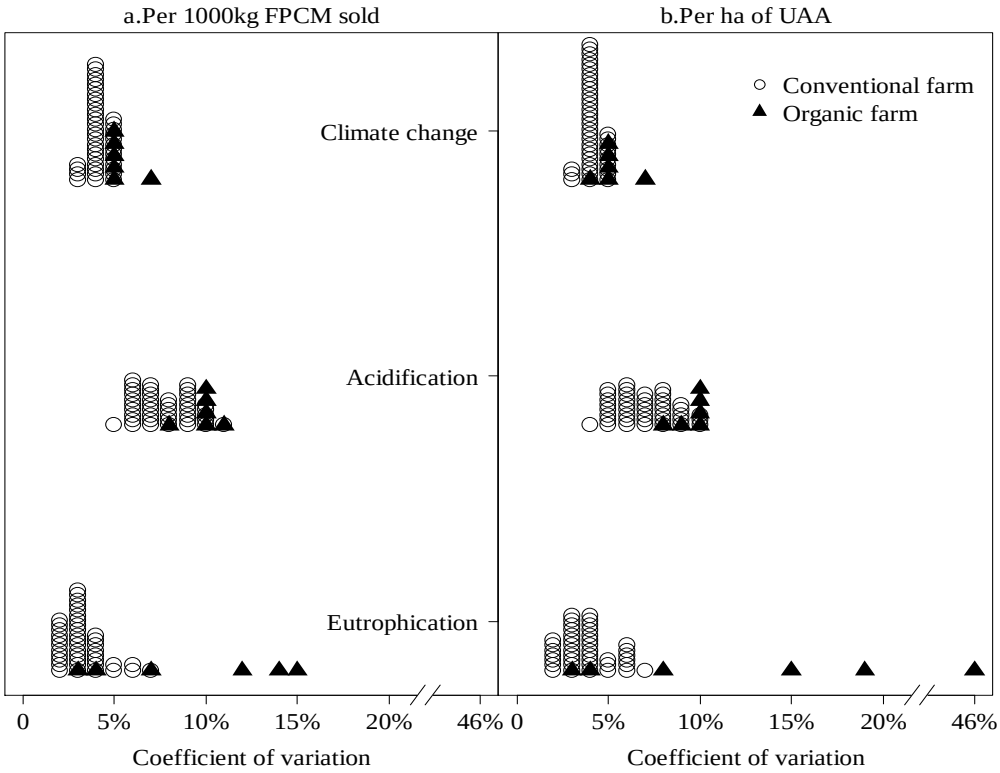

Figure 2. Strip plots of coefficients of variation (CVs) of total climate change, acidification, and eutrophication impacts (a) per 1000 kg fat-and-protein corrected milk (FPCM) sold and (b) per ha of usable agricultural area (UAA) of 41 conventional (circles) and 6 organic (triangles) dairy farms. Points represent uncertainties in impacts due to parameter uncertainty in emission factors, while their degrees of scatter for each impact category reflect inter-farm variability in CVs.

3.2 Impacts by farm type

Despite increased uncertainty in potential impacts by farm type caused by EF uncertainty, conventional farms always had higher direct and total climate change impacts than organic farms per ha of UAA ($p<0.033$, Table 2). In contrast, only total acidification and direct eutrophication impacts were always higher for conventional farms per ha of UAA ($p<0.008$ and $p<0.041$, respectively). The confidence intervals of their counterparts (direct acidification and total eutrophication) did not overlap but had confidence intervals of p-values that included $p=0.05$. Per 1000 kg FPCM, only direct climate

change and direct and total acidification had confidence intervals of p-values (albeit wide ones) that included p=0.05.

Confidence intervals of mean impacts, their variabilities, and p-values of differences in impact between farm types caused by EF uncertainty encompassed the corresponding deterministic values of the previous study, sometimes widely, indicating no change in mean impacts between studies (Table 2). However, for five of the 12 direct and total impacts (direct climate change and direct and total acidification per 1000 kg FPCM, direct acidification and total eutrophication per ha of UAA), the confidence intervals of p-values obtained from propagating uncertainty in EFs now included α=0.05 (and other commonly-used significance levels), indicating the potential to change interpretation of results. Instead of t-tests, cumulative distribution functions (CDFs) of p-values can be used to estimate the probability that significant differences exist between farm types. For example, if choosing α=0.05, probabilities of significant difference between impacts were 17% for total climate change per 1000 kg FPCM (Fig. 4a) and 60% for direct eutrophication per ha of UAA (Fig. 4b).

3.3 Contributions of source categories to uncertainty in impacts

According to the sensitivity analysis, the source categories whose uncertainty contributed most to uncertainty in impacts differed by impact and farm type, but these categories were similar for both functional units. Per 1000 kg FPCM (i.e., cash crops excluded), manure deposited in pasture contributed the most to variations in climate change impacts (mean CTV of 67% and 84% for conventional and organic farms, respectively) (Fig. 3). The source categories contributing most to variation in acidification impact were related to manure management: cattle housing and manure storage, manure deposited in pasture, and manure spreading (mean CTV of 66%, 20%, and 14% for conventional farms, respectively; 52%, 34%, and 14% for organic farms, respectively). For eutrophication, leachate NO_3 had a mean CTV of 96% and 99% for conventional and organic farms, respectively. Contributions to variance per ha of UAA (i.e., cash crops included) were almost exactly the same, except for a slightly higher contribution of mineral fertilization and a slightly lower contribution of manure deposited in pastures (5 percentage points each) to climate change impacts of conventional farms (data not shown).

Across impact categories and farm types, variation in emissions from mineral fertilization had no CTV for organic farms (since it is prohibited) and relatively small CTV for conventional farms (8% for climate change, 1% each for eutrophication) (Fig. 3). Since “other” emissions (e.g., fuel and plastic use) did not change when EFs varied, they had zero CTV. Confidence intervals of mean CTVs were relatively small for all impacts except acidification for organic farms (Fig. 3).

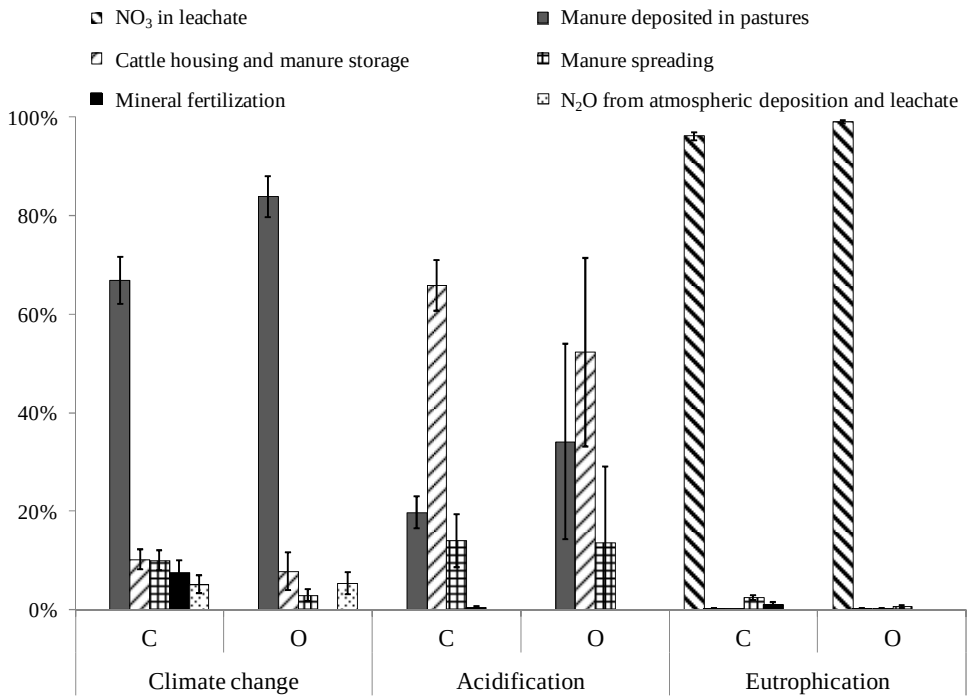

Figure 3. Mean contributions to variance (CTVs) and 95% confidence intervals (error bars) of seven categories of emission sources (due to epistemic uncertainty in emission factors) in direct climate change, acidification, and eutrophication impacts per ha of usable agricultural area of conventional (C) and organic (O) dairy farms in Brittany, France. Error bars reflect the combined effect of sample size and variability in CTVs due to differences in characteristics among farms.

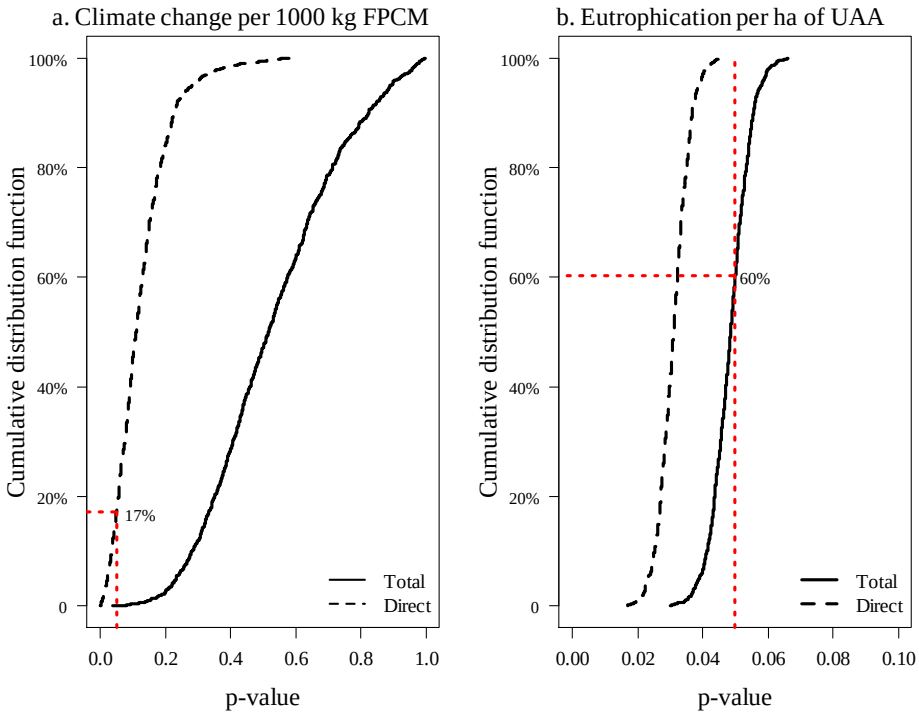

Figure 4. Cumulative distribution functions of p-values from 1000 Monte-Carlo simulation iterations for (a) total and direct climate change per 1000 kg fat-and-protein corrected milk (FPCM) and (b) total and direct eutrophication per ha of usable agricultural area (UAA). Dashed horizontal lines (red) indicate the probability of a difference in mean impact between farm types (conventional vs. organic) below a given significance level (here, α=0.05).

Table 2. Confidence intervals (95%) of mean values, their variabilities due to farm characteristics (coefficients of variation), and p-values of differences in means of three impacts per 1000 kg fat-and-protein-corrected milk (FPCM) sold and per ha of on-farm usable agricultural area (UAA) for conventional and organic dairy farms in Brittany, France, from Monte-Carlo simulation (MCS) and deterministic calculation (DC). Direct impacts consider only on-farm activities and hectares, while total impacts also include estimates of off-farm activities and hectares. Values in bold indicate differences between farm types with p-values always below 0.05. Values in italics indicate differences between farm types whose p-value confidence intervals include p=0.05.

				Per 1000 kg FPCM sold			**Per ha of UAA**		
Impact category	**Unit**	**Method**	**Type**	**Conventional farms**	**Organic farms**	**p**	**Conventional farms**	**Organic farms**	**p**
Climate change	kg CO_2-eq	MCS	Direct	*872-901 (14-18%)*	*937-1026 (7-17%)*	0.013-0.333	**5877-6243 (21-23%)**	**4422-4877 (14-24%)**	0-0.032
			Total	1024-1052 (13-16%)	1037-1126 (9-17%)	0.200-0.949	**6123-6440 (17-19%)**	**4690-5117 (13-22%)**	0.001-0.027
		DC	Direct	886 (15%)	981 (10%)	0.071	**6047 (21%)**	**4626 (18%)**	0.005
			Total	1038 (14%)	1081 (12%)	0.47	**6272 (17%)**	**4881 (16%)**	0.005
Acidification	kg SO_2-eq	MCS	Direct	*5.1-5.5 (14-20%)*	*5.4-6.4 (6-24%)*	0-0.833	*34.8-39.4 (20-28%)*	*25.3-30.7 (13-31%)*	0-0.077
			Total	*7.4-7.8 (15-20%)*	*6.3-7.3 (10-26%)*	0.013-0.675	**46.2-50.2 (15-21%)**	**28.4-33.5 (16-31%)**	0-0.007
		DC	Direct	5.3 (13%)	5.9 (10%)	0.062	**37.0 (21%)**	**28.0 (20%)**	0.007
			Total	7.6 (16%)	6.8 (15%)	0.135	**48.1 (16%)**	**31.0 (22%)**	0.001
Eutrophication	kg PO_4-eq	MCS	Direct	6.4-6.5 (39-41%)	4.4-4.9 (64-77%)	0.182-0.311	**41.2-43.0 (38-41%)**	**19.2-21.7 (81-97%)**	0.022-0.040
			Total	7.0-7.2 (36-38%)	4.8-5.3 (69-81%)	0.191-0.302	*39.2-40.8 (34-36%)*	*19.5-21.9 (81-96%)*	0.037-0.060
		DC	Direct	6.5 (40%)	4.7 (70%)	0.24	**42.1 (39%)**	**20.5 (88%)**	0.031
			Total	7.1 (37%)	5.0 (74%)	0.242	**40.0 (35%)**	**20.7 (88%)**	0.048

4. Discussion

4.1 Effects of adding uncertainty in emission factors to potential impacts

Propagating uncertainty in EFs with MCS added uncertainty to previously deterministic potential impacts for individual farms and also increased overall uncertainty in impacts by farm type. To clearly distinguish effects of EF uncertainty from those of farm-characteristic variability (expressed as CVs) on impacts by farm type, we chose to express the former differently, as confidence intervals, not only in mean impacts but in their variabilities and p-values of differences between them.

For individual farms, MCS-based impacts did not differ significantly from deterministic impacts from the previous study because default EF values used to calculate the latter corresponded to the means of the normal/log-normal EF distributions propagated. Individual farms of both types had relatively similar uncertainties in impact, except for higher eutrophication uncertainty for three organic farms, in which the calculation of NO_3 leaching was dominated by atmospheric N deposition and gaseous N emissions (and their uncertainty) due to their having smaller farm-gate N balances (mean = 18 kg/ha UAA) than those of other farms (mean = 71 kg/ha UAA). Using similar calculations, Payraudeau et al. (2007) also observed that variability in farm-gate N balance and uncertainty in EFs influenced uncertainty in NO_3 losses.

Impacts by farm type also did not differ significantly (α=0.05) between studies. Adding uncertainty to the previously calculated variability, however, revealed a potential to change the interpretation of differences between certain impacts by farm type, in particular total acidification per 1000 kg FPCM (now potentially significant) and total eutrophication per ha of UAA (now potentially non-significant).

4.2 Uncertainty analysis in other studies

Recent studies have used MCS in LCA-based approaches to assess effects of uncertainty in farm characteristics and/or EFs on climate change impacts (carbon footprints) of milk production. In a study of climate change impact of milk production in New Zealand, Basset-Mens et al. (2009) distinguished the variability of eight farm characteristics and eight EFs (estimated with standard deviations (SDs)) from uncertainties in their true values (estimated with standard errors of the mean (SEMs)) and analyzed their influence on climate change impact in 5000 MCS iterations. The 90% confidence interval (5^{th}-95^{th} percentiles) of climate change impact due to variability (~500-1582 kg CO_2-eq. per 1000 kg milk) was wider that that due to uncertainty (~856-1073 kg CO_2-eq. per 1000 kg milk).

Flysjö et al. (2011) modeled a representative dairy farm each in New Zealand and Sweden and estimated (via 5000 MCS iterations) the influence of uncertainties in a farm-specific EF for enteric CH_4 emission and three N_2O emission EFs on uncertainties in carbon footprints of milk. The 95%

confidence interval (2.5th-97.5th percentiles) of carbon footprint was wider for Swedish milk (828-1560 kg CO_2-eq. per 1000 kg energy-corrected milk (ECM)) than New Zealand milk (603-1520 kg CO_2-eq. per 1000 kg ECM). Using the same Swedish dairy-farm LCA model, Henriksson et al. (2011) varied seven farm characteristics (including the farm-specific CH_4 EF), based on surveys and national statistics, in 5000 MCS iterations to estimate their influence on carbon footprint. Their 95% confidence interval (940-1330 kg CO_2-eq. per 1000 kg ECM) was narrower than that of Flysjö et al. (2011) but reflected variability in farm characteristics rather than uncertainty in EFs.

While conclusions about the influence of uncertainty on milk-production impacts within or among studies that use the same models and assumptions appear valid, drawing conclusions from differences between different studies is challenging. The difficulty increases since many factors may differ, such as the type(s) of uncertainties assessed, input variables included, default values used, ranges and shapes determined for uncertainties, and whether and how milk production is corrected. That the confidence interval of mean climate change impact (due only to uncertainty in EFs) for conventional farms in our study (1024-1052 kg CO_2-eq. per 1000 kg FPCM) was narrower than corresponding confidence intervals in the other three studies may reveal more about differences in methodology (of both uncertainty analysis and LCA) than about differences in the systems studied. Uncertainty analysis thus adds an additional restriction to the fair comparison of LCA results from different studies: not only must their LCA models be similar, their uncertainty analyses must be similar, too.

Other methods for assessing the influence of multiple types of uncertainty exist and have been used in LCA. For example, Clavreul et al. (2013) combined probability distributions of variability and fuzzy intervals of epistemic uncertainty and used MCS to propagate them in an LCA of willow production for bioenergy. Combining probability distributions with fuzzy intervals yields a set of distributions with an even wider range of uncertainty than when only probability distributions are combined, due to lower precision (but potentially more complete representation of the state of knowledge) of fuzzy intervals.

4.3 Limitations of the study

Uncertainty analysis cannot escape some aspects of its underlying data. As in the previous study (van der Werf et al., 2009), the low variability in economic performance of the dairy farms surveyed (e.g., all were profitable) and the small sample size (n=47), especially of organic farms (n=6), limits the representativeness of results in this study, even for dairy farms in Brittany. Increasing the sample size of dairy farms would better represent the population, change the variability in impacts due to that in farm characteristics, and perhaps increase the precision of the prediction of results. In addition, since most of the emission-factor references used by EDEN-E are now relatively dated (1997-2007), emission factors or their uncertainty ranges that have changed in more recent references should be

updated in future studies using EDEN-E that are not explicitly attempting to compare results with previous studies.

We performed only 1000 MCS iterations per dairy farm, which increased the risks of insufficiently exploring the conceptual space of variable combinations or of a few extreme values skewing mean results. Increasing the number of MCS iterations from 1000 to 5000 for a few farms, however, increased the time necessary for MCS per farm far more (from 30 minutes to 90 minutes) than the corresponding increase in stability of estimates of mean values (data not shown). Thus, we considered 1000 iterations an acceptable trade-off.

Nonetheless, use of MCS in LCA has some limitations. First, it requires defining a probability distribution of each input variable based on statistical parameters (e.g., mean, dispersion), which becomes more difficult if empirical information is lacking (Payraudeau et al. 2007). When it is, expert judgment can help determine means and shapes of distributions (IPCC 2006c), including uniform or triangle distributions in extreme cases (Langevin et al. 2010; Morgan and Henrion 1992), but this represents an additional source of uncertainty. IPCC (2006c) favors normal and log-normal distributions, which represent many physical variables used in LCA relatively well (Geisler et al. 2005; Heijungs and Huijbregts 2004).

Most MCS is performed assuming that no correlations exist between input variables; thus, ignoring strong correlations that do exist between influential variables may lead to unrealistic combinations of input values and estimates of uncertainty in results (Bjorklund 2002). Including known or assumed correlations between input variables tends to decrease uncertainty in MCS results (Payraudeau et al., 2007), though some have reported that doing so increased it (e.g., Basset-Mens et al. (2009)). Although techniques for representing multiple correlations in MCS, such as variance-covariance matrices, have been developed in some LCA studies (e.g., Huijbregts et al. (2003)), they have been used less often in agricultural LCAs (e.g., Bojacá and Schrevens (2010)). By assuming no correlations between EFs in MCS, our results most likely reflect the largest uncertainties in impacts given the default values and ranges of EFs used (Chen and Corson 2013).

Due to EDEN-E and time constraints, this study did not explicitly estimate the influence on potential impacts of uncertainty in farm characteristics using MCS, as other studies (Basset-Mens et al. 2009; Henriksson et al. 2011) did. Doing so (with a different LCA model) would provide a more comprehensive assessment of the degree to which a variety of sources of uncertainty in input data influences impacts. Also, by examining only uncertainty (in EFs) and variability (in farm characteristics) in input data, this study excluded other potentially important sources of uncertainty, such as temporal, spatial, model, and scenario uncertainties. While the sample of all 47 farms covered the years 2003-2005, somewhat mitigating temporal uncertainty overall, each individual farm was sampled only once during those three years. Thus, variability in farm characteristics for each farm type

was based on only a single snapshot of each farm. Collecting data for each farm from multiple years would have decreased the influence of a particular year, especially if it had unusually extreme weather (e.g., 2003 in France) or market prices. A broader and more exhaustive study of uncertainty would need to include some of these other types, collecting data from additional regions or assessing the influence of specific models, methodological choices (e.g., allocation method), and assumptions (e.g., scenario characteristics). Sensitivity analysis can be used to test the influence of different models or allocation methods, while scenario analysis can test the influence of different characteristics or choices within scenarios (Hayashi et al. 2014).

4.4 Interpreting uncertainty in impacts

Expressing potential impacts as intervals yields imprecise predictions, which some decision makers might prefer (e.g., no oversimplified point estimates), but which others might find more challenging to interpret (Dubois and Guyonnet 2011). In particular, intervals of p-values (Fig. 4), while useful for close examination of differences between options, especially when the intervals include a preferred significance threshold (e.g., α=0.01 or 0.05), may be "too much information" for some individuals. Either way, the inclusion of additional types or sources of uncertainty assesses the state of knowledge about the system (or lack thereof) more completely. Decision makers can take this additional information into consideration, for example, using upper limits of impact intervals if they desire more conservative, precautionary decisions. When performing MCS in LCA, Basset-Mens et al. (2009) recommend that decision makers be presented with results based on "uncertainty" ranges (e.g., SEMs of input variables) rather than "variability" ranges (e.g., SDs of input variables) because variability represents something that they cannot reduce or control.

In contrast, epistemic uncertainty, as mentioned, can be reduced by collecting additional, more accurate, and/or more representative data. In this study, since overall uncertainty in EFs came from both epistemic uncertainty and variability (albeit in unknown proportions), confidence intervals of mean impacts and their variabilities could be narrowed by decreasing the epistemic uncertainty. If desired, acquiring higher-quality data to do so could begin with the emissions identified as most influential in the sensitivity analysis: N_2O and CH_4 from manure deposited in pastures for climate change, NH_3 and NO_x from cattle housing and manure storage for acidification, and NO_3 in leachate for eutrophication.

Uncertainty analysis need not be too intricate nor significantly increase the time required to perform LCAs. It is useful to first perform sensitivity analysis to identify which factors (e.g., farm characteristics, EFs) contribute most to uncertainty in potential impacts and then to focus on these factors in uncertainty analysis. Screening LCAs may accept higher levels of uncertainty and thus could perform more rapid, less-detailed uncertainty analyses and consider significant differences at higher significance levels (e.g., α=0.10).

5. Conclusions

Uncertainty analysis is crucial in LCA studies because consideration of uncertainty can make LCA results more reliable. Monte-Carlo simulation was an efficient probabilistic method to estimate effects of uncertainty in EFs and variability in farm characteristics on potential environmental impacts of dairy farms. Confidence intervals of mean impacts and their variabilities, due to uncertainty in EFs, resulted in wider ranges of predicted impacts, which gave the potential to change interpretation of differences in mean impacts between farm types. Nonetheless, how to express multiple types and sources of uncertainty and methods to combine them in the same LCA framework need further development to improve their understanding and interpretation by decision makers.

Acknowledgments

We thank two anonymous reviewers for their constructive criticism, which helped us improve the organization and clarity of the manuscript greatly.

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Chapitre 4.
Consideration of input correlations in Monte Carlo simulation when estimating enteric methane emissions in LCA

Paper prepared for submitting to International Journal of LCA;

Consideration of input correlations in Monte Carlo simulation when estimating enteric methane emissions in LCA

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Abstract

Purpose Monte Carlo simulation (MCS) is widely applied to analyze uncertainty in life cycle assessment (LCA). However, most LCA studies have ignored correlations among input variables by using independent univariate distributions in MCS, and doing so may under- or over-estimate the uncertainty in potential emissions. The objective of this study is to demonstrate a modified method based on the multivariate normal distributions (MND) that can maintain the correlations and different shapes of distributions of input variables.

Methods We applied a method that creates a sample matrix of correlated input variables in MCS to estimate enteric methane emissions from cattle, considering only variability among farm characteristics. Data were taken from a previous LCA study of conventional dairy farms in France. A simple model was created to calculate the emissions. For comparison, we used a sample-based calculation as a sample-based scenario and defined three MCS scenarios: random MCS without correlations, MCS with correlation based on Spearman rank-order correlations, and MCS with the modified MND-based method. The sample matrices generated and their influence on estimated emissions were compared among the sample-based scenario and the three MCS scenarios.

Results and discussion Since the random MCS scenario had no correlations among input variables, its predicted mean emissions were significantly higher and less realistic than those of the sample-based scenario. It had a wider range of uncertainty in emissions than the two MCS scenarios with correlations, which maintained the shapes of distribution of input variables. Of the two, the modified MND-based method is more flexible than the method based on Spearman correlations, because it can preserve both Pearson and Spearman correlations. However, the feasibility of correlation methods in LCA depends on the amount of information available about correlations. Lack of information about them, perhaps leading to arbitrary judgments, increases uncertainty in estimates of multivariable distributions. Therefore, one should carefully measure correlations among input variables to guarantee the feasibility of this method (i.e., test whether or not the correlation matrix is positive definite). In addition, considering only the strongly correlated input variables increases the computational efficiency of MCS.

Conclusion Consideration of correlations in MCS provides more realistic emission estimates than random simulation. The modified MND-based method maintains correlations (Pearson and Spearman) among input variables and the shapes of distribution that fit observed samples. To improve computational efficiency, it is recommended to choose only strongly correlated variables when applying correlated MCS in LCA studies, leaving weakly correlated variables randomly distributed. Finally, application of this method is feasible in LCA studies provided enough information about correlations exists. If not, random MCS provides more precautionary predictions.

Keywords Monte Carlo simulation; Multivariable normal distribution; Pearson and Spearman correlations; Cholesky factorization; life cycle assessment

1. Introduction

Monte Carlo simulation (MCS) is commonly used to analyze uncertainty in life cycle assessment (LCA) (Lloyd and Ries 2007). It generates a set of uncertain input variables (e.g., inventory data, characterization factors) using probabilistic distribution functions and estimates emissions and/or impacts (e.g., climate change, acidification) based on the values of input variables generated. Repeating the above process many times, the emissions or impacts are calculated as probability distributions, each of which has a mean (i.e., expected value of a population) and a variance (i.e., uncertainty range of a population). MCS has shown its feasibility and efficiency in uncertainty analysis in a complex LCA models, but most of studies using MCS assumed independent input variables (Basset-Mens et al. 2009; Steinmann et al. 2014). Failure to incorporate correlations among input variables may result in unrealistic predictions (Bjorklund 2002; Firestone et al. 1997; Lloyd and Ries 2007). Therefore, more attention should be paid to consideration of correlations in MCS in LCA studies.

In some LCA studies, the same variables (e.g., characterization factors) are used in more than one of the systems being compared. If MCS is run separately for each of these systems, results are likely to differ more than if MCS is run for all systems simultaneously, which can be done by introducing a comparison indicator (Sonnemann et al. 2003), recommended for considering this type of correlation (Huijbregts et al. 2003). Another type of correlation also exists among input variables, which is often ignored in MCS in LCA studies because the MCS requires independent values of input variables to generate the sample set of all possible combinations. However, assuming independence of input variables may under- or over-estimate output uncertainty (Bjorklund 2002). To avoid this problem, dependent variables should be modeled as a function of independent variables. Thus, dependent variables are no longer randomly distributed but vary with independent variables. Although a biophysical function between dependent and independent variables may not always exist, they may have a correlated relation (e.g., linear, monotonic). Based on this information, several methods have been developed to control correlations among input variables in MCS by generating a correlated sampling matrix.

Iman and Conover (1982) considered correlations between model inputs by inducing Spearman rank-order correlations. Helton and Davis (2003) described this method when using Latin Hypercube Sampling (LHS) to propagate uncertainty in models of complex systems. This correlation method allows for all distribution shapes, maintains rank-order correlations among input variables, and can be used with a stratified sampling technique (e.g., LHS) to generate samples. Indeed, when variables have nonlinear relations, Spearman rank-order correlations (monotonic) express them better than Pearson correlations (linear) (Berthouex and Brown 2002). Despite this method's advantages for controlling correlations in MCS, some analysts prefer to use Pearson correlations. The multivariate normal

distribution (MND) method was developed by Scheuer and Stoller (1962). It generates a set of variables whose Pearson correlations are controlled to be similar to desired correlations obtained from observations or empirical research (Cullen and Frey 1999; Morgan and Henrion 1992). IPCC (2000) mentioned both methods for controlling correlations but did not describe how to use them. Bojaca and Schrevens (2010) used MNDs in LCA uncertainty analysis of crop production and found that uncertainty in abiotic depletion and global warming impacts differed between simulations with correlations (multivariate) and without correlations (univariate). However, construction of MNDs requires that input variables have normal distributions; this may limit its application in LCA, because distributions of input variables vary depending on the information available about their shapes and the parameters (e.g., mean, variance) used to describe the distribution (Heijungs and Frischknecht 2005).

This study aimed to demonstrate a modified method based on the MND method. The method developed considered both Pearson and Spearman correlations among input variables in MCS and all shapes of distributions. It also illustrated the method based on Spearman rank-order correlations. Then, the correlations among input variables calculated by these methods and their influence on predictions were compared in a simple case study of methane emissions from cattle. Finally, the potential application of both methods in LCA studies is discussed.

2. Methods

2.1 Correlation control

Since classic MCS assumes that values of input variables are independent from one another, their values in each iteration ignore correlations among them. This process covers as many combinations of values as possible after many iterations. However, the degree of correlation among input variables may influence the variance of results. For instance, if $z = x + y$, the variance of z is calculated as follows:

$$\sigma_z^2 = \sigma_x^2 + \sigma_y^2 + 2\sigma_{xy} \quad \text{Eq. 1}$$

where σ_x^2 and σ_y^2 are variances of x_x and x_y, respectively, and σ_{xy} is their covariance. Denoting their Pearson correlation coefficients as ρ_{xy}, there is:

$$\rho_{xy} = \sigma_{xy} / \sqrt{\sigma_x^2 \sigma_y^2} \quad \text{Eq. 2}$$

If x and y are not correlated, ρ_{xy} equals zero; so, their covariance (σ_{xy}) equals zero. However, if a high correlation exists, σ_{xy} should not be ignored; doing so may yield significantly a different estimate of variance of z. Therefore, the variance of z is influenced by the variance of input variables (x and y) and their correlations.

The MND is a generalization of a one-dimensional normal distribution to higher dimensions. For a random vector $X=(x_1, x_2 \dots x_n)$, if each variable $x_n \in X$ is normally distributed with a set of mean values $\mu = (E[x_1], E[x_2] \dots E[x_n])$, and its variance-covariance matrix $\sum$ ($n*n$) is given based on empirical samples, the vector X corresponds to a n-dimensional random vector written as $X \sim N(\mu, \sum)$ (Scheuer and Stoller 1962):

$$X = Mz + \mu \quad \text{Eq. 3}$$

where z is a n-dimensional standard normal distribution ($z \sim N(0,1)$) and the matrix M is a lower triangular matrix of $\sum$ (symmetric and positive definite matrix[1]), which can be obtained by Cholesky factorization (Eaton and Olkin 1987). There is:

$$MM^T = \Sigma \quad \text{Eq. 4}$$

where the matrix M^T (an upper triangular matrix) is a conjugate transpose of M . Based on this theorem (Eq. 4. 2), the MND of vector X has density function:

$$f(X) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \exp\left(-\frac{1}{2}(X-\mu)^T \Sigma^{-1}(X-\mu)\right) \quad \text{Eq. 5}$$

As for the univariate normal distribution, the inverse of this density function allows n (the number of input variables) normal distributions of these variables to be generated, each with its own parameters (e.g., mean, variance and covariance), and whose variance-covariance matrix $\sum$ corresponds to their matrix of Pearson correlation coefficients (ρ_{ij} , $i, j \in n$) according to Eq. 2. Hence, the MND, which creates a matrix of input values with correlations similar to those in the empirical data, is often used in MCS uncertainty analysis. However, its assumption of a normal distribution of all input variables may be inappropriate in some case studies. In this study, we used an alternative method to transform normal distributions to other distributions. Like the original MND method, the method first constructs n-correlated standard normal units (z_i) of matrix Z ($B*n$, where B is the number of rows of Z) based on the desired Pearson correlation coefficients. Means of units in Z equal zero, and the variance-covariance matrix has the same values as the desired correlation matrix (Eq. 2) (i.e., variances equal one, covariance equals the Pearson correlations). If Spearman rank-order correlations (r_{ij}) are known instead, the normal "copulas" function (Nelsen 1999) can be used to transform r_{ij} into ρ_{ij}:

$$\rho_{ij} = 2\sin(\pi r_{ij}/6) \quad \text{Eq. 6}$$

Next, the correlated unit variables (z_i of Z) are used to obtain their desired distributions (Ferson et al. 2004):

[1] A symmetric $n*n$ real matrix M is called positive definite matrix if z^TMz (z^T is the transpose of z) is positive for every non-zero column vector z of n real numbers.

$$x_i = F^{-1}\big(\Phi(z_i)\big), i = 1, 2, \dots, n \quad \text{Eq. 7}$$

where $\Phi(z_i)$ is the standard normal distribution function of z_i and F^{-1} is the inverse of the desired distribution. Repeating the two steps for each row of matrix Z provides a matrix ($B*n$) of these variables. On one hand, the correlations are controlled by the MND-based method; on the other hand, the standard normal distribution function transforms the normal distributions of units into uniform distributions and then transforms them into the desired shapes of distribution. Hence, both correlations and distributions of variables are maintained when generating samples. In other words, any information about correlations and uncertainty (variance) in input variables is considered in the MCS.

Iman and Conover (1982) developed a different method, based on Spearman rank-order correlation coefficients (r_{ij}), to model correlated variables with different types of distributions. The main idea is to construct a standard matrix (using van der Waerden scores) whose rank-order correlations matrix has similar values as the desired rank-order correlations matrix (also based on Cholesky factorization) and then to rearrange the matrix of independently distributed variables into the same order as that of the standard matrix. Thus, the re-ordered matrix has the desired rank-order correlations, which reflect monotonic relations among the variables (More details in the appendix). To compare how these different methods control correlations in MCS, we applied them to a simple case study.

2.2 Data collection in a case study

Sample data were selected from a dataset of conventional Breton (France) dairy farms (n=41) collected previously by the LCA-based tool EDEN-E (Évaluation de la Durabilité des Exploitations) (van der Werf et al. 2009). Data for each farm include many input variables (e.g., number of animals, milk and meat production, energy use) and other factors (e.g., emission factors, characterization factors) used to build models to estimate the emissions and resource use of farm activities. For the sake of simplicity in this study, we chose a model from EDEN-E to estimate emissions of enteric methane (CH_4) from cattle, which are calculated as a function of the number of cattle in each age- or sex-based category and a corresponding emission factor. EDEN-E classifies cattle in five categories: dairy cows (i.e., lactating females), bulls, and heifers of three age classes (<1, 1-2 and >2 years old). We calculated the mean and standard deviation of each input variable based on the sample of 41 farms (Table 1) and assumed the number of bulls was zero because its mean value was less than one. To calculate mean annual enteric CH_4 emissions per animal category per year, EDEN-E applies the Tier 2 method of the IPCC (2006). In this study, we directly used the values calculated by EDEN. To avoid the influence of uncertainty in emission factors, all emission factors were kept as constant values for each farm except the emission factor corresponding to dairy cows, which is a function of mean milk yield per cow, which in EDEN is a function of the quantity of milk sold, the number of heifer calves (<1 year old) (to estimate the quantity of milk consumed on-farm) and the number of dairy cows.

Keeping emission factors constant focused on the influence of correlations in input variables (source of variability) on estimates of CH_4 emissions via MCS.

Table 1. Statistical descriptions of input variables and CH4 emission factors corresponding to heifer categories

Input variables	Unit	Mean	Standard deviation	Emission factor (kg CH_4/yr/head)
No. of dairy cows	head	43.5	9.47	*
No. of heifers (<1 year old)	head	11.0	7.81	37.2
No. of heifers (1-2 years old)	head	13.2	9.42	84.6
No. of heifers (>2 years old)	head	5.4	4.76	90.3
Quantity of milk sold	l	289 040	75 161	

**CH_4 emission factor of dairy cows varies as a function of quantity of milk sold, number of cows and number of heifer calves (<1 year old) on each farm.*

2.3 Monte-Carlo simulation with correlation

We created three MCS scenarios (S1, S2, and S3) to compare their predicted emissions to those calculated from sample data (S0: sample-based scenario). All three MCS scenarios determined distributions of input variables (i.e., means, standard deviations, correlation matrix, variance-covariance matrix) based on the data from the 41 farms. S1 used classic random-sampling MCS without correlation. Lognormal distributions were assumed for the number of dairy cows and the quantity of milk sold, according to goodness-of-fit tests. Truncated normal distributions were assumed for the other three input variables (number of heifers in each age class), since their values could not be negative. S2 used the samples generated from S1 and applied rank-order correlation coefficients to control Spearman correlations among input variables in MCS. S3 used a modified MND to model input variables according to their distributions (as in S1) and Pearson correlations. When considering Spearman correlations in S3, we first transformed the desired Spearman correlations into Pearson correlations (Eq. 6) and then generated a sample matrix that preserved Pearson correlations corresponding to the desired Spearman correlations. For all three MCS scenarios, the sampling process (10,000 MCS iterations) and statistical calculations (e.g., correlation matrix of input variables, mean of enteric CH_4 emissions) were performed using packages (e.g., “mnormt” for MND, “truncdist” for truncated distributions) of the R software (R Development Core Team 2012). The sample-based scenario and the three MCS scenarios calculated both Pearson and Spearman correlations among input variables. Estimated CH_4 emissions of all four scenarios were compared. Two-sample t-tests assuming unequal variance and two-sample Kolmogorov-Smirnov tests were applied to test for significant ($p<0.05$) differences in the means and fits of distributions of CH_4 emissions, respectively, between the sample-based scenario and the three MCS scenarios.

3. Results

3.1 Correlations between input variables

The three MCS scenarios each generated a matrix (10,000 rows × 5 columns) of input variables. The number of dairy cows in the sample-based scenario had strong correlations (Pearson's r and Spearman's $\rho \geq 0.5$) with the number of heifers <1 year old, the number of heifers 1-2 years old and quantity of milk sold (Table 2). In contrast, S1, the uncorrelated MCS scenario, had near-zero correlations (r and $\rho < 0.02$). S2, the method based on Spearman rank-order correlations, had Spearman correlations similar to those of the sample-based scenario (difference <0.02) but Pearson correlations less similar to those of the sample-based scenario, especially for the quantity of milk sold (difference >0.1). Nonetheless, its Pearson and Spearman correlations were similar to each other (difference <0.013). The Pearson correlations of S3, the modified MND-based scenario, were more similar than those of S2 to those in the sample-based scenario (difference <0.006). When Spearman correlations were calculated in S3, they were also similar to those of the sample-based scenario (difference <0.02). Furthermore, the linear regression line of quantity of milk sold versus the number of dairy cows for S3 when using Pearson correlations (adjusted $R^2 \approx 0.68$) overlapped that of the sample-based scenario ($R^2 = 0.69$) (Fig. 1). The same regression line for S3 when using Spearman correlations and for S2 also increased monotonically but deviated from that of the sample-based scenario ($R^2 \approx 0.50$ and 0.48, respectively). Ignoring correlations, the quantity of milk sold in S1 did not vary with the number of dairy cows ($R^2 \approx 0$). Thus, S2 and S3 each generated a matrix of input variables that was similar to the Spearman and Pearson correlation matrix of the sample-based scenario, respectively. Moreover, the MND-based method in S3 also preserved Spearman correlations. In contrast, the matrix of input variables generated in S1 did not represent the observed samples in the sample-based scenario.

Table 2. Pearson and, in parentheses, Spearman correlation coefficients between the number of dairy cows and the four other input variables for the sample-based scenario (S0) and three Monte-Carlo simulation scenarios: S1: truncated normal distributions and lognormal distributions without correlation, S2: method based on Spearman rank-order correlations, and S3: modified multivariate distributions with Pearson (Spearman) correlations.

Scenario	No. of heifers (<1 year old)	No. of heifers (1-2 years old)	No. of heifers (>2 years old)	Quantity of milk sold
S0	0.557 (0.494)	0.521 (0.548)	0.242 (0.307)	0.836 (0.700)
S1	0.007 (0.007)	-0.013 (-0.012)	-0.011 (-0.009)	-0.013 (-0.016)
S2	0.489 (0.477)	0.544 (0.531)	0.304 (0.298)	0.693 (0.681)
S3	0.555 (0.482)	0.507 (0.547)	0.232 (0.297)	0.834 (0.689)

3.2 Influence on enteric CH_4 emissions

Mean CH_4 emissions were significantly different ($p<0.05$) between the sample-based scenario and S1 but not between the sample-based scenario and S2 or S3 (Fig. 2). S1 overestimated CH_4 emissions, yielding a wider range of values and more uncertainty (coefficient of variation (CV) = 70%) than the sample-based scenario (CV = 39%) or the other two MCS scenarios (CV = 38% and 34%, respectively). In addition, all three MCS scenarios generated outliers beyond the higher whisker (the 75th percentile plus 1.5 times the interquartile range), probably because of the long tail of lognormal distributions assumed for the number of dairy cows and quantity of milk sold (Fig. 2). Cumulative density distributions of predicted CH_4 emissions in S2 and S3 (Pearson correlations only) were not significantly different from each other or to that in the sample-based scenario. In contrast, predicted CH_4 emissions in S1 deviated significantly from those in the sample-based scenario (Fig. 3).

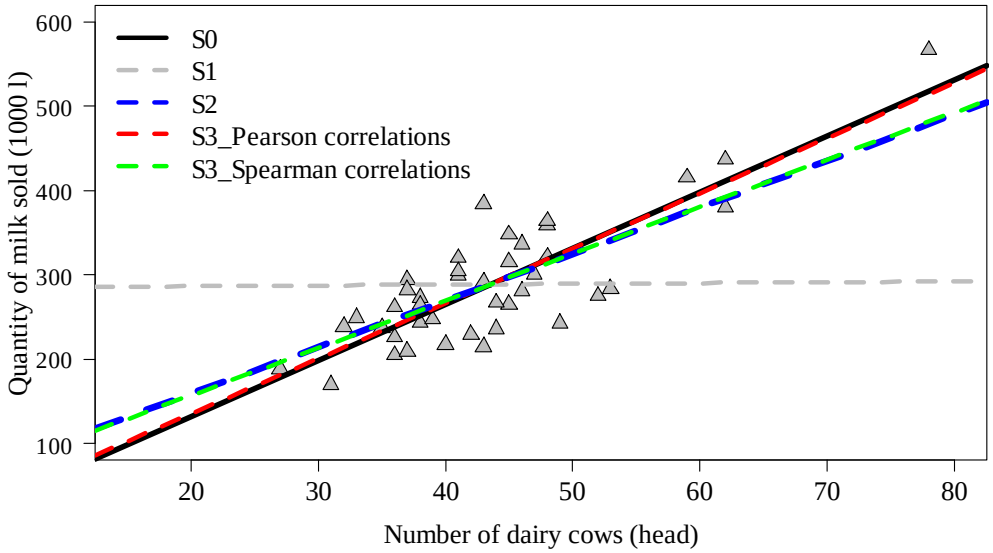

Figure 1. Quantity of milk sold (1000 l) versus the number of dairy cows (head) in the observed samples (triangles) and regression lines between them in observed samples (S0, solid black line) and three Monte-Carlo simulation scenarios: S1: truncated normal distributions and lognormal distributions without correlation (dashed gray line), S2: method based on Spearman rank-order correlations (dashed blue line), and S3: modified multivariate distributions with Pearson correlations (dashed red line) and with Spearman correlations (dashed green line)).

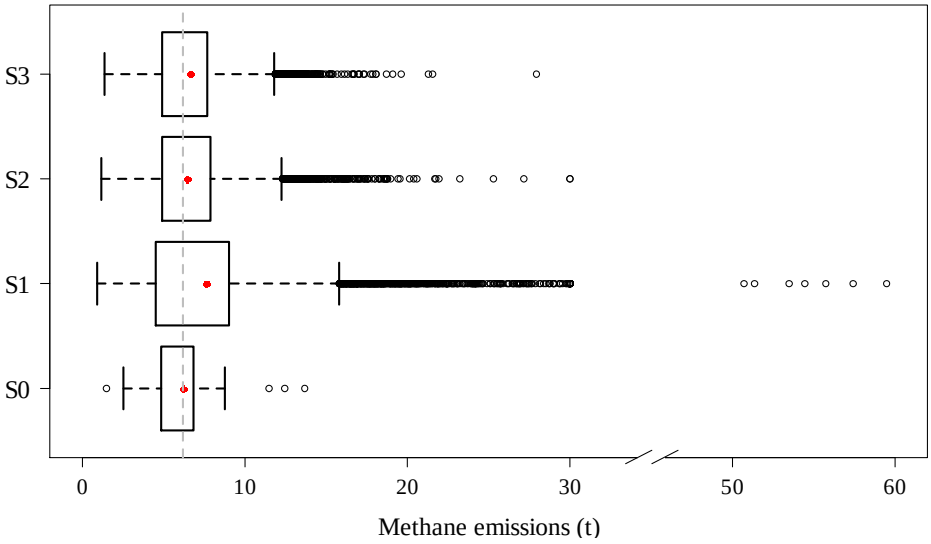

Figure 2. Box plots of methane emissions (t) from observed samples (S0) and three Monte-Carlo simulation scenarios: S1: truncated normal distributions and lognormal distributions without correlation, S2: method based on Spearman rank-order correlations, and S3: modified multivariate distributions with Pearson correlations. Red points indicate mean CH4 emissions. Ends of boxplot lower and higher whiskers represent the 25th percentile minus 1.5 times interquartile range and the 75th percentile plus 1.5 times interquartile range. The dashed gray line represents mean CH4 emissions from the sample-based scenario (a reference value). Points above or below the whiskers indicate outliers.

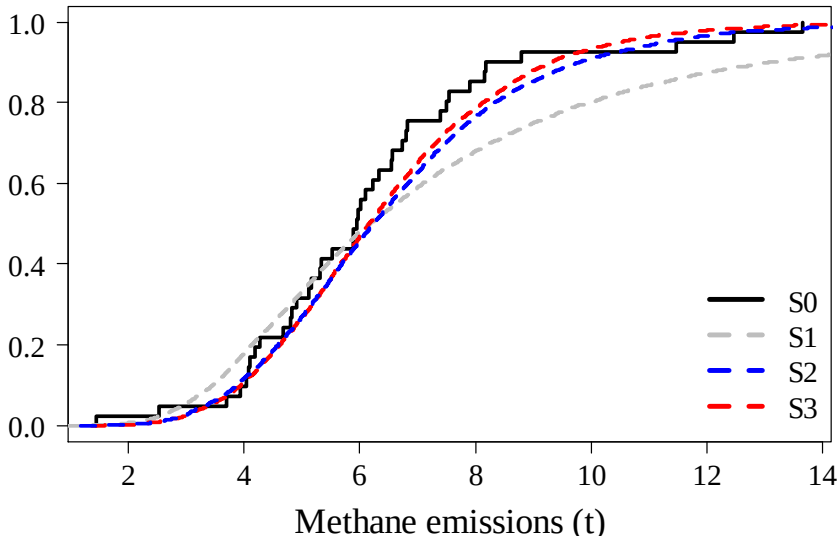

Figure 3. Cumulative density functions of enteric methane emissions (t) from cattle from observed samples (S0, solid black line) and three Monte-Carlo simulation scenarios: S1: truncated normal distributions and lognormal distributions without correlation (dashed gray line), S2: method based on Spearman rank-order correlations (dashed blue line), and S3: modified multivariate distributions with Pearson correlations (dashed red line).

4. Discussion

Incorporating correlations among input variables into MCS provided more realistic predictions of emissions and their uncertainty. For example, the samples generated in S2 and S3 maintained the shape of distribution of each input variable. Meanwhile, information about relations between variables was retained, such as the positive correlation between dairy cows and quantity of milk sold. While this relation is obvious, other systems analyzed in LCA have relations that are less obvious but no less influential, making retention of correlations potentially important. The method based on Spearman rank-order correlations preserves Spearman correlations, while the modified MND-based method is more flexible, preserving both Pearson and Spearman correlations. Both methods predicted emissions that were not significantly different and that had similar uncertainty ranges. It should note, however, that Pearson and Spearman correlations measure different aspects of variables. According to Hauke and Kossowski (2011), Pearson correlations measure the strength of linear relations among the variables and assumes that variables have a normal distribution. In contrast, Spearman correlations use rank scores rather than quantitative values to measure the strength of monotonic relations among variables without the assumption of a normal distribution. Therefore, one should be careful about the choice of type of correlation coefficient, selecting the one that better represents input variables in the model.

Either type of correlation coefficient (Pearson or Spearman) describes the degree(s) of relation between two or more variables but does not indicate causation between them (Berthouex and Brown 2002). Causation can only be addressed by knowing the mechanistic behavior of the system. For example, the emission factor for dairy cows was calculated as a function of milk production, which itself was a function of the number of dairy cows, the number of heifer calves (<1 year old) and the quantity of milk sold (independent variables). On the other hand, other strong correlations among input variables were observed in the observed samples, but their causation is unclear. Therefore, there is a need to incorporate information about correlations in LCA models; meanwhile, physical relations among variables should be studied to increase model accuracy.

The rank-order and MND-based methods used Cholesky factorization, which requires that variance-covariance matrices and correlation matrices be “positive definite” (Eaton and Olkin 1987). If they are not, upper triangular matrices cannot be found. Correlation matrices must be tested to ensure that they are positive definite. Ferson et al. (2004) argued that, except in cases of human error or small sample sizes, input values obtained from observed samples always have positive definite correlation matrices. In addition, problems may arise when input variables come from different studies or when arbitrary judgments about correlations are made. To address such cases, researchers (Higham 1988; Ince and Buongiorno 1991; Oren 1981) developed methods to build positive definite matrices that are similar to subjective correlation matrices or variance-covariance matrices. For instance, the R

package “corpcor” can compute the nearest positive definite matrix of a real symmetric matrix using the algorithm of Higham (1988). Since positive definiteness was not a problem in our study, we do not discuss details of these methods. However, we recommend confirming the positive definiteness of the desired matrix before applying the methods.

Although the case study illustrated only simple calculation of emissions, these methods can be applied to larger numbers of correlated input variables in the inventory assessment phase of LCA (Bojaca and Schrevens 2010). However, the difficulty of considering correlations in MCS may increase with LCA model complexity. First, neither method can be applied if information about the correlations is unknown. Even though expert judgment can provide indications about correlations, arbitrary values may introduce additional uncertainty (e.g., missing some possible combinations when generating the sample matrix). So, one should be careful about estimating correlations when empirical data are not available. When information about correlation among input variables is lacking, assuming that they are independent is more conservative but yields a wider range of predictions. Second, simultaneous consideration of many correlated input variables in LCA could decrease the efficiency of MCS. Since the strong correlations among input variables may influence predictions greatly, we suggest choosing only the strongly correlated variables when building the sample matrix, leaving the others weakly correlated distributed randomly.

5. Conclusions

The study demonstrated a modified method based on MNDs to preserve Pearson and Spearman correlations among input variables in MCS. This method maintained the correlations and shapes of distributions of input variables and yielded more realistic predictions of CH_4 emissions than those of classic uncorrelated MCS, depending on the reliability of the information about their correlations. For comparison, a method based on Spearman rank-order correlations was applied to the case study. Although emissions predicted by both methods were not significantly different, the sample matrix that each generated indicated different relations among input variables (linear versus monotonic), which can be chosen based on the analyst objectives. The modified MND-based method was more flexible, retaining correlations of both types of correlation coefficients. Both methods make it possible to consider correlations in uncertainty analysis via MCS, but the complexity of LCA studies (i.e., a large number of variables) may influence the feasibility of using these methods. Hence, we recommend choosing only strongly correlated variables in correlated MCS in LCA to improve computational efficiency, leaving weakly correlated variables randomly distributed. Finally, both methods require knowledge about the correlations. If this information is unknown due to lack of data, a classic random MCS provides more precautionary predictions by avoiding uncertainty due to arbitrary assumptions about correlations.

Appendix. Correlation control based on Spearman rank-order correlations

Suppose that there are n correlated variables $x_1, x_2 \dots x_n$, and we want to obtain a matrix ($k*n$) of these variables X, of which the desired rank-order correlation matrix C ($n*n$ positive definite matrix). The upper triangular matrix (P^T) of C can be found by Cholesky factorization:

$$PP^T = C \qquad \text{Eq. 8}$$

Next, we create a matrix S ($k*n$) and transform it to matrix S^*, whose rank-order correlation matrix has similar values as its Pearson correlation matrix, which itself has similar values as C:

$$S^* = SP^T \qquad \text{Eq. 9}$$

To do so, Iman and Conover (1982) suggested creating matrix S ($k*n$) by using van der Waerden scores $\Phi^{-1}(i/(k+1))$, $i=1, 2, ..., k$, where Φ^{-1} is the inverse function of the standard normal distribution. So, for each column of the matrix, we randomly permute these scores without replacement (i.e., each column includes the same scores but in different orders). Indeed, the use of van der Waerden scores makes the rank-order correlations of S have similar values as its Pearson correlations. The second prerequisite of this equation is that the Pearson correlation matrix of S be similar to the identity matrix (no correlation ($\rho_{ij} = 0$ for $i \neq j$) among the variables) (Helton and Davis 2003). This can be achieved by using correlation correction. So, denoting the Pearson correlation matrix as E (positive definite), according to Cholesky factorization, there is:

$$QQ^T = E \qquad \text{Eq. 10}$$

Next, S multiplied by $(Q^{-1})^T P^T$ (Q^{-1} is the inverse of the lower triangular matrix Q, T is the function that returns a given matrix to its transpose) transforms S into a matrix whose Pearson correlation matrix is the identity matrix, written as:

$$S^* = S(Q^{-1})^T P^T \qquad \text{Eq. 11}$$

Finally, we rearrange matrix X ($k*n$) of the n input variables, which are independently distributed and sorted in the same order as in matrix S^*. Hence, the Spearman rank-order correlations of transformed matrix X is similar to the desired matrix C.

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Chapitre 5.
Application of Dempster-Shafer theory to integrate methods to propagate variability and epistemic uncertainty in agricultural LCA

A shorter version of this paper presented in 2014 LCAFood conference in San Francisco

Application of Dempster-Shafer theory to integrate methods to propagate variability and epistemic uncertainty in agricultural LCA

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Abstract

Probability distributions are commonly used to represent variability in populations, while fuzzy intervals are an alternative approach for representing epistemic uncertainty in parameters when information is incomplete or imprecise. Combining both approaches, we represented variability and epistemic uncertainty in parameters separately, propagated them with Monte-Carlo simulation through the LCA model, and then used Dempster-Shafer theory to represent final results. We applied approaches to a case study of dairy farms to estimate their potential direct environmental impacts. Results indicated that consideration of incomplete information greatly increases overall uncertainty in impacts, as measured by a "relative interval width", which was useful for comparing the influence of input uncertainty among impact categories. Thus, our method provides conservative estimates of impacts by considering incomplete information, which is ignored by the classic probability method commonly used in LCA.

Keywords: life cycle assessment; Dempster-Shafer theory; variability; epistemic uncertainty

1. Introduction

Life Cycle Assessment (LCA) is a useful tool to estimate potential environmental impacts and resource use of farming systems (Thomassen et al. 2008; van der Werf and Petit 2002). The reliability of LCA results, which depends primarily on the quality of data and their pertinence for the system studied, is affected by uncertainty (Finnveden 2000; Weidema and Wesnaes 1996). Including uncertainty analysis in LCA may yield results that provide more useful information for decision making (Heijungs 1996; ISO 14040 2006). Therefore, there is a need to improve uncertainty analysis in LCA to increase the reliability of its results.

Uncertainty analysis includes a variety of methods that are used to express and propagate uncertainty in many fields, such as risk analysis (Vose 2008) and LCA (Benetto 2005; Bjorklund 2002). Most studies define two main types of uncertainty (variability and epistemic uncertainty), which have fundamental differences (Morgan and Henrion 1992). Variability (also called stochastic uncertainty) represents inherent differences among individuals in a population. It cannot be reduced but can be represented more precisely if more population data are available (De Rocquigny et al. 2008; Vose 2008). Probability distributions have been used widely in LCA (Basset-Mens et al. 2009; Henriksson et al. 2011; IPCC 2006b) to represent the variability due to randomness in the distribution of a given sample (e.g., with a mean, variance, and normal distribution). In contrast, epistemic uncertainty is defined as lack of knowledge (imprecise and incomplete information) about the true value of a variable or about the system mechanism. It can be decreased if more precise information or more accurate measurement becomes available. In LCA, epistemic uncertainty in parameters is often represented with probability distributions (Huijbregts 1998; Lloyd and Ries 2007), and both types of uncertainty are propagated by Monte-Carlo simulation (MCS), especially in complex models. MCS is an effective and robust way to estimate the uncertainty in predicted potential impacts (Payraudeau et al. 2007; Sonnemann et al. 2003). Some authors (Andre and Lopes 2012; Chevalier and Téno 1996; Mauris et al. 2001; Reza et al. 2013; Tan 2008), however, emphasize the difference between variability and epistemic uncertainty and argue that fuzzy-set theory (Zadeh 1978), with subjective degrees of plausibility/possibility, better represents uncertainty due to imprecise and incomplete information.

Since variability and epistemic uncertainty represent distinct states of knowledge, many studies have modeled them separately in the same framework. For example, Ferson et al. (2002) constructed “probability boxes” by combining probability theory and set theory. Baudrit et al. (2006) represented random variability and imprecision with probability and possibility distributions, respectively, and then propagated them for risk assessment. And Baraldi and Zio (2008) combined MCS and the possibilistic approach to propagate uncertainty. These three studies introduced the Dempster-Shafer

theory (Dempster 1966; Shafer 1976) to incorporate imprecise information into probabilistic models, making a bridge that combines different types of uncertainty (Yager 1987).

Although variability and epistemic uncertainty have been defined, and sometimes analyzed, separately in some LCA studies (Basset-Mens et al. 2009; Heijungs and Huijbregts 2004), few studies (Clavreul et al. 2013) have modeled them in the same framework. The aim of this study is to demonstrate how to combine two types of uncertainty, via Dempster-Shafer theory, to estimate potential environmental impacts of dairy farms. We then compare this method to classic probability methods.

2. Methods

We used probability distributions and fuzzy intervals to represent variability and epistemic uncertainty in parameters, respectively. These two types of uncertainty were propagated into LCA results by MCS and interval arithmetic using R software (R Development Core Team 2012). For each impact category, distributions of impact were represented by a Dempster-Shafer structure and mean impacts were represented by fuzzy intervals.

2.1 Representing variability with probability distributions

In a frequentist approach, a probability distribution assigns a probability of any possible event in a random experiment. It is often used to represent the variability of a variable. A random variable *X*, which is an element of all real numbers ($\mathcal{R}$), has a probability Pr(*x*) of having value *x*. In addition, the probability distribution can be described by its cumulative distribution function (CDF) and explained as the probability that *X* takes on a value less than or equal to *x*:

$$F(x) = Pr(X \leq x), for\ all\ X \in \mathcal{R} \qquad \text{Eq. 1}$$

In general, determining a distribution requires empirical data to identify its shape and basic parameters (e.g., mean and variance). If the amount of empirical data is sufficiently large, it can be considered to represent the entire population. However, since data acquisition is often limited by time and cost in LCA studies, probability distributions are generally determined subjectively based on the literature or expert judgment (Heijungs and Frischknecht 2005).

MCS is the most common method for propagating variability to estimate uncertainty in LCA studies. It consists of sampling input variables from their distributions and then calculating potential impacts through the model. By repeating the MCS many times, a CDF can be constructed to predict a probability range that represents overall uncertainty in impacts due to uncertainty in input variables.

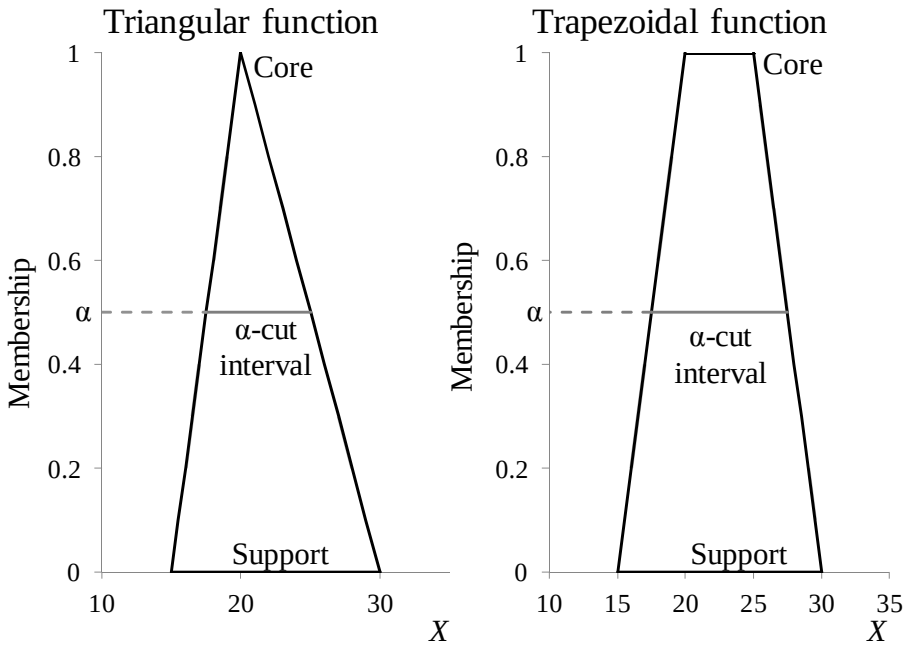

Figure 1. Triangular (left) and trapezoidal (right) fuzzy-interval membership functions for an uncertain variable X defined by core, support and α-cut intervals.

2.2 Representing epistemic uncertainty in parameters with fuzzy intervals

Fuzzy-set theory is an alternative approach to express epistemic uncertainty in parameters. In this approach, an uncertain variable is modeled by a set of "fuzzy" intervals, each with a level of possibility (α) that ranges from 0 (least possible) to 1 (most possible). Denoting each fuzzy interval as $\pi(\alpha_i)$, there is:

$$\pi(\alpha = 1) \subseteq \pi(\alpha_i \in [0,1]) \subseteq \pi(\alpha = 0) \quad \text{Eq. 2}$$

An uncertain variable can be mapped by a membership function defined by these "fuzzy" intervals and their corresponding levels of possibility. Commonly-used membership functions are shaped as triangles or trapezoids having minimum, maximum and mode values (mode intervals for the latter) (Fig. 1). For example, the minimum-maximum range of variable *X*, called the "support" (α=0), indicates all possible values of *X*. The mode (or mode interval), called the "core", indicates the most likely value(s) (α=1). At any given α level, there is a corresponding interval (called the "α-cut interval"). To propagate uncertainty, the fuzzy intervals of input variables are decomposed at each α level, and interval arithmetic is applied to generate a set of fuzzy intervals of the final result (Mauris et al. 2001).

2.3 Dempster-Shafer theory

Dempster-Shafer theory (DST) is a "mathematical theory of evidence" introduced by Dempster (1966) and further developed by Shafer (1976). It is a generalization of discrete probability theory in

which probabilities are assigned to sets of values rather than a single value. One important feature of DST is that imprecise information can be used to represent the state of knowledge quantitatively. It includes three basic functions: the basic probability assignment (bpa) function (or "mass function"), the belief function (Bel) and the plausibility function (Pl).

The bpa for a given set *A* (denoted *m(A)*) indicates the proportion of all available evidence that supports the supposition that a particular element of *x* belongs to set *A*. It has axioms such as:

$$m: 2^{\Omega} \rightarrow [0,1] \quad \text{Eq. 3}$$

$$m(\emptyset) = 0 \quad \text{Eq. 4}$$

$$\sum_{A \in 2^{\Omega}} m(A) = 1 \quad \text{Eq.5}$$

where 2^{Ω} is the power set that comprises all possible subsets, including the empty set ∅. *A* is any subset (called a "focal element") of power set. The belief and plausibility functions are defined from the bpa. The belief function of *A* is the sum of the bpa of all of the subsets (*B*) of *A* ($B \subseteq A$):

$$Bel(A) = \sum_{B \subseteq A} m(B), B \text{ is all of the subsets of } A, \text{and } B \neq \emptyset \quad \text{Eq. 6}$$

The plausibility function of *A* is the sum of the bpa of any subset (*C*) of power set with the condition that the intersection of *C* and *A is a non-empty set* ($C \cap A \neq \emptyset$):

$$Pl(A) = \sum_{C \cap A \neq \emptyset} m(C), C \in 2^{\Omega}, \text{and } C \neq \emptyset \quad \text{Eq. 7}$$

The three concepts can also be used in continuous probability distributions where any element of the uncertain parameter *X* is expressed as an interval ($[a_i, b_i]$) with bpa_i (where $a_i \leq b_i$ for all *i*). Thus, the power set of *X* is the collection of these intervals with their corresponding bpa_i, and the sum of bpa_i equals 1. So, Eq. 6 and 7 can be transformed as:

$$Bel(X \in]-\infty, x]) = Bel(x) = \sum_{b_i \leq x} m([a_i, b_i]) \quad \text{Eq. 8}$$

$$Pl(X \in]-\infty, x]) = Pl(x) = \sum_{a_i \leq x} m([a_i, b_i]) \quad \text{Eq. 9}$$

The belief and plausibility functions can be considered the lower and upper probability functions of *X* with a given value *x* (Ferson et al. 2002), respectively, and the true probability function of *X* (Pr(*x*)) lies inside them, interpreted as:

$$Bel(x) \leq Pr(x) \leq Pl(x) \quad \text{Eq. 10}$$

with an interval of the mean of *X*

$$\sum m_i a_i \leq E(X) \leq \sum m_i b_i \quad \text{Eq. 11}$$

If uncertain parameter X is determined by a set of single value ($a_i = b_i$ for all i) instead of intervals, the belief and plausibility functions converge on the same distribution, as in a classic CDF.

We used probability distributions and fuzzy intervals to represent random variables (x_1, $x_2 \ldots x_k$) and uncertain parameters (x_{k+1}, $x_{k+2} \ldots x_n$), respectively, and propagated them with MCS combined with interval arithmetic. Thus, assuming that impact category (y) is calculated by the model ($f(x_1, x_2 \ldots x_k, x_{k+1}, x_{k+2} \ldots x_n)$), we:

Generate a matrix (B rows (10,000) × k columns) of the first k variables using each one's probability distribution while preserving correlations between them: $M_b(x_1, x_2 \ldots x_k)$.

Select a possibility level α_i (e.g., assign values from 0 to 1 with step 0.1) and its corresponding fuzzy interval ($\pi^{k+1}, \pi^{k+2} \ldots \pi^{n}$) for the last n-k uncertain parameters (x_{k+1}, $x_{k+2} \ldots x_n$).

Using the variables in each row of $M_b(x_1, x_2 \ldots x_k)$, calculate minimum and maximum values of y with all possible combinations of the last n-k variables ($= 2^{(n-k)}$) in α_i, with a lower bound of L(y) = max [$f(x_1, x_2 \ldots x_n)$] and an upper bound of U(y) = min [$f(x_1, x_2 \ldots x_n)$]. For a model with only monotone functions, the computational optimization can be simplified by interval arithmetic.

Repeat steps 2 and 3 for all α_i to generate the fuzzy intervals of y_b ($[U(y), L(y)]_b$) and find the support of y_b (denoted $\pi\,(y_b)_{\alpha=0}$). Then attribute a mass ($m_b = 1/B$) to the support.

Repeat steps 2-4 B times to obtain a set of supports ($\pi_1, \pi_2, \ldots, \pi_B$) as focal elements, which is used to construct lower (belief function) and upper (plausibility function) bounds of y using Eq. 8 and 9.

Calculate the mean of the lower and upper bounds of y using Eq. 11 for each α to generate fuzzy intervals of the mean of y.

In this way, uncertainty in the value of an impact can be represented by a DST structure. For example, assume that impact indicator Y is modeled by a function with two uncertain parameters (X_1 and X_2), $Y = X_1 \times X_2$, where X_1 is normally distributed ($X_1 \sim N_{prob}(100,20)$) and X_2 is modeled by a triangular membership function ($X_2 \sim T_{fuzzy}(2, 6, 3)$). Thus, we construct the lower and upper bounds of Y and fuzzy intervals of the mean of Y at each α (Fig. 2) by following the above steps. Consequently, this procedure generates a set of intervals (11, in this study) with their corresponding α, and the mean of Y is represented as a membership function of this fuzzy set that is determined by its support, core and other α-cut intervals.

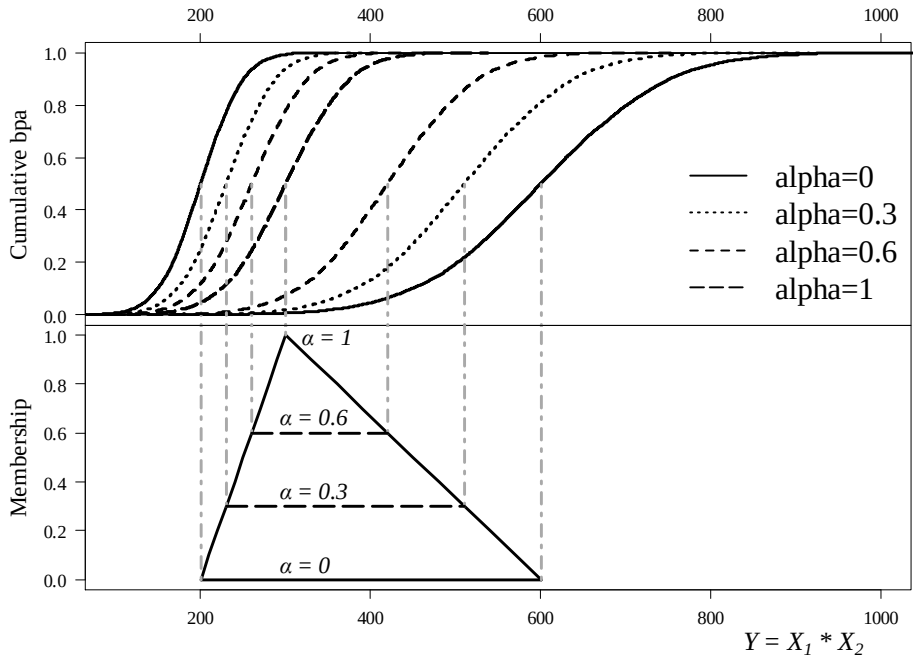

Figure 2. *Top:* Lower (belief) and upper (plausibility) bounds of indicator Y at different possibility levels (α); *Bottom:* fuzzy intervals of the mean of Y with support (α=0), core (α=1) and two α-cut intervals (at α=0.3 and 0.6).

2.4 Case study

We constructed an LCA model to estimate environmental impacts (climate change, acidification and eutrophication) of on-farm emissions of dairy farms. The functional unit was 1 metric ton of fat-and-protein corrected milk (FPCM). This model was based on the EDEN-E (Evaluation de la Durabilité des ExploitatioNs) tool, developed previously to estimate LCA-based environmental impacts of individual dairy farms (van der Werf et al. 2009). In this study, we focused only on direct impacts of the milk-production subsystem, because they were affected directly by uncertainty in emission factors. We used data from 41 conventional dairy farms from EDEN-E datasets. We obtained input variables such as animal production (e.g., meat, milk), number of animals by age and sex, and usable agricultural area. Other variables such as quantities of nitrogen (N) in farm inputs and outputs (e.g., fertilizers, feed, waste, and animals), energy agents (e.g., diesel, gasoline, and electricity), lubricants and plastics were also taken from EDEN-E. In addition, emission factors were used to estimate gaseous emissions; their default values and ranges of uncertainty were taken from the literature (EMEP-CORINAIR 2001; IPCC 2006a). These variables were used in the model to estimate direct impacts of conventional dairy farms. We considered two types of uncertainty in input variables: variability in structural characteristics of sampled farms and epistemic uncertainty in emission factors. Impact categories were calculated by multiplying emissions with the characterization factors of the CML-IA database (Guinée et al. 2002).

To compare results with those of the classic probability method, we made three scenarios to analyze uncertainty in the LCA model. For all scenarios, we used truncated normal or uniform distributions to represent variability in each farm characteristic because they provided only non-negative values. Means, standard deviations, and minimum/maximum values for each characteristic were determined from the empirical EDEN-E sample. Correlations between these variables were preserved using multivariable distributions (chapter 4). In the first scenario (S1), uncertainty in emission factors was ignored (default constants used). In the second scenario (S2), we considered uncertainty in emission factors with triangular probability distributions. In S2, default values and ranges of uncertainty were used as the mode and minimum/maximum values in the distribution, respectively. In the third scenario (S3), we used fuzzy intervals with triangular membership functions to represent uncertainty in emission factors. The same default values and ranges of uncertainty were used as the core and support in the membership function, respectively. Indeed, S1 can be considered a special case of S3 that considers only the core interval (α=1). Each emission factor was assumed to be independent. Scenarios S1 and S2 used MCS to propagate uncertainties, while S3 combined MCS and interval arithmetic to generate an interval distribution. Simulations were repeated 10,000 times. In S3, finding minimum and maximum impact values for each of the 10,000 replicates theoretically required calculating all possible combinations of emission factors (2^m combinations, m = number of emission factors), but doing so would have increased calculation time considerably. Therefore, since the LCA model was monotonic (emission factors used only addition and multiplication), calculations were optimized by using the minimum and maximum of each α-cut interval of emission factors.

Statistics (mean, 5th and 95th percentiles) of impact indicators were calculated as single values in S1 and S2 and as intervals in S3. To compare uncertainty in mean impact between categories, we calculated a "relative interval width" (RIW), equal to the maximum of a statistic's interval minus its minimum, divided by its mode. Thus, the RIW of mean impact in S3 was the width of the indicator's mean interval (i.e., its support) divided by its core (i.e., the most likely mean value). Because uncertainty in emission factors was assumed to be zero in S1 and a known distribution in S2, they were considered to have intervals of zero width.

3. Results

Statistics of the three impact categories differed by scenario (Table 1). For all three impact categories, the difference between the 5th and 95th percentiles ($I_{percentile}$) in S1 and S2 was narrower than the difference between the minimum of the 5th-percentile interval and the maximum of the 95th-percentile interval in S3, indicating higher overall uncertainty in S3. The increase in overall uncertainty was due to inclusion and representation of epistemic uncertainty in emission factors. The percentage increase in $I_{percentile}$ from S1 to S2 was 22% for climate change, 77% for acidification, and 0% for eutrophication, while that from S1 to S3 was 205% for climate change, 379% for acidification

and 29% for eutrophication. Thus, overall uncertainty in impacts increased greatly when uncertainty in emission factors was considered as imprecise information.

Table **1**. Statistics of potential climate change, acidification and eutrophication impacts per t of fat-and-protein-corrected milk (FPCM) in three scenarios that represented uncertainty in emission factors (EFs) differently: S1 - no uncertainty in EFs, S2 - probability distributions for EFs, S3 - fuzzy sets for EFs.

	Climate change (kg CO_2 eq./t FPCM)			**Acidification** (kg SO_2 eq./t FPCM)			**Eutrophication** (kg PO_4 eq./t FPCM)		
Statistics	**S1**	**S2**	**S3**	**S1**	**S2**	**S3**	**S1**	**S2**	**S3**
Lower limit (5th percentile)	668	746	[418, 1269]	8.3	9.6	[3.6, 18.4]	4.3	3.9	[2.5, 5.0]
Mean (support of the mean)	925	1075	[603, 1719]	10.8	14.3	[4.8, 24.5]	8.7	8.3	[6.7, 9.5]
Upper limit (95th percentile)	1275	1488	[861, 2271]	14.4	20.4	[6.3, 32.8]	14.1	13.7	[11.7, 15.1]

When visualized as CDFs (Fig. 3), S1 and S2 were represented by a single CDF each, while S3 was represented by two CDFs (plausibility and belief functions) defining upper and lower bounds of impact in each category (Fig. 3). These bounds were more widely separated for acidification and climate change impact than eutrophication.

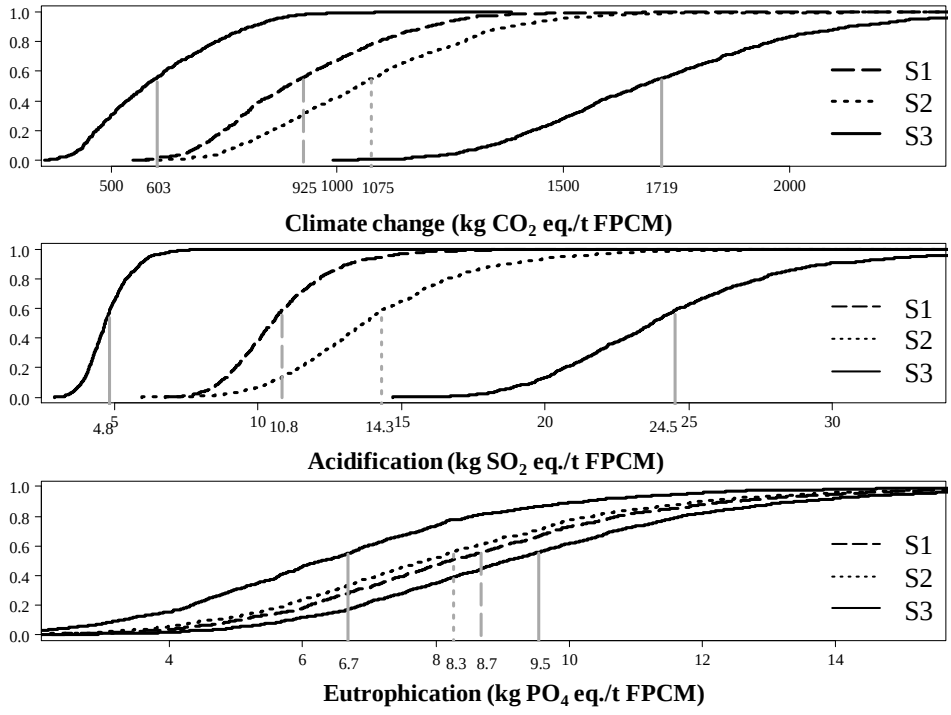

Figure 3. Cumulative density functions of direct (on-farm) climate change, acidification, and eutrophication impacts per t of fat-and-protein corrected milk (FPCM) in three scenarios that represented uncertainty in emission factors (EFs) differently: S1 - no uncertainty in EFs, S2 - probability distributions for EFs, S3 - fuzzy sets for EFs (solid curves bound 90% of possible values). Vertical gray lines indicate the mean impact (support of mean impact in S3) of each scenario.

Membership functions of mean impacts in S3 were nearly triangular, with minor skewness (Fig. 4). For example, the support of climate change ranged from 603-1719 kg CO_2 eq./t FPCM, with a core of 925 kg CO_2 eq./t FPCM. Note that the core of mean impact in S3 equaled the mean impact in S1, for which default values (considered as the true values) were used for emission factors. RIWs of mean impacts in S3 indicate that uncertainty in mean acidification impact (134%) was larger than that in mean climate change (96%) or eutrophication (35%) impacts (Table 1). However, S1 and S2 each had a single mean (e.g., 925 and 1075 kg CO_2 eq./t FPCM, respectively) and RIWs of mean impact of 0%.

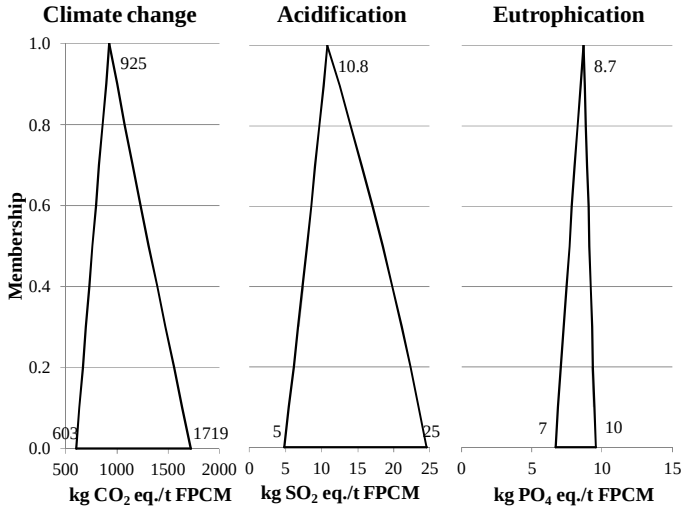

Figure 4. Fuzzy-interval distributions of means of climate change, acidification, and eutrophication impacts per t of fat-and-protein-corrected milk (FPCM) in scenario 3 (based on Dempster-Shafer theory).

4. Discussion

We focused on two sources of uncertainty in this case study: variability (in farm characteristics) and epistemic uncertainty (parameter uncertainty in emission factors). The classic probabilistic approach expresses both parameter uncertainty and variability with probability distributions; however, subjectively defining probability distributions may underestimate overall uncertainty. Therefore, unknown distributions should be considered as another source of uncertainty due to incomplete information and modeled with fuzzy intervals. If both probability distributions and fuzzy intervals exist in the same analysis, our DST-based method can combine them to estimate overall uncertainty in impact (S3). It provides a more conservative range of uncertainty (i.e. the interval between the minimum of the 5^{th} percentile and maximum of the 95^{th} percentile) than the classic probabilistic approach. Since S1 considered only variability in farm characteristics, the increase in overall uncertainty in impacts in S2 and S3 compared to S1 reflects the contribution of epistemic uncertainty in emission factors alone. Considering emission factors as fuzzy intervals (S3) increased overall uncertainty more than considering them as random values (S2). Unlike variability, epistemic

uncertainty in emission factors can be reduced when more precise information becomes available. For example, if the true values of emission factors (S1) or their distributions (S2) are known or assumed to be known, the real distribution of impact will be found inside the bounds of plausibility and belief, which yields a single mean value and a smaller range of uncertainty.

In parallel, the imprecision in emission factors was propagated into mean impacts, which were constructed from membership functions of their fuzzy sets. Those who used a similar propagation procedure in LCA (Clavreul et al. 2013) or risk assessment (Baudrit et al. 2006) studies considered all fuzzy intervals of impact as a set of random intervals with equal probability and then calculated a weighted-mean interval from upper and lower bounds of distributions. In contrast, we separated this process into two steps: (1) estimate the overall range of all possible impact values using the supports of emission factors and (2) model mean impacts with fuzzy intervals. Indeed, showing the membership function of mean impact instead of a weighted-mean interval provides more information to decision makers, such as the levels of possibility corresponding to the most likely mean impact and mean impacts of best- and worse-case scenarios based on the degree of possibility. This information allows a more precautionary approach than a simple interval of mean impact for evaluating the magnitude of and uncertainty in predicted impacts. For fuzzy intervals, the RIW of mean impact is a comparative indicator that reflects the influence of explicitly representing the knowledge of information as incomplete (an unknown distribution), unlike the classic probability method, which ignores this source of uncertainty. It enables the influence of epistemic uncertainty in different impacts to be compared when calculating a coefficient of variation is difficult or complex (e.g., in S3, which comprised multiple probability distributions). Comparing RIWs among impact categories illustrates the relative influence of epistemic uncertainty on overall uncertainty in the impacts of each. If overall uncertainty is hindering decision making, this information could lead decision makers to focus on reducing the sources of epistemic uncertainty that contribute the most to uncertainty in impacts. For example, since epistemic uncertainty in emission factors had a larger influence on acidification than eutrophication impacts in this study, more precise measurement of acidification-related emissions would have a relatively larger influence in reducing overall uncertainty in an impact.

For the sake of simplicity, we illustrated a simple LCA example based on a previous work. It had far fewer variables and parameters than a full LCA study; in addition, the model was monotonic, which simplified optimization of calculations in the simulation. However, when an LCA model is not monotonic, increasing the number of uncertain variables (especially imprecise variables) may increase the complexity of computation, because the number of iterations increases exponentially when searching for minimum and maximum impact values (i.e., 2^m combinations, where m=number of imprecise input variables), and even may make results virtually meaningless when considering too much imprecision. Therefore, performing an initial sensitivity analysis of the LCA model is

recommended (Heijungs 1996; Henriksson et al. 2013) to focus on the input variables that influence potential impacts the most. This decrease in the number of uncertain input variables may accelerate calculations, especially in more complex and non-monotonic models.

Correlations between random variables (i.e., inter-farm variability) were preserved in this study, while independence was assumed between random variables and imprecise parameters (emission factors). This assumption allowed a conservative confidence interval of impacts to be generated for all three scenarios, because all possible combinations of input variables were included in the stochastic simulation. However, representing dependence between random variables and imprecise parameters (if known) could improve the precision of predicted impacts. More research is needed on this issue to improve the validity of LCA results.

The DST-based method constructs two boundary distributions using belief and plausibility functions. This structure has been interpreted as "imprecise probability" (Ferson et al. 2002), which covers all possible probability distributions. Although it reflects the true state of knowledge (e.g., incomplete information about emission factors), an extremely wide range of potential impact is likely to be less useful for decision makers. Thus, simplifying interpretation of results by decision makers remains an open question. To address this problem in LCA, Clavreul et al. (2013) calculated a "confidence index" (Dubois and Guyonnet 2011) to generate a weighted probability distribution. Decision makers can choose this confidence index subjectively, depending on whether their decision policies are more optimistic (close to the upper bound) or pessimistic (close to the lower bound). We concur that this kind of confidence index is useful for decision making in LCA studies when uncertainty is modeled with imprecise and incomplete information.

5. Conclusion

The classic probability method is rigorous in that it requires precise information to express an uncertain variable, but subjective assumption about its distribution may underestimate uncertainty in the predicted result. In addition, it cannot separate epistemic uncertainty from variability, meaning that decision makers will have no information about the relative influence of each on overall uncertainty. Our proposed method overcomes this limit by integrating fuzzy intervals to represent imprecise data (e.g., emission factors) in probability models. As a consequence, a distribution with two bounds and fuzzy intervals of mean impact was generated. Combining the effects of variability and epistemic uncertainty yields a wider range of potential impacts, which may influence decision making. Fuzzy intervals of mean impact model the uncertainty in mean values. The RIW of mean impact, as a comparative indicator, reveals the influence of epistemic uncertainty on uncertainty in impacts, which may help decision makers adopt appropriate strategies if they want to improve the reliability of LCA results.

The paper demonstrated the application of DST in uncertainty analysis in a simple LCA study. Representing the lack of knowledge as fuzzy intervals differs from treating it as randomness. Thus, it provides a conservative but robust way to represent the state of knowledge in LCA studies when information is scarce. Its application in LCA is currently limited, however, due to its greater model complexity and, if epistemic uncertainty is large, greater difficulty in distinguishing potential differences among scenarios. Considering dependence among input variables is also important, since it gives more precise results, but techniques for doing so with fuzzy-interval variables are still in development. Therefore, more research is needed to focus on these issues to improve the feasibility of this method in LCA.

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Chapitre 6.
Synthèse générale, discussion et perspectives

Les objectifs initiaux de la thèse étaient d'identifier les sources d'incertitude dans les analyses du cycle de vie de systèmes de production agricole, et puis de proposer des démarches pour représenter et propager ces incertitudes jusqu'à l'incertitude totale sur les indicateurs d'impact à travers l'ensemble de la démarche de l'ACV. Pour atteindre ces objectifs, le travail de thèse a commencé par une revue bibliographique sur la méthodologie pour identifier et traiter les incertitudes différentes, et puis un arbre de décision a été proposé pour guider les analystes ACV à choisir les méthodes adaptées au traitement des incertitudes différentes. À l'aide de cet arbre de décision, le travail suivant s'est concentré sur l'application des méthodes différentes pour traiter la variabilité naturelle et les incertitudes paramétrique en ACV agricole, ainsi que sur l'interprétation des résultats en prenant en compte le degré de confiance. Ce dernier chapitre synthétise et discute les acquis du travail de thèse par rapport aux objectifs attendus de chaque chapitre et discute des perspectives qu'ouvre ce travail aux futures recherches sur l'incertitude dans le cadre de l'ACV.

6.1 Le choix des approches pour l'analyse des incertitudes dans l'ACV agricole

Le premier effort était de synthétiser une typologie des incertitudes et leurs définitions correspondantes dans le cadre de l'ACV (cf. chapitre 2). Cette typologie distingue en premier l'incertitude aléatoire (variabilité) et l'incertitude épistémique, dont les propriétés sont différentes par définition. La variabilité (incertitude aléatoire) représente la différence intrinsèque dans le système étudié, tandis que l'incertitude épistémique représente la limite des connaissances de ce système. Donc, l'incertitude épistémique peut être réductible en acquérant les informations supplémentaires (ex., plus d'échantillons, mesure améliorée), tandis que la variabilité est irréductible mais peut être mieux caractérisée en augmentant l'échantillonnage spécifiques (y compris, si nécessaire, temporelle ou spatiale). La typologie classifie six sous-catégories pour ces deux types d'incertitude, ce qui permet de mieux identifier les sources d'incertitude du système. Tous ces types d'incertitude, qui se présentent souvent dans toutes les étapes de l'ACV, ont une influence sur le résultat final. Malgré l'existence des terminologies différentes dans les sources, ce genre de typologie est générique et peut s'appliquer à toute analyse des incertitudes dans le cadre de l'ACV.

Sur la base de cette typologie des incertitudes, la prochaine étape était d'étudier les approches utilisées actuellement dans le cadre de l'ACV pour représenter et propager des incertitudes différentes. Ces approches se sont principalement appliquées à représenter la variabilité naturelle et l'incertitude paramétrique, bien que le traitement d'autres types d'incertitudes soit, au mieux, seulement mentionné. Parmi ces approches, l'approche probabiliste traditionnelle est la plus commune pour représenter la variabilité et l'incertitude paramétrique en ACV, mais sa limite conceptuelle pour représenter l'incertitude paramétrique appelle le développement d'autres méthodes. En outre, l'ignorance et

l'imprécision sont souvent ignorées dans l'analyse de l'incertitude en ACV ; or s'est un domaine où, leur influence peut s'exercer fortement. En conséquence, des approches alternatives (ex., l'intervalle flou, la probabilité imprécise, la théorie de Dempster-Shafer (DST)) ont été développées pour distinguer l'incertitude épistémique de la variabilité. Lorsque les informations viennent de sources différentes, les méthodes de combinaison basées sur la DST (ex., règle de combinaison de Dempster) permettent de représenter l'incertitude totale en tenant compte de toutes les sources d'information. Enfin, l'approche (semi-) qualitative peut évaluer la qualité de données, quand l'analyse quantitative n'est pas faisable. Comme cette approche introduit le dire d'experts pour évaluer le niveau de qualité des données et des modèles, son résultat est dépendant du contexte de l'étude et du groupe d'experts.

Dans la problématique de la propagation de l'incertitude, l'incertitude de modèle et la variabilité temporelle ou spatiale sont abordées : l'incertitude de scénario est traitée par l'analyse de scénario ; et des méthodes analytiques (ex., série de Taylor, arithmétique des intervalles) et stochastique (ex., simulation de Monte Carlo (MCS), bootstrap) peuvent être appliquées en propageant la variabilité naturelle et l'incertitude paramétrique selon leurs modes de représentation. Chaque méthode de représentation a ses propres avantages et ses limites. L'approche probabiliste, du point de vue pratique, est facile à mettre en œuvre dans les modèles ACV, notamment à travers de la MCS. Mais la détermination de la distribution est souvent subjective. L'intervalle flou et la probabilité imprécise sont appropriés pour représenter l'incertitude épistémique. La DST est suffisamment flexible pour intégrer des incertitudes différentes dans le même modèle et réussit à distinguer la variabilité et l'incertitude épistémique par l'interprétation de la structure de la DST. Pour ces dernières deux approches, cependant, le temps de calcul peut être considérable à cause de l'utilisation d'arithmétique des intervalles, notamment quand le modèle n'est pas monotone, ou les variables imprécises sont nombreuses. Par exemple, le temps de calcul était plus grand pour le scénario avec la DST (80 seconds) que pour celui avec l'approche probabiliste traditionnelle (10 seconds) dans le chapitre 5.

Ce chapitre offre une vision générale sur l'analyse des incertitudes par rapport à leurs avantages et limites en ACV. Afin de les mettre en œuvre en ACV, un arbre de décision a été établi, qui permet à la fois d'identifier les types d'incertitude des variables d'entrée et de conduire les analystes ACV à choisir les méthodes adaptées pour représenter les incertitudes différentes en considérant plusieurs facteurs (ex., les types d'incertitude, les informations disponibles, les objectifs de l'étude). Donc, en suivant les différentes branches de l'arbre de décision (Fig. 1), le deuxième effort s'est porté sur l'application de ces différentes méthodes pour l'analyse des incertitudes, notamment la variabilité naturelle et l'incertitude paramétrique, qui sont plus communes en ACV agricole.

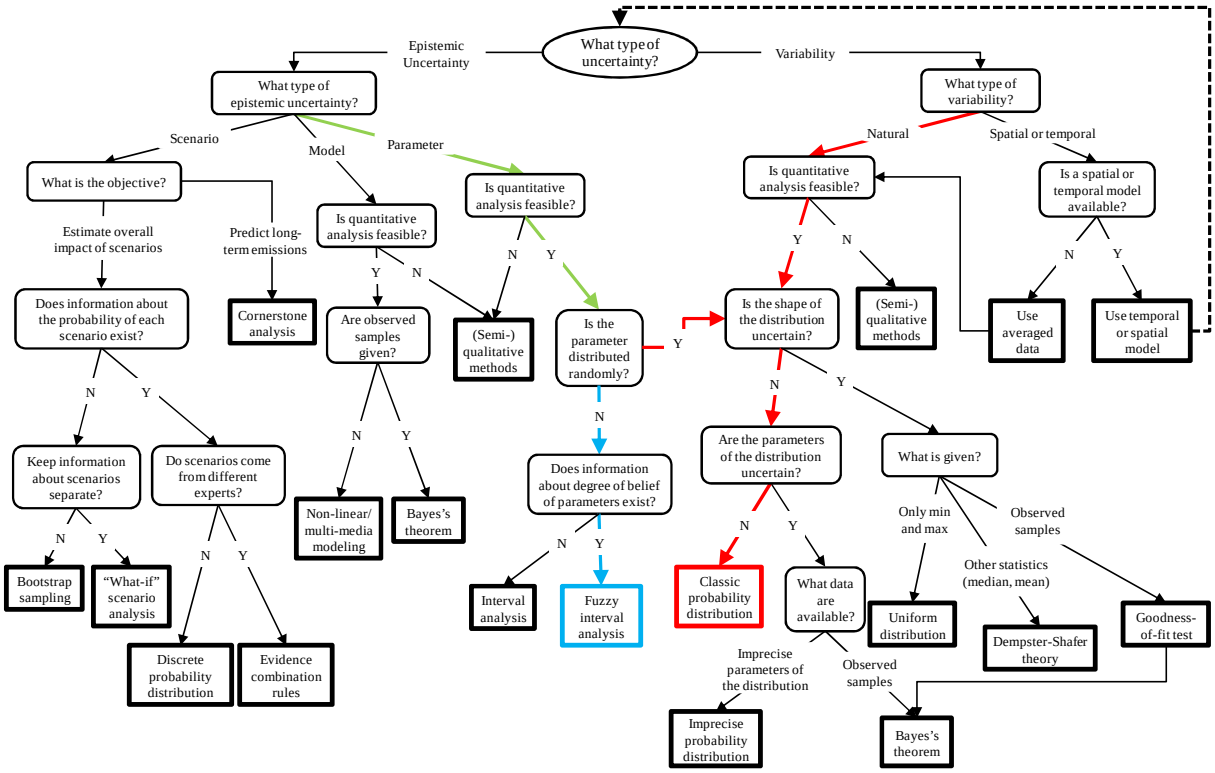

Figure 1. Arbre de décision pour choisir des méthodes appropriées pour représenter différents types d'incertitude (Fig. 5 dans le chapitre 2).

6.2 L'application de l'approche probabiliste classique avec simulation de Monte Carlo

La première branche suivie était l'approche probabiliste classique pour traiter l'incertitude paramétrique, (cf. chapitre 3), qui est actuellement largement appliquée par les analystes ACV. Cette approche a été utilisée dans une ACV d'une étude de cas agricole déjà réalisée sans prise en compte de l'incertitude paramétrique sur les facteurs d'émission. Les résultats de l'ACV étaient fortement affectés par la prise en compte de l'incertitude paramétrique, bien que les moyennes des impacts estimés ne changent pas de façon significative. L'augmentation de l'incertitude totale sur les impacts environnementaux qui en résulte est susceptible de modifier les conclusions des analyses dans le cadre d'une étude comparative. En effet, le test de significativité statistique est affecté par la prise en compte de l'incertitude paramétrique.

Pour distinguer clairement l'influence de l'incertitude épistémique et celle de la variabilité, elles ont été exprimées par intervalle de confiance et coefficient de variation (CV), respectivement. Donc la séparation de deux types d'incertitude a permis d'estimer la part d'incertitude sur les moyennes des impacts liée à l'incertitude sur les facteurs d'émission, et de prévoir les impacts potentiels liés à la variabilité sur les caractéristiques entre les fermes. Bien que ces expressions de l'incertitude soient imprécises, puisqu'on utilise une sorte « d'incertitude sur l'incertitude », qui est inhabituel pour

certains analystes ACV, la distinction des deux types d'incertitude peut servir à réduire l'incertitude épistémique en améliorant la technique de mesure pour obtenir des valeurs plus précises sur les variables d'entrée incertaines. D'autre part, la variabilité, issue d'information sur les échantillons observés, peut être utilisée pour prévoir les impacts potentiels. Parfois, la précision de mesure de la variabilité dépend des autres types d'incertitude (ex., incertitude paramétrique, incertitude de modèle). Par exemple, l'incertitude sur les facteurs d'émission a affecté les variances des impacts potentiels.

La MCS est mise en œuvre facilement pour propager les incertitudes des variables d'entrée vers l'incertitude de la variable de sortie. Cependant, il y a quelques limites à l'utilisation de MCS en ACV. D'abord, la MCS classique suppose que les variables d'entrée sont distribuées indépendamment afin que les valeurs des variables de sortie venant de toutes les combinaisons possibles puissent être représentées. Donc, le nombre d'occurrences des valeurs de chaque variable n'influence pas celles des autres. En conséquence, l'ignorance de fortes corrélations entre les variables d'entrée, qui existent souvent en ACV agricole, entraîne à surestimer ou sous-estimer l'incertitude. Afin de résoudre ce problème, une technique mathématique a été adaptée permettant de créer un jeu de variables d'entrée ayant une structure corrélative similaire à celle des données observées (cf. chapitre 4). De plus, on dispose souvent de peu d'information pour déterminer les distributions probabilistes des variables d'entrée. Donc le choix de la distribution est souvent subjectif, basé sur le dire d'experts. Celui peut introduire une incertitude supplémentaire issue du choix subjectif. Le choix de distributions doit être basé sur l'information disponible et les déterminations subjectives nécessitent un test (c.-à-d. test de qualité de l'ajustement) pour qu'elles soient cohérentes avec les échantillons observés. Lorsque ce genre d'information est indisponible, ou bien que les variables d'entrée sont affectées par une incertitude paramétrique, les approches non-probabilistes peuvent être appropriées (cf. chapitre 5). Enfin, puisque la MCS demande de nombreuses itérations pour fournir une distribution assez robuste, le temps de calcul informatique est souvent considérable, voire rédhibitoire. De ce fait, la puissance de calcul peut être un facteur limitant pour la prise en compte de l'incertitude.

6.3 La prise en compte des corrélations dans la simulation de Monte Carlo

Afin de prendre en compte des corrélations entre les variables d'entrée dans la MCS, ce chapitre a exploré une démarche basée sur la loi normale multidimensionnelle (cf. chapitre 4). La prise en compte des corrélations entre des variables d'entrée dans la MCS a permis d'acquérir une estimation réelle de l'incertitude sur les variables de sortie, en particulier dans le cas où les corrélations sont fortes. Cependant, il existe certains cas où les corrélations n'ont pas nécessairement besoin d'être considérées. Lorsque les corrélations entre les variables sont très faibles, leur influence sur l'incertitude du résultat est souvent négligeable. Par ailleurs, lorsque l'information sur les corrélations

n’est pas disponible, la MCS avec échantillonnage aléatoire est plus conservatrice, puisque toutes les combinaisons possibles des variables d’entrée sont générées.

De cette étude, seules les corrélations fortes entre des variables d’entrée ont été considérées. La méthode appliquée a la capacité à la fois de représenter l’information sur les corrélations entre des variables d’entrée à travers de la MCS, et de maintenir la forme de leurs distributions probabilistes, contrairement à la méthode d’origine, qui impose des distributions normales. De ce fait, on conserve la flexibilité du choix de la distribution, qui peut permettre d’éviter l’incertitude du choix subjectif. De plus, cette méthode est souple dans le sens qu’elle peut traiter la corrélation de Pearson mais aussi la corrélation de Spearman. L’utilisation de différents types de corrélation dépend de l’information disponible sur variables corrélées, ou bien de l’hypothèse que l’on fait sur ces corrélations : linéaire pour Pearson et monotone pour Spearman. En général, ce genre d’information provient d’études empiriques ou de dires d’expert, et l’établissement de la matrice de corrélations doit être faite avec précaution, car cette matrice doit être « définie positive » pour obtenir sa matrice triangulaire supérieure par la factorisation de Cholesky. Donc, je recommande aux analystes ACV de tester la faisabilité de la factorisation de Cholesky pour considérer les corrélations entre les variables d’entrée dans la MCS, avant de créer la matrice de corrélations des données de l’inventaire et les paramètres utilisés dans les processus d’évaluation des impacts.

En fait, dans le cadre de l’ACV, plusieurs critères (catégories d’impact) doivent être considérés pour la prise de décision. Les corrélations entre ces catégories d’impact fournissent des informations importantes aux décideurs. Par exemple, de fortes corrélations positives entre des impacts environnementaux (ex., changement climatique, acidification, eutrophisation) sont observées dans le système de production des truites en France (cf. Annexe 1). Dans la méthode proposée, l’ensemble de valeurs des variables d’entrée généré a un ordre de permutation spécifique déterminé selon les corrélations désirées entre ces variables. Ainsi, les distributions des impacts estimés possèdent un ordre spécifique correspondant à l’ordre des variables d’entrée. Donc, la MCS avec prise en compte des corrélations entre les variables d’entrée permet aussi de montrer les corrélations entre les impacts différents, si les variables utilisées pour calculer ces impacts sont corrélées fortement. Autrement dit, l’information sur les corrélations entre les impacts est conservée dans la MCS par cette méthode. Bien que les techniques pour contrôler la corrélation soient bien connues, leur application en ACV est encore peu développée pour cause d’insuffisance d’information et/ou de temps de calcul trop important. Nous pensons avoir démontré que l’effort vaut la peine d’être consenti eu égard à son impact sur la qualité des résultats.

6.4 L’application de la théorie de Dempster-Shafer

L‘arbre de décision a conduit à choisir des méthodes appropriées pour traiter des incertitudes différentes. Lorsqu’il existe à la fois une variabilité et une incertitude épistémique (plus précisément, l’incertitude paramétrique) dans le même cadre, l’approche probabiliste classique peut fusionner ces deux types d’incertitude au lieu de les séparer. Donc elle peut amener à sous-estimer l’incertitude sur le résultat final, car l’incertitude sur le choix de distribution est ignorée. Face à ce problème, la DST a été appliqué pour combiner deux approches différentes (la distribution probabiliste et l’intervalle flou) dans le même cadre d’étude (cf. chapitre 5). Ces deux approches ont été utilisées pour traiter la variabilité et l’incertitude paramétrique, respectivement, dans un contexte d’ACV agricole. En conséquence, les impacts potentiels et leurs incertitudes ont été estimés par une fonction de croyance (« belief function ») et une fonction de plausibilité (« plausibility function ») et illustrés par une paire de distributions cumulées inférieure et supérieure (p-box) qui contient la vraie distribution probabiliste du résultat. Cette forme de représentation estime un intervalle de probabilité sur les impacts potentiels (influence de la variabilité) et fournit une estimation plus conservatrice que l’approche probabiliste classique, parce qu’elle considère aussi l’imprécision sur l’état de connaissance en utilisant l’intervalle flou au lieu d’une distribution probabiliste supposée. En outre, la représentation de l’incertitude sur une valeur statistique (ex., moyenne) est influencée par l’expression de l’incertitude épistémique. Par exemple, les moyennes des impacts ont été exprimées par des intervalles flous. En théorie, l’incertitude sur la moyenne peut être éliminée lorsqu’il n’y a plus d’incertitude épistémique. C’est-à-dire, quand on sait soit la valeur réelle du paramètre, soit la vraie distribution du paramètre, le processus de MCS génère une seule distribution sur le résultat estimé avec la moyenne sous forme d’un point de valeur. Par conséquence, l’application de la DST permet d’identifier les influences de la variabilité et de l’incertitude épistémique sur l’estimation des impacts. La distance entre les deux bornes (inférieure et supérieure) indique l’espace potentiel à améliorer en réduisant l’incertitude épistémique.

Bien que la DST ait été développée depuis les années 1960 (Dempster 1967), l’utilisation de la DST est encore limitée en ACV. D’abord, le processus de propagation a besoin de déterminer les minima et les maxima du résultat associé avec des niveaux de possibilité en utilisant arithmétique des intervalles qui s’appuie sur les modèles ACV. Cependant, le temps de calcul peut devenir très grand pour un modèle compliqué ou non-monotone, en particulier avec de nombreuses variables incertaines exprimées par les intervalles flous. Ensuite, contrairement à l’approche probabiliste, il est difficile de conserver l’information sur les corrélations entre des paramètres incertains exprimés par l’intervalle ou l’intervalle flou. Sans considérer les corrélations entre ces paramètres, le résultat sous forme de p-box, qui contient toutes les combinaisons possibles, fournit une estimation conservatrice, mais la précision du résultat est plus ou moins affectée. Pour l’interprétation, les décideurs sont face à une situation

difficile, parce que les résultats sont exprimés sous forme d'intervalles (pour construire la structure de DST), plutôt que d'une seule distribution probabiliste. La décision basée sur les deux bornes inférieure et supérieure représente la situation optimiste et pessimiste. Cependant, un intervalle extrêmement large sur l'impact estimé peut être inutile pour prendre une décision significative. Face à ce problème, il est proposé d'utiliser un indice de confiance pour transformer les deux distributions cumulées à une distribution probabiliste pondérée en fonction de l'attitude du décideur, soit plus optimiste (proche de la borne inférieure), soit plus pessimiste (proche de la borne supérieure). Puisque l'indice de confiance intègre l'attitude du décideur subjective dans le résultat exprimé, cette étape doit être réalisée après l'évaluation de l'impact, et le choix de l'indice doit être jugé prudemment par les experts. Lorsque il n'existe pas d'information permettant de fixer l'indice de confiance, il est plus prudent d'employer l'intervalle pour exprimer le résultat afin éviter une décision trop subjective.

6.5 Découvertes principales and recommandations

Les travaux réalisés dans cette thèse amènent quelques contributions aux analystes pour aborder les incertitudes en ACV :

- L'analyse de l'incertitude elle-même est un moyen d'aider les analystes ACV à mieux connaître l'état des connaissances sur les données et les modèles utilisés dans un système. Elle ne permet pas de réduire l'incertitude, mais d'évaluer son influence sur le résultat. Donc les analystes ACV devraient éviter de faire trop d'hypothèses pour essayer d'avoir une étude sans incertitude, et plutôt se focaliser sur la représentation réelle des informations en prenant en compte de l'incertitude dans une étude réelle. Le processus d'analyse est itératif, afin de mettre à jour les résultats dès que de nouvelles informations deviennent disponibles (ex., sachant la vraie valeur ou la distribution d'une variable, sachant les corrélations entre des variables).

- L'analyse de l'incertitude, au lieu d'être une étape facultative adossée à la fin d'une ACV (comme elle l'est souvent actuellement), doit être considérée comme un processus important à réaliser dans toutes les étapes de l'ACV, et ce dès le début. On commence par identifier les sources d'incertitude dans l'étape « définition des objectifs et du champ de l'étude », qui va influencer le déroulement ou des choix dans les étapes qui suivent. Ensuite, les incertitudes sont représentées dans les modèles et les inventaires pour analyser leur influence sur les impacts. La propagation des incertitudes, à travers des étapes précédentes, donne des résultats qui intègrent les incertitudes sur les variables d'entrée. Enfin, l'interprétation des incertitudes et de leurs influences sur les résultats permet de compléter une étude ACV.

- Comme il n'existe pas de méthode polyvalente optimale pour analyser l'incertitude, cette thèse a visé à aider les analystes ACV à choisir des méthodes qui conviennent aux types d'incertitude

rencontrés. La diversité des méthodes possibles ouvre la possibilité de traiter tout type d'incertitudes, même s'il y a peu information disponible.

- À cause de leur différence conceptuelle, la variabilité et l'incertitude épistémique devraient être quantifiées séparément dans un même cadre du système. Cela demande une nouvelle visualisation de l'incertitude sur le résultat (ex., le « p-box », la structure DST), au lieu d'une distribution probabiliste. Par conséquent, l'interprétation du résultat doit distinguer leurs influences séparément sur le résultat. Parfois, la confiance jugée par les experts peut être ajoutée comme une information supplémentaire (ex., l'utilisation d'un indice de confiance) pour simplifier l'interprétation. En ce cas, une conclusion tirée sur le résultat doit préciser le niveau de confiance supposé.

- La DST permet d'établir un « pont » pour lier deux façons de représenter l'incertitude au point de vue objective (aléatoire) et subjective (épistémique). La structure DST est un moyen souple pour représenter l'incertitude, et la mise à jour des informations permet de la transformer à une distribution probabiliste (c.-à-d., considérer que la variabilité) ou à un/des intervalle/s flou/s (c.-à-d., ne considérer que l'incertitude épistémique).

- Les ACV réelles comportent souvent des modèles plus compliqués que l'étude de cas présentée dans la thèse. Donc le temps du calcul est considérable en utilisant la MCS, notamment quand plusieurs méthodes sont combinées pour représenter les incertitudes différentes. De ce fait, il vaut mieux faire un effort pour utiliser les algorithmes d'optimisation *ad hoc* afin d'augmenter l'efficacité de simulation. Par exemple, les modèles qui estiment les émissions des gaz, qui sont souvent relativement simples, peuvent être optimisés individuellement d'abord. Ensuite, les incertitudes sur les estimations des émissions de gaz, notamment celles qui sont représentées de manière imprécise, peuvent être regroupées pour évaluer les impacts potentiels là où les modèles de caractérisation (les émissions multipliées par leurs facteurs de caractérisation) sont souvent monotones croissants. Dans ce cas en effet, le minimum et le maximum des impacts peuvent être identifiés facilement selon l'arithmétique des intervalles. De plus, la réduction du nombre des variables imprécises peut également diminuer le temps de calcul des incertitudes. Pour ce faire, une analyse de sensibilité peut être mise en place a priori pour identifier les variables les plus influentes sur l'incertitude finale (Heijungs 1996).

6.6 Limites et perspectives

Afin d'approfondir les recherches méthodologique présentées dans cette thèse, il est nécessaire de réfléchir à quelques points critiques sur l'application des méthodes pour traiter des incertitudes en ACV agricole dans les futures recherches. Les travaux réalisés lors de la thèse amènent aux conclusions suivantes :

- Cette thèse n'a traité que trois catégories d'impact liés aux émissions d'azote et de méthane. Cependant, il serait intéressant de prendre en compte l'influence de l'incertitude sur d'autres catégories d'impact (ex. toxicité, utilisation d'énergie, biodiversité). Par exemple, la biodiversité est menacée par des impacts (ex. pollution de l'air et de l'eau, dégradation du sol, déforestation) au sein des activités d'élevage (Steinfeld et al. 2006). En ce cas, la prise en compte de l'incertitude sur la biodiversité concerne plusieurs facteurs de ces différentes sources d'impact. Donc, un futur travail pourrait étudier d'autres catégories d'impact pour lesquelles les influences des incertitudes des variables entrées sont probablement plus complexes que celles des trois catégories d'impact étudiées dans cette thèse.

- Pour valider la méthode DST dans le contexte ACV agricole, il sera nécessaire de l'appliquer dans des études supplémentaires. D'abord, l'étude de cas dans la thèse s'est limitée à considérer seulement la variabilité naturelle et l'incertitude paramétrique. Cependant, il existe d'autres types d'incertitudes en ACV (ex., allocations ou modèles différents), qui n'ont pas été traités dans cette thèse. En fait, les méthodes de combinaison basées sur la DST sont capables de combiner les différentes sources d'évidence (incertitudes de scénario) dans le même modèle, mais elles n'ont pas été appliquées dans les études de cas ACV. Donc un futur travail devra considérer ces types d'incertitude et propager leur influence sur l'incertitude sur les sorties pour tester sa pertinence dans les cas d'ACV réels. Par exemple, la méta-analyse étudie les données venant d'études différentes (ex., en agronomie) afin d'avoir une analyse plus précise des données (Philibert et al. 2012). Comme les données proviennent des sources différentes (c.-à-d. variabilité entre les études individuelles), il serait intéressant d'employer les règles de combinaisons pour exprimer les résultats d'une méta-analyse dans le cadre de l'ACV.

- Une technique a été appliquée pour contrôler les corrélations entre des variables dans le processus de propagation. Cependant, cette technique ne s'applique qu'à l'approche probabiliste traditionnelle. Lors de l'utilisation des intervalles ou des distributions probabilistes imprécises, cette technique n'est plus valable dans la MCS. Donc il sera nécessaire d'étudier l'intégration des informations sur les corrélations et les dépendances entre des variables dont les représentations des incertitudes sont imprécises. Pour cela, le travail de Ferson et al. (2004) sur la dépendance en modélisation probabiliste dans le domaine de l'analyse des risques pourra offrir de bonnes pistes pour les travaux à venir.

- La mise en œuvre de l'approche probabiliste s'applique en ACV pour évaluer la qualité des données avec l'aide de la matrice de pédigrée. Cependant, la méthode actuelle fusionne l'incertitude sur la qualité (c.-à-d., incertitude épistémique) avec celle de base (c.-à-d., variabilité) (Weidema et al.

2013). Donc il sera intéressant d'étudier l'application de la DST en quantifiant séparément l'incertitude sur la qualité, afin de distinguer son influence sur les résultats en sortie.

- Dans cette thèse, des méthodes ont été implémentées pour représenter et propager les incertitudes à l'aide des outils informatiques. Cependant, il n'y a pas de logiciel ACV qui intègre plusieurs méthodes pour que les analystes ACV puissent choisir les méthodes appropriées pour traiter les incertitudes. Donc la considération des incertitudes différentes demande le développement de logiciels ACV en intégrant plusieurs méthodes de traitement. Cet outil informatique devra fournir un guide pour choisir les méthodes. De plus, il devra être capable d'effectuer la simulation en propageant les incertitudes à travers le modèle ACV.

En conclusion, un arbre de décision a été proposé pour guider les analystes ACV en choisissant les méthodes possibles pour traiter les incertitudes différentes et à démontrer leurs applications dans le cadre de l'ACV agricole. Le choix des méthodes doit être fait prudemment, en fonction des études de cas spécifiques. Les applications de chaque méthode et l'efficacité du calcul doivent être améliorées dans les futures recherches, notamment pour la DST, qui prouve sa flexibilité en combinant les approches probabiliste et non-probabiliste. Il est à espérer que ces travaux exploratoires ont permis d'atteindre les objectifs initiaux et fournissent une base et une vision intéressante pour engager les recherches futures.

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Annexe.
Environmental assessment of trout farming in France by life cycle assessment: using bootstrapped Principal Component Analysis to better define system classification

Journal of Cleaner Production in 2014 (in press)

Environmental assessment of trout farming in France by life cycle assessment: using bootstrapped Principal Component Analysis to better define system classification

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Abstract

Trout farming is the main fish production system in France. This article describes a system to classify trout farms based on environmental impacts calculated by life cycle assessment and technical and economic indicators. Since the number of surveyed farms was too small for a robust assessment, we combined principal component analysis (PCA) with a non-parametric bootstrap technique. French trout farms were surveyed to collect technical and economic indicators. The representativeness of the survey was verified by comparing it to a national inventory. Life cycle assessment was used to estimate environmental impacts of farms and the contribution of each production stage to impacts. PCA was used to evaluate both technical-economic and environmental indicators of the trout farms, which were separated into three groups based on the size of fish produced (pan-size, large and mixed-size, and very large). Non-parametric bootstrap was used to compare the groups and to test the significance of PCA results. Results validated the fish-farm classification system based on the size of fish produced and indicated that farm operations and fish feeding contributed the most to environmental impacts. The PCA method distinguished three groups via their technical indicators, with non-significant differences among the groups in environmental impacts. However, environmental indicators showed strong links with technical and economic indicators. In conclusion, bootstrapped PCA offers the ability to assess groups of trout production system when the sample size is too small and provides more conservative results by considering uncertainty. Future studies should focus on providing reliable data to reduce uncertainty.

Keywords: life cycle assessment; non-parametric bootstrap; principal component analysis; trout farming system

1. Introduction

Trout farming is the main aquaculture production system in France. It is primarily based on farming rainbow trout (Oncorhynchus mykiss) in flow-through systems, in which inlet water is diverted from a river, passed once through the rearing tanks and then returned to the river. All nutrients are provided by exogenous formulated feed containing fish meal, fish oil and plant-based ingredients. Production is carried out in small (10 t/year) to large farms (900 t/year). The farms have different production objectives responding to different markets. For example, some farms produce pan-sized trout or large trout for filets; other farms produce fish for restocking rivers or ponds for angling. These different production strategies imply different practices (e.g., feed type, feeding management, oxygen supply, rearing densities, and water treatment). The trout farms in France are spread widely throughout the country, but their number is small (around 600) comparing to livestock systems. Since trout farming uses water of good quality, farm practices and the quality of water at their outlets are watched closely.

Despite the rapid growth of fish farming throughout the world (mean increase of fish production volume of 12%/year in the last ten years) (FAO, 2012), trout production decreased in France from 47 000 t in 1997 to 37 000 t in 2007 (Agreste, 2011). This production suffers from economic competition from other aquatic products and the application of water-quality regulations (e.g., European Union Water Framework Directive), which can cause farmers to abandon fish production. The decrease in the number of farms and the corresponding decline in production led the French aquaculture producer organization (CIPA) to assess the sustainability of French trout farming. To do so, different approaches were applied: development of indicators of economic, social and environmental sustainability; environmental assessment of farms based on biological and chemical-physical measurements (Aubin et al., 2011); and life cycle assessment (LCA). This paper focuses on the definition of a trout-farm classification system using LCA indicators and certain technical and economic indicators.

LCA is a holistic method designed to estimate potential impacts associated with a product or service based on the resources consumed and pollutants emitted into the environment at all stages of its life cycle, from raw material extraction to its end-of-life (Guinée et al., 2002). It is an internationally accepted method described in ISO standards (ISO 14040 (2006), ISO 14044 (2006)). LCA has been adapted to fish farming (Papatryphon et al., 2004b) and applied in several studies to estimate environmental impacts of aquaculture in different contexts (Aubin, 2013; Cao et al., 2013; Henriksson et al., 2012). Salmonid production has been studied in particular, since it is common in Europe and North America. Moreover, it is a simple and well-controlled rearing system which fits with the industrial ecology rationale of LCA. Some studies about salmon production have investigated different rearing and feeding practices (Ayer and Tyedmers, 2009; Pelletier and Tyedmers, 2007;

Pelletier et al., 2009). Other studies have investigated trout production (Aubin et al., 2009; Gronroos et al., 2006; Papatryphon et al., 2004b; Samuel-Fitwi et al., 2013). All of these studies helped to understand the contribution of system components to environmental impacts and showed the overwhelming influence of feed composition and management. Nevertheless, these studies were based on small numbers of farms.

To better understand the influence of rearing practices in trout farming, Papatryphon et al. (2004b) classified production systems into three classes according to the size of fish produced (pan-size, large trout, and very large trout). They observed high variability in the impact categories (relative variation ranged from 41% in biotic resource use to 87% in energy demand). Moreover, variability in impacts was associated with different production techniques; for example, variation in eutrophication was related mainly to differing feed efficiency among farms. However, the small number of farms investigated (n=8) did not allow broader conclusions. As mentioned by Henriksson et al. (2012), the number of farms investigated often raises the question about the representativeness of aquaculture systems in LCA. As a consequence, environmental assessment of fish farms is relatively weak, making extrapolation of their potential environmental impacts delicate. To better characterize heterogeneous populations, especially in agricultural and aquacultural production, building classification systems is a common practice (Lazard et al., 2010). These classification systems are often based on surveys and statistical analysis, such as Principal Component Analysis (PCA).

PCA reduces the dimensionality of an observed dataset with many correlated variables by transforming them into a new set of variables, named principal components (PCs), which retain as much as possible the variation of the observed dataset (Jolliffe, 2005). It is used to extract the most important information from the dataset to get an overview of it in a small number of dimensions (e.g., two or three) described by their eigenvalues (measures of variation in samples explained by the PCs), loadings (coordinates of original variables in the PCs) and scores (coordinates of individuals in the PCs). PCA is commonly used to represent the variability in observed samples. However, a small sample size ($n<30$) may not allow conclusions to be extrapolated to the entire population when the standard error of the mean is large (Berthouex and Brown, 2002). Hence, the consideration of uncertainty in the results due to small sample size is an important subject in statistical analysis. Indeed, this type of uncertainty can be expressed with a confidence interval (CI) or standard error (Luo et al., 2013; Melia et al., 2012).

Bootstrap sampling is a numerical method used to quantify uncertainty due to random sampling errors without assumptions about a variable's distribution (Efron, 1979). A bootstrapped sample is created by randomly sampling from an observed sample repeatedly. Bootstrap sampling can be applied, for example, to estimate the accuracy and stability of PCA results by providing a CI for eigenvalues and loadings (Babamoradi et al., 2013; Daudin et al., 1988; Timmerman et al., 2007).

However, there are two shortcomings when using bootstrap-based PCA. First, the coordinates of component loadings and scores are arbitrary (Jackson, 1995; Jolliffe, 2005; Mehlman et al., 1995), which may overestimate the CI of loadings (reflection). Second, PCs may have a similar eigenvalues in a bootstrapped sample, which may change the order of PCs compared to the observed sample (re-ordering) (Timmerman et al., 2007). To address these problems, reflection and re-ordering corrections are performed on each bootstrapped sample (more details in Peres-Neto et al. (2003) and Babamoradi et al. (2013)).

In this study, we decided to bypass the problem of the small sample size of trout farms by using non-parametric bootstrap. This method has the advantage of being more robust than parametric bootstrap when the distribution of observed data fails a normality test. Therefore, to better understand the characteristics of French trout farms, this study used PCA to validate a classification system of French trout farms based on their types of commercial products. This system classifies trout farms based on their estimated environmental impacts and production techniques. The accuracy of PCA results (CI) is evaluated with the bootstrap method.

2. Materials and methods

2.1 Sample survey and national inventory

A sample of 24 trout farms throughout France was selected based on the size of fish produced, hydrogeological characteristics of the environment, and farmer agreements. The farms were surveyed from 2007 to 2011, recording data such as farm production (types and quantities of products), farm inputs (types, quantities and origins, especially of energy sources, feed, juveniles, and water), infrastructure and equipment, and water quality (Aubin et al., 2011). Annual trout production of the farms varied from 20 to 667 t. Farms were divided into three groups according to the size of fish produced, as performed by Papatryphon et al. (2004b): G1, pan-size trout (250-400 g); G2, large and mixed-size trout (e.g., different sizes from 200 to 3000 g); and G3, very large trout (>2000 g). The number of farms per group was 5, 9 and 10, respectively. To check the representativeness of the trout farm sample in the survey, we compared it to a classification of trout farms (defined by the amount of feed consumed) available in a 2007 inventory of French trout farms (Agreste, 2009).

2.2 Life Cycle Assessment

LCA was conducted according to the four steps and general requirements of the methodology proposed by ILCD (European Commission, 2010). The methodology was adapted to characteristics of fish farming. The goal and scope of this study is the environmental assessment of trout farming in France at the farm scale in order to adapt improvement strategies as a function of farm type. The boundary of the production system mainly contains farm operations, feed production (including ingredient production and transportation), production of juveniles, infrastructure construction,

equipment manufacturing, and production of medicines and other inputs, such as liquid oxygen and energy carriers (Fig. 1). Despite the existence of thousands of processes in LCA of trout production, these processes are the most important contributors to overall impacts, according to the literature (Aubin, 2013).

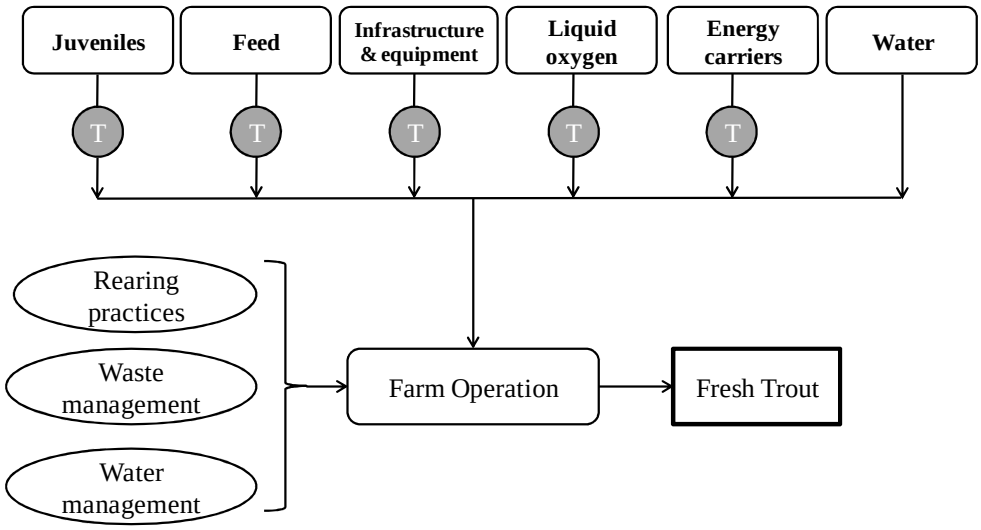

Figure 1. System boundary of trout farming in France. Rounded rectangles represent processes of the production system. Ellipses represent management factors of fish farms. "T" means transportation.

The life cycle was defined up to the farm gate, and the functional unit (impact calculation basis) was one t of raw fish. Emissions of farm metabolic wastes (i.e., nitrogen and phosphorus compounds, suspended solids) into the aquatic environment were calculated using the mass-balance approach described by Papatryphon et al. (2005) and adapted by Aubin et al. (2011) to take into account internal dynamics of waste inside the farm. Specific information about feed ingredients came from Boissy et al. (2011). Economic allocation was used to divide environmental burdens among co-products in feed-ingredient production. Secondary data (e.g., transport and electricity use) were extracted from the ecoinvent v. 2.2 database. LCA impact categories were selected to address a variety of environmental issues of fish farming. Climate change (kg CO_2-eq.), acidification (kg SO_2-eq.), eutrophication (kg PO_4-eq.) were calculated using the characterization factors of CML2 baseline 2000 v. 2.03 (Guinée et al., 2002). To consider the contribution of fish farming to land use, we selected a land occupation (m^2*y) indicator. Energy use of fish farming (energy demand (GJ)) was calculated according to the Cumulative Energy Demand method, v. 1.03 (Frischknecht et al., 2005). Water requirements of the activity (water dependence (m^3)), including water consumption and water passing through the fish farm, was calculated according to Aubin et al. (2009). Net Primary Production Use (NPPU) (t C), which indicates the pressure of fish farming on biotic resources (especially marine resources), was calculated according to Papatryphon et al. (2004b). These LCA impact categories were selected based on previous studies and guidelines in the field of aquaculture LCAs (Aubin, 2013; Aubin et al., 2009;

Henriksson et al., 2012; Pelletier and Tyedmers, 2007). The calculation of LCA impact categories was performed with SimaPro v. 7. Other indicators of rearing performances were added to reflect technical and economic characteristics of the systems: annual production level (t), feed conversion ratio (FCR) and annual liquid oxygen consumption (t). In addition, on-farm human labor (human.day) was included to highlight the relationship between production factors and labor on trout farms.

2.3 Comparing differences in group means with the bootstrap method

To identify significant differences among the three groups, we used the bias-corrected and accelerated (BCa) bootstrap method (see appendix) to calculate 95% CIs around the differences in group means, because it adjusts both bias and skewness in the bootstrap distribution and provides a reasonably accurate CI. Significant differences were assumed at $p<0.05$. The re-sampling procedure was performed 1000 times (B=1000) using R (R Development Core Team, 2012). Thus, we assumed that each group was independent and taken randomly from its own population. The differences between groups were considered significant if the bootstrapped 95% CIs around the differences included zero. In other words, the null hypothesis (H_0) was that differences between group means equaled zero. We chose a non-parametric bootstrap method to test differences between indicator means, because some of them (e.g., production level, liquid oxygen consumption, and acidification) might not satisfy normality or homogeneity of variance, two conditions required for parametric tests such as analysis of variance (ANOVA).

2.4 PCA method

To address the comparison problem due to the small sample size, we applied PCA (R "princomp" function) to a matrix of eleven independent variables (n=11) from observed samples (m=24) and bootstrapped samples (m*=24) (Fig. 2). Through PCA, three vectors were generated: eigenvalues, loadings and scores. The BCa method was used to estimate 95% CIs for the eigenvalues of PCs to determine how many PCs to keep (bootstrapped Kaiser-Guttman criterion (Lambert et al., 1990)). So, only the components whose 95% CI for the eigenvalues exceeded 1 (mean of eigenvalues) were retained. The loadings of original variables and the scores of individuals from the observed sample were mapped. We also used bootstrapped PCA (B=1000) with re-ordering and reflection corrections to generate the component loadings and scores (Peres-Neto et al., 2003). The significance of correlations between variables was tested by calculating BCa 95% CIs for correlation coefficients. The significance of variable loadings was tested by calculating p-values. They were calculated as the number of bootstrapped loadings smaller (when the original loadings were positive) or greater (when the original loadings were negative) than zero, divided by B (Peres-Neto et al., 2003). Thus, variables were associated with the corresponding components when $p<0.05$. The individual scores of the three farm groups were distinguished by confidence regions (R "ellipse" package) of the centroids of bootstrapped scores at a 90% confidence level (Dehlholm et al., 2012).

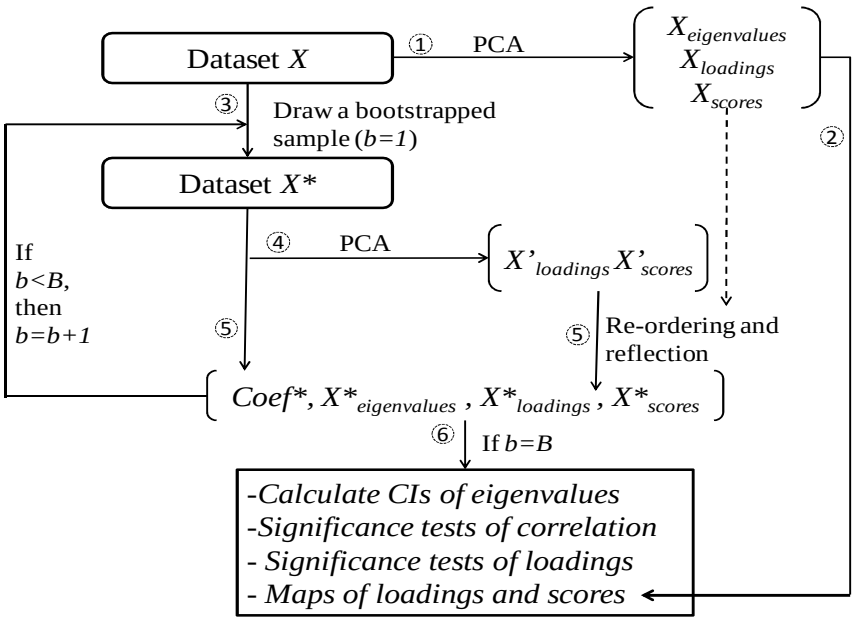

Figure 2. Bootstrapped Principal Component Analysis (PCA) procedures with re-ordering and reflection corrections.

3. Results

3.1 Farm sample representativeness

The observed sample included trout farms from all classes in the inventory except farms consuming less than 25 t of feeds per year (Table 1). Since this class represents only 6% of national feed consumption, it was not taken into account in our sample. The representativeness of the survey (expressed as the percentage of total national feed consumption) increased with the class size. The highest representativeness (40%) was for farms consuming more than 500 t of feed per year, while the lowest representativeness (5%) was for farms consuming 25-50 t/year. The larger farms (feed consumption more than 300 t/yr) are specialized in large trout production. Some of smaller farms (feed consumption less than 300 t/yr) are specialized in pan-size trout, while the others produced a combination of all sizes.

Table 1. Number of trout farms in each class (based on annual feed consumption (Q)) in the French inventory (Agreste, 2009) and this study's survey of farms grouped by the size of fish produced (G1: pan-size fish, G2: large and mixed-size fish, G3: very large fish).

	National inventory		**Trout survey**					
Class	Number of farms	Total feed cons. (t/yr)	Number of farms	Total feed cons. (t/yr)	Percentage of national total (%)	G1 (%)	G2 (%)	G3 (%)
Q < 25 t	366	2627	0	0	0	0	0	0
25 t ≤ Q < 50 t	59	2174	3	99	5	0	100	0
50 t ≤ Q < 100 t	56	4143	4	239	6	27	73	0
100 t ≤ Q < 200 t	56	7908	5	697	9	38	36	26
200 t ≤ Q < 300 t	27	6819	3	769	11	34	35	31
300 t ≤ Q < 500 t	25	9986	4	1686	17	21	0	79
Q ≥ 500 t	11	10 090	5	4046	40	0	0	100
Total	600	43 747	24	7535	17*			

** Percentage of feed consumptions of trout samples in national feed consumptions*

3.2 Contribution analysis

Among trout-production stages, feed (i.e., feed production, milling, and transport) was the main contributor to mean impacts, such as NPPU (≈94%), land occupation (>92%), climate change (67-73%), acidification (63-69%) and energy demand (50-59%) (Fig.3). Farm running (i.e., farm operations and on-farm emissions) was the main contributor to eutrophication (81-82%) and water dependence (89-93%) and influenced energy demand (20-26%). Fry (i.e., production and transport of trout eggs or juveniles) contributed to acidification, eutrophication, climate change, energy demand and water dependence at a level of 7-14%. It had a slight contribution (1-6%) to NPPU and land occupation. The infrastructure and equipment (i.e., infrastructure, tank and building construction, equipment manufacturing and transport) only contributed to acidification, climate change and energy demand and their contributions were greatly variable among farm groups (2-16%), with the highest levels always observed in group G2. Liquid oxygen (i.e., liquid oxygen production and transport) had higher contribution to acidification, climate change and energy demand (7-10%) in groups G1 and G3 than in group G2. Chemicals (i.e., production and transport of medicines, cleaning products and other chemicals) had negligible contribution (<1%). Except for land occupation and energy demand, all impacts decreased in this order: G2, G1, G3.

3.3 Environmental impacts and rearing performance of the three groups

Means and coefficients of variation (CV) of indicator values were calculated per group in the observed sample (Table 2). G1 had lower variability in acidification (12%), eutrophication (6%) and climate change (6%) than G2 and G3 (>20%). G2 had higher variability in most indicators than the other two groups, except for FCR and land occupation. Variability in liquid oxygen consumption was much higher in G2 (260%) than in the other two groups (76% and 67%, respectively).

There were no significant differences in environmental impacts (e.g., acidification, eutrophication and climate change) or resource use (e.g., land occupation, energy demand and water dependence) between groups when comparing them with those of the bootstrap-based method (Fig. 3). However, there were significant differences in technical parameters between the groups, such as production level, feed consumption, liquid oxygen consumption, NPPU, water dependence and human labor. Although production level was significantly higher in G3 (440 t) than in G2 (79 t) and G1 (168 t), FCR was not significantly different among the three groups. In addition, G2 had significantly higher NPPU and water dependence than G3, while no significant difference was found between G1 and the other two groups. For human labor, G2 required significantly more working time than the other two groups.

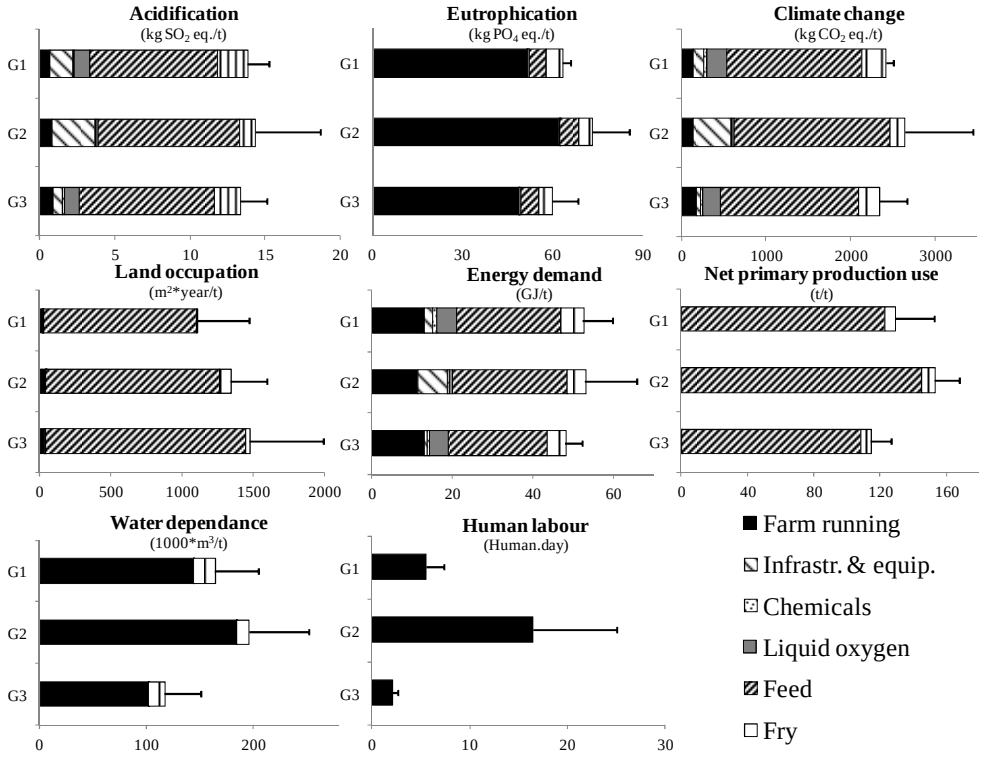

Figure 3. Contribution of system production stages to LCA impacts for trout farms grouped by the size of fish produced: G1 (pan-size), G2 (large and mixed-size) and G3 (very large). Error bars represent 95% confidence intervals around the means of total impacts.

Table 2. Means of environmental impacts, technical and economic indicators and their coefficients of variation (CV) for trout farms grouped by the size of fish produced: G1 (pan-size), G2 (large and mixed-size), and G3 (very large). Superscript letters indicate significant ($p<0.05$) differences between groups.

		G1		G2		G3	
Indicator	Unit	Mean	CV	Mean	CV	Mean	CV
Production level	t	168[a]	56%	79[b]	94%	440[c]	42%
Feed conversion ratio		1.09	8%	1.17	14%	1.2	18%
Acidification	kg SO_2-eq.	14	12%	14	26%	13	23%
Eutrophication	kg PO_4-eq.	63	6%	73	27%	60	21%
Climate change	kg CO_2-eq.	2425	6%	2647	28%	2344	20%
Land occupation	m^2*year	1099	53%	1339	34%	1472	56%
Energy demand	GJ	53	15%	53	29%	48	18%
Water dependence	1000 m^3	164[ab]	40%	196[a]	51%	117[b]	49%
Human labor	human.day	5.5[b]	58%	16.5[a]	89%	2.1[b]	60%

3.4 PCA results

The eigenvalues of the first three PCs in the bootstrapped PCA were 3.8, 2.6 and 1.8, respectively. Since the lower limits of 95% CIs calculated with the BCa method were less than 1, the first three PCs were selected, which explained a mean of 75% of the total variation in the observed sample, with a 95% CI of 71-82%. Significance tests of loadings indicated that acidification, eutrophication, climate change and energy demand were associated with the first PC (PC1); production level, liquid oxygen consumption, NPPU and human labor were associated with the second PC (PC2); and only FCR was associated with the third PC (PC3) (Table 3).

Acidification, eutrophication, climate change and energy demand had strong and significantly positive correlations ($r>0.5$, $p<0.05$) with each other, while NPPU, water dependency and human labor had significant negative correlations with production level and liquid oxygen consumption (Table 4). Eutrophication and climate change were significantly and negatively correlated with production (-0.416 and -0.362, respectively). In addition, FCR had strong significant correlations with land occupation ($r=0.610$) and NPPU ($r=0.405$). Also, NPPU was significantly correlated with human labor ($r=0.526$), but not with water dependence.

The sample-based variable loadings and individual scores of PC1 versus PC2 were mapped (Fig. 4). Considering the confidence regions around centroids of each group, farms of G2 and G3 had a wider distribution on the map and were distinguished by technical and economic indicators, while those of G1 and G2 overlapped, which indicates similar characteristics. Some farms had extreme values, such as farms 4 and 10 in G3, which contributed strongly to PC1 and had high production but low environmental impacts. Farms 9 (G3) and 13 (G2) contributed strongly to PC2 but had different

properties: the former consumed much more liquid oxygen, while the latter required more working time. Also, farm 18 in G2 had the highest environmental impacts.

Table 3. Matrix of p values of the first three principal components of 11 technical and environmental indicators. Bold values mean variables are significantly ($p<0.05$) associated with corresponding PC via the bootstrap method.

Variable	PC1	PC2	PC3
Production level	0.085	**0.029**	0.150
Feed conversion ratio	0.096	0.482	**0.032**
Liquid oxygen consumption	0.143	**0.019**	0.147
Acidification	**0.017**	0.165	0.305
Eutrophication	**0.011**	0.388	0.233
Climate change	**0.015**	0.170	0.366
Land occupation	0.162	0.269	0.067
Energy demand	**0.034**	0.164	0.273
Net primary production use	0.216	**0.030**	0.160
Water dependence	0.117	0.135	0.364
Human labor	0.259	**0.015**	0.271

Table 4. Correlation matrix of 11 technical and environmental indicators of French trout farms. Bold values indicate significant ($p<0.05$) correlation between variables via the bootstrap method.

	Prod.	FCR	Oxygen	AC	EU	CC	Land	Energy	NPPU	Water	Labor
Prod.	1.000										
FCR	**-0.044**	1.000									
Oxygen	**0.828**	0.146	1.000								
AC	-0.378	0.235	-0.125	1.000							
EU	**-0.416**	0.455	-0.255	**0.706**	1.000						
CC	**-0.362**	0.231	-0.134	**0.934**	**0.758**	1.000					
Land	0.118	**0.610**	0.218	0.182	0.188	0.261	1.000				
Energy	-0.243	**-0.014**	-0.096	**0.668**	0.432	**0.771**	0.241	1.000			
NPPU	**-0.410**	**0.405**	**-0.355**	-0.180	0.169	**-0.041**	0.184	**-0.027**	1.000		
Water	**-0.493**	0.144	**-0.321**	0.207	0.198	0.188	-0.099	0.140	0.425	1.000	
Labor	**-0.523**	0.139	**-0.414**	-0.065	0.047	-0.081	-0.090	-0.262	**0.526**	0.192	1.000

Prod: production level; FCR: feed conversion ration; Oxygen: liquid oxygen consumption; AC: acidification; EU: eutrophication; CC: climate change; Land: land occupation; Energy: energy demand; NPPU: Net primary production use; Water: water dependence; Labor: Human labor.

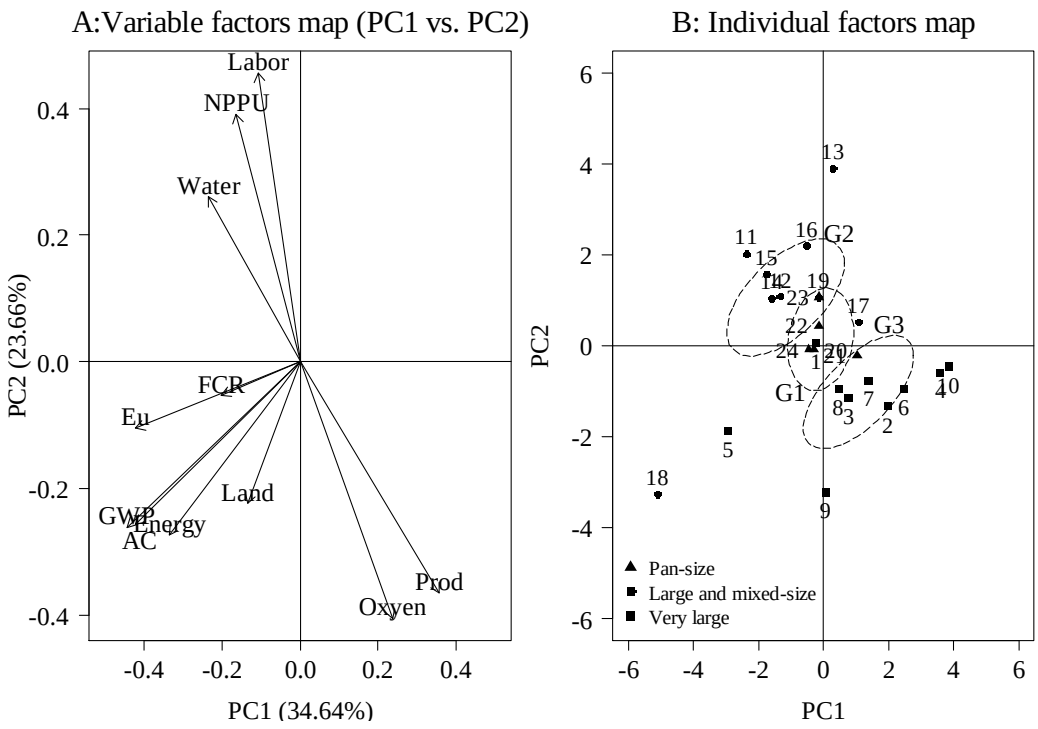

Figure 4. (A) Variable factors map of the first principal component (PC1) versus the second principal component (PC2) and (B) plot of individual farms (*m*=24) scores of PC1 versus PC2. The individuals were classified into three groups based on the size of fish produced: pan-size, large and mixed-size and very large. Dashed ellipses indicate 90% confidence regions of the bootstrapped scores for each group.

4. Discussion

4.1 Representativeness of the survey

Since nearly all farm classes reported in the national inventory are represented in our survey, we consider the representativeness of the survey sufficient, especially for large farms. However, the national inventory did not collect data about the size of trout produced. Even though the results of this study tend to indicate that large and specialized farms have the best performances, it would be interesting to obtain information about the commercial size of trout produced in a larger survey or a future inventory.

4.2 Comparison of impacts with previous studies

Comparison of LCA results with those from previous studies is always a delicate question due to methodological differences, especially in definition of system boundaries and allocation of burdens among co-products (Aubin, 2013; Henriksson et al., 2012). Fortunately, most impact categories in LCA studies of salmonid farming are identical and based on the CML2 baseline 2000 v. 2.03 impact assessment method (Guinée et al., 2002). Therefore, one can compare the orders of magnitude of impacts in the same categories for similar types of production.

Mean acidification in our study ranged from 13 to 14 kg SO_2-eq./t, which lies in the same order of magnitude as those in other studies of trout farming: 10.6-16.5 kg SO_2-eq./t in Papatryphon et al. (2004b), 19.2 kg SO_2-eq./t in Aubin et al. (2009), and 10.8 kg SO_2-eq./t in Samuel-Fitwi et al.(2013). Mean eutrophication in our study ranged from 60 to 76 kg PO_4-eq./t, which lies in the same order of magnitude as those of other studies of flow-through trout farms: 74 kg PO_4-eq./t in Papatryphon et al. (2004b) and 60 kg PO_4-eq./t in Samuel-Fitwi et al. (2013). These eutrophication impacts are higher than those observed in trout reared in recirculating aquaculture systems: 18-21 kg PO_4-eq./t in Roque d'Orbcastel et al. (2009) and 42-48 kg PO_4-eq./t in Boissy et al. (2011). Mean climate change in our study (2344-2647 kg CO_2-eq./t) is similar to that in Samuel-Fitwi et al. (2013), somewhat higher than that in Papatryphon et al. (2004b) (1540-2410 kg CO_2-eq./t), higher than that in Boissy et al. (2011) (2220 kg CO_2-eq./t), and lower than that in Aubin et al. (2009) (2753 kg CO_2-eq./t). Mean energy demand in our study (48-53 GJ/t) is within the range of that in Paptryphon et al. (2004b) (31.0-78.4 GJ/t) and lower than those in Aubin et al. (2009) (78 GJ/t) and Boissy et al. (2011) (55-55.7 GJ/t). All values of acidification, eutrophication, climate change and energy demand in our study are higher than those in Papatryphon et al. (2004a), whose boundaries encompassed only feed production. NPPU in our study (114-153 t C/t) was at the same level as standard salmon (145 t C/t) and trout (112 t C/t) in the Boissy et al. (2011) study. The high variation in NPPU found in our study is due to the variability in feed composition and improvements in data on fish meal composition.

4.3 Farm classification and contribution analysis

The three groups had similar environmental impacts and were distinguished mainly by technical and economic indicators (e.g., production level, liquid oxygen consumption, NPPU, water dependence, and human labor). G1 farms show intermediate performances. These farms benefit from the biological performances of small trout, combined with more traditional practices than farms from the two other groups. G2 farms show the lowest efficiency of inputs, with high levels of water dependence, NPPU and human labor to produce 1 t of fish. Moreover, this group has less homogeneous characteristics, with higher variability in production level, liquid oxygen consumption and human labor. These characteristics reflect the lower level of specialization of the farms through the different markets they supply: small and large trout for food or restocking markets. These more opportunistic and variable strategies lead to lower rearing performances. These strategies can be driven not only by economic considerations, but by choices about quality of life by the farmers. They have the lowest mean production level. In contrast, G3 farms display high efficiency. Their water dependence and NPPU were the lowest of the three groups, and other indicators such as energy use and FCR were not significantly different from the two other groups, although their specialization in producing very large trout induces an increase in the biological FCR and the duration of the production cycle. These farms are the largest of the three groups and they use liquid oxygen to

optimize fish performances. These farms aim for maximum efficiency of inputs, including the human labor necessary to produce 1 t of fish, which is the lowest of the three groups. They generally have a high technical level and use genetically improved trout strains.

4.4 Correlations among variables and bootstrapped PCA results

The negative correlation between production level and FCR, climate change, energy demand, NPPU, water dependence and human labor indicates that farm production level strongly influenced technical and environmental efficiencies. Economies of scale exist, which lead to an appropriate level of production that balances economic constraints and environmental laws. The significant negative correlation between production and some environmental impacts (e.g., eutrophication, climate change, energy demand, and NPPU) indicates that increasing the size of fish produced tends to reduce these environmental impacts per t of fish. Therefore, an optimal level of production in each group that maximizes production while minimizing environmental impacts could be calculated using optimization modeling. NPPU was positively and significantly correlated with production level and FCR, which shows that the feed system has an important direct influence on trout production but a large indirect influence in regions where feed ingredients are produced. The positive correlations between acidification, eutrophication, climate change and energy demand show that improving the production system could improve all of these impact categories simultaneously.

We used the bootstrapped Kaiser-Guttman criterion (the lower limit of CI for eigenvalues >1) (Guttman, 1954; Lambert et al., 1990) to determine which PCs to retain because this method considers the random sampling error that may influence the distribution of eigenvalues, in which mean value may be below the criterion value (i.e., equals 1). In such cases, the bootstrap-based method may be less arbitrary than the traditional Kaiser-Guttman criterion. However, although the bootstrapped Kaiser-Guttman criterion reduces the number of PCs, it may still overestimate that number (Jackson, 1993). Our study shows that projecting the loadings of original variables and individual scores onto two or three PCs more clearly describes correlations among variables and identifies the most influential individuals. However, the explanation based on the observed sample may be less meaningful because its small sample size lacked normality, a prerequisite of PCA. Therefore, the bootstrap-based method shows advantages for interpreting the significance of PCA results. However, more attention should be paid to avoid the re-ordering and reflection problems during the resampling procedure. To overcome these problems, we applied the technique proposed by Peres-Neto et al. (2003) in this study, though orthogonal rotation is an equivalent method (Milan and Whittaker, 1995; Timmerman et al., 2007).

4.5 Bootstrap method

Most significance tests (e.g., student t-test and ANOVA) assume that the population mean is normally distributed, especially when the expected value and variance of the population are known. Although the mean and standard deviation of observed samples are usually used to represent the expected value and the square root of variance of the population, it generally requires a sufficiently large sample size (n>30) or that the parameters of its distribution be known. However, this is not always the case in aquaculture studies (Henriksson et al., 2012; Papatryphon et al., 2004b). Several studies have compared tests of equality to overcome this shortcoming (Boos and Brownie, 2004; Efron and Tibshirani, 1993; Lim and Loh, 1996; Reiczigel et al., 2005). In our study, we used non-parametric bootstrap to perform the significance tests. The 95% CIs around the differences in group means were used to judge whether or not the null hypothesis was rejected. Bootstrapped results were more conservative and realistic than those from the sample-based calculation because random sampling error was taken into account. Also, the non-normality of some indicators (e.g., production, liquid oxygen consumption, and acidification) suggests that non-parametric bootstrap was more robust than a parametric bootstrap (Potvin and Roff, 1993) because there was no assumption about the true distribution of indicators to represent the whole population. Another advantage of the bootstrap method is its ability to estimate CIs around some statistics which cannot be obtained from the observed sample. In this study, for example, BCa was used to estimate CIs for the correlations, which were used to validate their significance. As concluded by Medulsee (2003), non-parametric bootstrap was a robust method for estimating CIs for Pearson's correlation coefficients.

As an approximation method, however, the bootstrap method is designed to estimate uncertainty in any statistical value (e.g., mean, median and correlation coefficient), and the accuracy of bootstrapped results depends on the quality and quantity of the observed sample (Luo et al., 2013; Wisz et al., 2008). Nevertheless, when parametric assumption is justified (satisfying normality and homogeneity of variance), Efron (1988) suggested using parametric bootstrap, which is more accurate than non-parametric bootstrap. To do so, more data are required to increase the reliability of parametric bootstrap. In addition, the quality of secondary data used in an analysis may result in additional uncertainty (e.g., inaccurate measurement and unrepresentative data). Thus, increasing data quality could reduce parameter uncertainty and provide more accurate results (Henriksson et al., 2013; Weidema and Wesnaes, 1996).

5. Conclusion

In this study, a small sample of survey data was used to compare three types of trout production systems. The results showed strong links between technical/economic and environmental indicators. Non-parametric bootstrap and BCa-based CIs were applied to better estimate uncertainty in the

statistical values. PCA showed the relative influences of variable indicators and individual scores. Technical/economic indicators (production level, human labor) were the main drivers and were correlated with environmental impacts such as eutrophication and climate change. So, improving rearing performances is one way to decrease environmental impacts. The remaining variability in indicators within farm groups showed that there is room to improve farm management and decrease environmental impacts, especially in G2, whose less specialized production led to less control over management parameters. Feed and liquid oxygen consumption are the main factors that influence the environmental impacts. Furthermore, these indicators reflect practices such as the monitoring of fish growth, water quality, and feeding practices. The three groups had few differences in environmental impacts. Despite the small sample size, our bootstrapped PCA method reinforces this overall conclusion.

Consideration of uncertainty in LCA is an improvement that is frequently cited. We applied a method to address the uncertainty due to a small sample size in an LCA-based case study. For the first time, non-parametric bootstrapped PCA has been used to assess groups of trout farms, and it is able to express uncertainty in statistical parameters of indicators. In the future, to provide reliable results, data quality and other types of uncertainty should be considered throughout the entire system.

Acknowledgements

The authors thank Michael Corson for reviewing earlier versions of this manuscript and helping improve its English content.

Appendix. Bias-corrected and accelerated (BCa) bootstrap method

The BCa method is used to estimate the confidence interval of a statistic of interest θ (e.g., mean and median) at significance level α (Efron and Tibshirani, 1993). Its lower and upper limits are found at the $100\alpha_1$th and $100\alpha_2$th percentile of bootstrap distribution, respectively:

$$\alpha_1 = \Phi(z_0 + \frac{z_0 + z^{\alpha}}{1 - a(z_0 + z^{\alpha})}) \quad \text{Eq. 1}$$

$$\alpha_2 = \Phi(z_0 + \frac{z_0 + z^{(1-\alpha)}}{1 - a(z_0 + z^{(1-\alpha)})}) \quad \text{Eq. 2}$$

where Φ is the standard normal cumulative distribution function, z^{α} is the 100αth percentile point of Φ, and z_0 is calculated as:

$$z_0 = \Phi^{-1}(\frac{\theta_i^* < \theta}{B}) \quad \text{Eq. 3}$$

where Φ^{-1} is the inverse of the standard normal cumulative distribution function, θ_i* is the ith bootstrap estimate of θ, and B is the number of the iteration.

Skewness is corrected by the "accelerated indicator" a, which is calculated as:

$$a = \frac{\sum_{n=1}(\theta' - \theta_n)^3}{6 * (\sum_{n=1}(\theta' - \theta_n)^2)^{3/2}} \quad \text{Eq. 4}$$

where θ_n is the estimated statistic of interest from the observed sample without the nth row (jackknife replicate) and $\theta'$is the mean of θ_n.

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