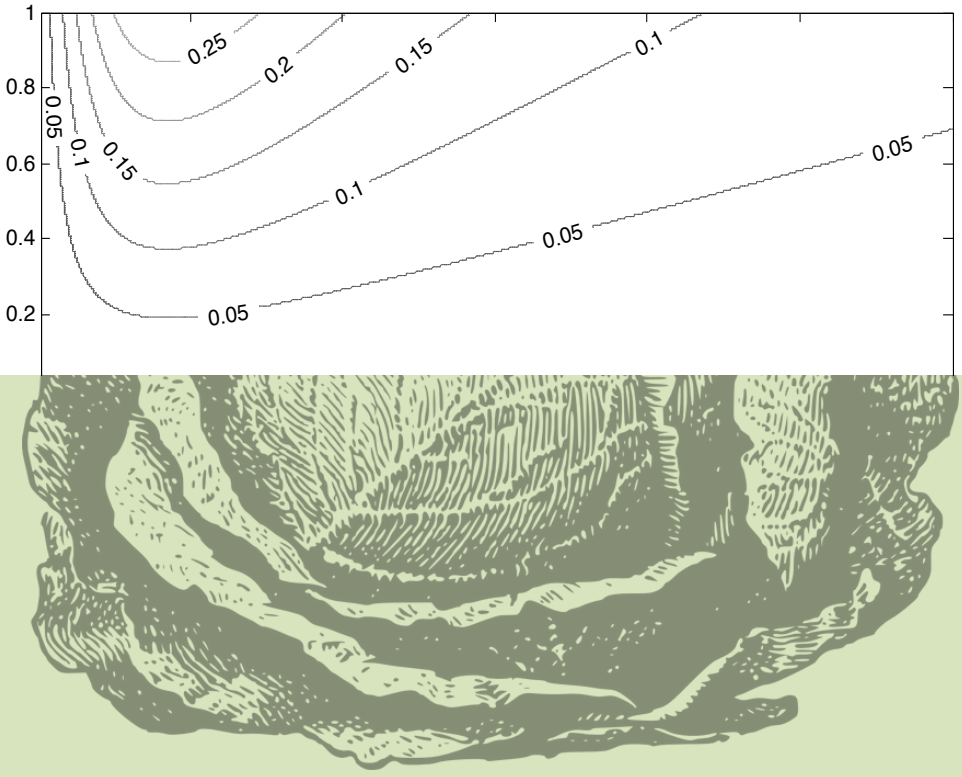
AN UNCERTAIN CLIMATE

the value of uncertainty and sensitivity analysis in environmental impact assessment of food



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ABSTRACT

Production of food contributes to climate change and other forms of environmental impact. Input data used in environmental impact assessment models, such as life cycle assessment (LCA) and nutrient balance (NB) analysis, may vary due to seasonal changes, geographical conditions or socio-economic factors (i.e natural variability). Moreover, input data may be uncertain, due to measurement errors and observational errors that exist around modelling of emissions and technical parameters (i.e. epistemic uncertainty). Although agricultural activities required for food production are prone to natural variability and epistemic uncertainty, very few case studies in LCA and NB analysis made a thorough examination of the effects of variability and uncertainty. This thesis aimed to enhance understanding the effects of variability and uncertainty on the results, by means of uncertainty and sensitivity analysis. *Uncertainty analysis* refers to the estimation of the uncertainty attribute of a model output using the uncertainty attributes of the model inputs. There are three types of sensitivity analyses: (I) a *local sensitivity analysis* addresses what happens to the output when input parameters are changed, i.e. the intrinsic model behaviour of a parameter; (II) a *screening analysis* addresses what happens to the output based on the uncertainty range of the different input parameters; and (III) a *global sensitivity analysis* addresses how much the uncertainty around each input parameter contributes to the output variance. Both the screening analysis and the global sensitivity analysis combine the intrinsic model behaviour with the information of uncertainty around input parameters. Applying uncertainty analysis and sensitivity analysis can help to reduce the efforts for data collection, support the development of mitigation strategies and improve overall reliability, leading to more informed decision making in environmental impact assessment models. Including uncertainty in environmental impact assessment models showed that: (1) the type of uncertainty analysis or sensitivity analysis applied depends on the question to be addressed and the available information; (2) in some cases it is no longer possible to benchmark environmental performance if epistemic uncertainty is included; (3) including correlations between input parameters during uncertainty propagation will either increase or decrease output variance, which can be predicted beforehand; (4) under specific characteristics of the input parameters, ignoring correlation has a minimal effect on the model outcome. Systematically combining a local and global sensitivity analysis in environmental impact assessment models: (1) resulted in more parameters than found previously in similar studies (for the case studies discussed in this thesis); (2) allowed finding mitigation options, either based on innovations (derived from the local sensitivity analysis) or on management strategies (derived from the global sensitivity analysis); (3) showed for which parameters reliability should be improved by increasing data quality; (4) showed that reducing the (epistemic) uncertainty of the most important parameters can affect the comparison of the environmental performance.

Contents

CHAPTER 1

General introduction

1.1 Background

Food is essential to sustain and enhance human life. Nowadays, food production is generally acknowledged as one of the drivers of environmental pressure [Tilman and Clark, 2014]. Agricultural land, for example, covers approximately one third of the earth's land that is not permanently frozen [Bajželj et al., 2014]. The majority of this land is used for production of animal-source food [Steinfeld et al., 2006]. The agricultural sector not only uses natural resources, such as land, energy, water and fossil phosphorus, but also contributes to climate change, acidification, water pollution and biodiversity loss. The global livestock sector, for example, contributes to approximately 14.5% of all anthropogenic greenhouse gas emissions, mainly via emissions of carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) [Gerber et al., 2013]. An increase in the demand for food products is still expected, because of the growth of the global human population, growing incomes and changes in diets. The challenge to produce this food in an environmentally friendly way, therefore, becomes even more urgent. To develop strategies to produce food with a low environmental impact, the environmental impact of food needs to

be quantified.

Quantifying the environmental impact of agricultural activities, such as crop or livestock production, requires great care, since the input data naturally vary due to, for example, seasonal changes, geographical conditions and socio-economic factors. Moreover, uncertainties, such as measurement errors in observations, exist around modelling of emissions and technical input parameters. Once you acknowledge that variability and uncertainties exist, questions arise such as: *how does variation of input parameters influence the results? Which input parameters explain most of the variation of the model output? Do input uncertainties have an effect on the comparison between the environmental impacts of two products?* To answer the questions raised by the acknowledgement of variability and uncertainty, one is naturally led to the field of uncertainty and sensitivity analysis.

1.1.1 Quantification of environmental impact

Quantification of environmental impact originating from the production and use of materials, substances or products from a chain perspective, based on physical principles, can be divided into two main approaches [Wrisberg et al., 2002]. (I) *Region-oriented approaches*, where the system boundary of a specific area and time interval (e.g., The Netherlands, 01/01/2015 until 31/12/2015) is the starting point to determine which activities are included. Region-oriented approaches can concern a specific year and economic sector, or all processes controlled by one company, such as a farm. Four examples of region-oriented approaches are: (1) material flow analysis, concerning material flows through a region or company, e.g. iron or plastics; (2) substance flow analysis, concerning specific elements such as nitrogen or phosphorus; (3) nutrient balance analysis, concerning input and output of nutrients or substances through a region or a farm; and (4) environmental input-output analysis, focusing on pollution of industrial trade of, e.g. a country. (II) *Function-oriented approaches*, where the function of the product is the starting point and defines the system boundary, ideally from cradle-to-grave. Function-oriented approaches can be time independent, but often consider the production of the final product for a specific year, and only processes from power plants, companies or farms are considered that belong to the studied production chain. Examples of function-oriented approaches are life cycle assessment and cumulative energy requirement analysis.

A region-oriented approach widely used in agriculture is a nutrient balance analysis. A nutrient balance is computed as the difference between nutrients entering a system and leaving the system; the system itself is considered as a black box. The difference between nutrient inputs and outputs is generally called the nutrient surplus, and is assumed lost to the environment [Sutton et al., 2013]. Nutrient losses contribute to, for example, eutrophication, acidification, emission of greenhouse gas emissions [Sutton et al., 2013], and depletion of fossil phosphorus [Suh and Yee, 2011]. A nutrient balance can be computed at a range of levels, varying from crop or animal, to farm or, for example, the entire European Union [Aarts et al., 1992; Schröder et al., 2003; Lesschen et al., 2011]. Nutrients generally considered in agriculture are nitrogen and phosphorus, because these nutrients are essential for plant growth. A nutrient balance can be used to identify where and why losses occur, and to develop mitigation strategies to reduce these losses.

A function-oriented approach widely used in agriculture is life cycle assessment (LCA), which quantifies relevant resource use and emissions of a product over the entire production chain. LCA can be used to quantify all different types of environmental impacts (e.g. eutrophication, climate change, eco-toxicity), and is increasingly applied in agriculture [Guinée et al., 2010]. An environmental impact that is often considered related to livestock production is climate change, due to the large contribution of livestock to the global anthropogenic emissions of greenhouse gases [Gerber et al., 2013]. In such cases, one often speaks of the carbon footprint of an agricultural activity or product. An LCA can be used to identify where in the chain most emissions occur, and develop mitigation strategies to reduce these emissions.

1.1.2 Origins of variability and uncertainty in environmental modelling

Nutrient balance analysis and life cycle assessments can both be used to develop a model that quantifies environmental impact. Collecting data for environmental impact assessment models is often perceived as a laborious task [Lloyd and Ries, 2007; Björklund, 2002]. Moreover, required data contains uncertainty due to measurement errors, or can vary widely due to natural circumstances. Most studies that quantify environmental impact, do not consider the impact of variability or uncertainties of input data on their results. Many studies aim at quantification of, for example, the carbon footprint of one

kilogram of food. Most of these studies use only point values (i.e. a singles value that represents each data point in the environmental impact assessment model) and overlook the range of possible realisations, and could therefore be misleading [Björklund, 2002], or might provide a false sense of accuracy [De Koning et al., 2010]. For example, nutrient balances can be used to benchmark farms, by means of quantifying the nutrient use efficiency (NUE). The NUE of one farm then is used to compare its environmental performance to other farms within the peer group. A higher NUE means that the farm is performing better. In such a situation, the peer group can learn from this farm, and incorporate similar mitigation strategies to improve their NUE. When incorporating measurements uncertainties in the calculation of the NUE, however, it might no longer be possible to rank the NUE of farms anymore, as it might not be possible to make a distinction in NUEs between the farms.

Origins of variability and uncertainty in environmental impact assessment models can be divided into two broad categories: (I) natural variability and (II) epistemic uncertainty.

Natural variability relates to *observable* variation, which means it is inherent to the system and therefore cannot be reduced [Walker et al., 2003]. Although it is possible to strive for reduction of natural variability in time or space, the *observed* variation cannot be reduced. An example of natural variability in agriculture is variation between annual crop yields of wheat, which exist in time, i.e. across years, and in space, i.e. across countries or soil types. Another example is the variation in diet preferences amongst consumers, which makes it impossible to calculate the carbon footprint of one day of food.

Epistemic uncertainty originates from a lack of knowledge and can be reduced by gaining more or better data [Walker et al., 2003]. Epistemic uncertainty includes errors from measurement instruments, or those introduced by the observer. For example, in case a weighting scale is not available to determine the weight of a cow, the weight can be estimated based on body measurements, such as body length, heart girth and height [Francis et al., 2004; Lesosky et al., 2012]. Literature shows that body weight can be estimated from single heart girth measurements with reasonable accuracy. Heart girth measurements, however, can result in measurement errors because the positioning of the cow can easily affect the result [Heinrichs et al., 1992]. More sources of natural variability and epistemic uncertainty are found in Table 1.1.

The theoretical distinction made between natural variability and epistemic uncertainty, however, may be not so clear in practice. An example is the epis-

Table 1.1: Examples of natural variability and epistemic uncertainty.

Category	Examples of sources
Natural variability	Climate variability, soil type, genetic differences, variation in temperature, differences in management strategies, geographical differences, consumer preferences
Epistemic uncertainty	Measurement errors, errors in observations, errors of measurement instruments, estimates of experts, lack of knowledge

temic uncertainty ranges that are given by the intergovernmental panel on climate change (IPCC) around the emission factors of N_2O from application of fertiliser. This range is often interpreted as epistemic uncertainty, but might include also natural variation due to differences in climate conditions or soil types, which is in fact caused by natural variability. Both natural variability and epistemic uncertainty are also found for the parameter annual milk yield per cow. Annual milk yield per cow can vary naturally due to genetic differences, or differences in feeding strategies, whereas milk yields can also be prone to the same measurement error (i.e. epistemic uncertainty).

Many experience natural variability or epistemic uncertainty around data for input parameters in environmental assessment models, making the exact environmental impact difficult to quantify.

1.2 Incorporating variability and uncertainty in environmental impact assessment

Uncertainty analysis can be used to propagate epistemic uncertainties and natural variability of input parameters through an environmental impact assessment model (Table 1.2). From now on, when the term uncertainty analysis is used, it can refer to the analysis of the magnitude and consequences of both epistemic uncertainty and natural variability of the input parameters. The term *uncertainty* in uncertainty analysis can be interpreted as a quantitative value either representing epistemic uncertainty or natural variability. An uncertainty analysis quantifies the uncertainty of the output based on the uncertainty of the input parameters. For example, *what is the uncertainty around*

greenhouse gas emissions of 1 kg of milk? These types of methods require the knowledge of a distribution function (e.g. a normal distribution), or a least a parameter of dispersion, such as the variance, to propagate the input uncertainties through the environmental impact assessment model.

In addition to the uncertainty analysis, a sensitivity analysis can be used to study the effect of input uncertainties on the output of an environmental impact assessment model. Two commonly used approaches for sensitivity analysis are local sensitivity analysis and global sensitivity analysis. Terminology often used in case of uncertainty analysis and sensitivity analysis is defined in Table 1.2.

Most studies of environmental impact assessment models assume that the input parameters can vary independently [Lloyd and Ries, 2007; Bojacá and Schrevens, 2010]. However, in certain cases correlations exist between input parameters, for example, a correlation can be expected between crop yield and fertiliser. This means that if fertiliser rate is increased, crop yield (to some extent) also increases. Including correlations in the sampling design can answer questions such as: *what is the effect of including correlations between crop yield and fertiliser on the model output? What is the effect of including correlations between input parameters on the global sensitivity analysis?* Including correlations can affect both uncertainty analysis and sensitivity analysis, but requires information of the presence of correlations coefficients of the input parameters, such as the variance for uncorrelated parameters or a covariance for correlated parameters, to propagate the input uncertainties through the environmental impact assessment model.

A local sensitivity analysis quantifies the effect on the output when an input parameter is changed. For example, *what would be the effect on greenhouse gas emissions per kg of milk when a cow would produce 5% more milk with the same amount of feed?* In general, these type of methods consider the effect of a change independent of other input parameters and do not consider the actual range over which the input parameters can vary (Figure 1.1). These types of methods are especially useful when data availability is limited to point values.

A screening analysis quantifies the effect on the output when an input parameter is changed according the to uncertainty range of an input parameter. For example, *what would be the effect on greenhouse gas emissions per kg of pork when variation of manure production in pigs vary with 3%?* In general, this type of method also considers the effect of a change independent from other input parameters. These types of methods are especially useful when only little

Table 1.2: Uncertainty versus sensitivity: definitions of uncertainty (analysis) and sensitivity (analysis).

Concept	**Definition**
Uncertainty	a property attributable to an input parameter or an output parameter. In the context of this thesis it relates to quantitative uncertainty. Uncertainty of the input parameters can be given as a probability distribution function (for instance, a normal distribution with a specified mean and standard deviation).
Uncertainty analysis	refers to the estimation of the uncertainty attribute of a model output using the uncertainty attributes of the model inputs.
Sensitivity	a property attributable to how a model output behaves as the result of the variation of an input parameter [Saltelli et al., 2008]. There are three types of *sensitivity analyses*.
Local sensitivity analysis	addresses what happens to the output when input parameters are changed, i.e. the intrinsic model behavior of a parameter. The parameters that have the largest effect on the model output are referred to as the most *influential parameters*.
Screening analysis	addresses what happens to the output based on the uncertainty range of the different input parameters.
Global sensitivity analysis	addresses how much the uncertainty around each input parameter contributes to the output variance [Saltelli et al., 2008]. Both the screening analysis and the global sensitivity analysis combine the intrinsic model behaviour with the information of uncertainty around input parameters. The parameters that change the model output most or explain most of the output variance are referred to as the most *important parameters*.

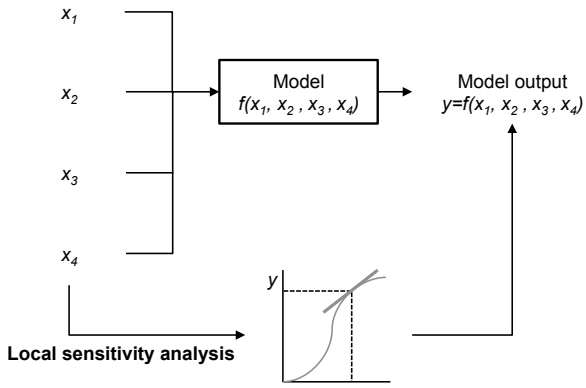

Figure 1.1: An illustration of a local sensitivity analysis for a model with four input parameters $(x_1, \ldots, x_4)$. Each input parameter is changed independently; the influence of parameter x_1 for example, can be expressed as the effect of changing x_1 on the output y.

information is available on the input uncertainties.

A global sensitivity analysis can be seen as an extension of uncertainty propagation: it determines how much each input parameter contributes to the output variance. A global sensitivity analysis considers the actual variation over all input parameters simultaneously (Figure 1.2). For example, *how much does the annual variation around crop yield of wheat contribute to the uncertainty around the greenhouse gas emissions? What is the impact of incorporation of covariance on the global sensitivity analysis?* In general (but not always), these methods require full knowledge of the input uncertainties (i.e. distribution functions) and information regarding the covariance if the input parameters are correlated.

Incorporating uncertainty in an environmental impact assessment model will strengthen the model outcomes. It will provide knowledge about the range of model outputs, which enables more informed decision-making. At present, however, a standardised methodology how to propagate uncertainties or which type of sensitivity analysis to use, is missing.

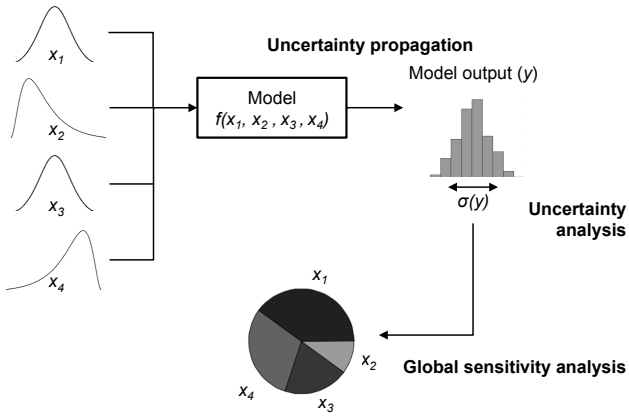

Figure 1.2: An illustration of a global sensitivity analysis for a model with four parameters: the variance decomposition (pie chart) explains the output variance (histogram), given the distribution functions of the four input parameters on the left hand side of the figure.

1.3 Knowledge gaps

To determine the effect of input uncertainties on the output, most environmental impact assessment studies that performed a local sensitivity analysis use a straightforward method, i.e. a one-at-a-time (OAT) approach. An OAT approach varies an input parameter with, e.g. 5 or 10%, and subsequently quantifies the impact on the model output [Suh and Yee, 2011; Van Middelaar et al., 2012; Van Zanten et al., 2015a; Yang et al., 2011]. This procedure is usually repeated for a limited number of input parameters. The input parameters that cause most change in model output are considered to be the most influential parameters. The OAT approach, however, has two weaknesses. First, the number of input parameters assessed is usually a subset of the total available input parameters, implying that potential influential parameters might be overlooked. Second, the actual uncertainty ranges of input parameters are ignored: some input parameters may vary only with 5%, while others may vary with a factor ten or hundred. Their impact on the model output, therefore, might be under- or overestimated. The OAT approach is often chosen because of its simplicity, as it is not necessary to gather additional data or to derive, for example, ranges or distribution functions for all input parameters [Björklund, 2002]. Moreover, data availability for environmental impact assessment models is often very limited. Even with limited data, however, it is still possible to perform uncertainty or sensitivity analysis.

Even in case no other data are available than the point values used in the model, a local sensitivity analysis can be performed. The multiplier method [Heijungs and Suh, 2002; Heijungs, 2010] (MPM), for example, determines the local sensitivity of all input parameters in an LCA model, and does not require actual ranges over which input parameters can vary. The MPM, therefore, accommodates the first weakness of OAT methods mentioned, as it systematically explores the sensitivity of all input parameters. MPM can be used to explore areas of potential mitigation options [Heijungs, 1996]. Once these parameters are indicated, a further examination is required to see if these parameters can be improved, by e.g. technical innovations or by improving management. However, since MPM only quantifies the intrinsic sensitivity of the input parameters within the model, and does not include the actual uncertainty of the input parameters, this method is not suitable to make comparisons.

In case only limited amount of data is available, for example, the ranges

of input parameters are known, we can perform a screening analysis. The method of elementary effects [Saltelli et al., 2008; Campolongo et al., 2007] (MEE), for example, calculates the sensitivity of input parameters based on their actual ranges, by exploring model outputs of those ranges. MEE can be used to determine how uncertainty around the input parameters affects the output. MEE does include an uncertainty range for each input parameter, and, therefore, partly accommodates the second weakness of the OAT approach. Also, this screening analysis can be used to indicate important parameters that contain opportunities for improvement regarding environmental performance [Saltelli et al., 2008; Campolongo et al., 2007]. Since MEE is a screening analysis, it is can also be used to find parameters that should be taken into account in a subsequent global sensitivity analysis, i.e. it focuses the data collection to the most important parameters before performing a global sensitivity analysis. As only the ranges are used of the input parameters, because the distribution functions could not (yet) be defined, the uncertainty of the model output is of limited value. For example, the model output of the MEE method cannot be used to determine significant differences between two product alternatives, which can be done with uncertainty propagation of distributions functions using Monte Carlo simulation.

So far, no study combined the MPM and MEE in an environmental impact assessment model, to see if a combination of methods leads to more insight in parameters that can contain potential improvement options, or if their uncertainty needs to be reduced to improve the reliability of the results.

In case full knowledge about the uncertainties is available, including the distribution function (e.g. a normal distribution), mean and a parameter of dispersion (e.g. standard deviation), uncertainty propagation can be performed by means of a simulation on the basis of stochastic sampling. Current practice in LCA is dominated by one type of sampling, namely Monte Carlo sampling [Lloyd and Ries, 2007], but there are several other methods to propagate uncertainties [Lloyd and Ries, 2007], such as Latin hypercube sampling, which uses a smart sampling design that can potentially reduce the sample size of the simulation, just as (randomised) quasi Monte Carlo sampling. Fuzzy interval arithmetic [Lloyd and Ries, 2007], makes use of only three data points (mean, minimum and maximum value) to propagate uncertainties. Analytical uncertainty propagation [Heijungs, 1996], uses only the mean and a parameter of dispersion to propagate uncertainties. However, these methods have not been compared in a consistent manner to see if one of

these methods performs better than the other.

After uncertainty propagation, a global sensitivity analysis can be performed that can be used to explain where the output uncertainty comes from, i.e. which parameters are most important in explaining the output variance. A global sensitivity analysis can also be used to determine which of the input parameters contribute only minor to the output variance and thus can be set to a fixed value to simplify data collection of similar future studies [Saltelli et al., 2008]. In LCA literature, different methods for global sensitivity analysis have been used that quantify the contribution to output variance. Sampling-based methods employ regression-like techniques that use the distribution function, such as the squared standardised regression coefficients and the squared Pearson correlation coefficient or squared Spearman (rank) correlation coefficient [Saltelli et al., 2008]. In contrast, analytical methods (the so-called key issue analysis; [Heijungs, 1996]) only require a parameter of dispersion to calculate the contribution to the output variance for each parameter. Outside the LCA domain, a much wider set of methods have been developed and applied, such as random balance design and the Sobol' method [Sobol', 2001; Saltelli et al., 2008], which also both use the distribution functions. So far, the application of different methods for global sensitivity analyses in environmental impact assessment models, such as LCAs and nutrient balances, have been limited. For these methods, it is not known if there is one method that performs better than the other methods.

A common strategy in environmental impact assessment models, is to look for improvement options, and to do so, two product alternatives are compared. A suitable approach is to use a discernibility analysis [Henriksson et al., 2015; Heijungs and Kleijn, 2001], where random drawings from two sampling (e.g. Monte Carlo) runs are compared and a frequency distribution is determined of how much one alternative is better than the other. Incorporating uncertainties in this way, improves environmentally friendly decision-making and benchmarking. So far, no study has yet combined the knowledge of a global sensitivity analysis in a benchmarking study in environmental impact assessment models, such as a nutrient balance, to see if reducing input uncertainties influence the result of benchmarking.

In addition, very few studies incorporated correlations in the sample design of environmental impact assessment models [Wei et al., 2014; Bojacá and Schrevens, 2010]. So far, no study has yet included the effect of correlations on the global sensitivity analysis in environmental impact assessment model

and applied it to a case study of food production. Moreover, none explored how to quantify the effect of ignoring correlations between input parameters on the output variance and in global sensitivity analysis.

Even though case studies of food production are especially prone to natural variability and epistemic uncertainties, very few case studies made a thorough examination of all the parameters in the model. Therefore, I come to the overall aim of this thesis:

> The aim of this thesis is to explore how uncertainty and sensitivity analysis can help to reduce the efforts for data collection, support the development of mitigation strategies and improve overall reliability of informed decision-making in environmental impact assessments models.

To do so, the following topics were addressed:

- Comparing different methods for uncertainty propagation and sensitivity analysis that include uncertainty, and find their applicability, for example by combining results of different methods;
- Determining the effect of correlations in uncertainty propagation and global sensitivity analysis;
- Application to case studies in food production systems.

An overview of the applied methods in each chapter can be found in Figure 1.3.

1.4 Thesis outline

In Chapter 2, a local sensitivity analysis and a screening analysis are applied in an LCA case study of pork. Input uncertainties in pork production systems come from epistemic uncertainties around emission factors, and natural variability around technical parameters such as crop yields and feed intake. The results the screening analysis (which requires ranges) was combined with the results of the local sensitivity analysis (which requires only point values), to provide improvement options related to data quality and management strategies.

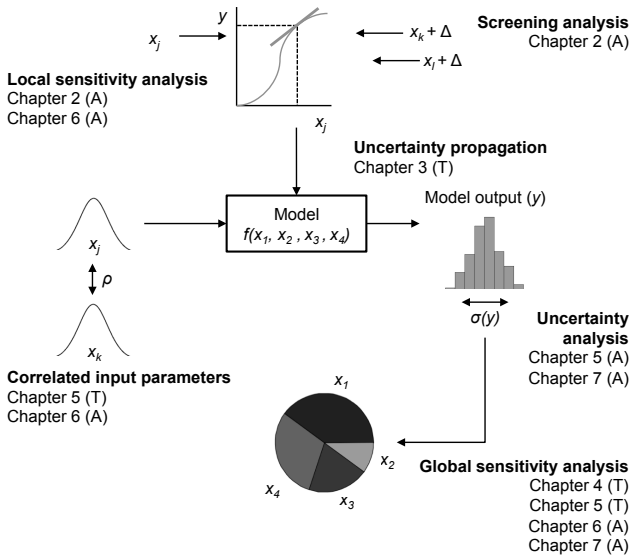

Figure 1.3: Main methodological focus in each chapter. T: theory, A: application.

In Chapter 3, methods for uncertainty propagation are compared on their data requirements, accuracy and efficiency, applied to artificial case studies of electricity production and wild caught fish.

In Chapter 4, methods for global sensitivity analysis are compared, based on data requirements and capability to explain the output variance. The methods will be applied to an artificial case study of wild-caught fish and electricity production.

In Chapter 5, a novel method is introduced that quantifies the effect of including or ignoring correlations in the sampling design on the output uncertainty and global sensitivity analysis. The method can be used when both correlation between two input parameters and the variance (of one of) the input parameters is unknown. To show how the method can be used, the method is applied to an artificial case study of electricity production.

In Chapter 6, a local and a global sensitivity analysis is applied to a case study of milk production in Germany. Uncertainties are caused by epistemic uncertainty around emission factors and natural variability around technical parameters such as crop yield and dry matter feed intake. Also, correlation between fertiliser rate and crop yields, and feed intake and milk yield are taken into account. The aim is to identify input parameters that can be set to a fixed value to reduce data collection efforts, by combining the results of a local and a global sensitivity analysis.

In Chapter 7, epistemic uncertainties are incorporated in benchmarking of nutrient use efficiency of dairy farms. First, the effect of incorporating the uncertainties on the ranking of the farms is determined. Second, parameters are identified which explain most of the output variance for different farm typologies. Third, the uncertainties of the most important parameters are reduced; to see if reducing the input uncertainties influence benchmarking.

In Chapter 8, the value of uncertainty and sensitivity analysis in environmental assessment models is discussed, and recommendations are given towards future research.

CHAPTER 2

Sensitivity analysis of greenhouse gas emissions from a pork production chain

Joint work with:
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R. Heijungs
E.A.M. Bokkers
I.J.M. de Boer
(submitted)

Abstract

This study aimed to identify the most essential input parameters in the assessment of greenhouse gas emissions (GHG) along the pork production chain. We identified most essential input parameters by combining two sensitivity-analysis methods: the multiplier method and the method of elementary effects. The former shows how much an input parameter influences assessment of GHG emissions, whereas the latter shows the importance of input parameters on uncertainty in the output. For the method of elementary effects, uncertainty ranges were implemented only for input parameters that were identified as being most influential based on the multiplier method or that had large uncertainty ranges based on the literature. Results showed that the most essential input parameters are the feed-conversion ratio, the amount of manure, CH_4 emissions from manure management and crop yields, especially of maize and barley. Combining the results of both methods allowed derivation of mitigation options, either based on innovations (e.g. novel feeding strategies) or on management strategies (e.g. reducing mortality rate), and formulation of options for improving reliability of the results. Mitigation options based on innovations were shown to be most effective when directed at improving the feed-conversion ratio; decreasing the amount of manure produced by pigs; improving maize, barley and wheat yields; decreasing the number of sows or piglets per growing pig needed and improving efficiency of N-fertiliser production. Mitigation options based on management strategies were shown to be most effective when farmers strive to reduce feed intake, reduce the application of N fertiliser to maize and barley, and reduce the number of sows per growing pig needed towards best practices. Finally, the method of elementary effects showed that reliability of assessing GHG emissions of pork production could be improved when uncertainty ranges are reduced, for example, around direct and indirect N_2O emissions of the main feed crops in the pig diet and the CH_4 emissions of manure. Also the reliability could be improved by improving data quality of the most essential parameters. Combining two types of sensitivity-analysis methods identified the most essential input parameters in the pork production chain. With this combined analysis, mitigation options via innovations and management strategies were derived, and parameters were identified that improved reliability of the results.

2.1 Introduction

Environmental impacts of the agri-food industry have been of increasing concern; in particular awareness about environmental impacts of animal production are increasingly acknowledged [Steinfeld et al., 2006]. The livestock sector, for example, is responsible for about 15% of the total anthropogenic emis-

sions of greenhouse gases [Gerber et al., 2013]. Worldwide, pork production explains about 9% of greenhouse gas (GHG) emissions of the livestock sector [Gerber et al., 2013].

In general, the environmental impact of pork production is quantified using life cycle assessment (LCA) [Baumann and Tillman, 2004]. To quantify GHG emissions of the entire pork production chain, we need to define values for input parameters, such as feed-conversion ratios, crop yields, nitrogen application ratios, and emission factors. Uncertainty around these input values can cause a large variation in GHG emissions estimates. For example, within the IPCC Tier 1 framework, direct N_2O emissions of N from fertiliser and manure and crop residues vary by a factor of ten: 0.003 to 0.03 kg N_2O per kg N applied [IPCC, 2006c].

To quantify to what extent environmental impacts of the pork production chain varied and to explore the robustness of the results, Basset-Mens and Van Der Werf [2005]; Basset-Mens et al. [2005]; Van Der Werf et al. [2005] identified ranges of some of their input parameters and assessed the effect of these ranges on the output. Basset-Mens and Van Der Werf [2005] for example, concluded that N_2O emissions of feed crops caused large uncertainty around estimates of total GHG emissions, indicating that the impact of the feed crops is high, as are the uncertainty ranges around their emissions. None of these studies systematically explored the effect, or contribution, of each individual input parameter to the output. However, it is possible to assess the importance of each individual parameter in an LCA model by performing a sensitivity analysis.

Most LCA studies that performed a sensitivity analysis used a straightforward method, i.e. a one-at-a-time (OAT) approach. An OAT approach selects an input parameter and changes it e.g. 10%, and subsequently quantifies the effect on model output [Suh and Yee, 2011; Van Middelaar et al., 2012; Van Zanten et al., 2015a; Yang et al., 2011]. By exploring the impact of input parameters on the output, the robustness of the results is explored. The input parameters that cause most change in model output are considered to be the most *influential* parameters.

The OAT approach is often chosen because of its simplicity as it is not necessary to gather additional data or to derive, for example, ranges or distribution functions for all input parameters [Björklund, 2002]. However, the OAT approach has two weaknesses. First, the number of input parameters assessed is usually a subset of all input parameters, implying that potential

influential parameters might be overlooked. Second, the arbitrary choice of 10% may not reflect the actual uncertainty range of the input data. Some input parameters may vary only 5%, while others may vary by a factor of ten. Therefore, the actual effect on the output might be under- or overestimated.

Two methods for sensitivity analysis are available that overcome these weaknesses. The multiplier method (MPM) determines the influence of all input parameters in an LCA model, and, therefore, accommodates the first weakness. MPM was first introduced in LCA by Heijungs [1994], but to our knowledge has not been applied to an agricultural case study in LCA. MPM can be used to determine areas of potential mitigation options [Heijungs, 1996] but does not take into account the actual ranges over which the input parameters can vary.

In contrast, the method of elementary effects (MEE) does include an uncertainty range for each input parameter, and, therefore, accommodates the second weakness mentioned. MEE calculates the importance of the input parameters based on their actual ranges, by exploring model outputs within these ranges. MEE can be used to determine how much the uncertainty around the input parameters affects the output. The parameters that affect the output most, based on their uncertainty range, are referred to as the most *important* parameters. It should be noted that although MEE provides a sampled model output, it is primarily used for sensitivity analysis belonging to the area of screening methods [Saltelli et al., 2008]. MEE was originally designed by Morris [1991] and expanded by Campolongo et al. [2007]. To our knowledge, MEE has only been applied to LCA studies outside livestock production e.g. cocoa production by Mutel et al. [2013] and detergent production by De Koning et al. [2010].

This study aims to identify the most *essential* parameters in an LCA model of GHG emissions of pork production by combining results of the two sensitivity-analysis methods. First, MPM is applied, including all input parameters in the model, and second MEE is applied, which explores consequences of actual ranges in uncertainty. Combining results of both methods may help to formulate potential mitigation options and increase reliability of LCA results.

2.2 Material and methods

2.2.1 Matrix formulation in LCA

To facilitate the use of the sensitivity-analysis methods applied in this study, we used matrix-based LCA [Heijungs and Suh, 2002]. The inventory totals equal:

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} \tag{2.1}$$

Input parameters of an LCA consist of technical parameters and emissions or resource use. The technology matrix **A** contains the technical parameters of various production processes included in the chain, such as production of feed or storage of manure, presented as a set of linear equations. Each column represents a production process. The associated emissions are found in the **B**-matrix, e.g. the kg CH_4 per kg manure storage per year. The **A**-matrix is scaled to produce the amount given by the functional unit **f** (e.g. kg of growing pig). To calculate the total environmental impact per impact category (**h**), the inventory result (**g**) is multiplied by the characterisation matrix (**Q**):

$$\mathbf{h} = \mathbf{Q}\mathbf{g} \tag{2.2}$$

In this case, **Q** contains the characterisation factors of GHG emissions for global warming potential (GWP) on a 100-year time interval: carbon dioxide (CO_2), biogenic methane ($CH_{4,bio}$): 28 kg CO_2 e/kg biogenic methane, fossil methane ($CH_{4,fossil}$): 30 kg CO_2 e/kg fossil methane; and nitrous oxide (N_2O): 265 kg CO_2 e/kg nitrous oxide [Myhre et al., 2013], thus reducing to a vector $\mathbf{q}'$, and **h** to a scalar h. All modelling in this paper is done in MATLAB, and the code is available upon request to the authors. We only considered elements in **A** and in **B** to contain uncertainty; **f** and **Q** remained fixed.

2.2.2 Multiplier method

MPM predicts the change in the result h of a small change around the default value of each input parameter in **A** or **B**. A derivation of the method can be found in Heijungs [2010]. MPM uses the first-order partial derivatives $\frac{\partial(h,m)}{\partial(A,i,j)}$ and $\frac{\partial(h,m)}{\partial(B,i,j)}$ to estimate the influence around each input parameter. To compare the influence of the input parameters, the partial derivatives are normalised

with respect to their original value A_{ij} and B_{kj}, where A_{ij} and B_{kj} are elements of **A** and **B** respectively, and h_m are the impact categories in h. The multipliers equal:

$$\eta(h,m;A,i,j) = \frac{A_{ij}}{h_m}\frac{\partial(h,m)}{\partial(A,i,j)} \tag{2.3}$$

$$\eta(h,m;B,k,j) = \frac{B_{kj}}{h_m}\frac{\partial(h,m)}{\partial(B,k,j)} \tag{2.4}$$

Full expressions of the multipliers of Equations (2.3) and (2.4) are given in Heijungs [2010]. The multiplier will give not only the magnitude but also the direction of change, and can either be positive or negative. The multipliers can be interpreted as how much a 1% change in the input will affect the output (in %). For illustrational purposes, we will also use the absolute effect, given by $|\eta|$.

2.2.3 Method of elementary effects

MEE uses the actual ranges of each input parameter. A range is defined as a minimum and a maximum for each parameter, and can originate from variability or epistemic uncertainty. Variability in input parameters arises from e.g. variation in crop yields or N-fertiliser rates over years; it is inherent to the data and cannot be reduced. Epistemic uncertainty comes from unknowns around an input parameter [Walker et al., 2003], and is for example found for the IPCC emission factors of N_2O emissions of fertiliser application. Gaining more knowledge about an input parameter, e.g. by better measurements, can reduce epistemic uncertainty [Chen and Corson, 2014].

The minimum and maximum value for each input parameter can be used to calculate the combination of all minima and maxima, but in the case of 100 parameters, this would lead to $2^{100} \approx 10^{30}$ calculations. This approach may not be feasible, especially for large models. To overcome this problem, MEE selects two points within the range for each input parameter and calculates the change in the output based on this change in the input parameter, changing each parameter only once. To perform MEE, the range of each input parameter is divided into three equal parts (it does not use the default value, as MPM does). If a parameter ranges from 0 to 1, for example, the division would lead to (0; 1/3); (1/3; 2/3); (2/3; 1). It is possible to create smaller or larger

divisions, but this is a common choice [Campolongo et al., 2007; Saltelli et al., 2008]. Starting from an arbitrary starting point, one parameter is selected at random and changed with a predefined step size $\delta_{A,i,j}$ or $\delta_{B,k,j}$, set to 2/3 of the range of each input parameter [Campolongo et al., 2007]. This is repeated until each parameter has changed once (one trajectory has been performed) and the elementary effects $EE(A,i,j)$ and $EE(B,k,j)$ can be calculated for each parameter A_{ij} and B_{kj} by dividing the change in output by the step size Δ (equal to 2/3):

$$EE(A,i,j) = \frac{h(A_{ij} + \delta_{A,i,j}) - h(A_{ij})}{\Delta} \tag{2.5}$$

$$EE(B,k,j) = \frac{h(B_{kj} + \delta_{B,k,j}) - h(B_{kj})}{\Delta} \tag{2.6}$$

The above procedure is repeated several times. A measure of importance is found by calculating μ^*, which is the (absolute) mean of the average elementary effects[1]:

$$\mu^*(A,i,j) = \frac{1}{R}\sum_{r=1}^{R} |EE(A,i,j)| \tag{2.7}$$

$$\mu^*(B,k,j) = \frac{1}{R}\sum_{r=1}^{R} |EE(B,k,j)| \tag{2.8}$$

where R is the number of trajectories (usually set to 10). The set of μ^* values can be ranked from the most to the least important parameter[2].

2.2.4 Framework for combining MPM and MEE

We combined MPM and MEE based on a figure in Heijungs [1996], which distinguished between the *influence* and the *importance* of input parameters

[1] As the trajectories are chosen at random, one can imagine that the choice of the trajectories can be closer or further apart. In an optimal situation, one would like the trajectories to be as far apart as possible. Campolongo et al. [2007] proposed a brute force approach that selects e.g. ten more optimal trajectories from a set of 100. As this model is linear, e.g. the ranking of the parameters did not change for multiple runs, we did not include this part of the methodology as it takes much more computational effort in terms of run-time and memory usage.

[2] Another indicator that can be calculated is the σ, which is an indicator for the interaction or non-linear effects: if the elementary effect of a certain parameter changes for different trajectories, the magnitude of the elementary effect depends on either the configuration of the model or the presence of nonlinear effects, but this will not be discussed in this paper.

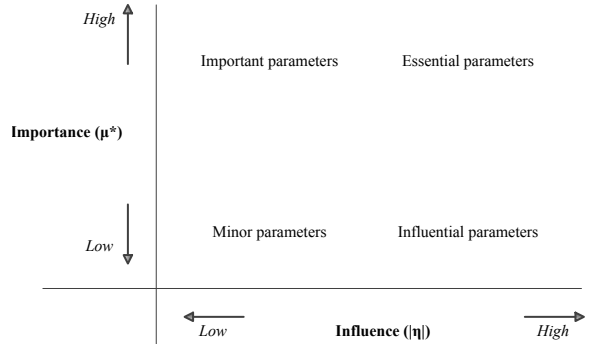

Figure 2.1: Framework for combining MPM and MEE. The most influential and important parameters are shown in the top right corner (essential parameters). Adapted from Heijungs [1996].

on output uncertainty. If an input parameter is both influential and important, the parameter is considered as *essential* (Figure 2.1). We used MPM to determine the influence and MEE to determine the importance of each input parameter.

We adapted the figure from Heijungs [1996], to identify mitigation options based on innovations or management strategies (Figure 2.1). The horizontal axis ranks the most influential parameters, which therefore could have most impact if they are reduced. These mitigation options reflect innovations in the production chain. The vertical axis ranks the parameters that are most important to output uncertainty, caused by their variability due to e.g. differences in management practises, or epistemic uncertainties. Input parameters that are highly important and highly influential can be used to identify potential mitigation strategies (i.e. essential parameters, Figure 2.1, top right corner). Environmental impacts of the livestock sector, for example, can be reduced if farmers adapt their management strategies towards those farmers, with a relatively low environmental impact. In addition, reliability can be improved by reducing the epistemic uncertainties that are shown to be important, which are also found in the direction of the vertical axis. Reducing the epistemic

uncertainty ranges of input parameters that affect the output highly would lead to smaller ranges of uncertainty around the output, hence more reliable conclusions. Epistemic uncertainties can be reduced by better measurements. Reliability can also be improved by improving data quality of the most essential parameters.

2.2.5 Case study: pork production chain

Pork production system

The pig production model is based mainly on Van Zanten et al. [2015b] and the functional unit is one kg body weight of a growing pig. The model of Van Zanten et al. [2015b] describes a growing-pig production chain in the Netherlands in which soya bean meal is replaced by rapeseed meal. Environmental impacts of the following processes in the pig chain were considered and are explained below: production of crop inputs (e.g. fertiliser), feed processing (e.g. milling), piglet production (rearing), manure management, pig housing, and enteric fermentation from pigs (Figure 2.2). The supplementary material (Table 2.6) provides the compositions of diets for growing pigs, piglets, gilts and sows.

Diet compositions were an average representation for the year 2012 and were composed based on the procedure described by Bikker et al. [2011]. The average diet contained four diets, one for each quarter of the year. The diets were formulated using a commercial linear programming tool for feed (i.e. Bestmix®, Adifo, Maldegem, Belgium), which optimises a diet by minimising the cost of the diet [Nuscience, 2012]. The diets had to meet the average nutritional requirements for the pigs in Dutch practice, e.g. growing pig diets contained 9.68 MJ net energy per kg feed. To assess the average growth performance (aligned with the nutritional content of the diet), annual average company data of Dutch pig farms were used [Agrovision, 2012]. Piglets had a start weight of 25 kg. After 118 days, growing pigs were ready for slaughter, weighing 118 kg on average. In case of a multifunctional process (e.g. production of soya bean oil and soya bean meal), economic allocation was used, which is the partitioning of environmental impacts between co-products based on the relative economic value of the outputs [Guinée, 2002]. Economic allocation is used most commonly in LCA studies of livestock products [De Vries and De Boer, 2010].

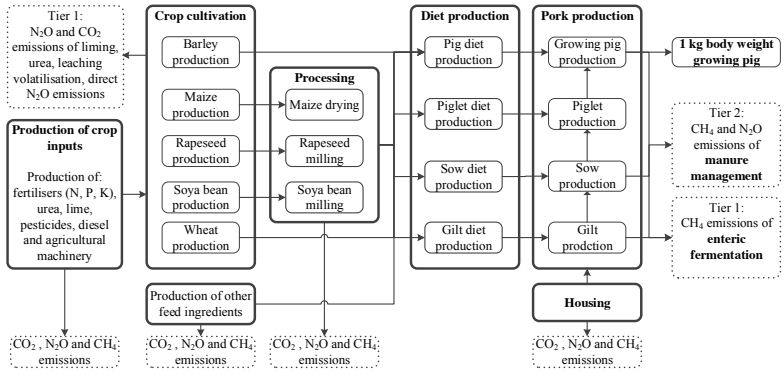

Figure 2.2: Production processes in the pork production chain; solid boxes are production processes, while dotted boxes refer to emissions.

Inventory

Data were collected for each of the stages in the production process of pork (Figure 2.2): (1) production of crop inputs; (2) crop cultivation, including transportation and processing; (3) feed production; (4) pork production; (5) manure management; (6) enteric fermentation and (7) housing of the pigs (supplementary material, Table 2.7). For MPM, all default data can be found in the supplementary material. For MEE, we tried but were unable to determine ranges for all input parameters. Based on the literature (e.g. uncertainty ranges around direct N_2O emission factors) and our own analysis with MPM (Section 2.3.2), we identified the most important parameters to be included. Input parameters (technical parameters and emissions) for which we could quantify uncertainty ranges are discussed in more detail below (Table 2.1 to 2.4).

The pork production chain contained 354 input parameters; all were analysed in MPM, and 46 were considered in MEE. Ranges for MEE were based on variability in farm data and epistemic uncertainties around the input parameters.

Table 2.1: Default values of the feed composition of five ingredients that were largest in mass-share for pig, gilt, sows and piglets, including a range in the total feed intake of the growing pig.

	Pig production	**Gilt production**	**Sow production**	**Piglet production**
Feed intake (kg)	244 (234-352)[3,4]	403[5]	1174[6]	29[7]
Barley (%)	12.9	6.78	13.7	32.1
Maize (%)	26.7	25.0	21.1	21.5
Rapeseed meal (%)	10.2	10.0	1.30	n/a
Soya bean meal (%)	7.50	4.25	3.70	12.9
Wheat (%)	20.9	20.4	12.4	11.0
Other (%)	21.8	33.6	47.8	22.5

Production of crop inputs and crop cultivation

Diets of growing pigs, piglets, sows and gilts consisted of 31 ingredients in total (supplementary material, Table 2.6) and represented a mean feed intake of 244 kg, ranging from 234-352 kg (Table 2.1), including feed intake related to mortality of growing pigs (Table 2.7). Uncertainty ranges were assumed only for the five ingredients that contributed most to GHG emissions in the diet of the growing pig, identified with the MPM method. These five ingredients were barley, maize, rapeseed (meal), soya bean (meal) and wheat. Data on feed processing and feed transportation are given in the supplementary material (Table 2.8).

Default values and ranges for yields and N-fertiliser applications for the five main ingredients in the pig diet were defined (Table 2.2). Ranges are caused by (natural) variability around the input parameters. The default data of the technical parameters that were fixed, e.g. inputs for crop production, are given in in the supplementary material (Table 2.8).

[3]Personal communication M. Dolman (May 11, 2015)
[4]kg feed per growing pig
[5]kg feed per gilt
[6]kg feed per sow per year
[7]kg feed per piglet

Table 2.2: Default values and ranges of yields and fertiliser application rates per crop type per year.

Ingredient	**Yield** (kg DM[8]/ha)		**N-fertiliser application** (kg N/ha)	
	Default[9]	Range[10]	Default[9]	Range[11,12]
Barley	5520	4824 – 5809	130	76 – 130
Maize	7621	5917 – 7621	150	64 – 294
Rapeseed	3040	2800 – 3477	73.4	49 – 78[13]
Soya bean	4800	4342 – 5099	9	0 – 12[14]
Wheat	6010	5245 – 6451	55	43 – 64[13]

Table 2.3: Emission factors for CO_2 emissions and direct/indirect N_2O emissions based on IPCC Tier 1 per crop per year.

Emission factor (kg/crop yr)	**Default**	**Range**
CO_2 from liming	0.12	0.06 – 0.12
CO_2 from urea	0.2	0.1 – 0.2
Direct N_2O	0.01	0.003 – 0.03
Indirect N_2O from leaching	0.0075	0.005 – 0.025
Indirect N_2O from volatilisation	0.01	0.002 – 0.05

Direct and indirect N_2O and CO_2 emissions due to liming and urea application were quantified, including their ranges according to IPCC Tier 1 (supplementary material, Equations (2.9) - (2.17)). The ranges are caused by epistemic uncertainties around the emission factors given in IPCC [2006c]. For the other feed ingredients, default values were included [Vellinga et al., 2013]. CO_2 emission factors from urea application and liming, direct and indirect N_2O emission factors of the five main ingredients (barley, maize, rapeseed, soya bean and wheat), and their ranges, were also included (Table 2.3).

[8]DM: dry matter

[9]Default: Garcia-Launay et al. [2014]

[10]Range: FAOSTAT (based on 5 years: 2009 - 2013) for France (barley, maize, rapeseed, wheat) and Brazil (soya bean)

[11]Minimum: Basset-Mens and Van Der Werf [2005] (red label, solid manure for barley, maize and wheat converted to N)

[12]Maximum: Meul et al. [2012], except for barley: Garcia-Launay et al. [2014]

[13]Adjusted for N area and N fertiliser

[14]For two harvests per year

Table 2.4: Emission factors for direct and indirect N_2O emissions and CH_4 emissions from manure per animal per growing period (110 days). D: default; R: range.

Emission factor	**Type**	**Pig production**	**Gilt production**	**Sow production**	**Tier**
Direct N_2O	D	0.0127	0.0162	0.0306	2[15]
(kg N_2O/animal)	R	0.0064 – 0.0254	0.0081 – 0.0323	0.0153 – 0.0612	
Indirect N_2O [16]	D	0.0159	0.0202	0.0382	2[15]
(kg N_2O/animal)	R	0.0019 – 0.0953	0.0024 – 0.1212	0.0046 – 0.2294	
CH_4	D	1.36	0.933	3.66	2
(kg CH_4/animal)	R	1.36 – 5.33	0.933 – 31.1	3.66 – 31.1	
CH_4 fermentation	D	1.5	1.5	1.5	1
(kg CH_4/animal)	R	0.75 – 2.25	0.75 – 2.25	0.75 – 2.25	

Emissions due to manure management and enteric fermentation

Handling and storage of manure causes emissions of CH_4 and direct and indirect N_2O emissions (Table 2.4). Emissions from manure were based on IPCC rules: for CH_4 and N_2O a Tier 2 approach was used, whereas for enteric fermentation a Tier 1 approach was used. Ranges are caused by epistemic uncertainties around the emission factors given in IPCC [2006b] and IPCC [2006c]. An extended table can be found in the supplementary material (Table 2.9).

In summary, we identified ranges due to variability in the total feed intake of growing pigs, yields and N-fertiliser application rates of the five main ingredients of pig diets, and the number of sows and gilts needed per growing pig (the replacement rate). The mortality rate of the sows and gilts was included in the replacement rate. In addition, ranges due to epistemic uncertainties were found for CO_2 and N_2O emissions of feed-crop production, CH_4 emissions due to enteric fermentation and N_2O, and CH_4 emissions of manure management based on the IPCC Tier 1 and Tier 2 frameworks. We assumed that all input parameters could vary independently; however, three

[15] N excretion in manure was specific for the Netherlands; for emission factors and the gas fractions of volatilisation, default values of the IPCC were used.

[16] Indirect N_2O emission due to volatilisation was not considered because all pigs were indoors.

exceptions were made:

- In general, when feed intake increases, manure production and N excretion increases as well [CBS, 2010]. Therefore, we assumed a proportional relation between feed intake and manure production, i.e. the amount of manure produced (and N excreted) was increased in direct proportion to feed intake, e.g. if feed intake increased 10%, manure production of the growing pig also increased 10%.
- In general, when N fertilisation increases, crop yield increases. Therefore, we assumed that the random values drawn for N fertilisation and crop yield followed a similar sampling pattern, e.g. when a high value for N-fertilisation was drawn, this resulted in a high value for crop yield and vice versa. This means that if one randomly draws a sample at 2/3 of the uncertainty range for N fertilisation, also for crop yield a sample at 2/3 of the range is selected. But if crop yield is selected first in the trajectory, for example at 1/3 of the uncertainty range, for N fertilisation a sample at 1/3 of the uncertainty range is selected as well.
- The random values drawn for N fertilisation and crop yield were used to calculate the emissions from cultivation (i.e. CO_2 emission from liming and urea application, direct and indirect N_2O emissions). The emission factors of the CO_2 and N_2O emissions of cropping were still assumed to vary independently from the N fertilisation and the crop yield, because the emission factors also depend on temperature and soil type, etc. Also, the N_2O and CH_4 emission factors from manure management varied independently from the amount of manure, because the emission factors depended not only on the amount of manure but other external factors such as climate conditions [IPCC, 2006b].

2.3 Results and discussion

2.3.1 Pork production

GHG emissions per kg body weight (BW) of a growing pig were 2.61 kg CO_2 e per kg BW, of which 21% came from crop inputs and 46% came from feed production (Figure 2.3). Manure management contributed 17% of the total emissions, housing 11%, and enteric fermentation 4.7% (Figure 2.3). These results

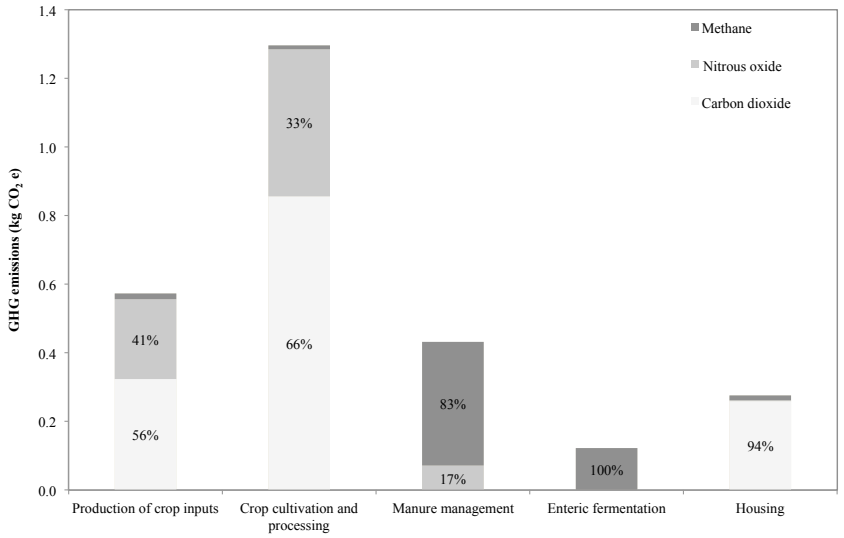

Figure 2.3: Greenhouse gas emission of 1 kg growing pig emitted during its growing period (110 days).

corresponded to those found in the literature, in which feed production (crop cultivation, production of crop inputs) and manure management explained most of the emissions [Basset-Mens and Van Der Werf, 2005; Dalgaard, 2007; Van Zanten et al., 2015b].

Based on minimum and maximum values (Table 2.1 to 2.4), minimum and maximum GHG emissions were were 1.83 and 5.00 kg CO_2 e per kg growing pig, respectively. Estimates for pork production chains are demonstrated to vary from 3.9 - 10 kg CO_2 e per kg meat [De Vries and De Boer, 2010], converted to kg edible product, this resulted in 3.5 - 9.5 kg CO_2 e per kg edible product.

2.3.2 Multiplier method

First we applied MPM, considering the default data only. The most influential parameters were *feed intake (input feed)*, followed by *manure produced by the growing pig (manure output)* and *yield of maize (maize output)* (respectively #1, #2

and #3, Table 2.5). Regarding crop inputs, the most influential parameter was the *output of N fertiliser*, which can be interpreted as the efficiency of the N fertiliser production. Regarding crop cultivation, *yield of maize (maize output)*, followed by *yield of barley (barley output)* and *yield of wheat (wheat output)* were most influential. Regarding manure management and fermentation, *manure produced by the growing pig* was most influential, followed by *CH_4 emissions due to manure and enteric fermentation of the growing pig*.

2.3.3 Method of elementary effects

As described (Section 2.2.5), defining the ranges for MEE depended on results of MPM (Table 2.5), and the literature. Based on results of the MPM, we defined ranges for the yields of the five main ingredients of pig diets and N-fertiliser application. Even though indirect N_2O emissions did not show up in the top ten most influential input parameters of the feed ingredients of MPM, we included them as well because Basset-Mens and Van Der Werf [2005] showed that the uncertainty ranges of these emissions are high and will influence the results. We defined ranges for the methane emissions of manure and fermentation, and also for the N_2O emission of manure. A range for feed intake of the growing pig was defined, but not for the maize ratio in the pig diet, because the diets were fixed. We were not able to define ranges for the parameters related to crop inputs, such as N-fertiliser production.

Parameters with the highest elementary effect contributed most to the uncertainty in the results and are considered the most important input parameters: feed intake of the growing pig (input feed) (#1, Figure 2.4), followed by methane emissions from manure (#2, Figure 2.5), followed by N-fertiliser input for maize cultivation (#3, Figure 2.6).

2.3.4 Discussion of the sensitivity-analysis methods

Applying MPM for sensitivity analysis overcomes arbitrary choices of selecting a subset of input parameters, as done in traditional OAT sensitivity-analysis methods. One disadvantage of MPM is that the effect of uncertainty ranges around input parameters on model output is not included. MEE allowed us to include the uncertainty ranges of input parameters that were

[17]Number of sows required per pig is based on the replacement rate of the sows and on the number of piglets per sow per year.

Table 2.5: Multipliers (η) of the most influential parameters, whose values can be interpreted as follows: increasing an input parameter (i.e. N-fertiliser output) by 1% will change the global warming potential (GWP) –0.097%. The ten most influential parameters of the LCA model are shown in bold-italic print. Rank 1 identifies the most influential parameter (i.e. with the largest multiplier). Only parameters with a relatively high influence, i.e. $|\eta| > 0.03$, are shown. FCR: Feed Conversion Ratio.

Stage	Process	Flow	Multiplier	Rank within stage	Overall rank	Interpretation
Production of crop inputs	N-fertiliser production	Fertiliser output	–0.097	1	8	Efficiency of fertiliser production
		N_2O emission	+0.061	2		n/a
		CO_2 emission	+0.034	5		n/a
	Diesel production	Diesel output	–0.042	3		Efficiency of diesel production
		CO_2 emission	+0.040	4		n/a
	Urea fertiliser production	Urea fertiliser output	–0.030	6		Efficiency of urea fertiliser production
Crop cultivation and processing	Production of maize	Maize output	–0.14	1	3	Yield of maize
		Input N-fertiliser	+0.048	5		N-fertiliser rate
		Direct N_2O emission	+0.034	7		n/a
	Production of barley	Barley output	–0.097	2	9	Yield of barley
	Production of wheat	Wheat output	–0.093	3	10	Yield of wheat
		Direct N_2O emission	+0.030	8		n/a
	Production of soya bean meal	Soya bean meal output	–0.053	4		Milling yield of soya bean
	Production of soya bean	Soya bean output	–0.039	6		Yield of soya bean before milling
	Production of rape meal	Rapeseed meal production	–0.034	9		Milling yield of rapeseed
Production of other feed ingredients	Production of phytase	Phytase output	–0.033	1		n/a
		CO_2 emission	+0.033	2		n/a
Feed production	Pig feed production	Input maize	+0.11	1	5	Maize ratio, pig diet
		Input wheat	+0.091	2		Wheat ratio, pig diet
		Input barley	+0.062	3		Barley ratio, pig diet
Pork production	Pig production	Input feed	+0.52	1	1	Feed conversion ratio
		Input piglets	+0.11	2	6	Number of piglets per pig; piglet mortality
		Input sows	+0.10	3	7	Number of sows per pig[17]
	Sow production	Input feed	+0.081	4		FCR, sow
	Piglet production	Input feed	+0.077	5		FCR, piglet
Manure management	Manure production, pig	Manure output	+0.15	1	2	Production of manure by growing pig
		CH_4 emission	+0.12	2	4	n/a
Enteric fermentation	Enteric fermentation, pig	CH_4 emission	+0.043	1		n/a
Housing pig	Energy use	Energy input	+0.064	1		n/a
		CO_2 emission	+0.060	2		n/a

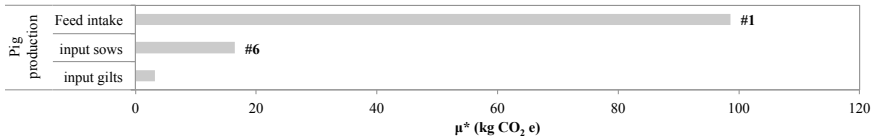

Figure 2.4: Elementary effects (μ^*) of technical parameters. Feed intake is the most important parameter in the LCA model. Numbers at the end of the bars indicate the overall rank of the 10 parameters that contributed most to output uncertainty.

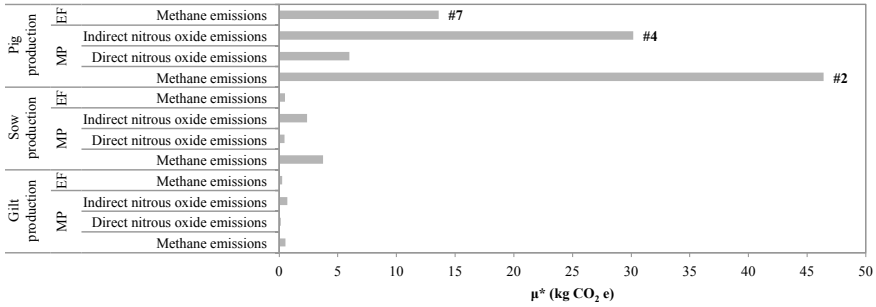

Figure 2.5: Elementary effects (μ^*) of parameters causing most uncertainty in the results of manure management and enteric fermentation. MP: manure production; EF: enteric fermentation. Numbers at the end of the bars indicate the overall rank of the 10 parameters that contributed most to output uncertainty.

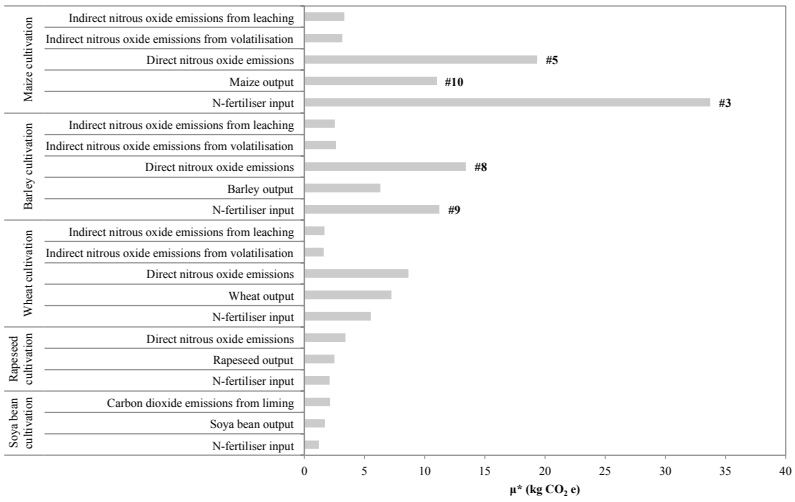

Figure 2.6: Elementary effects (μ^*) of parameters causing most uncertainty (i.e. $|\mu^*| > 1$) in the result of crop cultivation. Numbers at the end of the bars indicate the overall rank of the 10 parameters that contributed most to output uncertainty.

available in the single-issue LCA model. However, one disadvantage of MEE is that it is based only on minimum and maximum values, thus excluding a distribution function or an average value. Other methods for sensitivity analysis are available which belong to the area of global sensitivity analysis, such as squared standardised regression coefficients [Saltelli et al., 2008], which quantify how much each input parameter contributes to output variance [Campolongo et al., 2007; Saltelli et al., 2008]. To apply a global sensitivity analysis, more data are required, such as the standard deviation and a distribution function. Because these types of data were not available in this study, we could not apply this method. However, we were interested mainly in influential input parameters that could give direction for future innovations; important parameters that could improve farm management strategies and improve reliability of results, which could also be derived with MEE.

There are two disadvantages to the way in which we applied MEE. First, we were not able to identify ranges for all input parameters; therefore, we might have missed potentially important input parameters. Second, we assumed that all input parameters either varied independently, or were directly related (i.e. N fertiliser and crop yield), which probably overestimates what happens in reality. However, MEE is less suitable for implementing correlations than more data-intensive global sensitivity-analysis methods, such as using the squared standardised regression coefficients as a proxy for a sensitivity index.

One of the most influential input parameters was the amount of manure produced by the growing pig, which was directly related to feed intake. That increased feed intake resulted in increased manure production and N excretion is plausible; however, assuming that it does so in direct proportion remains questionable. In addition to feed intake, factors such as water intake can also change the amount and N content of manure. However, ignoring a relation between feed intake and manure production and N excretion would have resulted in underestimating CH_4 and indirect and direct N_2O emissions. To what extent manure production and N excretion are over- or underestimated in relation to feed intake, however, remains unclear.

2.3.5 Combining MPM and MEE

The results of MPM identified a different set of parameters than MEE. By combining results of the two sensitivity-analysis methods, we could extract

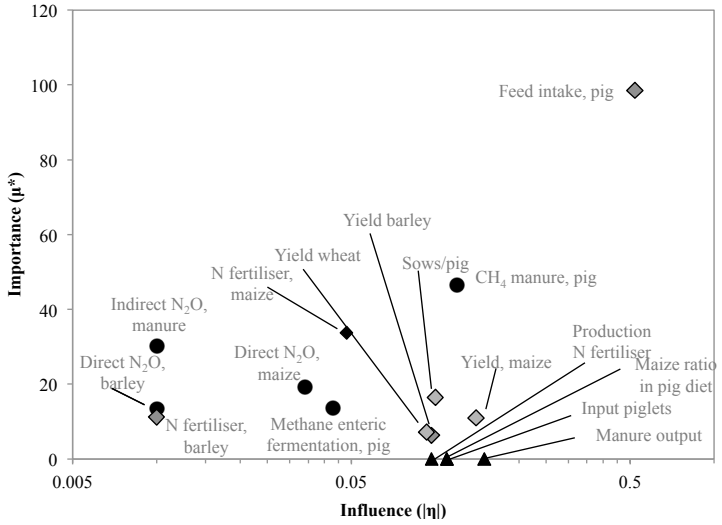

Figure 2.7: Most essential parameters in the LCA model of pork production. Parameters along the horizontal axis (log-scale) are the most influential parameters identified by MPM. Parameters along the vertical axis are the most important parameters identified by MEE. *Circles:* parameters containing epistemic uncertainty; *diamonds:* parameters containing variability. Parameters on the horizontal axis (*triangles*) are those for which no ranges could be defined. MPM: multiplier method; MEE: method of elementary effects.

the most essential parameters to identify GHG mitigation strategies for pork production and improve reliability of the results. The most influential parameters are *feed intake of the growing pig*, followed by *manure produced by the growing pigs* and *yield of maize* (Figure 2.7), while the most important parameters are *feed intake of the growing pig*, followed by *methane emissions of manure* and by *N fertiliser of maize*. *Feed intake of the growing pig* is therefore considered the most essential parameter in the LCA model of GHG emissions of pork production. A change in feed intake immediately affects the amount of feed produced and the corresponding emissions of the feed ingredients.

Parameters with input uncertainties that affect the output (i.e. high importance), such as the direct N_2O emissions of barley and maize (from leeching and volatilisation), have in fact a low influence. Applying only MPM would have led to overlooking these parameters. In contrast, parameters that have relatively high influence, but for which no uncertainty ranges could be defined (e.g. N-fertiliser production), might have been underestimated if only MEE had been applied.

2.3.6 Formulating mitigation options and improving reliability

The most influential parameters (Figure 2.7, horizontal axis), have the most impact when they are reduced. Innovation options to improve the most influential parameters, such as decreasing feed intake of growing pigs, decreasing the amount of manure produced, increasing yields of feed ingredients in pig diets, decreasing the number of sows needed per growing pig, decreasing piglet mortality, and increasing efficiency of N-fertiliser production, will have a large effect on results. These mitigation strategies result in increased efficiency that will have an effect throughout the production chain.

Mitigation options via e.g. management strategies can be formulated by looking at the most important parameters (Figure 2.7, vertical axis) affected by natural variability (Figure 2.7, *diamonds*), such as feed intake and fertiliser application. Natural variability in parameters can be caused by variability in climate, soil types or temperature, or differences in genetics, geography or farm management. Farmers can strive to reduce environmental impacts of the pig production chain by adapting their management strategies towards those of the most successful farmers. For example, farmers can improve the feed conversion ratio (kg dry matter feed intake/kg growth), but doing so is not easy, because it depends on several factors, such as feed quality, feed access, pig health, and climate conditions e.g. temperature and humidity of the stalls.

Reliability of GHG assessments can be improved by looking at parameters with epistemic uncertainties (Figure 2.7, *circles*). Epistemic uncertainties around emission factors for indirect N_2O emissions and CH_4 emissions of manure, and direct N_2O emissions of maize and barley cultivation have the most effect on the reliability of results. Decreasing uncertainty ranges of these emission factors would decrease those around the output, hence provide more reliable conclusions. However, reducing uncertainty around the indirect

N_2O emission of maize production would not mean that GHG emissions are actually reduced, only that the results are more reliable. Estimates can be improved by taking measurements in the field. Reliability could be also be improved by improving data quality of the most essential parameters.

Mitigation strategies, either in the form of technical innovations or improved management practices related to feed intake, would reduce GHG emissions the most. Feed cultivation has higher impact than other stages of pork production. However, our results showed that besides feeding strategy, mitigation strategies related to manure management are also important. If feed-related mitigation strategies are assessed, possible trade-offs with manure management should also be considered, as they might have a high impact on the results.

2.4 Conclusion

We applied two methods for sensitivity analysis, MPM and MEE. Combining both methods allowed us to determine the most essential parameters in the model, from which we could derive mitigation options based on innovation and management strategies, and to formulate options for improving reliability of estimates of GHG emissions of a pork production chain. Mitigation options based on innovation (e.g. novel feeding strategies) would be suggested for the most influential parameters in the model (identified by MPM): feed intake, amount of manure produced by growing pigs, crop yields of the main feed ingredients, number of sows required for one growing pig and fertiliser-production efficiency. Mitigation options based on management strategies (e.g. reducing mortality rate) would be suggested for technical parameters with high variability (identified by MEE) such as feed intake, crop yields and number of sows per pig. The uncertainty ranges can be used as margins of improvement within the pork production chain. In addition to that, MEE showed that reliability could be improved most when uncertainty ranges around direct and indirect N_2O emissions of the main feed crops in the pig diet and the CH_4 emissions of manure production are reduced.

Combining two sensitivity-analysis methods identified the most essential input parameters in the pork production chain, while allowing for uncertainties around input data. With this combined analysis, potential targets for mitigation options via innovations and management strategies were derived,

and parameters were identified that improved reliability of the results.

Acknowledgements

We would like to thank Mark Dolman (LEI Wageningen UR) for providing us with information about feed conversion ratios. We would also like to thank the two anonymous reviewers whose inputs considerably improved this paper.

Supplementary material

Data required determining technical parameters

Table 2.6: Average diet composition pigs, gilts, sows and piglet; the five main ingredients are given in bold. Reference: Van Zanten et al. [2015a] and for growing pigs Bikker et al. [2011].

Ingredient	**Pig** (%)	**Gilt** (%)	**Sow** (%)	**Piglet** (%)
Animal fat	2	2	0.7	2
Barley	12.9	6.78	13.7	32.1
Bread meal	2.75	2.25	1.58	1.75
Maize	26.7	25	21.1	21.5
DL-Methionine	0.03	0.02	0.01	0.14
Lactic Acid	n/a	n/a	n/a	1
Limestone	1.06	0.9	1.11	1
L-Lysine HCL	0.34	0.3	0.24	0.45
L-Threonine	0.06	0.05	0.07	0.12
L-Tryptofaan	0.02	n/a	n/a	n/a
Monocalciumphosphate	0.13	0.11	0.38	0.66
Palm kernel expeller	1	n/a	3.25	n/a
Phytase	0.62	0.65	0.65	0.65
Potato protein	n/a	n/a	n/a	1.35
Premix	0.4	0.4	0.4	0.4
Rapeseed expeller	1	n/a	0.84	n/a
Rapeseed meal	10.2	10	1.3	n/a
Salt	0.32	0.3	0.54	0.6
Soya bean hulls	n/a	2.54	6	n/a
Soya bean meal	7.5	4.25	3.7	12.9
Soya beans heat treated	n/a	n/a	n/a	0.11
Sugar beet pulp	n/a	5	8.82	1
Sugarcane molasses	2.9	2	2.4	1.44
Triticale	1.5	1.13	n/a	n/a
Wheat	20.9	20.4	12.4	11
Wheat middling	3.69	10.2	15.7	5
Sunflower oil	0.69	0.41	0.49	0.5
Sunflower seed meal	3.29	5	3.49	3
Whey powder	n/a	n/a	n/a	1

Table 2.7: Default values and ranges for breeding and housing Van Zanten et al. [2015a]

	Value	**Ranges**	**Unit**
Breeding[18]	0.01731	0.01454 - 0.02363	Number of gilts/pig
	0.03397	0.02853 - 0.04637	Number of sows/pig
	1.022	n.a.	Number of piglets/pig
Housing[19]	0.8	n.a.	m^2/pig
	2.25	n.a.	m^2/gilt
	2.25	n.a.	m^2/sow
	0.35	n.a.	m^2/piglet

[18]The amount of sows and gilts required for the production of one pig included death rate.

[19]For piglets, gilts and sows we compensated for the difference in m^2 used per animal place in comparison with the m^2 used per finishing pig place based on Dutch regulations (policy document, 2007)

Table 2.8: Technical parameters for crop production. Sum of transportation of crop ingredients (N, P, K, lime, pesticides) to the farm, transportation of to the feed factory or drying (barley, maize and wheat) or to feed mill (rapeseed, soy), and from the factory to the Netherlands.

	Barley	**Maize**[20]	**Rapeseed**	**Soya bean**	**Wheat**	**Ref.**
Land of origin	France	France	France	Brazil[21]	France	GL[22]
cr_{yield} (kg dm/ha year)	5520	6518	3040	4800	6010	GL[22]
Allocation (%)	n/a	n/a	0.25	0.59	n/a	CvM[20]
Seeds (kg/ha year)	125	20	3	110	140	GL[22]
Pesticides (kg act. sub./ha year)	8.96	1	1.13	5	1.97	GL[22]
N fertiliser (kg/ha year)	130	150	73.4	9	55	GL[22]
Urea (kg N/ha year)	24.7	0	91.6	18	110	CvM[20]
P fertiliser (kg/ha year)	37	56.8	50	180	26	GL[22]
K fertiliser kg/ha year	34	63	50	180	24	GL[22]
Lime (kg/ha year)	298	298	298	2160	298	CvM[20]
N manure (kg/ha year)	10	101	16	0	10	GL[22]
Diesel (kg/ha year)	84	85	92	160	83	GL[22]
Agricultural machinery (kg/ha year)	18.7	21.7	20.4	39	18.6	GL[22]
Yield before drying (kg dm/ha year)	n/a	7621	n/a	n/a	n/a	CvM[20]
Electricity for drying (kWh/kg)	n/a	0.008	n/a	n/a	n/a	CvM[20]
Lorry (tkm)	785	1130	420	529	785	CvM[20]
Rail (tkm)	8416	10948	3661	0	8808	CvM[20]
Sea (tkm)	0	0	0	45492	0	TS[23]

Crop production

The direct N_2O emissions from crop production are quantified using Equation 11.1 [IPCC, 2006c] (adjusted amount of N in mineral soils that is mineralised is zero: $F_{som} = 0$):

$$N_2O_{\text{direct,cropproduction}} = \frac{44}{28}\left(N_{sf} + N_m + N_{cr}\right) EF_1 \tag{2.9}$$

where: N_{sf} (kg N/year) is the amount of N in synthetic fertiliser, N_m (kg N/year) the amount of N in manure, N_{cr} (kg N/year) the amount of N in crop residues en EF_1 (kg N_2O - N/(kg N year)) the emission factor of direct N from fertiliser, manure and crop residues. The amount of N in crops (N_{cr}) is estimated by Equation 11.6 (adjusted: no area burnt $area_{\text{burnt}} = 0$, pastures are renewed every year $frac_{renew} = 1$, considering 1 hectare: $area = 1$:

$$N_{cr} = cr_{yield}\left[R_{ag} \cdot N_{ag}\left(1 - frac_{rem}\right) + R_{bg} \cdot N_{bg}\right] \tag{2.10}$$

where: cr_{yield} (kg dm/ha) is the crop yield, R_{ag} (kg dm/dm) the ratio of above ground residue dry matter to the harvest yield, N_{ag} (kg N/kg dm) is the N content of above-ground residues, $frac_{rem}$ (%) is the fraction of above-ground residues that is removed,

[20] Van Middelaar et al. [2012]
[21] Central-West Brazil
[22] Garcia-Launay et al. [2014]
[23] TS: Assumptions in this study.

R_{bg} (kg dm/kg dm) is the ratio of below-ground crop residues to harvested yield and N_{bg} (kg N/kg dm) the N content of below-ground crop-residues. R_{ag} is calculated by:

$$R_{ag} = \frac{AG_{DM} \cdot 1000}{cr_{yield}} \tag{2.11}$$

where AG_{DM} (Mg/ha) is the above-ground residue, which can be estimated by:

$$AG_{DM} = \frac{cr_{yield} \cdot slope}{1000} + intercept \tag{2.12}$$

and R_{bg} can be estimated by:

$$R_{bg} = R_{BG-BIO} \cdot \frac{AG_{DM} \cdot 1000 + cr_{yield}}{cr_{yield}} \tag{2.13}$$

where R_{BG-BIO} (%) is the ratio of below-ground residues to aboveground biomass.

The indirect N_2O emissions from crop production come from leaching and volatilisation. Leaching is quantified using Equation 11.10 (adjusted, leaching of mineralised N and N leaching from urine and dung is zero: $F_{som} = 0$ and $F_{PRP} = 0$:

$$N_2O_{leaching,cropproduction} = \frac{44}{28}\left(N_{sf} + N_m + N_{cr}\right) \cdot Frac_{leach} \cdot EF_5 \tag{2.14}$$

where $Frac_{leach}$ (%) is the fraction of N added to managed soils and EF_5 (kg N_2O/kg leached) is the emission factor for N_2O emissions from leaching. The indeirect N_2O emissions due to volatilisation are calculated with Equation 11.9 (adjusted, $F_{PRP} = 0$):

$$N_2O_{volatilisation,cropproduction} = \frac{44}{28}\left(N_{sf} \cdot Frac_{gasf} + N_m + Frac_{gam}\right) \cdot EF_4 \tag{2.15}$$

where $Frac_{gasf}$ (%) is the fraction of synthetic fertiliser that volatilises, $Frac_{gam}$ (%) is the fraction of manure that volatilises and EF_4 (kg N-N_2O/(kg NH_3-N+NO_x-N volatilised)) is the emission factor of N_2O emissions of atmospheric deposition of N.

The CO_2 emission factor for liming are calculated using Equation (11.12) (adjusted, no dolomite liming $M_{dolomite} = 0$):

$$CO_{2_{liming}} = 1000 \cdot \frac{44}{12} \cdot M_{lime} \cdot EF_{lime} \tag{2.16}$$

where M_{lime} (ton C/year) is the annual amount of limestone ($CaCO_3$) and EF_{lime} (ton C/ton limestone) is the emission factor. The annual CO_2 emissions due to urea fertilisation are given by:

$$CO_{2_{ureafertilisation}} = 1000 \cdot \frac{44}{12} \cdot M_{urea} \cdot EF_{urea} \tag{2.17}$$

where M_{urea} (ton C/year) is the amount of urea applied per year and EF_{urea} (ton C/ton urea) is the emission factor.

Manure management

Table 2.9: Direct and indirect N_2O and CH_4 emissions IPCC Tier 2. Values are given for the growing period (kg / year).

	Pig	Gilt	Sow	Reference
Manure (kg)	356	420	1649	RIVM[24]
N-content (%)	0.0114	0.0122	0.0059	RIVM
N-content (kg)	4.04	5.14	9.73	
EF_3 (kg N_2O/kg N)	0.002 (0.001 – 0.004)	0.002 (0.001 – 0.004)	0.002 (0.001 – 0.004)	Table 10.21[25]
Direct N_2O (kg N_2O/year)	0.0127 (0.0064 – 0.0254)	0.0162 (0.0081 – 0.0323)	0.0306 (0.0153 – 0.0612)	
EF_4 (kg N_2O-N/kg N)	0.01 (0.01 – 0.05)	0.01 (0.01 – 0.05)	0.01 (0.01 – 0.05)	Table 11.3[26]
$Frac_{gam}$ (%)	0.25 (0.15 – 0.3)	0.25 (0.15 – 0.3)	0.25 (0.15 – 0.3)	Table 10.22[25]
Indirect N_2O (kg N_2O/year)	0.0159 (0.0019 – 0.0953)	0.0202 (0.0024 – 0.1212)	0.0382 (0.0046 – 0.2294)	
V_S	15.29	10.51	41.22	
B_0 (m^3 CH_4/kg manure)	0.34	0.34	0.34	
MCF	0.39	0.39	0.39	
CH_4 (kg CH_4/year)	1.36 (1.36 – 5.33)	0.933 (0.933 – 31.1)	3.66 (3.66 – 31.1)	

Direct N_2O emissions from manure management (Equation 10.25, adjusted) [IPCC, 2006b]:

$$N_2O_{direct,manure} = \frac{44}{28} N_{ex} EF_3 \tag{2.18}$$

where N_{ex} is the amount of excreted N in manure per animal per year and EF_3 is the emission factor for direct N_2O emissions from manure (kg N_2O/kg).

Indirect N_2O emissions from manure management (Equation 10.26 and 10.27, adjusted)

$$N_2O_{indirect,manure,volatilisation} = \frac{44}{28} N_{ex} \cdot Frac_{gam} \cdot EF_4 \tag{2.19}$$

where $Frac_{gam}$ is the fraction of manure that volatilises. The CH_4 emission for manure management was available for Tier 2 (Equation 10.23, adjusted):

$$CH_{4_{manure}} = V_S \cdot 365 \cdot B_0 \cdot 0.67 \cdot \frac{MCF}{100} \tag{2.20}$$

[24] Coenen et al. [2012]
[25] IPCC [2006b]
[26] IPCC [2006c]

where V_S is the daily volatile solid excreted (kg DM/day), B_0 maximum methane producing capacity for manure (m^3 CH_4/kg), MCF the methane conversion factor (%). Results can be found in Table 2.9.

CHAPTER 3

Methods for uncertainty propagation in life cycle assessment

Joint work with:
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Environmental Modelling & Software, 2014

Abstract

Life cycle assessment (LCA) calculates the environmental impact of a product over its entire life cycle. Uncertainty analysis in LCA is usually performed using Monte Carlo sampling. In this study, Monte Carlo sampling, Latin hypercube sampling, quasi Monte Carlo sampling, analytical uncertainty propagation and fuzzy interval arithmetic were compared based on e.g. convergence rate and output statistics. Each method was tested on three LCA case studies, which differed in size and behaviour. Uncertainty propagation in LCA using a sampling method leads to more (directly) usable information compared to fuzzy interval arithmetic or analytical uncertainty propagation. Latin hypercube and quasi Monte Carlo sampling provide more accuracy in determining the sample mean than Monte Carlo sampling and can even converge faster than Monte Carlo sampling for some of the case studies discussed in this paper.

Software and data availability

All modelling done in this paper is done in MATLAB®; the code and data can be forwarded by the first author upon request. In addition, software for life cycle assessment calculations based on matrix representation is available at CML, and was developed by Reinout Heijungs, Leiden University. The software CMLCA can be downloaded free of charge from: www.cmlca.eu, programming language Delphi, system requirement Windows XP or higher (32 bits), no special hardware requirements.

3.1 Introduction

Life cycle assessment (LCA) is an established method to calculate the environmental impact of a product over its entire life cycle [Curran, 2012]. It has also been applied in areas such as business strategy, product innovation, policy development and eco-labelling [Cooper and Fava, 2006]. It has been used to quantify environmental emissions of production systems [e.g. Whittaker et al., 2013], and to make decisions about potential options to reduce the environmental impact of products [Carvalho et al., 2012; Levis et al., 2013; Tillman, 2000]. According to the ISO 14040 standardised framework for (environmental) life cycle assessment, an LCA consists of four phases: goal and scope definition, inventory analysis, impact assessment and interpretation. The goal and scope phase includes definition of the boundary of the product life cycle, the functional unit (main output of the system) and allocation method. In

the inventory analysis, data about resource use and emissions related to each production process are collected and are translated to environmental impacts. During the final phase the results are presented and interpreted.

During the inventory analysis, data are collected from different systems along the chain. These data can be highly variable, especially if they originate from systems that depend on weather conditions, like agriculture [Brentrup et al., 2000]. Results of an LCA, therefore, are uncertain due to lack of knowledge about the true value of its model parameters [Björklund, 2002; Heijungs and Huijbregts, 2004]. LCAs that demonstrate a single point value as their result, overlook the range of possible realisations of output data, and could therefore be misleading [Björklund, 2002], or might provide a false sense of accuracy [De Koning et al., 2010]. At present, a standardised definition for uncertainty in LCA [Björklund, 2002; Heijungs and Huijbregts, 2004; Finnveden et al., 2009] and a standardized methodology how to propagate uncertainties are missing. Application of uncertainty propagation in LCA might be hampered due to long calculation time [Ciroth et al., 2004], caused by the large amount of data elements (i.e. input parameters); lack of consensus about relevant applicable methods or missing information on the required descriptive statistics of input parameters [Björklund, 2002]. Incorporating uncertainty, however, increases reliability of results and improves decision making.

Various types and sources of uncertainty can be distinguished [Björklund, 2002; Heijungs and Huijbregts, 2004; Finnveden et al., 2009]. In this paper, we focus on parameter uncertainty, following the definition of Björklund [2002] and Heijungs and Huijbregts [2004]. Parameter uncertainty includes e.g. inaccuracy of measurements, erroneous data, incomplete data, round-off errors and (natural) variability. A comprehensive paper of Lloyd and Ries [2007] showed the broad scope of techniques and methods available to researchers in LCA towards propagation of (parameter) uncertainty. Uncertainty propagation is currently dominated in LCA literature by one type of method (i.e. Monte Carlo sampling), but there are several other methods on propagating uncertainties [Lloyd and Ries, 2007]. These methods would be better at coping with the large size of LCA inventories and considerably reduce computational effort (i.e. calculation time and memory usage) [Heijungs, 2010], or can be applied when limited knowledge about the input uncertainties is present [Heijungs et al., 2005].

So far, these methods of uncertainty propagation have not been compared in a consistent manner. Methods examined in this paper were selected from

Lloyd and Ries [2007], because they are most commonly applied. The following methods were selected: Monte Carlo sampling (MCS) and (standard) Latin hypercube sampling (LHS), analytical uncertainty propagation (AUP) and fuzzy interval arithmetic (FIA) [Lloyd and Ries, 2007]. In addition, we also selected another type of sampling method: (randomised) quasi Monte Carlo sampling (QMCS) that showed promising results (e.g. Subramanyan et al. [2008] in LCA and Tarantola et al. [2012] more in general).

The performance of these uncertainty propagation methods may depend on size, behaviour of the case study (linear or non-linear) and properties of the input parameters [Saltelli et al., 2010; Tarantola et al., 2012]. To illustrate the performance of the methods, we therefore examined different input parameters for three case studies that differed in size and behaviour. Two small artificial case studies were selected that differed with respect to their behaviour and a bigger linear case study representing an existing production system of a northeast Atlantic fishery.

This study aims to (1) give more insight into Monte Carlo sampling, Latin hypercube sampling, quasi Monte Carlo sampling, fuzzy interval arithmetic and analytical uncertainty propagation, and (2) compare the uncertainty propagation methods to show the performance, advantages and disadvantages of each method used when applied in LCA. We start with a recap of matrix representation in LCA, followed by an introduction to each of the five uncertainty propagation methods. Subsequently, all five methodologies are applied to the case studies and their results are compared on different criteria.

3.2 Materials and methods

3.2.1 Preliminary on notation and terminology

In order to calculate the environmental impact ($\mathbf{g}$) corresponding to a functional unit ($\mathbf{f}$), a model of the following form is constructed [Heijungs, 2002]:

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} \tag{3.1}$$

The (square) technology matrix $\mathbf{A}$ represents production processes which are given in each column, the rows represent product flows. The matrix is constructed in such a way that e.g. in the first column electricity is produced that is subsequently used for fuel production in the second column. This results

in a large matrix with interlinked production processes, which is scaled to produce the amount given by the functional unit vector **f** (the scaling vector **s** equals: $\mathbf{s}=\mathbf{A}^{-1}\mathbf{f}$). The intervention matrix **B** represents the input of raw materials and output of emissions corresponding to each production process of the technology matrix **A**. In most LCAs a readily available database is used for **A**, like the ecoinvent v2.2 database [ecoinvent, 2010], which is currently made up out of 4087 processes. The size of this square **A**-matrix, therefore, is large, although many elements are zero. When using readily available databases like the ecoinvent database, as is quite common in LCA, the size of **A** causes calculation of the environmental impact to be of high computational effort. This is due to the calculation of the inverse of **A**, which slows down the calculation. Especially when performing an uncertainty analysis using a stochastic approach and large amounts of simulations are required. This illustrates the exploration of low demanding sampling methods to decrease calculation time and memory usage.

3.2.2 Uncertainty propagation methods

In the next section five uncertainty propagation methods will be discussed: MCS, LHS, QMCS, AUP and FIA. Subsequently, a description of the case studies and their model parameters are given, followed by a description of how the methods are compared.

Monte Carlo sampling

Uncertainty propagation using a sampling approach started with the development of MCS in 1949 [Metropolis and Ulam, 1949], quickly becoming widespread [Burmaster and Anderson, 1994; Helton et al., 2006]. MCS consists of drawing (pseudo-) random numbers from a set of input parameters (k) with known distribution functions to obtain the sampled distribution of the output parameter [Helton et al., 2006]. While MCS might be computationally demanding, it has the advantage that it can be used to compare output statistics like the mean or parameter of dispersion between two studies. A disadvantage is the long calculation time due to a large number of simulations that have to be performed before the output uncertainty can be determined. The standard error of the mean (SEM) can be used as a measure of the convergence rate of the sampling method. The SEM describes how much variation

Table 3.1: Descriptive statistics and additional requirements for implementation of Monte Carlo sampling (MCS), Latin hypercube sampling (LHS), quasi Monte Carlo sampling (QMCS), Fuzzy interval arithmetic (FIA) and analytical uncertainty propagation (AUP) in life cycle assessment.

Method	Inputs	Outputs	Additional requirements
MCS	pdf, μ, ϕ[1]	e.g. $\bar{x}$, s	(pseudo-) Random sample generator
LHS	pdf, μ, ϕ	e.g. $\bar{x}$, s	Stratified sampling approach, (pseudo-) random sample generator
QMCS	pdf, μ, ϕ	e.g. $\bar{x}$, s	Quasi-random numbers, randomisation method
FIA	S, v_c, $\delta^{\pm}$	$\bar{v}_c$, $\bar{\delta}^{\pm}$	Construction of a possibility function
AUP	σ	σ	First order Taylor approximation

is expected around the sample mean for a specific sample size. In theory, the standard error of the mean of MCS convergences as $\mathcal{O}(s/\sqrt{N})$, where s is the standard deviation of the sample and N is the sample size. This means that the convergence rate does not depend on the amount of input parameters. In order to apply MCS, the following input is required: the type of distribution function (e.g. log-normal, triangular) of each input parameter, a central value (such as the mean (μ)) and a parameter of dispersion (ϕ), such as the standard deviation (σ) of the probability density function in case of normal distributions. The result of applying this method is a sampled distribution of $\mathbf{g}$ (Table 3.1).

Latin hypercube sampling

LHS is a variant of Monte Carlo sampling employing a stratified sampling approach. The distribution functions of the input variables are divided in equally probable (i.e. stratified) subgroups from which random numbers are drawn, which are subsequently combined at random [Helton et al., 2006]. The idea behind LHS is that input parameters are sampled more uniformly than (psuedo-) random sampling, resulting in a faster convergence rate. LHS has been suggested, therefore, as a promising alternative to MCS for uncertainty

[1] pdf: probability density function (distribution function) μ: mean; ϕ: parameter of dispersion; $\bar{x}$: mean of the sample; s standard deviation of the sample; S: shape; v_c: core value; $\delta^{\pm}$: upper and lower bound; σ: standard deviation.

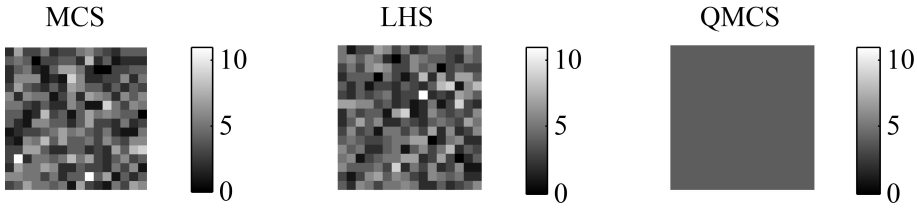

Figure 3.1: Density plot for MCS, LHS and (unscrambled) QMCS in two dimensions. Each plot is divided into a 16x16 grid, showing exactly 4 points in each grid cell in case of QMCS. MCS and LHS result in less equally distributed samples; N=1024.

propagation in LCA by Heijungs [2010] and Peters [2007], and it is used in LCA amongst others by Basson and Petrie [2007]; De Koning et al. [2010]; Geisler et al. [2005] and Huijbregts et al. [2000]. Many improvements have been made to the original LHS design, such as maximin LHS [Morris and Mitchell, 1995] and Latin supercube sampling [Tarantola et al., 2012], but we will only focus on the original design, referred to in this paper as standard LHS. In order to apply this method, similar type of information as for MCS is required (Table 3.1).

Quasi Monte Carlo sampling

The QMCS procedure is similar to MCS, but uses quasi-random numbers to sample from the distribution functions [Sobol', 1967; Saltelli et al., 2010]. Quasi-random numbers are deterministic numbers that are equally distributed for a given distribution function [Tarantola et al., 2012]. The convergence rate can be faster than MCS, the standard error of the mean converges approximately as $\mathcal{O}(s/N)$ [Caflisch, 1998]. There are many types of quasi-random numbers, but in this paper we have chosen for the Sobol' sequence, because this method outperformed the (improved) LHS design for many test cases [Tarantola et al., 2012]. The quasi-random numbers are scrambled (i.e. randomised) to allow for calculation of the standard error later on, and performs optimal when the sample size equals a power of 2, i.e. $N = 2^i$, where i is a non-negative integer. To illustrate the difference in the sampled distributions of MCS, LHS and (unscrambled) QMCS, three density plots are given for two

uniformly distributed parameters in Figure 3.1. The sample space is divided into a grid of 256 squares and one counts how many points are present in each square of the grid. QMCS corresponds to exactly four points for each square in the grid, while the amount of points for both MCS and LHS range from zero to ten. This means that in case of two input parameters the output distribution using QMCS remains equally distributed, while MCS and LHS do not. For an overview of the required inputs, see Table 3.1.

Analytical uncertainty propagation

Analytical uncertainty propagation (AUP) can be used to determine the variance of the output uncertainty based on the variance of each uncertain input variable (Table 3.1). The variance of the output is described as a function of the variances of the uncertain input parameters. This function is given by a Taylor series expansion of Equation (3.1), and therefore is an approximation of the output uncertainty. In this study, we have chosen for the method according to Heijungs [2010] because it only demands information about the variance of the input data, whereas the shape of each distribution function is not required. This is an advantage when limited knowledge about the input data is available. Another advantage of AUP is that it is not computationally demanding [Heijungs, 2010]. One of the disadvantages is that a first order approximation is considered here, therefore it is suitable for small input uncertainties, but may not be for large input uncertainties [Heijungs, 2010]. AUP has been used by for example Heijungs et al. [2005], and in a slightly different form by Hong et al. [2010] and Imbeault-Tétreault et al. [2013].

Fuzzy interval arithmetic

Fuzzy interval arithmetic (FIA) determines the output uncertainty by assigning possibility functions to each input variable. This is done by assigning a possibility of one to the most plausible value(s) (i.e. the core value(s)) and zero to the most unlikely values (beyond the upper and lower bounds). In order to propagate the possibility functions, intervals described by the lower (δ^-) and upper bounds (δ^+) are created for different heights of each possibility function (so-called α-cuts) and these intervals are simultaneously propagated through the model [Cruze et al., 2013]. The main advantage of this method is that only a few α-cuts (e.g. 10 or 20) are needed to give insight into the output

uncertainty; therefore, this approach is not seen as computationally demanding. In order to apply this method, the following information is required: the core value, the upper and lower bound of the possibility function, and the type of possibility function of each input variable, which is usually triangular or trapezoid shaped (Table 3.1). In this paper, core values are set equal to the means of the probability density functions. For the upper and lower bounds, a distance of ± 10 and $\pm$ 60% of the mean was taken and a triangular shape was selected. The result of applying this method is a possibility function with a core value of height equal to one, and an upper and lower bound. This is contrary to probability functions where the total area under the probability function equals one, and it is therefore not possible to compare this result directly to stochastic results or to perform statistical tests based on probability theories. This is seen as a disadvantage, but nevertheless, it has been used on several occasions in LCA (see e.g. Clavreul et al. [2013]; Tan et al. [2004]; Tan [2008]). Transformation of probability functions to possibility functions are for example described in André and Lopes [2012] or Mauris et al. [2001]. To be able to compare the FIA to the results of the sampling methods, we followed André and Lopes [2012] to transform the fuzzy interval to the most likely probability density function [Eq. 15 in André and Lopes, 2012], to which a 6^{th} order polynomial was fitted. The polynomial will be compared to a normal distribution coming from MCS.

3.2.3 Description of the case studies

Case study 1

Case study 1 is a small artificial model describing 1 MWh electricity production containing input parameters (k=5; see Figure 3.2). Details of case study 1 and 2 can be found in e.g. Heijungs [2002]. The model shows linear behaviour for small changes in the input parameters. All input parameters were assumed to be either from a normal distribution or a log-normal distribution function. In the results, input uncertainties are indicated as a coefficient of variance (CV=σ/μ). The CV of all input parameters were assumed to be 5% in case of normal distribution, because larger CV can reverse the sign of the input parameters, resulting in unrealistic drawings. In case of a log-normal (log-N) distribution, the CV was assumed to be 5% or 30%. Table 3.2 gives an overview of the distributions of the input parameters for each case study

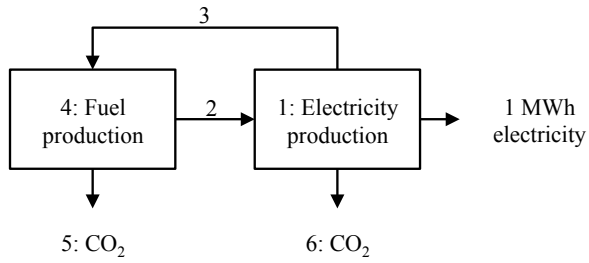

Figure 3.2: Flow diagram of case study 1 and 2, describing a product system producing 1 MWh electricity, only in case study 2 electricity production is required for fuel production (arrow 3).

Table 3.2: Type of distribution function of all of the input parameters for each case study (the coefficient of variation is given between brackets).

Case study 1	**Case study 2**	**Case study 3**
Normal (5%)	Normal (5%)	Normal (5%)
Log-N (5%)	Log-N (5%)	Log-N (5%)
Log-N (30%)	-	Log-N (30%)

studied in this paper. In case of FIA, the possibility function and boundaries are described in Section 3.2.2.

Case study 2

Case study 2 is similar to case study 1 but adjusted in such a way that it shows non-linear behaviour by assuming that 300 kWh of electricity is required for fuel production (see Figure 3.2). As a consequence, small changes in the input parameters will result in large changes in the output. All input parameters (k=6) were assumed to be from a normal distribution or a log-normal distribution. The CV's of all input parameters were assumed to be 5% in case of normal distribution and log-normal distributions, because larger CV can reverse the sign of the input parameters, resulting in unrealistic drawings. In case of FIA, the possibility function and boundaries are described in Section 3.2.2.

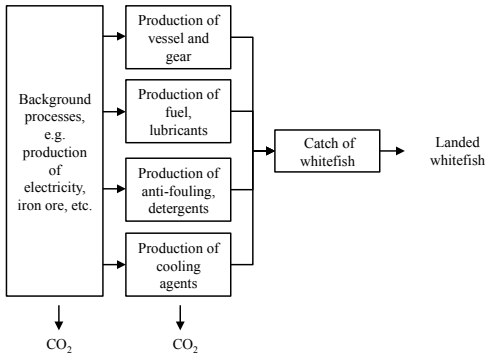

Figure 3.3: Flow diagram of case study 3, describing the production of 1 kg landed white fish, only catch and on-board processing are within the scope of this case study.

Case study 3

Case study 3 describes a large production system of a northeast Atlantic whitefish trawling fishery. We used a production system of fish as our case study because environmental impact of fisheries has been of increasing interest [e.g., Ziegler et al., 2003; Vázquez-Rowe et al., 2010] and the daily catch is associated with high natural variability. For this paper a Norwegian bottom trawl fishery targeting cod and haddock in the northeast Atlantic was considered. The supply chain is limited to fishing by a single vessel, operating from Northern Norway and going out on fishing trips of one to two weeks. The fish is landed in various ports along the Norwegian coast. Twice-daily data was provided on fuel use and fish production for 2011 and 2012. Detergent and other chemical use, the lifespan and construction material of the vessel were provided on an annual basis. Environmental impact of background processes, e.g. the production of iron ore for the production of steel of the vessel, were taken from ecoinvent v2.2 [ecoinvent, 2010]. The goal of this LCA was to assess the greenhouse gas emissions of 1 kg landed white fish. All greenhouse gas emissions were allocated to the landed white fish, which were headed and gutted at sea. The boundary of the life cycle and the production chain is given in Figure 3.3. We assessed the impact of landed white fish on climate

Table 3.3: Selection of data used to calculate the CO_2 e of 1 kg of whitefish. The global warming potential (GWP) is given in kg CO_2 e/kg

Description	Amount[2]	Unit	GWP	Reference
Life time vessel	30.0	years	n/a	n/a
Reinforcing steel	2.03	kt	1.45	ecoinvent [2010]
Chromium steel	226	t	4.50	ecoinvent [2010]
Life time rigg	1.00	year	n/a	ecoinvent [2010]
Life time trawls	0.33	year	n/a	ecoinvent [2010]
Rubber parts	4.24	t	5.76	ecoinvent [2010]
Chain and iron	4.06	t	1.47	ecoinvent [2010]
Sweaper	16.0	t	2.11	ecoinvent [2010]
Polyethylene netting	1.24	t	1.93	ecoinvent [2010]
Dynema (ropes)	46.0	kg	2.32	ecoinvent [2010]
Nylon twine	67.0	kg	9.68	ecoinvent [2010]
Combination rope	564	kg	2.32	ecoinvent [2010]
Plastic balls	1.25	t	5.76	ecoinvent [2010]
Sack	2.25	t	2.32	ecoinvent [2010]
Flexigrid	450	kg	2.32	ecoinvent [2010]
Anti-fouling	362	kg/year	2.89	ecoinvent [2010]
Tap-water use	1.39	kt/year	$3.14 \cdot 10^{-4}$	ecoinvent [2010]
Cooling agent	180	kg/year	2.11	ecoinvent [2010]
Detergents	1.40	t/year	0.886	ecoinvent [2010]
Fuel use in port	36.7	t/year	3.73	Cooper [2004]
Lubricating oil	13.9	t/year	4.27	Cooper [2004]
Fuel use fishing	3.12	kt/year	3.73	Cooper [2004]
Total landings	6.18	kt/year	n/a	n/a

change, by summing the greenhouse gases emissions of carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O) to their CO_2 equivalent (CO_2 e), using a global warming potential (GWP) of 100 years [IPCC, 2007]. There was no uncertainty placed on the GWP-values; biogenic emissions were not taken into account. An overview of the (aggregated) data of the foreground system can be found in Table 3.3. The production process of fish resulted in a technology matrix **A** of size 35x35. We considered only the greenhouse gas equivalents for the intervention matrix **B**. In total k=115 input parameters were considered. All input parameters including the ones from the ecoinvent database, were assumed to be either normally or log-normally distributed. The CV of all input parameters were assumed to be 5% in case of a normal distribution, because larger CV can reverse the sign of the input parameters, resulting in unrealistic drawings. In case of a log-normal distribution, CV was assumed to be 5% or 30% (Table 3.2). In case of FIA, the possibility function and boundaries are described in Section 3.2.2.

3.2.4 Ways of analysis

The methods for uncertainty propagation were compared based on the following criteria:

[2]WhiteFish [2013]

- **Convergence rate:** the convergence rate can be determined using the standard error of the mean (SEM) for an increasing sample size. The SEM is calculated by taking the standard deviation of the distribution of the sample means. When two SEM's are compared, the sample with the smallest SEM reflects the true mean more accurately. The empirical standard error of the sample mean is plotted with respect to the sample size, and compared to the theoretical predictions. This can only be done for the sampling approaches. The sample size (N) increases from 32 to 1024. For each run (R), the sample mean is calculated from an independent sample of Nxk random or quasi random numbers, each run is repeated fifty times.
- **Descriptive statistics:** several descriptive statistics can be derived from the five methods. In this paper, the mean and standard deviation are given for MCS, LHS and QMCS. In case of AUP only the standard deviation can be derived; in case of FIA we present the core value and the upper and lower bound of the model output.
- **Computational effort:** for each method the amount of memory usage and calculation time were discussed.

3.3 Results

All five methods were applied to the three case studies. FIA will be discussed separately, as it is not possible to compare the results directly to the other four methods.

3.3.1 Results of case study 1

Figure 3.4 shows the standard error of the sample mean for MCS, LHS and QMCS (with increasing sample size). All five input parameters are normally distributed with a CV of 5%. For each method, the points in the graph are derived as follows: first, the mean is calculated from a sample size of 32, this is repeated 50 times. Subsequently, the standard error of the fifty sample means is calculated and plotted in the figure. This procedure is repeated for each sample size. The theoretical convergence rate (TCR) of $s/\sqrt{N}$ for MCS and

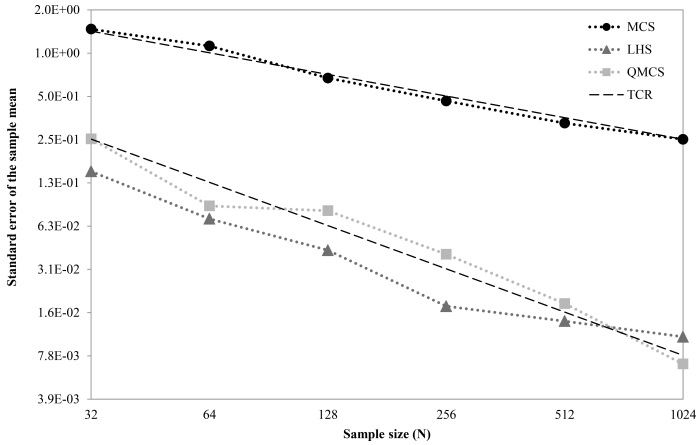

Figure 3.4: Convergence rate of the standard error of the sample mean for MCS, LHS and QMCS applied to case study 1 (k=5, CV=5%) on a log-log scale (base 2). All input parameters are normally distributed; TCR: theoretical convergence rate.

the approximate theoretical rate of s/N for QMCS are also presented, where s is based on the standard deviation in case R=50, N=1024 for MCS and QMCS respectively (Table 3.4). Figure 3.4 shows that the standard error of MCS converges as $s/\sqrt{N}$, whereas the standard error of LHS and QMCS convergence as approximately s/N. LHS and QMCS converge, therefore, faster than MCS, i.e., the slope of the LHS and QMCS plot is steeper. Moreover, LHS and QMCS start at a smaller standard error, indicating higher accuracy of the sample mean. Subsequently, the distributions of the input parameters were changed from normal to log-normal. Figure 3.5 shows the standard error of the sample mean when all input parameters are log-normally distributed with a CV of 5%. Again LHS and QMCS converge faster than MCS and show a higher accuracy. Figure 3.6 shows the convergence rate when all input parameter are log-normally distributed with a CV of 30%. In that case, QMCS converges faster than MCS and LHS for each sample size. LHS seems to converge at a similar rate as MCS, but with a higher accuracy.

Table 3.4 shows the mean and standard deviation for fifty independent runs (R=50); each run having a sample size of 1024, for a CV of 5% or 30%

Table 3.4: Greenhouse gas emissions (kg CO_2 e/MWh electricity) of four methods explored (the standard deviation is shown between brackets) for different *CV*'s of the input parameters; *R*=50, *N*=1024, *k*=5. Analytical uncertainty propagation (AUP) is based on a single calculation.

	Normal (5%)	**Log-N** (5%)	**Log-N** (30%)
Monte Carlo sampling	120 (8.05)	120 (8.01)	133 (54.2)
Latin hypercube sampling	120 (8.08)	120 (8.05)	133 (54.1)
Quasi Monte Carlo sampling	120 (8.07)	120 (8.03)	133 (54.3)
Analytical uncertainty propagation	120 (8.00)	120 (8.00)	120 (48.0)

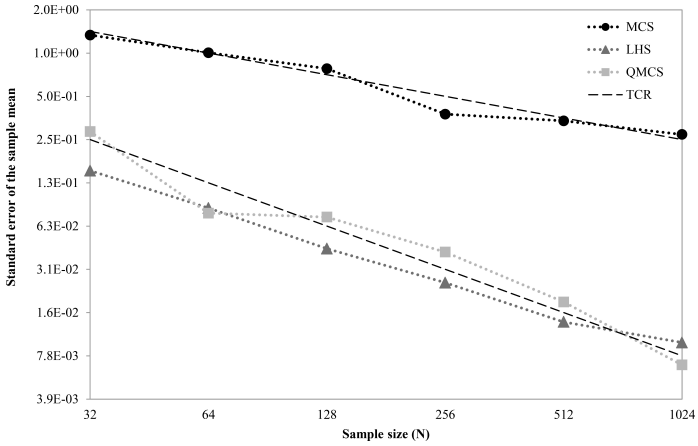

Figure 3.5: Convergence rate of the standard error of the sample mean for MCS, LHS and QMCS applied to case study 1 (*k*=5, *CV*=5%). All input parameters are log-normally distributed.

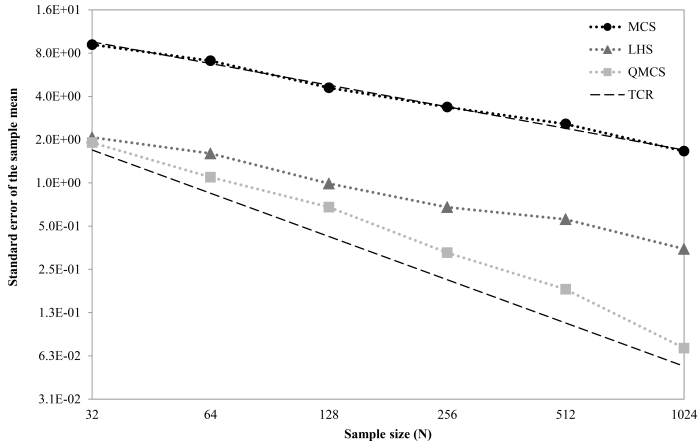

Figure 3.6: Convergence rate of the standard error of the sample mean for MCS, LHS and QMCS applied to case study 1 (k=5, CV=30%). All input parameters are log-normally distributed.

and different distributions of the input parameters (normal or log-normal). The standard deviation calculated with AUP is also shown, together with the deterministic output. Results show that the means and standard deviations are rather similar for all three sampling methods, regardless of the distribution of the input parameters. In case of small uncertainties in the input parameters (CV=5%), AUP and the sampling methods give approximately the same results for the standard deviation.

3.3.2 Results of case study 2

Figure 3.7 shows the standard error of the sample mean for MCS, LHS and QMCS (with increasing sample size). All six input parameters are normally distributed with a CV of 5%. Results shows that QMCS convergence faster than MCS. LHS seems to converge at a similar rate as MCS, but with a higher accuracy. Subsequently, the distribution of the input parameters was changed from normal to log-normal. Figure 5.25 shows the standard error of the sample mean when all input parameters are log-normally distributed with a CV

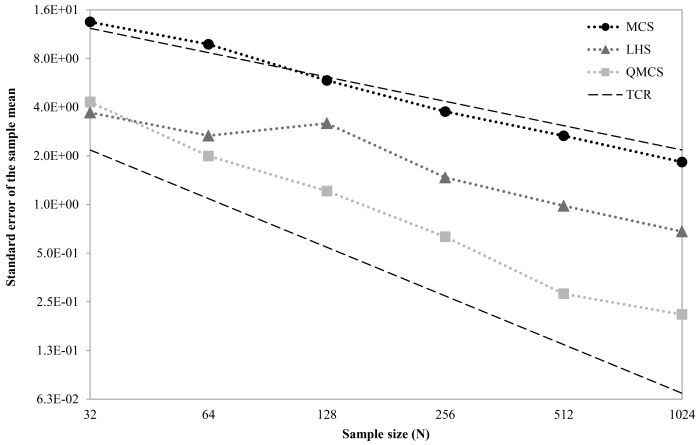

Figure 3.7: Convergence rate of the standard error of the sample mean for MCS, LHS and QMCS applied to case study 2 (k=6, CV=5%). All input parameters are normally distributed.

of 5%. In that case, QMCS converges faster than MCS and LHS for (almost) each sample size. LHS seems to converge at a similar rate as MCS, but with a higher accuracy. Table 3.5 shows the mean and standard deviation for fifty independent runs (R=50); each run having a sample size of 1024, for a CV of 5% and different distributions of the input parameters (normal or log-normal). The standard deviation calculated with AUP is also shown, together with the deterministic output. Results show that the means and standard deviations are rather similar for all three sampling methods, regardless of the distribution of the input parameters. AUP gives a lower value for the standard deviation than the sampling methods.

3.3.3 Results of case study 3

Figure 3.9 shows the standard error of the sample mean for MCS, LHS and QMCS (with increasing sample size). All 115 input parameters are normally distributed with a c_v of 5%. Results show that the standard error of MCS converges as $s/\sqrt{N}$. The standard error of LHS and QMCS convergences as approximately s/N, hence LHS and QMCS converge faster than MCS. LHS

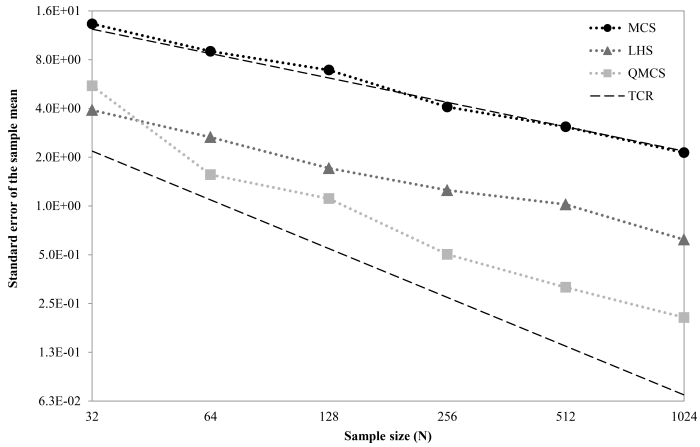

Figure 3.8: Convergence rate of the standard error of the sample mean for MCS, LHS and QMCS applied to case study 2 (k=6, CV=5%). All input parameters are log-normally distributed. The standard error of 50 runs is shown for increasing sample size.

Table 3.5: Greenhouse gas emissions (kg CO_2 e/MWh electricity) of four methods explored (the standard deviation is shown between brackets) for different CV's of the input parameters; R=50, N=1024, k=6. Analytical uncertainty propagation (AUP) is based on a based on a single calculation.

	Normal (5%)	**Log-N** (5%)
Monte Carlo sampling	313 (69.6)	313 (69.8)
Latin hypercube sampling	313 (69.7)	313 (69.6)
Quasi Monte Carlo sampling	313 (70.5)	313 (69.6)
Analytical uncertainty propagation	300 (57.7)	300 (57.7)

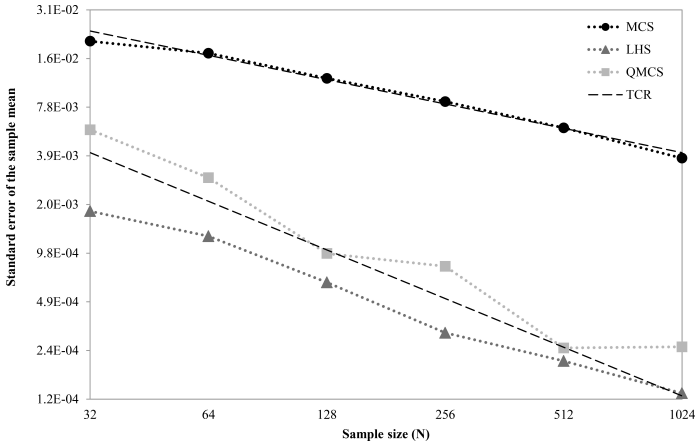

Figure 3.9: Convergence rate of the standard error for MCS, LHS and QMCS applied to case study 3 (k=115, CV=5%). All input parameters are normally distributed. The standard error of 50 runs is shown for increasing sample size.

shows a higher accuracy than QMCS for each sample size. Subsequently, the distribution of the input parameters was changed from normal to log-normal. Figure 3.10 shows the convergence rate when input parameters are log-normally distributed with a CV of 5%, and Figure 3.11 shows the convergence rate when input parameters are log-normally distributed with a CV of 30%. In case of CV of 5%, LHS and QMCS converge faster than MCS, and LHS shows a higher accuracy for each sample size than QMCS. In case of CV of 30%, LHS and QMCS converge at a similar rate as MCS, but show a higher accuracy. Table 3.6 shows the mean and standard deviation for fifty independent runs (R=50); each run having a sample size of 1024, for a CV of 5% or 30% and different distributions of the input parameters (normal or log-normal). The standard deviation calculated with AUP is also shown, together with the deterministic output. Results show that the means and standard deviations are rather similar for all three sampling methods, regardless of the distribution of the input parameters. In case of small uncertainties in the input parameters (CV=5%), AUP and the sampling methods give the same results for the standard deviation.

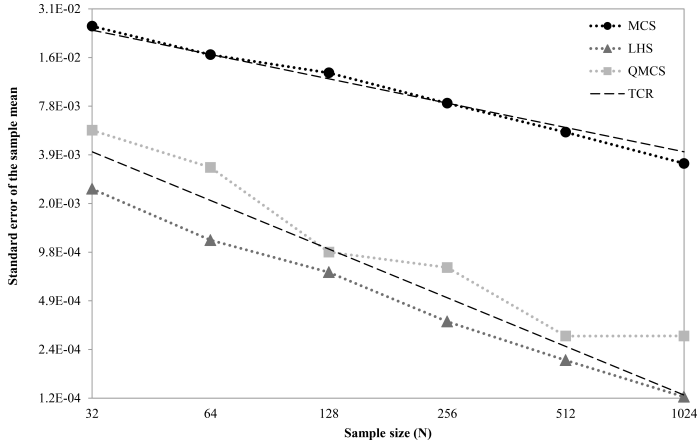

Figure 3.10: Convergence rate of the standard error for MCS, LHS and QMCS applied to case study 3 (k=115, CV=5%). All input parameters are log-normally distributed. The standard error of 50 runs is shown for increasing sample size.

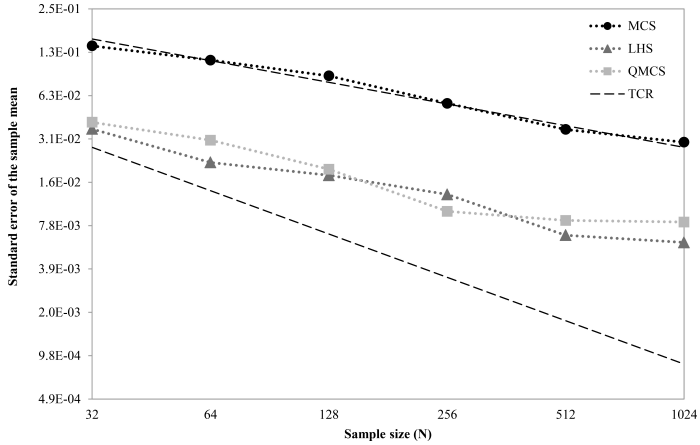

Figure 3.11: Convergence rate of the standard error for MCS, LHS and QMCS applied to case study 3 (k=115, CV=30%). All input parameters are log-normally distributed. The standard error of 50 runs is shown for increasing sample size.

Table 3.6: Greenhouse gas emissions (kg CO_2 e/kg whitefish) of four methods explored (the standard deviation is shown between brackets) for different CV's of the input parameters; R=50, N=1024, k=115. Analytical uncertainty propagation (AUP) is based on a based on a single calculation.

	Normal (5%)	**Log-N** (5%)	**Log-N** (30%)
Monte Carlo sampling	1.95 (0.13)	1.96 (0.13)	2.16 (0.87)
Latin hypercube sampling	1.96 (0.13)	1.96 (0.13)	2.16 (0.88)
Quasi Monte Carlo sampling	1.96 (0.13)	1.96 (0.13)	2.16 (0.88)
Analytical uncertainty propagation	1.95 (0.13)	1.95 (0.13)	1.95 (0.78)

3.3.4 Results FIA

Table 3.7 shows the results of FIA for case study 1, 2 and 3. Core values remain the same, but the upper and lower bounds diverge with an increase in range. For a range of $\delta^{\pm}$=60%, for example, the core value, especially for case study 3, lies no longer in the centre of the range. This is caused by a large range of (one of) the input parameters. It indicates that one or more parameters are approaching the asymptote as described by Cruze et al. [2013]. It is not possible to compare the results of FIA directly to the sampling methods. First, a transformation from a possibility function to a probability function has to be made, as described in Section 3.2.2. The results of FIA of case study 3 for input parameters with a range of $\pm$ 10% were transformed to a probability density function. Figure 3.12 shows the triangular fuzzy interval of case study 3. From the fuzzy interval, the most likely probability function (ml pdf) is constructed, through which a polynomial is fitted [André and Lopes, 2012]. The polynomial can be compared to the result of a probability density function constructed from MCS from which all input parameters are normally distributed with a CV of 5%, the mean and standard deviation of the sample distribution are given in Table 3.6. The fitted polynomial and the probability density function produce roughly the same result. This means that the output of FIA with a range of 10% of the input parameters gives roughly

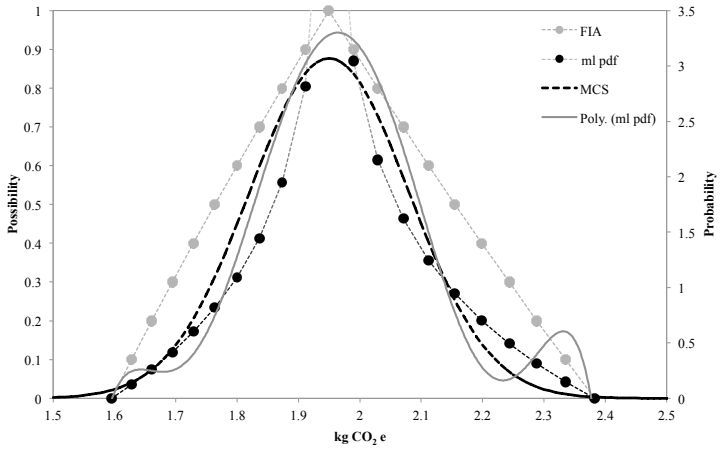

Figure 3.12: Fuzzy interval transformed to most likely probability density function for case study 3; ml pdf: most like probability density function.

the same result as MCS with normally distributed input parameters with a *CV* of 5%.

Table 3.7: Core value (kg CO_2 e/functional unit) for the output of case study 1, 2 and 3, the range is shown between brackets

Range	Case study 1	Case study 2	Case study 3
10%	120 (98.2-147)	300 (245-367)	1.95 (1.59-2.38)
60%	120 (30.0-480)	300 (75.0-1.20 $\cdot 10^3$)	1.95 (0.49-7.80)

3.3.5 Computational effort of propagation methods

Computational effort of uncertainty propagation methods is relevant when large amount of input parameters are considered that potentially slow down the calculation. LHS and QMCS come with additional calculations compared to MCS and might therefore increase calculation time. Random numbers that are drawn for each sample in case of MCS, can be overwritten for the next

Table 3.8: Comparison of convergence rates for MCS, LHS and QMCS, for case study 1, 2, and 3 for different properties of the input parameters.

	Case study 1 ($k = 5$)	**Case study 2** ($k = 6$)	**Case study 3** ($k = 115$)
Normal (5%)	LHS∼QMCS>MCS	QMCS>LHS[3]∼MCS	LHS[4]∼QMCS>MCS
Log-N (5%)	LHS∼QMCS>MCS	QMCS>LHS[3]∼MCS	LHS[4]∼QMCS>MCS
Log-N (30%)	QMCS>LHS[3]∼MCS	n/a	LHS[5]∼QMCS[5]∼MCS

random number, keeping memory use constant. Calculation time, therefore, increases linearly with the amount of random drawings. In case of LHS, however, memory use increases linearly with the sample size because it is not possible to draw only one random number from each equally probable subgroup without knowing (i.e. storing) from which subgroup previous random numbers are drawn. Also in case of QMCS calculation time increased. An indication of the difference in calculation time for MCS versus QMCS is given for case study 3. Applying QMCS when 115 parameter were considered, for a sample size of 1024, took about twice as long compared to MCS.

Calculation time as well as memory usage of FIA and AUP are low compared to the other sampling methods. AUP requires only a single calculation; FIA requires about 11 calculations to generate an output, which was far less than even the fastest converging sampling method that was studied here.

3.4 Discussion

The uncertainty propagation methods were compared based on convergence rate, descriptive statistics and computational effort. Convergence rate could be determined for sampling methods only. Table 3.8 presents an overview of the results of the sampling-based methods. Comparing our results to publications outside the LCA domain, Helton et al. [2006] found that LHS did not outperform MCS, but they applied the sampling methods to non-linear

[3]LHS shows a higher accuracy than MCS.
[4]LHS shows a higher accuracy than QMCS.
[5]LHS and QMCS show a higher accuracy than MCS.

functions. We also found comparable convergence rates of LHS and MCS, although LHS showed a higher accuracy in determining the sample mean in our case. Deutsch and Deutsch [2012], Kollig and Keller [2002] and McKay et al. [1979] showed an improvement of LHS over MCS for several test cases. Tarantola et al. [2012] showed that QMCS method outperformed Latin supercube sampling (an improvement of the standard LHS design) for most of the test functions. Based on our results, and the results we found in literature, we conclude that LHS or QMCS can converge faster than MCS, but it depends on specific characteristics of the model (size, behaviour) and properties of the input parameters.

Regarding AUP, we want to point out an LCA-paper of Heijungs and Lenzen [2014], who made a comparison between MCS and AUP. The authors also concluded that AUP in form of a first order Taylor approximation will work best for small uncertainties.

There are also some limitations on the case studies described here. First, case study 1 and 2 represent an artificial production system and might, therefore, not represent the behaviour of actual case studies in LCA. Second, in each case study, we had to assume the type of distribution function and their dispersion parameters. Although the most common type of distribution functions were chosen [Lloyd and Ries, 2007], other distribution functions might influence the performance of sampling methods. Third, in each case study we assumed that all parameters are independent. This leads to either over- or underestimation of the output uncertainty. Most studies in LCA neglect correlations [Lloyd and Ries, 2007]. This might not be realistic for each parameter; e.g. a higher fossil fuel consumption would lead to higher CO_2 emission. This knowledge could be incorporated by creating a covariance matrix, however, this was ignored.

3.5 Conclusions

From the results in this paper, we concluded:

- For each LCA case study that was considered in this paper, LHS and QMCS outperformed MCS in terms of accuracy in determining the sample mean, regardless the type of distribution function or the coefficient of variation of the input parameters.

- Characteristics (size, behaviour) of the LCA case study and the properties of the input parameters influenced the convergence rate. For example, LHS converged faster than MCS in case study 3 (large, linear) but equally fast as MCS in case study 2 (small, non-linear).
- AUP works best for small uncertainties of the input parameters and linear case studies; it required less memory than the sampling methods.
- FIA uses less memory compared to the sampling methods. Other conclusions for FIA are less explicit. A characteristic of FIA is that it is a deterministic process, this can be seen as an advantage (no extreme values) or a disadvantage (not comparable to sampling methods or determine a statistical difference between two scenarios). Moreover, transforming FIA to a probability framework takes up additional calculations.
- Uncertainty propagation in LCA using a sampling-based method leads to more (directly) usable information compared to FIA or AUP. AUP can be favourable over the sampling methods when large amount of input parameters are considered and input uncertainties are small. LHS and QMCS provide more accuracy in determining a sample mean than MCS and can even converge faster for some of the case studies discussed in this paper.

Acknowledgements

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CHAPTER 4

Methods for global sensitivity analysis in life cycle assessment

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Abstract

Input parameters required to quantify environmental impact in life cycle assessment (LCA), can be uncertain due to e.g. temporal variability or unknowns about the true value of emission factors. Uncertainty of environmental impact can be analysed by means of a global sensitivity analysis to gain more insight into output variance. This study aimed to: (1) give insight into and (2) compare methods for global sensitivity analysis in life cycle assessment. Five methods that quantify the contribution to output variance were evaluated: standardised regression coefficient, Spearman correlation coefficient, key issue analysis, Sobol' method and random balance design. To be able to compare the performance of global sensitivity methods, two case studies were constructed: one small hypothetical case study describing electricity production, that is sensitive to a small change in the input parameters, and a large case study describing a production system of a northeast Atlantic fishery. Input parameters with relatively small and large input uncertainties were selected. The comparison of the sensitivity methods was based on four aspects: (I) sampling design, (II) output variance, (III) explained variance, and (IV) contribution to output variance of individual input parameters. The evaluation of the sampling design (I) relates to the computational effort of a sensitivity method. Key issue analysis does not make use of sampling and was fastest, whereas the Sobol' method had to generate two sampling matrices, and therefore, was slowest. The total output variance (II) resulted in approximately the same output variance for each method, except for key issue analysis, which underestimated the variance especially for high input uncertainties. The explained variance (III) and contribution to variance (IV) for small input uncertainties, was optimally quantified by standardised regression coefficients and the main Sobol' index. For large input uncertainties, Spearman correlation coefficients and the Sobol' indices performed best. The comparison, however, was based on two case studies only, which might not be representative. Most methods for global sensitivity analysis performed equally well, especially for relatively small input uncertainties. When restricted to the assumptions that quantification of environmental impact in LCAs is linear, standardised regression coefficients, Spearman correlation coefficients or key issue analysis can be used for global sensitivity analysis. The choice for one of the methods depends on the available data, the magnitude of the uncertainties in input data and aim of the study.

4.1 Introduction

LCA calculates the environmental impact of a product or production process along the entire chain. Input parameters required to describe the production chain, can be uncertain due to e.g. temporal variability or unknowns about the

true value of emission factors. Uncertainty in the input parameters will cause an uncertainty around the outcome of an LCA. In this paper, uncertainty can refer to variability or epistemic uncertainty [Chen and Corson, 2014; Clavreul et al., 2013] of the input parameters. Variability (e.g. natural, temporal, geographical) is inherent to natural systems such as agriculture and cannot be reduced. Epistemic uncertainty refers to unknowns in the system and can be reduced by gaining more knowledge about the system. Analysing this uncertainty can be done by means of a sensitivity analysis, and can help to gain more insight into the robustness of the result, to prioritise data collection or to simplify an LCA model. Many LCA studies have been performed over the last decade, and interest in addressing uncertainty propagation is increasing [Groen et al., 2014; Heijungs and Lenzen, 2014; Lloyd and Ries, 2007]. Few studies, however, apply a systematic and consistent sensitivity analysis to address the effect of input uncertainties on the output [Mutel et al., 2013]. An explanation might be that ISO 14044 recommends a sensitivity analysis as part of the LCA framework to identify the importance of the input uncertainties, but does not recommend a specific technique.

A sensitivity analysis can be performed by varying an input parameter and, as such, determine the effect on the result. Furthermore, if the distributions function of the input parameters is known, it is possible to calculate the contribution to the output variance. The first approach belongs to the area of local sensitivity analysis. A local sensitivity analysis determines the effect of a (small) change in one of the input parameters at a time. The second approach belongs to the area of global sensitivity analysis. A global sensitivity analysis can be seen as an extension of uncertainty propagation: it determines how much each input parameter contributes to the output variance. The main differences between a local and global sensitivity analysis are illustrated in Table 4.1. In this paper we focus on global sensitivity analysis, which requires a case study of which the distribution functions of the input parameters are known.

In Figure 4.1, the procedure of a global sensitivity analysis is illustrated with a schematic LCA model, containing four input parameters. First, the input parameters and their uncertainties are represented by probability density functions (step 1). Second, uncertainty propagation is performed with e.g. Monte Carlo simulation, which propagates uncertainty through the LCA model (step 2) to obtain a distribution function of the output. Third, the variance of the output is calculated (step 3). After the uncertainty propagation is

Table 4.1: Main differences in requirements of input data and of results of a sensitivity analysis between local and global sensitivity analysis.

	Local sensitivity analysis	**Global sensitivity analysis**
Synonyms	One at a time approach; differential analysis; marginal analysis; perturbation analysis	Contribution to variance; variance-based sensitivity analysis; key issue analysis
Requirements	Point value (central value)	Central value, parameter of dispersion and probability density function; method for uncertainty propagation
Result	Ranking of sensitive input parameters	Contribution to output variance of each input parameter; uncertainty distribution of output; ranking
Examples	Partial derivatives; change due to methodological choice or input parameter	Regression or correlation techniques; Taylor approximation; Sobol' indices

performed, a method for global sensitivity analysis is selected (step 4), which determines how much each input parameter contributes to the output variance (step 5). In the example of Figure 4.1, the sensitivity analysis shows that parameter 1 and to a lesser extent parameter 2 are the ones that contribute most to the output variance.

In LCA literature, five methods for global sensitivity analysis have been mentioned that quantify the contribution to output variance: (1) (standardised) regression coefficients, as was suggested by Huijbregts et al. [2001], and applied in LCA by e.g. Aktas and Bilec [2012]; Basset-Mens et al. [2009]; Sugiyama et al. [2005]; Vigne et al. [2012]; (2) Pearson correlation coefficient [Heijungs and Lenzen, 2014; Onat et al., 2014]; (3) Spearman (rank) correlation coefficient [Chen and Corson, 2014; Geisler et al., 2005; Heijungs and Lenzen, 2014; Mattila et al., 2012; Mattinen et al., 2014; Sonnemann et al., 2003; Wang and Shen, 2013]; (4) key issue analysis, which applies a first order Taylor expansion around the LCA model to estimate the output variance, thus avoiding sampling; key issue analysis in LCA has been developed by Heijungs [1996] and applied in LCA by e.g. Heijungs et al. [2005]; Jung et al. [2014]; and (5)

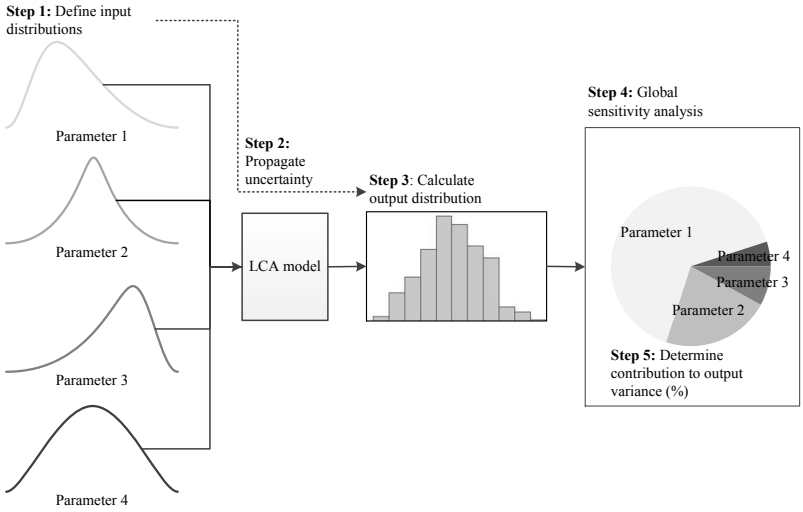

Figure 4.1: Illustration of global sensitivity analysis in LCA (based on Saltelli et al. [1999])

Fourier amplitude sensitivity test has been applied by De Koning et al. [2010].

Outside the LCA domain, a much wider set of approaches have been developed and applied, such as random balance design and the Sobol' method, that also quantify the contribution to output variance [Saltelli et al., 2008; Sobol', 2001; Tarantola et al., 2012, 2006]. The random balance design is closely related to the Fourier amplitude sensitivity test. To our knowledge, random balance design has been not yet been applied in LCA. The application of the Sobol' method in LCA has been limited, see for example [Wei et al., 2014], and for a characterisation model that can be applied in LCA [Cucurachi et al., 2014].

For most of the methods, it is not known under which conditions they perform optimally, or if there is a method that performs better than the other methods in LCA. The aim of this study is two-fold: (1) to study the applicability of a number of previously suggested methods for global sensitivity analysis to LCA and (2) to compare the methods based on their ability to explain the output variance. To be able to compare the performance of global sensitivity methods, two case studies were constructed: one small hypothetical case study describing electricity production, that was sensitive to a small change in the input parameters, and a large case study describing a production system of a northeast Atlantic fishery.

4.2 Methods for global sensitivity analysis in LCA

4.2.1 Sampling procedure with matrix based LCA

In this paper, we use matrix formulation for LCA (for an explanation see Heijungs and Suh [2002]). A matrix formulation of the LCA model will facilitate the use and discussion of the global sensitivity methods. Matrix based LCA quantifies the total emissions and resource use (g) of a product over its entire life cycle by:

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} \tag{4.1}$$

The production processes are represented by $v = 1$ to y columns in the square technology matrix $\mathbf{A}$ (size $x \times y$), the rows ($u = 1$ to x) represent a specific product flow. For example, if electricity is produced in one column, other production processes given in other columns can use it as input. The inventory matrix $\mathbf{B}$ (size $z \times y$) consists of use of resources and emissions

Table 4.2: Meaning of symbols.

Symbol	Meaning	Symbol	Meaning
$\mathbf{A}$ or a_{uv}	Technology matrix	$\mathbf{P}$ or p_{ij}	Sampling matrix for uncertain input parameter in $\mathbf{A}$ and $\mathbf{B}$
$\mathbf{B}$ or b_{wv}	Intervention matrix	$\mathbf{Q}$	Sampling matrix
$\mathbf{b}'$ or b_v	Intervention vector in case $w = 1$	$\mathbf{R}$	Sampling matrix column j comes from $\mathbf{Q}$ and all other $k-1$ columns come from $\mathbf{P}$
c_j	Regression coefficients	r	Correlation coefficients
e_i	Error or residual term	S_j	Sensitivity index for parameter j
$\mathbf{f}$	Final demand vector	$\mathbf{s}$	Scaling vector
$\mathbf{g}$	Inventory vector containing sample of CO_2 values	u	Row of $\mathbf{A}$
i	Index variable of sample matrix $\mathbf{P}$	v	Column of $\mathbf{A}$ or $\mathbf{B}$
j	Input parameter	w	Row of $\mathbf{B}$
k	Total number of input parameters	x	Number of rows in $\mathbf{A}$
l	Total number of input parameters (Sobol' method)	y	Number of columns in $\mathbf{A}$ and $\mathbf{B}$
M	Maximum oscillation frequency	z	Number of rows in $\mathbf{B}$ and $\mathbf{g}$
N	Sample size	γ	$\mathbf{b}'\mathbf{A}^{-1}$
p_j	All input parameter $\mathbf{A}$ and $\mathbf{B}$	ω	frequency

corresponding to each production process. Using the final demand vector $\mathbf{f}$ (size $w = 1$ to z), the production processes are scaled to produce the desired amount. In this paper we will only consider CO_2 emissions from each production process (so $z = 1$, transforming $\mathbf{B}$ into a row vector $\mathbf{b}$ (size y). The main LCA equations in this paper is therefore

$$g = \mathbf{b}'\mathbf{A}^{-1}\mathbf{f} \tag{4.2}$$

where the prime (') indicates transposition. An overview of the symbols introduced in this section can be found in Table 4.2.

Because elements of $\mathbf{A}$ and $\mathbf{b}'$ will be uncertain, we developed general formulas based on a row vector $\mathbf{p}'$ that contains all elements of $\mathbf{A}$ and $\mathbf{b}'$.

Thus:

$$p_{v+(u-1)y} = a_{uv}$$

and

$$p_{xy+v} = b_v$$

We may choose to restrict $\mathbf{p}'$ to contain uncertain elements of $\mathbf{A}$ and $\mathbf{b}'$ only, to save memory. Using this notation, Equation (4.2) can be conceived as

$$g = \gamma(\mathbf{p})\mathbf{f}$$

where $\gamma(\mathbf{p})$ is a function based on combining the underlying matrices $\mathbf{A}$ and $\mathbf{b}'$. All global sensitivity methods applied in this paper, except for key issue analysis, require sampling for uncertainty propagation. In this paper, we used Monte Carlo sampling to generate random numbers, and a random balance design to generate equi-distributed numbers, from the distribution functions of the input parameters to generate an output distribution (Figure 4.2). The sampling matrix $\mathbf{P}$ (size $N \times k$) contains $i = 1$ to N random numbers drawn for each input parameter $j = 1$ to k of matrix $\mathbf{A}$ and $\mathbf{b}'$. For example, Monte Carlo sampling could lead to drawing the following random numbers: 1.04, 0.96, 0.92 for the first three parameters. Combining these values and the realisations for the other parameters in Equation (4.2) will lead to the first realisation of 5.1 kg CO_2. This procedure is repeated N times, the whole simulation is repeated 50 times. In this section, six measures, also called sensitivity indices, that quantify the contribution to output variance are introduced. The mathematical notations in case of matrix based LCA are given, the full derivation can be found in the supplementary material. All sensitivity methods are programmed in MATLAB and can be forwarded by the first author upon request. Calculating sensitivity indices, there are four aspects that can differ per method. The comparison of the sensitivity methods will be based on these four aspects:

(I) The sampling design (i.e., how the rows of $\mathbf{P}$ are constructed);

(II) The total output variance;

(III) The total output variance (II) that is explained by the method (this is ideally 100%);

(IV) The contribution to (III) of the individual input parameters.

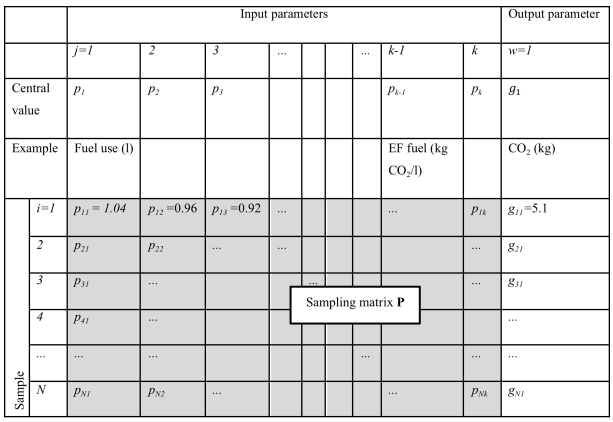

Figure 4.2: Monte Carlo sampling approach for matrix based calculations in LCA, EF: emission factor.

The relation between the output variance (II), explained variance (III) and the contribution to variance (IV), is visualised in Figure 4.3.

In general, the variance of the model output in Equation (4.2) is given by the conditional variance of parameter p_j and a residual term (or error term):

$$\text{var}(g) = \text{var}\left(E(g|p_j)\right) + E\left(\text{var}(g|p_j)\right) \tag{4.3}$$

The conditional variance $\text{var}\left(E(g|p_j)\right)$ is the "expected reduction in variance that would be obtained if parameter could be fixed" [Saltelli et al., 2010]. E is the expected value and $\text{var}(g) = \frac{1}{N-1}\sum_i (g_i - \overline{g})^2$, and $\overline{g} = \frac{1}{N}\sum_i g_i$. The variance explained by each of the parameter can be given by the correlation ratio [McKay et al., 1999] and [Saltelli et al., 2008, Equation 1.25]:

$$S_j = \frac{\text{var}\left(E(g|p_j)\right)}{\text{var}(g)} \tag{4.4}$$

Where the ratio S_j is the (main) sensitivity index. A derivation of the sensitivity index and why it is equal to the standardised regression coefficient

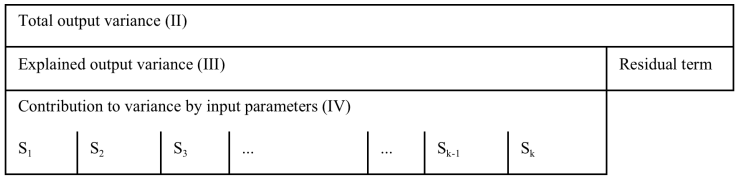

Figure 4.3: Relation between total output variance, explained output variance and contribution to variance by the individual input parameters.

can be found in the supplementary material, Equations (4.21) to (4.24). The expressions for the sensitivity indices for each method are found in the boxed equations in the next subsections.

4.2.2 Regression- or correlation based methods for sensitivity analysis

The contribution to variance can be quantified using regression or correlation. First the general framework of a regression model is introduced. According to the theory of multiple linear regressions, g can be described by:

$$g_i = c_0 + \sum_{j=1}^{k} c_j p_{ij} + e_i \tag{4.5}$$

Where the constant c_0 represents the intercept, c_j the slope (or regression coefficient) and e_i the error term, which is assumed to be normally distributed with a constant variance. The sensitivity index using standardised regression coefficients (SRC) is equal to:

$$S_j^{SRC} = \frac{\text{var}(p_j)}{\text{var}(g)}(c_j)^2 \tag{4.6}$$

Where $\text{var}(p_j) = \frac{1}{N-1}\sum_i (p_{ij} - \overline{p_j})^2$ and $\overline{p_j} = \frac{1}{N}\sum_i p_{ij}$. The full description of Equation (4.6) is given in the supplementary material, Equations (4.25) - (4.29).

The S_j^{SRC}, similar to the Pearson correlation coefficient squared, are not robust to outliers [Hamby, 1994; Saltelli and Sobol', 1995]. An alternative to the Pearson correlation coefficient is using its rank transformed counterpart, in the form of the Spearman rank correlation coefficient. The Spearman correlation coefficient (SCC) calculates the linear dependence between the input and output parameter. Each draw of input parameter p_{ij} is rank-transformed to $p_{(i)j}$, and g_i is rank-transformed to $g_{(i)}$. The SCC is calculated as follows:

$$r_j^{SCC} = \frac{\sum_i \left(p_{(i)j} - \overline{p_j}\right)\left(g_{(i)} - \overline{g}\right)}{\sqrt{\sum_i \left(p_{(i)j} - \overline{p_j}\right)^2 \sum_i \left(g_{(i)} - \overline{g}\right)^2}} \tag{4.7}$$

The sensitivity index using SCC is equal to:

$$S_j^{SCC} = (r_j^{SCC})^2 \tag{4.8}$$

The full description of Equation (4.8) is given in the supplementary material, Equation (4.30). In this paper, sensitivity indices based on SRC and SCC are calculated from the same simulations.

4.2.3 Key issue analysis using a first order Taylor expansion

Key issue analysis (KIA) is a method for analytically determining the contribution to variance (or variance decomposition) by means of a first order Taylor expansion. The first order Taylor expansion around the central values ($\overline{p_j}$) of Equation (4.2) results in:

$$g_j = g(p_j) = g(\overline{p_j}) + \left(\frac{\partial g(\overline{p_j})}{\partial p_j}\right)(p_j - \overline{p_j}) \tag{4.9}$$

Because the total output variance var(g) is estimated by the first order Taylor expansion, the variance explained by the individual parameters will always be equal to 100% (Figure 4.3). The variance according to KIA, therefore, may be of a different magnitude than the output variance obtained by

sampling. The sensitivity index using KIA is equal to:

$$S_j^{KIA} = \frac{\text{var}(p_j)}{\text{var}(g)} \left(\frac{\partial g}{\partial p_j} \right)^2 \tag{4.10}$$

The full derivation of Equation (4.10) is given in the supplementary material, Equations (4.31)-(4.33).

4.2.4 Variance decomposition methods for sensitivity analysis

Sobol' indices

In case of variance-based methods for sensitivity analysis, the variance of Equation (4.2) is rewritten as the sum of the variance of all first order conditional variances and higher order terms (supplementary material, (4.35)-(4.36)):

$$\begin{aligned} \text{var}(g) = &\sum_j \text{var}\left(E(g|p_j)\right) + \\ &\sum_l \sum_{j>l} \left(\text{var}\left(E(g|p_j, p_l)\right) - \text{var}\left(E(g|p_j)\right) - \text{var}\left(E(g|p_l)\right)\right) + \cdots \end{aligned} \tag{4.11}$$

To calculate the conditional variances of Equation (4.4), we have adopted the sampling algorithm described by [Saltelli et al., 2010]. The sampling algorithm fixes one parameter to calculate the variance reduction in the output. The sampling algorithm requires two sampling matrices. In addition to the sampling matrix $\mathbf{P}$, a second sampling matrix $\mathbf{Q}$ is generated in the same way, independent of $\mathbf{P}$. From $\mathbf{P}$ and $\mathbf{Q}$ a third sampling matrix is derived $\mathbf{R}$, from which column j comes from $\mathbf{Q}$ and all other $k-1$ columns come from $\mathbf{P}$. For each matrix $\mathbf{P}$, $\mathbf{Q}$ and $\mathbf{R}$, output of the model is calculated using Equation (4.2), resulting in $g(\mathbf{P})$, $g(\mathbf{Q})$ and $g(\mathbf{R})$. The variance is calculated through the identity: $\text{var}(g) = E(g^2) - E^2(g)$. The variance equals:

$$\text{var}(g) = \frac{1}{N} \sum_i (g(\mathbf{P})_i)^2 - \left(\frac{1}{N} \sum_i g(\mathbf{P})_i \right)^2 \tag{4.12}$$

Likewise, the conditional variance is given by:

$$\text{var}\left(E(g|p_j)\right) = \frac{1}{N}\sum_i g(\mathbf{Q})\left(g(\mathbf{R}^j)_i - g(\mathbf{Q})_i\right) \tag{4.13}$$

The sensitivity index, applying Sobol's main effect (SME) index (supplementary material, Equation (4.38)), is equal to:

$$S_J^{SME} = \frac{\frac{1}{N}\sum_i g(\mathbf{Q})\left(g(\mathbf{R}^j)_i - g(\mathbf{Q})_i\right)}{\frac{1}{N}\sum_i \left(g(\mathbf{P})_i\right)^2 - \left(\frac{1}{N}\sum_i g(\mathbf{P})_i\right)^2} \tag{4.14}$$

The Sobol' total effect index (STE) calculates how much input parameter j explains of the output variance, including all possible interactions with other parameters:

$$S_j^{STE} = S_j + S_{jl} + S_{jm} + \cdots + S_{jlm} + \cdots S_{jlm\cdots k} \tag{4.15}$$

The total effect index equals the "expected variance that would be left if all [parameters] but [parameter p_j] could be fixed" [Saltelli et al., 2010]), and is based on the quantification of the residual term in Equation (4.3):

$$E\left(\text{var}(g|p_{\sim j})\right) = \frac{1}{2N}\sum_i \left(g(\mathbf{P})_i - g(\mathbf{R}^j)_i\right)^2 \tag{4.16}$$

The Sobol' total effect index (supplementary material, Equation (4.40)), is equal to:

$$S_j^{STE} = \frac{\frac{1}{2N}\sum_i \left(g(\mathbf{P})_i - g(\mathbf{R}^j)_i\right)^2}{\frac{1}{N}\sum_i \left(g(\mathbf{P})_i\right)^2 - \left(\frac{1}{N}\sum_i g(\mathbf{P})_i\right)^2} \tag{4.17}$$

In case of an LCA model without outliers, all interaction terms (e.g. S_{jl} and other higher order terms in Equation (4.15)) are approximately zero, so: $S_j^{STE} \approx S_j^{SME}$, in case of models containing outliers, $S_j^{STE} > S_j^{SME}$. This also means that the sum of the total sensitivity index for an LCA model containing outliers can be larger than 100 % (supplementary material, Equations (4.41)-(4.42)).

Random balance design

The theory of Fourier series states that any (periodic) function can be written as a sum of wave functions. Random balance designs (RBD) calculate the conditional variance by rewriting the LCA model in Equation (4.2) in terms of sums of sine and cosine functions. We use complex numbers to facilitate notation of sine and cosine, thus using $e^{\sqrt{-1}\omega}$, where we prefer to write $\sqrt{-1}$ over i, allowing us to remain using i as an index variable. For this method, we use the discrete Fourier transformation to convert an equally spaced periodic function of size N. The model output of Equation (4.2) in terms of Fourier coefficients are given in the supplementary material, Equation (4.45). The Fourier coefficients are given by:

$$g(p_\omega) = \frac{1}{N} \sum_{i=0}^{N-1} g(p_{ij}) e^{-\sqrt{-1}\pi\omega i/N} \tag{4.18}$$

where ω represents the frequency domain, which is divided in equally spaced segments: $\omega = 1$ to $N-1$. The parameters that contribute most to the output variance will resemble the wave-like shape of the input parameter. This means that the most sensitive parameters have the highest amplitude and that the amplitude of the wave of the output is a measure of the conditional variance of input parameter j. The total variance is given by:

$$\text{var}(g) = \left(\frac{1}{N} \sum_{\omega=1}^{N-1} |g(p_\omega)| \right)^2 \tag{4.19}$$

A similar expression is found for the conditional variance of each input parameter (Equation (4.49)). The sensitivity index using RBD is equal to:

$$S_j^{RBD} = \frac{2 \left(\sum_{\omega=1}^{M} |g^j(p_\omega)| \right)^2}{\left(\sum_{\omega=1}^{N-1} |g(p_\omega)| \right)^2} \tag{4.20}$$

Where M is equal to the maximum oscillation frequency and $g^j(p_\omega)$ is the reordered model output for parameter j. The derivation of the sensitivity index in Equation (4.20) can be found in the supplementary material, Equations (4.44)-(4.50).

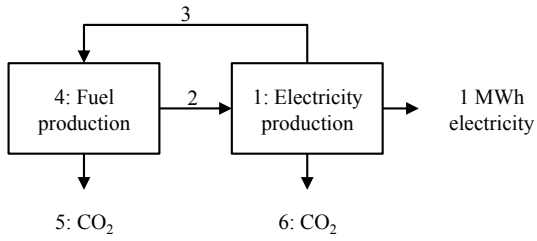

Figure 4.4: Case study 1: production of 1 MWh electricity [Groen et al., 2014].

4.3 Case studies

A hypothetical of the production of 1 MWh of electricity was selected (the original version of the case study appeared in [Heijungs and Suh, 2002]). The case study consisted of two processes: fuel production and electricity production (Figure 4.4). In Figure 4.4, parameter 1 equals the electricity production, parameter 2 equals fuels use for electricity production, parameter 3 equals electricity use of fuel production, parameter 4 equals fuel production, parameter 5 equals CO_2 emissions during fuel production and parameter 6 equals CO_2 emissions during electricity production. The case study is set up in such a way that a small change in one of the input parameters, results in a large change of the output.

We assumed that the input parameters were log-normally distributed and the relative standard deviation (i.e. coefficient of variation: $CV = \sigma/\mu$) equalled: 5% or 30% for two different scenarios. All input parameters are assumed log-normally distributed to avoid drawing random numbers with an incorrect sign. This is admittedly a weak argument, but our main purpose is to construct a toy example to study the sensitivity indices, not to build a realistic system. We selected a relatively small and large coefficient of variation because we wanted to explore if the Sobol' total sensitivity indices and the Spearman correlation coefficients would explain more of the output variation in case of outliers.

The second case study describes a whitefish fishery in the northeast Atlantic. The functional unit equalled 1 kg landed whitefish. The flow diagram shown in Figure 4.5. Five input parameters we wish to highlight are parameter

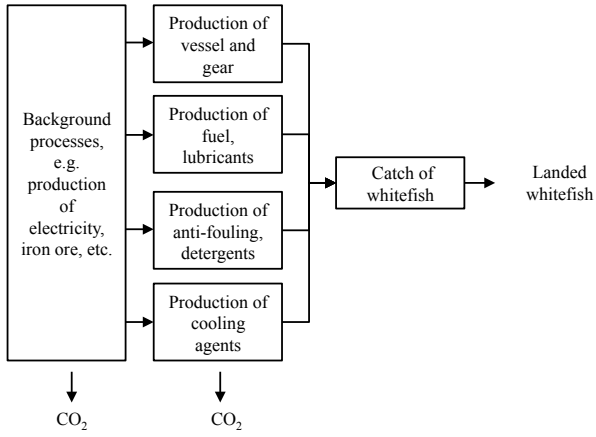

Figure 4.5: Case study 2: production of 1 kg of landed whitefish from the northeast Atlantic [Groen et al., 2014].

α: total amount of landed fish; parameter β: emission factor fuel combustion; parameter γ: fuel production; parameter δ: emission factor fuel production, and parameter ϵ: fuel use. The fishery consists of a single vessel, making trips of approximately two weeks, landing their fish in Tromsø, Norway. Data comprised of annual averages of the vessel and gear, fuel, lubricants, anti-fouling, detergents, cooling agents, and total catch and were collected by the vessel owner. Background data, such as the CO_2 emissions during steel production from the vessel, came from the ecoinvent database v2.2 [ecoinvent, 2010]. In total 115 input parameters were considered. Also in this case study, we assumed that all input parameter were log-normally distributed with a CV of 5 or 30%.

4.4 Results

In this section we will discuss the sampling design (I); total output variance (II); the explained variance (III) and the contribution to the output variance of the individual input parameters as given by the sensitivity indices S_j (IV).

Table 4.3: Sample design and calculation of the output variance for the six sensitivity indices.

Methods	**Uncertainty propagation**	**Sampling design (I)**	**Runs**
Standardised regression coefficient	Sampling	Random	N
Spearman correlation coefficient	Sampling	Random	N
Key issue analysis	Analytical	N/A	1
Sobol' main effect	Sampling	2x Random	$2N$
Sobol' total effect	Sampling	2x Random	$2N$
Random balance design	Stratified sampling	Wave-like, equally distributed and of size $2N$	N

4.4.1 Sampling design

The differences in uncertainty propagation methods requires differences in sample designs and, therefore, in computational effort between methods (Table 4.3). SRC, SCC and RBD both require N runs, but for the Sobol' indices (SME and STE) $2N$ runs are needed to calculate the indices. This means that this method is more computationally demanding than the other sampling methods. Although KIA requires only a single calculation, it does not produce a distribution function of the output, making it more difficult to compare two or more studies. RBD is using the discrete Fourier series, which allowed us to use the *Fast Fourier Transformation* algorithm, which is computationally fast [Frigo and Johnson, 2005].

4.4.2 Output variance and explained variance

Table 4.4 shows the mean, total output variance (II) and variance explained by the global sensitivity method (III) of case study 1, in case of a parameter of dispersion of CV=5% and CV=30%, for a sample size of N=4096 and 50 repetitions. In order to make a proper comparison, we ran an additional Monte Carlo simulation where we calculated the output variance based on $N = 10^6$, and we considered this as the best approximation of the output variance.

Table 4.4: Mean and variance for CO_2 using different sensitivity methods for case study 1 (N=4096; 50 repetitions), using standardised regression coefficients (SRC); Spearman correlation coefficients (SCC); key issue analysis (KIA); Sobol' main effect (SME); Sobol' total effect (STE); and random balance design (RBD). II: total output variance; III: variance explained.

$CV = 5\%$	$N = 10^6$	**SRC**	**SCC**	**KIA**	**SME**	**STE**	**RBD**
Mean (kg CO_2)	128	128	128	128	128	128	128
II (kg^2)	80.8	80.7	80.7	80	80.8	80.8	81
III (%)	-	99.6	94.9	100	97.8	101	90.6
Residual (%)	-	0.04	5.1	n/a	2.2	n/a	9.4
$CV = 30\%$							
Mean (kg CO_2)	145	145	145	128	145	145	145
II (10^3 kg^2)	4.3	4.27	4.27	2.88	4.35	4.35	4.29
III (%)	-	81.7	94	100	91.6	110	79.7
Residual (%)	-	18.3	6	n/a	8.4	n/a	20.3

For CV=5%, all methods produced approximately the same mean and output variance for this case study. Variance explained by most methods added up to approximately 100%, suggesting that very few outliers were present. For CV=30%, most methods produced approximately the same mean and output variance. However, KIA estimated the total output variance considerably lower than the sampling based methods. Furthermore, SRC explained less than SCC, which suggested the presence of outliers. STE also showed a value much larger than 100%, which also suggested the presence of outliers. RBD explained less of the output variance than other methods. Note that the mean value for CO_2 is larger when the CV is larger, although the mean value of the input parameters is the same. This is an effect of the asymmetric distribution used. KIA neglects the shape of the distribution and therefore misses this effect.

Table 4.5 shows the mean and the output variance (II) for case study 2 in case of a parameter of dispersion of $CV = 5\%$ and $CV = 30\%$. Case study 2 contains 115 parameters, the variance explained (III) is shown of the 5 most contributing parameters and the for all 115 parameters, because all other parameters contribute $\ll 1\%$.

For $CV = 5\%$, all methods produced approximately the same mean and output variance. Most methods explained approximately 100% of the vari-

ance, suggesting that very few outliers were present. For $CV = 30\%$, most methods produced approximately the same mean and output variance, except for KIA. KIA estimated the total output variance considerably lower than the sampling based method. In case of RBD, the output explained by 5 or by 115 parameters differed considerably, suggesting that RBD overestimated the sensitivity indices of low contributing parameters.

Table 4.5: Mean, output variance and variance explained by 5 or 115 parameters for CO_2 using different sensitivity methods for case study 2 ($N = 4096$; 50 repetitions), using standardised regression coefficients (SRC); Spearman correlation coefficients (SCC); key issue analysis (KIA); Sobol' main effect (SME); Sobol' total effect (STE); and random balance design (RBD). II: total output variance; III: variance explained.

$CV = 5\%$	$N = 10^6$	**SRC**	**SCC**	**KIA**	**SME**	**STE**	**RBD**
Mean (kg CO_2)	1.96	1.96	1.96	1.95	1.96	1.96	1.96
II (kg^2)	0.017	0.017	0.017	0.0168	0.0169	0.0169	0.017
III [1] (%) - 5	-	99.2	95.4	100	95.1	101	90.2
III [2] (%) - 115	-	99.2	95.5	100	95.2	101	101
Residual (%)	-	0.80	4.50	n/a	4.80	n/a	und.[3]
$CV = 30\%$							
Mean (kg CO_2)	2.16	2.16	2.16	1.95	2.16	2.16	2.16
II (kg^2)	0.76	0.758	0.758	0.606	0.775	0.775	0.766
III[1] (%) - 5	-	87.2	94.4	100	93.6	103	83.3
III[2] (%) - 115	-	87.3	94.5	100	93.6	103	94
Residual (%)	-	12.7	5.5	n/a	6.4	n/a	6

4.4.3 Sensitivity index

Figure 4.6 shows the sensitivity index (IV) of each parameter of case study 1 for a parameter of dispersion of $CV = 5\%$ and $CV = 30\%$, scaled to the benchmark output variance computed with $N = 10^6$. We scaled the graphs

[1]Variance explained by five most contributing parameters.

[2]Variance explained by all 115 parameters.

[3]und: undefined. Because the explained variance was more than 100% due to an overestimation of the sensitivity indices of the low contributing parameters, the residual could not be defined.

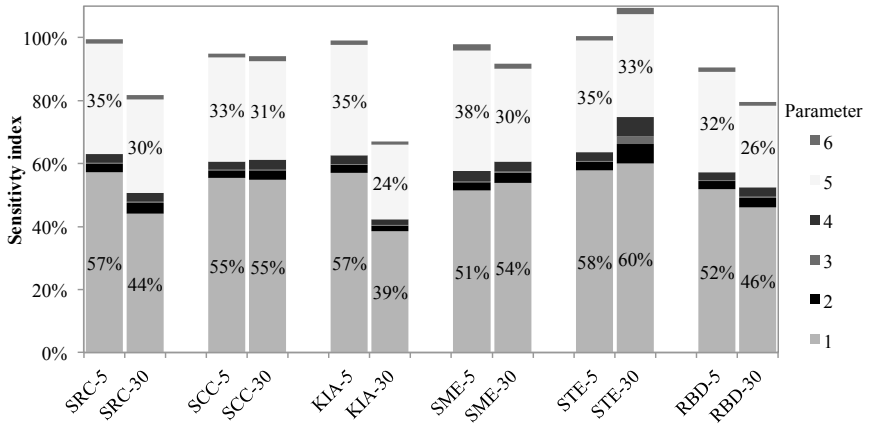

Figure 4.6: Contribution to output variance for sensitivity methods applied to case study 1 (N=4096; 50 repetitions; CV=5% or CV=30%) for the sensitivity index (SRC, SCC, KIA, SME, RBD) or total sensitivity index (STE) for each parameter (1-6) is shown. SRC: standardised regression coefficient; SCC: Spearman correlation coefficient; KIA: key issue analysis; SME: Sobol' main effect index; STE: Sobol' total effect index; RBD: random balance design; 1: electricity production; 2: fuels use electricity production; 3: electricity use fuel production; 4: fuel production; 5: CO_2 emissions fuel production; 6: CO2 emissions electricity production.

to this benchmark to compensate for methods that predicted a lower output variance. For example, for a CV of 30%, KIA arrived at an output variance of 0.606, which is approximately 20% lower than the output variance with a sample size of $N = 10^6$. In case of applying SRC to case study 1 (CV = 5%), parameter 1 was responsible for 57% of the output variance. For each method, parameter 1 and 5 contributed most to the output variance, the exact contribution, however, differed per method. Parameter 2, 4 and 6 each have a contribution of approximately 1-6%, parameter 3 contributed less than 0.7% to the output variance. There are some differences in the ranking of parameter 2, 4 and 6 between the various methods.

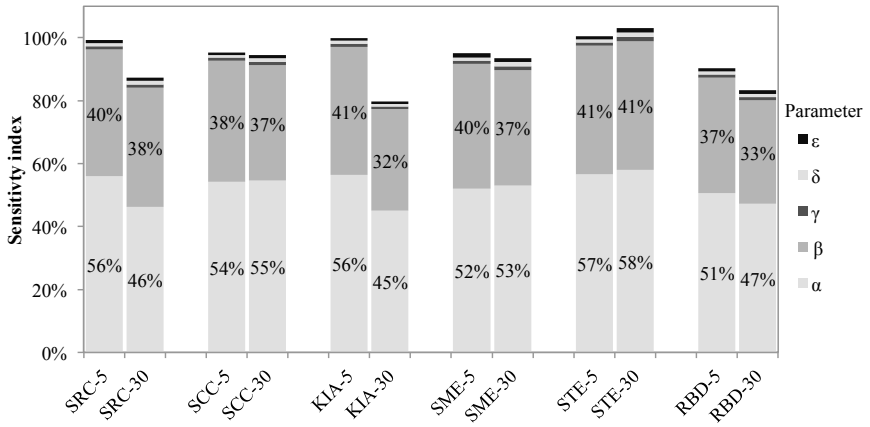

Figure 4.7: Contribution to output variance for sensitivity methods applied to study 2 (N=4096; 50 repetitions; CV=5% or CV=30%) for the sensitivity index (SRC, SCC, KIA, SME, RBD) or total sensitivity index (STE) for each parameter (α-ϵ) is shown. SRC: standardised regression coefficient; SCC: Spearman correlation coefficient; KIA: key issue analysis; SME: Sobol' main effect index; STE: Sobol' total effect index; RBD: random balance design; α: catch of whitefish; β: emission factor fuel combustion; γ: production of fuel; δ: emission factor fuel production; ϵ: fuel use.

Figure 4.7 shows the sensitivity index (III) of the five most dominant parameter in case of a parameter of dispersion of $CV = 5\%$ and $CV = 30\%$. The sensitivity indices (III) are shown only for the five most contributing parameters, because all other parameters contribute $\ll 1\%$. Although for each method, parameter α and β contributed most to the output variance, the exact contribution differed per method. All methods agreed on the much smaller contribution (around 1%) of parameter γ, δ and ϵ, although there are differences in the precise value, as well as in the ranking.

4.5 Discussion

Table 4.6 gives an indication of performance of the sensitivity methods, applied to the two case studies, under conditions of small ($CV = 5\%$) and large input uncertainties ($CV = 30\%$). The evaluation of the sampling design (I) relates to the computational effort of a sensitivity method: KIA does not make use of sampling and was fastest. RBD was faster than SRC and SCC due to the implementation of the Fast Fourier Transformation algorithm. SME and STE have to generate two sampling matrices, and therefore, were slowest. The total output variance (II) calculated with each method resulted in approximately the same output variance, except for KIA, which underestimated the output variance especially in case of high input uncertainties. The variance that is explained by each method (III) is equal to the sum of the sensitivity coefficients (IV). In case of small input uncertainties, SRC and SME performed best, whereas in case of large input uncertainties, SCC or SME in combination with STE performed best.

Table 4.6: Performance of the sensitivity methods on a scale from poor (−−), insufficient (–), neutral (0), sufficient (+) to good (++). SRC: standardised regression coefficient; SCC: Spearman correlation coefficient; KIA: key issue analysis; SME: Sobol' main effect index; STE: Sobol' total effect index; RBD: random balance design.

	SRC	**SCC**	**KIA**	**SME**	**STE**	**RBD**
Sample design (computational effort) (I)	–	–	++	−−	−−	0
Ability to calculate total output variance (II):						
Small input uncertainty (CV=5%)	++	++	+	++	++	++
Large input uncertainty (CV=30%)	++	++	−−	++	++	++
Ability to explain output variance (III) and calculate sensitivity indices (IV):						
Small input uncertainty (CV=5%)	++	+	+[4]	++	+	+
Large input uncertainty (CV=30%)	–	+	−−[4]	+	++	–

[4]Although strictly speaking, KIA explains 100% of the variance, this 100% of the variance that is calculated, which is shown to be an underestimation.

There were some limitations to the case studies that were used to evaluate the sensitivity methods. First, all parameters are assumed to be uncorrelated, which is a simplification because of lack of data. When correlations are present, including correlated inputs will increase the accuracy of the outcome of the global sensitivity analysis [Jacques et al., 2006; Xu and Gertner, 2008b]. Models with correlated inputs can be found in Xu and Gertner [2008b]) for SRC, in Jacques et al. [2006] for the Sobol' indices and in Xu and Gertner [2008a] for RBD. Second, the performance indicators in Table 4.6 are based on two case studies with two different sets of input parameters, which is limited. Other types of distributions functions or case studies with more input parameters, for example, were not considered. Third, we only considered the inventory stage in this paper. Usually, an LCA includes a midpoint or even an endpoint assessment. In general, the midpoint to inventory calculation step is assumed to be linear, but the inventory to midpoint or midpoint to endpoint relations could be nonlinear, in these cases the Sobol' methods might be preferred because it is better able to include nonlinear effects [Iooss and Lemaître, 2014; Sobol', 2001]. An illustrative example is given in [Cucurachi et al., 2014], where sensitivity indices were quantified in case of impact assessment of noise on human health, resulting in high values for STE compared to SME, illustrating the benefit of using Sobol' indices as a measure of global sensitivity.

Figure 4.8 gives an overview of the best performing methods in case of large ($CV = 30\%$) or small ($CV = 5\%$) input uncertainty and a situation being sensitive (case study 1) or not sensitive (case study 2) to small changes in the input parameters. In practice, LCAs are usually insensitive to small changes in the input parameters, because the underlying mathematical model is constructed from a set of linear equations. When restricted to the assumptions that LCAs are linear up to the midpoint assessments, SCC, SRC or KIA could be used for global sensitivity analysis. The choice for a global sensitivity method, however, also depends on: (1) data availability to the LCA practitioner; (2) the magnitude of the uncertainties in the input data, and (3) the aim of the study. If only a parameter of dispersion could be defined and not a probability distribution function, applying KIA is a feasible option, especially when input uncertainties are small. If probability distribution functions are provided, either SRC (low input uncertainties) or SCC (large input uncertainties causing outliers) are most feasible.

If the goal of the LCA is to determine whether there is a significant dif-

	Insensitive to small changes (case study 2)	Sensitive to small changes (case study 1)
Large input uncertainty (cv = 30%)	SCC	SME & STE
Small input uncertainty (cv = 5%)	SRC or KIA	SRC or KIA

Figure 4.8: Overview of the best performing methods in case of large ($CV = 30\%$) or small ($CV = 5\%$) input uncertainty and sensitive (case study 1) or not (case study 2) to small changes in the input parameters.

ference between scenarios or innovations, SRC or SCC can determine the input parameters which contribute most to the output variance and, therefore, should be known most accurately before calculating P-values. When interested in the performance of a single production system, SRC, SCC or KIA can help to indicate parameters that could contain opportunities for improvement regarding environmental performance [Heijungs, 1994]. When repeating an LCA of similar goal and scope, the input parameters that contribute only minor to the output variance according to SCC, SRC or KIA, can set to a fixed value to simplify data collection.

4.6 Conclusion

The aim of this study was two-fold: (1) to study the applicability of a number of previously suggested methods for global sensitivity analysis to LCA and (2) to compare the methods based on their ability to explain the output variance, using a number of case studies. Five methods that quantify the contribution to output variance were evaluated: standardised regression coefficient (SRC), Spearman correlation coefficient (SCC), key issue analysis (KIA), Sobol' indices (STE and SME) and random balance design (RBD). Most methods performed approximately equally well for quantifying output variance and contribution to variance of the input parameters, especially for relatively small input uncertainties. In case of large input uncertainties, methods robust to outliers such as Spearman correlation coefficient or the Sobol' indices

performed better than the other methods.

When restricted to the assumptions that quantification of environmental impact in LCAs is linear, standardised regression coefficients, Spearman correlation coefficients or key issue analysis can be used for global sensitivity analysis. The choice for one of the methods depends on the available data, the magnitude of the uncertainties in the input data and the aim of the study.

Acknowledgements

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Supplementary Material

General framework for sensitivity indices

If we consider a linear function $Y(X)$:

$$E(Y|X) = cX + c_0 \tag{4.21}$$

Then c is given by the regression coefficient (Equation (4.28)):

$$c = \frac{\text{cov}(X, Y)}{\text{var}(X)} \tag{4.22}$$

Use: $\text{var}(cX) = c^2\text{var}(X)$. The variance of Equation (4.21) is given by:

$$\text{var}\left(E(Y|X)\right) = \text{var}\left(cX + c_0\right) = c^2\text{var}(X) \tag{4.23}$$

The correlation ratio, in case of a linear function, is given by:

$$\frac{\text{var}\left(E(Y|X)\right)}{\text{var}(Y)} = \frac{c^2\text{var}(X)}{\text{var}(Y)} = \frac{\text{cov}(Y, X)^2}{\text{var}(X)\text{var}(Y)} = S_j \tag{4.24}$$

Which is equal to the squared correlation coefficient in Equation (4.30). Equation (4.24) shows that in case of a linear function, the correlation ratio, or the explained variance, is equal to the standardised regression coefficients (Equation (4.29)) and the squared correlation coefficient (4.30), without the rank transformation.

Standardised regression coefficients

The part of the output variance that is explained by the linear regression model is given by:

$$\text{var}(g) \approx \text{var}(\mathbf{Pc}) \tag{4.25}$$

Equation (4.25) can be rewritten as:

$$\text{var}(g) \approx \sum_j c_j^2 \text{var}(p_j) \tag{4.26}$$

Subsequently, we divide both sides of Equation (4.26) by the variance $\text{var}(g)$. Equation (4.26) becomes:

$$1 \approx \sum_j c_j^2 \frac{\text{var}(p_j)}{\text{var}(g)} \tag{4.27}$$

Where the unstandardised regression coefficient, found by least square fitting, equals:

$$c_j = \frac{\sum_i (p_{ij} - \bar{p}_j)(g_i - \bar{g})}{\sum_j (p_{ij} - \bar{p}_j)^2} \tag{4.28}$$

The sensitivity index is found by standardising the regression coefficient by the standard deviations of $\mathbf{P}$ and $\mathbf{g}$, and taking its square:

$$\begin{aligned} S_j^{SRC} =& \frac{\left(\sum_i (p_{ij} - \bar{p}_j)(g_i - \bar{g})\right)^2}{\sum_i (p_{ij} - \bar{p}_j)^2 \sum_j (p_{ij} - \bar{p}_j)^2} \frac{\left(\frac{1}{N-1}\sum_i (p_{ij} - \bar{p}_j)\right)^2}{\left(\frac{1}{N-1}\sum_i (g_i - \bar{g})\right)^2} \\ =& \frac{\left(\sum_j (p_{ij} - \bar{p}_j)(g_i - \bar{g})\right)^2}{\sum_i (p_{ij} - \bar{p}_j)^2 \sum_i (g_i - \bar{g})^2} \end{aligned} \tag{4.29}$$

Spearman rank correlation

The sensitivity index for the parameters are found by squaring the correlation coefficient in Equation (4.6):

$$S_j^{SCC} = r_j^2 = \frac{\left(\sum_i (p_{(i)j} - \bar{p}_j)(g_{(i)} - \bar{g})\right)^2}{\sum_i (p_{(i)j} - \bar{p}_j)^2 \sum_i (g_{(i)} - \bar{g})^2} \tag{4.30}$$

When comparing Equation (4.29) to Equation (4.30), expect for the rank transformation, the expression are exactly the same. This means that the squared standardised regression coefficient S_j^{SRC} is equal to the squared Pearson correlation coefficient.

Key issue analysis

The variance of $\mathbf{g}$ of Equation (4.9) equals:

$$\text{var}(g) = \sum_j \text{var}\left(\bar{p}_j + \frac{\partial g}{\partial p_j}\right)(p_j - \bar{p}_j) \tag{4.31}$$

Use: $\text{var}(x + c) = \text{var}(x)$ and $\text{var}(cx) = c^2\text{var}(x)$, where c is a constants, to arrive at:

$$\text{var}(g) = \sum_j \left(\frac{\partial g}{\partial p_j}\right)^2 \text{var}(p_j) \tag{4.32}$$

Dividing both sides by $\text{var}(g)$, results in:

$$1 = \sum_j \left(\frac{\partial g}{\partial p_j} \right)^2 \frac{\text{var}(p_j)}{\text{var}(g)} \tag{4.33}$$

The derivatives are determined using matrix perturbation theory [Heijungs and Suh, 2002]:

$$S_j^{KIA} = \begin{cases} \frac{\text{var}(p_j)}{\text{var}(g)} (\mathbf{B}\mathbf{A}^{-1}\mathbf{s})^2 & j \in \mathbf{A} \\ \\ \frac{\text{var}(p_j)}{\text{var}(g)} (\mathbf{s})^2 & j \in \mathbf{B} \end{cases} \tag{4.34}$$

Sobol' method

In case of variance-based methods for sensitivity analysis, Equation (4.1) is rewritten as the following ANOVA decomposition:

$$g = \bar{g} + \sum_j g_j + \sum_l \sum_{j>l} g_{jl} + \dots g_{jl..k} \tag{4.35}$$

Where the input parameters are represented by $j = 1$ to k and $l = 1$ to k and $\bar{g}$ equals the mean (or expectancy) of g. The variance of Equation (4.35) is given by ($\bar{g}$ drops out because it is a constant):

$$\begin{aligned} \text{var}(g) =& \text{var} \left(\bar{g} + \sum_j g_j + \sum_l \sum_{j>l} g_{jl} + \dots g_{jl..k} \right) \\ =& \sum_j \text{var}(g_j) + \sum_l \sum_{j>l} \text{var} g_{jl} + \dots \end{aligned} \tag{4.36}$$

Which in turn equals Equation (4.11). The sensitivity indices are found by dividing both sides of Equation (4.11) by $\text{var}(g)$:

$$1 = S_j + \sum_l \sum_{j>l} S_{jl} + \dots S_{jl..k} \tag{4.37}$$

If only variance contribution up to the first order term (or main sensitivity index) S_j is considered, Equation (4.37) reduces to:

$$S_j^{SME} = \frac{\text{var}\left(E_{p \sim j}(g|p_j) \right)}{\text{var}(g)} \tag{4.38}$$

which is the conditional variance or the *expected reduction in variance that would be obtained if parameter p_j could be fixed* [Saltelli et al., 2010]. Note that Equation (4.38) is of a similar form as Equation (4.24), which was our general framework for the sensitivity indices. When we follow the best practise approach described by Saltelli et al. [2010] for the sampling algorithms available to calculate the conditional variance, Equation (4.38) is given by Equation (4.14). The total sensitivity index (S_j^{STE}) calculates how much input parameter p_j explains of the output variance, including all possible interactions with other parameters:

$$S_j^{STE} = S_j + \sum_l \sum_{j>l} S_{jl} + \dots S_{jl..k} \tag{4.39}$$

The total sensitivity index (S_j^{STE}) equals the *expected variance that would be left if all [parameters] but [parameter p_j] could be fixed* [Saltelli et al., 2010]. The total sensitivity index is given by:

$$S_j^{STE} = \frac{E_{p\sim j}\left(\text{var}_{p_j}(g|p_{\sim j})\right)}{\text{var}(g)} \tag{4.40}$$

For example, in case of three input parameters the total sensitivity of Equation (4.39) index becomes for parameter 1:

$$S_1^{STE} = S_1 + S_{12} + S_{13} + S_{123} \tag{4.41}$$

And parameter 2:

$$S_2^{STE} = S_2 + S_{21} + S_{23} + S_{213} \tag{4.42}$$

Explaining why the sum of the total sensitivity index for an LCA model containing outliers will be: $\sum_j S_j^{STE} > 100\%$.

Random balance design

A random balance design (RBD) is an alternative to the Fourier Amplitude Sensitivity Test (FAST) [Tarantola et al., 2006]. The idea behind RBD is that the output of our model given by the identity: $\text{var}(g) = E(g^2) - E^2(g)$, can be quantified by the so-called Fourier coefficients. The theory of Fourier series states that any periodic function can be written as a sum of wave functions. For this method, we use the discrete Fourier transformation to convert an equally spaced periodic function of size N. First, a periodic sampling design is applied to the distribution functions of the input parameters in Equation (4.1). To that end, N equally spaced sample points are generated over $[-\pi, \pi]$ for each parameter p_j:

$$t_{ij} = -\pi + \frac{2\pi}{N}(i-1) \tag{4.43}$$

Subsequently, k random permutations are created and the sample points (t_{ij}) are translated to a wave. The (stratified) sample matrix equals:

$$p_{ij}^{RBD}(t_{ij}) = F_j^{-1}\left(\frac{1}{2} + \frac{1}{\pi}\arcsin(\sin(t_{ij}))\right) \tag{4.44}$$

Where F_j^{-1} corresponds to the inverse distribution function of each parameter. The output $g(p_{ij}^{RBD})$ is calculated. To calculate the output variance, the model output is expanded using the discrete Fourier transform:

$$g(p_{ij}) = \sum_{\omega=0}^{N-1} g(p_\omega) e^{\sqrt{(-1)}\pi\omega i/N} \tag{4.45}$$

And the discrete Fourier coefficients are given by:

$$g(p_\omega) = \frac{1}{N}\sum_{i=0}^{N-1} g(p_{ij}) e^{-\sqrt{(-1)}\pi\omega i/N} \tag{4.46}$$

The total variance is given by $\text{var}(g) = E(g^2) - E^2(g)$:

$$\text{var}(g) = \frac{1}{N}\sum_{i=0}^{N-1} g(p_{ij})^2 - (g(p_{\omega=0}))^2 \tag{4.47}$$

Parseval's identity is used:

$$\begin{aligned}\text{var}(g) =& \frac{1}{N^2}\sum_{\omega=0}^{N-1}|g(p_\omega)|^2 - \frac{1}{N^2}|g(p_{\omega=0})|^2 = \frac{1}{N^2}\sum_{\omega=1}^{N-1}|g(p_\omega)|^2 \\ =& \left(\frac{1}{N}\sum_{\omega=1}^{N-1}|g(p_\omega)|\right)^2\end{aligned} \tag{4.48}$$

To calculate the conditional variance for each input parameter, the model output is reordered with respect to t_i in increasing order (which is the inverse permutation): $g^j(p_{ij})$. When you look at the reordered model output$g^j(p_{ij})$, we expect for dominant parameters that they highly resemble the wave-like shape of the input parameter, as was given in Equation (4.44). This also means that the most sensitive parameters have the highest amplitude. For the conditional variance, the summation goes up to $M = 4$ [Tarantola et al., 2006], and because M is smaller than the Nyquist frequency $(N/2)$,

the conditional variance is multiplied by a factor two:

$$\text{var}\left(E_{p\sim j}(g|p_j)\right) = 2\left(\frac{1}{N}\sum_{\omega=1}^{M}|g^j(p_\omega)|\right)^2 \tag{4.49}$$

Where $g^j(p_\omega)$equals the re-ordered model output for parameter p_j. The sensitivity index is equals:

$$S_j^{RBD} = \frac{2\left(\sum_{\omega=1}^{M}|g^j(p_\omega)|\right)^2}{\left(\sum_{\omega=1}^{N-1}|g(p_\omega)|\right)^2} \tag{4.50}$$

CHAPTER 5

Ignoring correlation in uncertainty and sensitivity analysis in life cycle assessment: what is the risk?

Joint work with:
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Abstract

Life cycle assessment (LCA) is an established tool to quantify the environmental impact of a product. Incorporation of uncertainty propagation in LCA is nowadays widely acknowledged. Currently, most LCA studies that include uncertainty analysis ignore correlations between input parameters during uncertainty propagation, due to e.g. unfamiliarity with methods that include correlations or lack of data. The effect of ignoring these correlations on the output variance, however, remains unclear: it is not known if and under which conditions it can lead to erroneous conclusions. Two approaches to include correlations between input parameters during uncertainty propagation are studied: an analytical approach and a sampling approach. The use of both approaches is illustrated for an artificial case study of electricity production. Results demonstrate that that both approaches yield approximately the same output variance and sensitivity indices for this specific case study. Furthermore, we demonstrate that the analytical approach can be used to quantify the risk of ignoring correlations between input parameters during uncertainty propagation in LCA. We demonstrate that: (1) we can predict if including correlations among input parameters in uncertainty propagation will increase or decrease output variance; (2) we can quantify the risk of ignoring correlations on the output variance and the global sensitivity indices. Moreover, this procedure requires only little data regarding the input parameters.

5.1 Introduction

Life cycle assessment (LCA) is an established tool to quantify the environmental impact of a product [Curran, 2012]. The presence of uncertainty and variability around data, such as input parameters in LCA, is widely acknowledged [Lloyd and Ries, 2007; Björklund, 2002], and several studies implemented uncertainty propagation by means of, for example, Monte Carlo simulation [Lloyd and Ries, 2007; Finnveden et al., 2009; Imbeault-Tétreault et al., 2013]. Data collection for LCA is perceived as the most time consuming step [Björklund, 2002] and even if the presence of uncertainty and variability is acknowledged, data might not always be available to construct distribution functions needed for uncertainty analysis. An additional complication is the potential presence of correlations between input parameters. For example, when both fuel combustion and the corresponding emissions of CO_2 are considered as stochastic input parameters, a correlation might be present a between fuel combustion and the emissions of CO_2. Although the amount of CO_2 emissions relates directly to the carbon content of fuel, other (external) factors,

such incomplete combustion for low temperatures or quality of the fuel, can cause a presence of a correlation between the two parameters. Currently, in most LCA case studies that include uncertainty propagation, correlations between input parameters are ignored [Björklund, 2002], even though the effect of ignoring these correlations on the output variance is unclear [Bojacá and Schrevens, 2010; Wei et al., 2014]. There can be several reasons why correlations are ignored: (1) there is no data available on the correlation coefficients, (2) including correlation coefficients in uncertainty propagation complicates the subsequent uncertainty and sensitivity analysis, which is usually not available in standard LCA software, or (3) unfamiliarity with methods that include correlations during uncertainty propagation. To our knowledge, in only three studies [Cucurachi et al., 2015; Bojacá and Schrevens, 2010; Wei et al., 2014] correlations between input parameters were included.

Ignoring correlations between input parameters in the sample design, however, could lead to under- or overestimation of the output variance. This can lead to incorrect decision making regarding environmental mitigation strategies, or more tangible, to ecological or health risks [Tukker, 2002; Cowell et al., 2002]. For example, a common strategy in LCA is to look for improvement options, and to do so, two product alternatives are compared. A suitable approach is to use a *discernibility analysis* [Heijungs and Kleijn, 2001; Henriksson et al., 2015], where random drawings from two Monte Carlo runs are compared and the percentage is given how often one alternative is better than the other. If the output variance of greenhouse gas emissions of a reduction strategy is overestimated due to ignoring correlations between input parameters, this could lead to false negatives. This means the actual variance is lower and the comparison between both products would have led to different results if correlations had been taken into account. Another example concerns the application of a *threshold analysis*, where due to e.g. legal boundaries for ammonia emissions on farms or toxicity levels in soils, a certain thresholds may not be exceeded. Ignoring correlations could lead to an underestimation of the output variance and therefore it can appear that the emissions of a product remain under the threshold, while in fact they are not.

In this paper, we first show how to handle correlations between input parameters for uncertainty propagation and global sensitivity analysis in LCA, by using an analytical approach and a sampling approach. Subsequently, we demonstrate that the analytical approach can be used to quantify the risk of ignoring correlations between input parameters during uncertainty propaga-

tion in LCA, based on minimum data requirement. To this end, a hypothetical case study about electricity production is formulated on which the procedure is applied.

5.2 Methods for uncertainty propagation and global sensitivity analysis for correlated input parameters in LCA

Methods for global sensitivity analysis describe how much of the output variance can be explained by the variance of each uncertain or variable input parameter. In linear models (such as LCA), a global sensitivity index is represented by a ratio explaining how much each input parameter contributes to the output variance. For LCAs with uncorrelated input parameters, the squared standardised regression coefficients can be used as a global sensitivity index [Groen et al., 2015a; Mutel et al., 2013; Saltelli et al., 2008]. For more complicated, non-linear impact assessment methods, advanced methods such as the Sobol' method can be used [Cucurachi et al., 2015].

In case of correlated input parameters in the LCA model, the regression model no longer holds [Xu and Gertner, 2008b] and should be adjusted [Xu and Gertner, 2008b]. In this paper, matrix-based notation for LCA is introduced, followed by the corresponding notation for global sensitivity indices with correlated input parameters [Xu and Gertner, 2008b], for an analytical and a sampling approach. The analytical approach is later on used to determine criteria for ignoring correlation in LCAs.

5.2.1 Matrix-based LCA

To facilitate the use of both approaches, matrix-based LCA [Heijungs, 2002] is used, where all production processes are described in the **A**-matrix and the accompanying resource use and emissions in the **B**-matrix. To compare the analytic and stochastic approach for correlated input parameters in LCA, first an artificial case study is introduced to show how both approaches work. In this example, we will look at the production of electricity. The production of 10 kWh electricity requires 2 liter of diesel. For the production of 10 kWh electricity 1 kg CO_2 is emitted, for the production of 100 liter diesel, 10 kg

CO_2 is emitted. In matrix notation this looks like:

$$\mathbf{A} = \begin{pmatrix} 10 & 0 \\ -2 & 100 \end{pmatrix} \tag{5.1}$$

The **A** matrix contains three parameters unequal to zero. The corresponding CO_2 emissions can be given by:

$$\mathbf{B} = \begin{pmatrix} 1 & 10 \end{pmatrix} \tag{5.2}$$

The **B**-matrix contains two input parameters. In this example, we are interested in the production of 1000 kWh electricity. The functional unit is given in the **f**-vector:

$$\mathbf{f} = \begin{pmatrix} 1000 \\ 0 \end{pmatrix} \tag{5.3}$$

To calculate the total CO_2 emissions for the production of 1000 kWh electricity, the inverse of the **A** needs to be calculated:

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} = \mathbf{B}\mathbf{s} \tag{5.4}$$

Where **s** equals the scaling vector. In general, not only CO_2 emissions can be considered here, but many more emissions, but to simplify the example we used a single type of emissions turning the **B**-matrix into a row-vector **b** and the **g**-vector into a scalar g. The locations and names of the input parameters can be found in Table 5.1.

5.2.2 Including uncertainty and variability in LCA

We assumed that all the input parameters were normally distributed. To that end, we made a slight adaptation to the original matrix-based LCA notation. We now assume that the elements in the **A**-matrix and the **B**-matrix are replaced by normally distributed stochastic variables, and that the original values of the elements in the **A**-matrix and the **B**-matrix are now the means of the corresponding normal distributions. For example, this means that the first element of the stochastic **A**-matrix, is now a stochastic variable:

$$a_{11} \sim N(\mu_{A,1,1}, \sigma_{A,1,1}) \tag{5.5}$$

Table 5.1: The location of the distribution functions in the LCA model are given as a triplet: first the matrix is specified, matrix (**A** or **B**), followed by the row index (i or k), and column index (j) in **A** and **B**. The corresponding mean (μ), standard deviation (σ), and coefficient of variation (CV) of the input parameters are also given.

Element	μ	σ	$CV(\%)$
$A,1,1$	10	0.09	0.9
$A,2,1$	-2	0.23	11.5
$A,1,2$	0	0	n/a
$A,2,2$	100	12	12
$B,1,1$	1	0.15	15
$B,1,2$	10	1.2	12

The new notation, including the mean (μ), standard deviation (σ) and coefficient of variation: $CV = \frac{\sigma}{|\mu|}$, are found in Table 5.1. Furthermore, we assumed a correlation between the parameter found at $A,1,1$ and $B,1,1$; and between the parameter at $A,2,2$ and $B,1,2$ given by the Pearson correlation coefficient of $\rho_{A,1,1;B,1,1} = 0.8$ and $\rho_{A,2,2;B,1,2} = 0.9$ respectively. For example, the variance of the parameter at $A,1,1$ equals:

$$\sigma_{A,1,1;A,1,1} = \sigma^2_{A,1,1} = 0.09^2 = 0.0081 \tag{5.6}$$

And the covariance between parameter $A,1,1$ and $B,1,1$ equals:

$$\sigma_{A,1,1;B,1,1} = \sigma_{B,1,1;A,1,1} = \rho_{A,1,1;B,1,1} \cdot \sigma_{A,1,1} \cdot \sigma_{B,1,1} = 0.8 \cdot 0.09 \cdot 0.15 = 0.0108 \tag{5.7}$$

The covariance matrix ($\mathbf{\Sigma}$) has a general structure of:

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}(\mathbf{A},\mathbf{A}) & \mathbf{\Sigma}(\mathbf{A},\mathbf{B}) \\ \mathbf{\Sigma}(\mathbf{B},\mathbf{A}) & \mathbf{\Sigma}(\mathbf{B},\mathbf{B}) \end{pmatrix} \tag{5.8}$$

Where $\mathbf{\Sigma}(\mathbf{A},\mathbf{B}) = \mathbf{\Sigma}(\mathbf{B},\mathbf{A})$. This leads the the covariance matrix ($\mathbf{\Sigma}$) of:

$$\mathbf{\Sigma} = \begin{pmatrix} 0.0081 & 0 & 0 & 0 & 0.0108 & 0 \\ & 0.0529 & 0 & 0 & 0 & 0 \\ & & 0 & 0 & 0 & 0 \\ & & & 144 & 0 & 12.96 \\ & & & & 0.0225 & 0 \\ & & & & & 1.44 \end{pmatrix} \tag{5.9}$$

Our main interest lies in determining the variance of stochastic output parameter $\sigma^2(g,k)$, which can be approximated using an analytical approach $\tilde{\sigma}^2(g,k)$and a sampling approach $\hat{\sigma}^2(g,k)$.

5.2.3 Sensitivity indices for correlated input parameters

Two approaches were used to calculate the sensitivity indices, an analytical approach (represented by a tilde) and a sampling approach (represented by a hat). For the analytical and the sampling approach, the total partial variance contribution (σ_T^2) of each individual input parameter ($p \in \{(A,1,1),...(B,1,2)\}$) can be given by an uncorrelated part (σ_U^2) and a correlated part (σ_C^2):

$$\sigma_T^2(g,k;p) = \sigma_U^2(g,k;p) + \sigma_C^2(g,k;p) \tag{5.10}$$

The total ($S_T(g,k;p)$), uncorrelated ($S_U(g,k;p)$) and correlated ($S_C(g,k;p)$) sensitivity indices for the analytical and sampling approach respectively, are given by:

$$\tilde{S}_T(g,k;p) = \frac{\tilde{\sigma}_T^2(g,k;p)}{\tilde{\sigma}^2} \qquad \text{or} \qquad \hat{S}_T(g,k;p) = \frac{\hat{\sigma}_T^2(g,k;p)}{\hat{\sigma}^2} \tag{5.11}$$

$$\tilde{S}_U(g,k;p) = \frac{\tilde{\sigma}_U^2(g,k;p)}{\tilde{\sigma}^2} \qquad \text{or} \qquad \hat{S}_U(g,k;p) = \frac{\hat{\sigma}_U^2(g,k;p)}{\hat{\sigma}^2} \tag{5.12}$$

$$\tilde{S}_C(g,k;p) = \frac{\tilde{\sigma}_C^2(g,k;p)}{\tilde{\sigma}^2} \qquad \text{or} \qquad \hat{S}_C(g,k;p) = \frac{\hat{\sigma}_C^2(g,k;p)}{\hat{\sigma}^2} \tag{5.13}$$

Where $\tilde{\sigma}^2$ is equal to the *output* variance approximated up to first order by the analytical approach in Equation (5.14) and $\hat{\sigma}^2$ is estimated by the sampling approach given in Equation (5.26).

Analytical approach

The variance of Equation (5.4), including the correlations, can be given using a first order Taylor approximation [Heijungs, 2010]:

$$\tilde{\sigma}^2(g,k) \approx \overbrace{\sum_{i,j}\left(\frac{\partial(g,k)}{\partial(A,i,j)}\right)^2 \sigma^2_{A,i,j} + \sum_{j}\left(\frac{\partial(g,k)}{\partial(B,k,j)}\right)^2 \sigma^2_{B,k,j}}^{\tilde{\sigma}^2_U(g,k)}$$
$$\overbrace{+2\sum_{i,j,l,m}\frac{\partial(g,k)}{\partial(A,i,j)}\frac{\partial(g,k)}{\partial(A,l,m)}\sigma_{A,i,j;A,l,m}}^{\tilde{\sigma}^2_C(g,k)}$$
$$+2\sum_{j,m}\frac{\partial(g,k)}{\partial(B,k,j)}\frac{\partial(g,k)}{\partial(B,k,m)}\sigma_{B,k,j;B,k,m}$$
$$+2\sum_{i,j,m}\frac{\partial(g,k)}{\partial(A,i,j)}\frac{\partial(g,k)}{\partial(B,k,m)}\sigma_{A,i,j;B,k,m} \tag{5.14}$$

Where $\frac{\partial(g,k)}{\partial(A,i,j)} = \frac{\partial g_k}{\partial a_{ij}}$, etcetera. Please note that $\tilde{\sigma}^2_C(g,k)$ is equal to the last three terms in this equation. Although the analytical expression in Equation (5.14) contains a number of elements to be filled, we can already notice several things. First, there is no need to define distribution functions, only a mean and a standard deviation or variance is sufficient to propagate the input uncertainties (or variability of the input parameters) up to first order. Second, the first two elements in Equation (5.14) are equal to the output variance if no correlations were involved. Third, the effect of the correlations, given in the third, fourth and fifth element in Equation (5.14), are added to the variance. This means that given a positive or negative covariance, and the sign of the derivatives, we can derive if the output variance will decrease or increase. We come back to this in Section 5.4.2.

Sampling approach

The sampling approach for uncertainty propagation and the ensuing global sensitivity analysis consists of several steps. First, the distributions functions, means and standard deviations of the input parameters are determined, to-

gether with correlations. We assume all input parameters are normally distributed. Second, the input parameters are described as joint distributions functions, using the covariance matrix (Equation (5.9)). Third, uncertainty and variability of input parameters were propagated through the LCA model by means of Monte Carlo simulation, or alternative sampling strategy. Details can be found in the supplementary material. Subsequently, the total partial variance ($\hat{\sigma}^2_T(g,k;p)$), uncorrelated partial variance ($\hat{\sigma}^2_U(g,k;p)$) and the correlated partial variance ($\hat{\sigma}^2_C(g,k;p)$) are calculated. Finally, the sensitivity indices are calculated based on Equations (5.11) - (5.13), using Equation (5.26).

5.2.4 Quantifying the effect of correlation in uncertainty propagation

Using Equation (5.14), we can determine if a correlation between two parameters will either increase or decrease the output variance, depending on the sign of the correlation coefficient and the partial derivative. Subsequently, we can determine how much the output variance is under- or overestimated considering the correlations at hand. We return to the example given in Section 5.2.2, and we only consider the correlation between parameter at location $A,1,1$ and $B,1,1$. For reasons of comprehensibility, we removed the correlation between parameter at locations $A,2,2$ and $B,1,2$ (i.e. $\rho_{A,2,2;B,1,2} = 0$). We will use this example to determine how much the output variance is under- or overestimated as a function of the correlation coefficient ρ and the relative variance CV of the parameter at $B,1,1$ (variance of the parameter at $A,1,1$ is fixed to 0.9%). This approach is based on the work of Smith et al.[Smith et al., 1992]. The measure of under- or overestimation is given by:

$$\tilde{\eta}(CV,\rho) = \log(\tilde{\sigma}^2_U/\tilde{\sigma}^2) \qquad \text{or} \qquad \hat{\eta}(CV,\rho) = \log(\hat{\sigma}^2_U/\hat{\sigma}^2) \tag{5.15}$$

The logarithm is taken to make sure that a factor of 2 and a factor of 0.5 appear as equal.

5.2.5 Quantifying the effect of correlation on global sensitivity analysis

To quantify the effect of the correlation coefficients on the global sensitivity analysis, a comparison is made between the total sensitivity index (S_T) coming

from the correlated model (Equation 5.11) and the sensitivity index ignoring correlations ($S_{U;\rho=0}$):

$$\tilde{S}_{U;\rho=0}(g,k;p) = \frac{\tilde{\sigma}^2_{U;\rho=0}(g,k;p)}{\tilde{\sigma}^2_U} \quad \text{or} \quad \hat{S}_{U;\rho=0}(g,k;p) = \frac{\hat{\sigma}^2_{U;\rho=0}(g,k;p)}{\hat{\sigma}^2_U} \tag{5.16}$$

Where $\rho = 0$ refers to an LCA model in which there is no correlation between any two pairs of input parameters.

5.3 Comparing the analytical and sampling approach

The output variance from the analytical approach ($\tilde{\sigma}^2 = 206.7$) and the sampling approach ($\hat{\sigma}^2 = 207.2$) were almost equal. The sensitivity indices from the analytical and sampling approach are compared in Table 5.2. The derivation of the sensitivity indices of the analytical approach are described in equations (5.17) - (5.25). In the case of our example ($k = 1$), the uncorrelated partial variance of each input parameter is given by [Xu and Gertner, 2008b]:

$$\tilde{\sigma}^2_U(g,1;A,1,1) = (1-0.8^2)\left(\frac{\partial(g,1)}{\partial(A,1,1)}\right)^2 \sigma^2_{A,1,1} \tag{5.17}$$

$$\tilde{\sigma}^2_U(g,1;A,2,1) = (1-0)\left(\frac{\partial(g,1)}{\partial(A,2,1)}\right)^2 \sigma^2_{A,2,1} \tag{5.18}$$

$$\tilde{\sigma}^2_U(g,1;A,1,2) = 0 \tag{5.19}$$

$$\tilde{\sigma}^2_U(g,1;A,2,2) = (1-0.9^2)\left(\frac{\partial(g,1)}{\partial(A,2,2)}\right)^2 \sigma^2_{A,2,2} \tag{5.20}$$

$$\tilde{\sigma}^2_U(g,1;B,1,1) = (1-0.8^2)\left(\frac{\partial(g,1)}{\partial(B,1,1)}\right)^2 \sigma^2_{B,1,1} \tag{5.21}$$

$$\tilde{\sigma}^2_U(g,1;B,1,2) = (1-0.9^2)\left(\frac{\partial(g,1)}{\partial(B,1,2)}\right)^2 \sigma^2_{B,1,2} \tag{5.22}$$

Note that the uncorrelated partial variance for parameter $A,2,1$ is equal to the partial variance if no correlation had been present. The correlated partial

Table 5.2: Comparing output variance and sensitivity indices for correlated input parameters, using the analytical method (tilde) and the sampling method (hat), $N = 5000$.

Element	$\tilde{S}_T$	$\tilde{S}_U$	$\tilde{S}_C$	$\hat{S}_T$	$\hat{S}_U$	$\hat{S}_C$
$A,1,1$	0.5769	0.0020	0.5749	0.5734	0.0021	0.5713
$A,2,1$	0.0256	0.0256	0	0.0240	0.0255	-0.0016
$A,1,2$	0	0	0	0	0	0
$A,2,2$	0.0003	0.0053	-0.0050	0.0005	0.0053	-0.0048
$B,1,1$	0.9668	0.3919	0.5749	0.9671	0.3940	0.5730
$B,1,2$	0.0003	0.0053	-0.0050	0.0003	0.0053	-0.0050

variance is equal to:

$$\tilde{\sigma}^2_C(g,1;A,1,1) = \tilde{\sigma}^2_C(g,1;B,1,1) = 2\frac{\partial(g,1)}{\partial(A,1,1)}\frac{\partial(g,1)}{\partial(B,1,1)}\sigma_{A,1,1;B,1,1} + 0.8^2\left(\frac{\partial(g,1)}{\partial(A,1,1)}\right)^2\sigma^2_{A,1,1} + 0.8^2\left(\frac{\partial(g,1)}{\partial(B,1,1)}\right)^2\sigma^2_{B,1,1} \quad (5.23)$$

$$\tilde{\sigma}^2_C(g,1;A,2,1) = \tilde{\sigma}^2_C(g,1;A,1,2) = 0 \quad (5.24)$$

$$\tilde{\sigma}^2_C(g,1;A,2,2) = \tilde{\sigma}^2_C(g,1;B,1,2) = 2\frac{\partial(g,1)}{\partial(A,2,2)}\frac{\partial(g,1)}{\partial(B,1,2)}\sigma_{A,2,2;B,1,2} + 0.9^2\left(\frac{\partial(g,1)}{\partial(A,2,2)}\right)^2\sigma^2_{A,2,2} + 0.9^2\left(\frac{\partial(g,1)}{\partial(B,1,2)}\right)^2\sigma^2_{B,1,2} \quad (5.25)$$

The sensitivity indices are calculated based on equations (5.11) - (5.13). As can be seen in Table 5.2, the total (S_T), uncorrelated (S_U) and correlated (S_C) contribution of each parameter p are almost the same for the analytical and the sampling approach. Although this is what we would have expected, the exercise of deriving both methods adds to understanding how a correlated sampling approach works. However, the analytical approach has the advantage that it is less data intensive, only covariance matrix needs to be constructed and it requires only a single calculation to calculate the output variance. The main disadvantage is that there is no output distribution formed during the calculation process (e.g in the form of a histogram), as is the case for the sampling approach. As LCA is often used to compare two types of products, comparing two distribution functions can be very helpful during decision making or to

highlight similarities between products.

5.4 Risks of ignoring correlation

5.4.1 Update on notation

In Section 5.3 we showed that the analytical approach and the sampling approach resulted in approximately same results for the output variance and the sensitivity indices. Therefore, from here on we continue the notation in a more general sense, i.e. we omit the use of hat and tilde from now on, as we assume that either the analytical approach (tilde) and the sampling approach (hat) will both result in the same outcome.

5.4.2 The effect of ignoring correlation in uncertainty propagation

As mentioned in Section 5.2.3, it is possible to determine how much the output variance will increase or decrease based on the signs of the partial derivatives and covariance in Equation (5.14). In Table 5.3, we listed all the possible combinations of the partial derivatives in case of positive ($\rho > 0$) and negative ($\rho < 0$) correlations between two input parameters. The first thing we notice is that a positive correlation between two parameters does not necessarily mean that the output variance increases. But there is more to be said, both on the location of the correlations and the sign of the partial derivatives. In theory, every stochastic parameter can be correlated with any of the other stochastic parameters. In case of n model parameters, using symmetry, $(n^2 - n)/2$ potential correlations could be identified. For a small (but realistic) LCA with 250 input parameters, this is equal to 31,125 potential correlations coefficients. Collecting data on covariances of more than $30,000$ input parameters, however, would be an appalling task. But when we look at what the parameters actually represent, a great number of these correlations can be assumed zero. Each production process in the **A**-matrix (and the corresponding emissions in the **B**-matrix) is represented by a single column, it could be argued that *in most cases*, correlations appear within a column as the production processes itself are independent. For example, it can be expected that correlations either appear between an element in **A** and **B** (e.g. more fuel leads to more CO_2

Table 5.3: Effect of including correlation on the output variance of the most common partial derivatives, + means that the output variance increases when a correlation is included between two input parameters, − means that the output variance decreases when a correlation is included.

		$\frac{\partial(g,k)}{\partial(A,l,m)} < 0$	$\frac{\partial(g,k)}{\partial(B,k,m)} > 0$
$\rho > 0$	$\frac{\partial(g,k)}{\partial(A,i,j)} < 0$	+	−
	$\frac{\partial(g,k)}{\partial(B,k,j)} > 0$	−	+
$\rho < 0$	$\frac{\partial(g,k)}{\partial(A,i,j)} < 0$	−	+
	$\frac{\partial(g,k)}{\partial(B,k,j)} > 0$	+	−

emissions) or between two elements in **A** (e.g. more fertilizer input leads to higher yields); or between two elements from **B** in one column (e.g. more CO_2 emissions are associated with more N_2O emissions). Applying such rules of the thumb can decrease the amount of potential correlations to be assessed drastically. Regarding the signs of the partial derivatives, in most cases:

- The partial derivative $\frac{\partial(g,k)}{\partial(B,k,j)}$ is positive, because it is equal to the (positive) scaling factor **s** [Heijungs, 2010], which is only negative for e.g. avoided emissions;
- The partial derivative $\frac{\partial(g,k)}{\partial(A,i,j)}$ is negative, because it is equal to a negative factor multiplied with the (positive) scaling factor [Heijungs, 2010].

For all combinations of the (most common) derivatives and the sign of the correlation coefficient the effect on the output variance is given in Table 5.3.

Let us consider the example of Section 5.2.2, where we considered a positive correlation between the production of fuel (an element of **A**) and CO_2 emissions (an element of **B**). The partial derivative $\frac{\partial(g,k)}{\partial(A,i,j)}$ is negative, and $\frac{\partial(g,k)}{\partial(B,k,j)}$ is positive. Combining this with the positive correlation, means that the covariance term in Equation (5.14) will be negative and thus decrease the total output variance when the correlations were taken into account. The contour plot in Figure 5.1 shows how much we under- or overestimate the output variance, as a function of the correlation coefficient ρ and the magnitude of the CV of the parameter at location $(B, 1, 1)$. The correlation coefficient varied

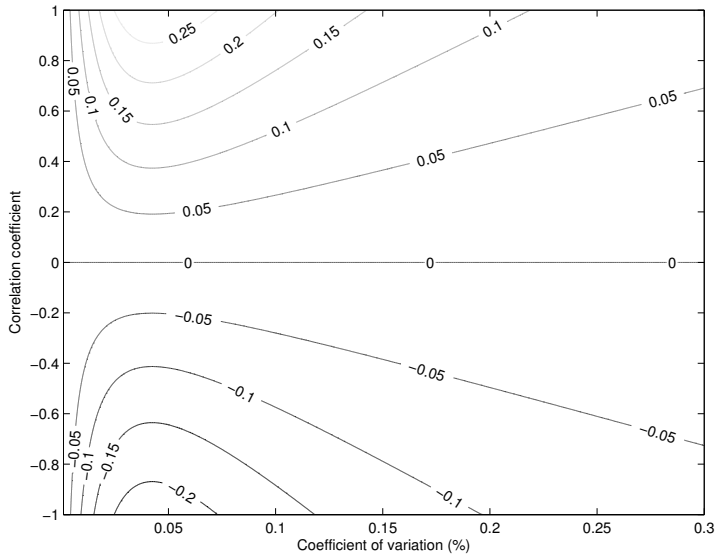

Figure 5.1: Log-ratio between output variance of an uncorrelated and a correlated model as given by Equation (5.15) as function of the correlation coefficient (ρ) and the coefficient of variation (CV) of the parameter at location $(B, 1, 1)$; $\eta = 0$: both models predict the same output variance, $\eta < 0$ output variance is underestimated when correlations are ignored; $\eta > 0$: output variance is overestimated when correlations are ignored.

between $\rho = -1$ and $\rho = 1$, the CV of the parameter at location $(B, 1, 1)$ varied between $CV = 0\%$ and $CV = 30\%$. When the correlation equals zero, both models predict the same output variance. When the values of the contour plot are negative, the output variance is underestimated when correlation is ignored. Figure 5.1 shows that there is a region on the contour map, where results are only slightly under- or overestimated, which, depending on the research at hand, could be considered as acceptable.

Figure 5.1 shows that including correlation is most important for a relatively small variance of the parameter at location $(B, 1, 1)$ ($CV \approx 4\%$) and a large correlation coefficient ($|\rho| > 0.5$). This can be explained: for a large CV of the parameter at location $(B, 1, 1)$ (i.e. CV is close to 30%), parameter $(B, 1, 1)$ becomes so dominant in explaining the variance, that the effect of the correlation with the parameter at location $(A, 1, 1)$ can be ignored. In contrast, for a very small CV of the parameter at location $(B, 1, 1)$, the parameter at location $(A, 1, 1)$ becomes more dominant in explaining the output variance, and the contribution of the parameter at location $(B, 1, 1)$ can be ignored. Only when both parameters contribute, the effect of their correlation becomes present as seen in Figure 5.1. The effect also becomes stronger when the correlation increases.

5.4.3 The effect of ignoring correlation in sensitivity analysis

Considering the effect of correlations in more detail, we look at the uncorrelated and correlated sensitivity indices (S_U and S_C). The effect of the magnitude of the correlation (ρ) and the CV on the sensitivity indices S_U and S_C is shown for the parameter at location $(B, 1, 1)$ in Figure 5.2 and Figure 5.3 respectively. The correlation coefficient ρ is varied between -1 and 1 and the CV is varied between 0 and 30%. In case of the uncorrelated sensitivity index ($S_U(B, 1, 1)$) in Figure 5.2, the contribution of this index is largest when the correlation coefficient is close to zero and the CV is relatively large (Figure 5.2). In case of the correlated sensitivity index ($S_C(B, 1, 1)$) in Figure 5.3, the contribution of this index is largest when the correlation is strong (close to -1 or $+1$) and when the CV is relatively large (Figure 5.3).

The correlated sensitivity index is negative for positive correlations and a relatively small CV ($< 10\%$), which can be explained by looking at Equation (5.23): the second and third term are alway positive, the first term is negative for positive correlations. For relatively small CV-values, the first term will

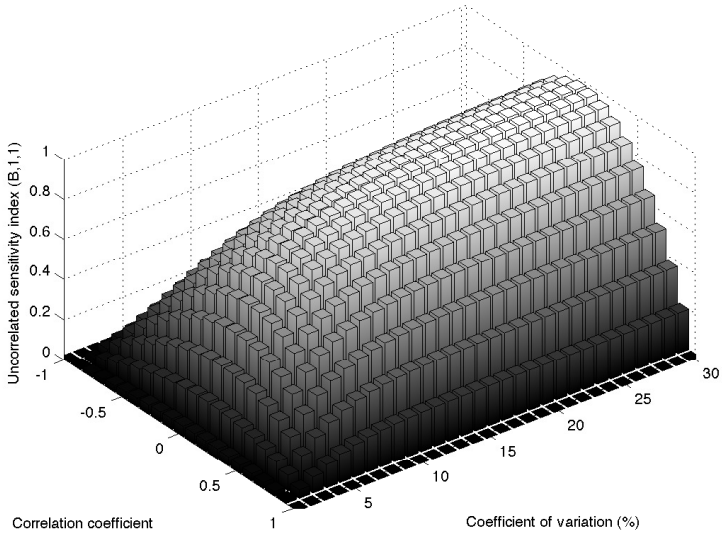

Figure 5.2: The uncorrelated sensitivity index ($S_U(B,1,1)$) as a function of the correlation coefficient (ρ) and coefficient of variation (CV).

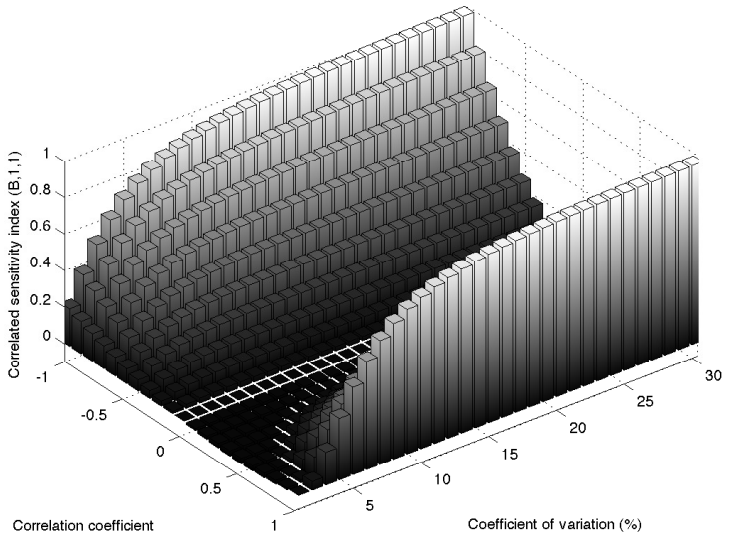

Figure 5.3: The correlated sensitivity index ($S_C(B,1,1)$) as a function of the correlation coefficient (ρ) and coefficient of variation (CV).

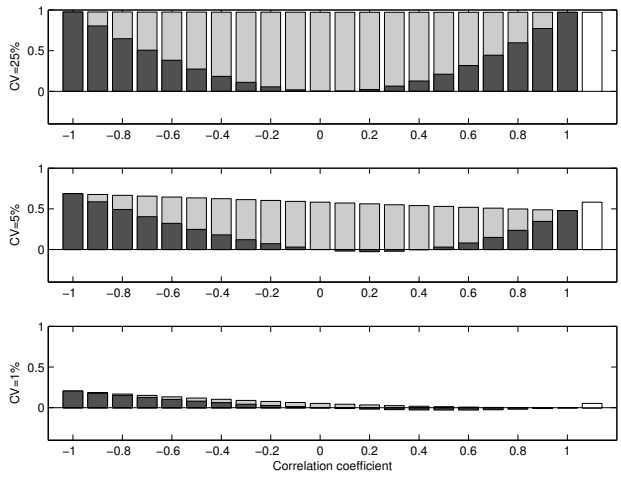

Figure 5.4: The total sensitivity index ($S_T(B,1,1)$) in light grey, the correlated sensitivity index ($S_C(B,1,1)$) in dark grey and the sensitivity index from the uncorrelated model ($S_{U;\rho=0}(B,1,1)$) in white, with a CV of 25%, 5% and 1%; CV of the parameter at location$(A,1,1)$ is 0.9 %

be larger than the second and third term combined, leading to a negative contribution of the correlated sensitivity index.

For uncertainty propagation, correlations seemed especially important for large correlation coefficients ($|\rho| > 0.5$) and for relatively small CV ($\approx$ 4%; Figure 5.1). For the global sensitivity analysis, the uncorrelated and correlated sensitivity indices contribute most for relatively large CV ($>$ 5%), which seems partly contradictory at first sight. To that end, a comparison is made between the total sensitivity index (S_T) coming from the correlated model (Equation (5.11)) and the sensitivity index ($S_{U;\rho=0}$) coming from the uncorrelated model for the parameter at location $(B,1,1)$ using Equation (5.16).

In Figure 5.4 the total sensitivity index (S_T) in light grey, the correlated sensitivity index (S_C) in dark grey and on the righthand side the sensitivity index from the uncorrelated model ($S_{U;\rho=0}$) is shown in white for a CV of 25%, 5% and 1%. Figure 5.4 shows that for a CV of 25%, the uncorrelated

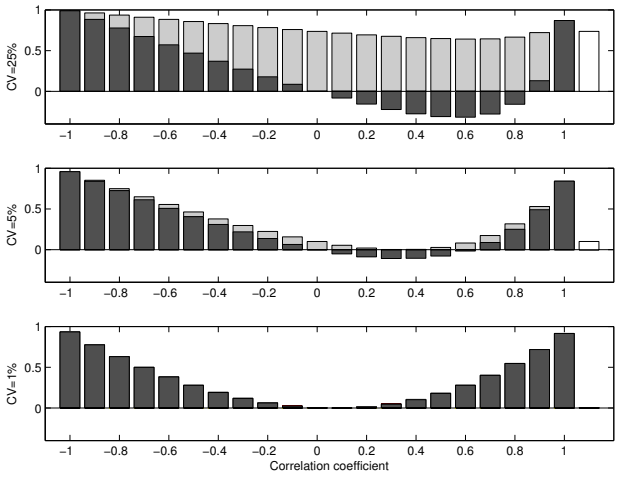

Figure 5.5: The total sensitivity index ($S_T(B,1,1)$) in light grey, the correlated sensitivity index ($S_C(B,1,1)$) in dark grey and the sensitivity index from the uncorrelated model ($S_{U;\rho=0}(B,1,1)$) in white, with a CV of 25%, 5% and 1%; CV of the parameter at location $(A,1,1)$ is 12%.

and the correlated model show the same sensitivity index, which confirms our findings from Figure 5.1. However, for a CV of 5%, the uncorrelated model overestimates the sensitivity index of the parameter at location $(B,1,1)$ for positive correlation, and underestimates the sensitivity index for negative correlation, in accordance with Figure 5.1. For a relatively small CV of 1%, the uncorrelated model overestimates the sensitivity index of the parameter at location $(B,1,1)$ for positive correlation, and underestimates the sensitivity index for negative correlation.

In Figure 5.1 and Figure 5.4, the relative variation of the parameter at location $(A,1,1)$ was relatively small: 0.9%. Figure 5.5 shows what happens when we make the parameter $(A,1,1)$ more important, i.e. the relative variation is set to 12%. In that case, the uncorrelated sensitivity index, shown by the white bar in Figure 5.5, underestimates the sensitivity indices, especially for relatively small variations of $CV = 1\%$ and $CV = 5\%$. Note also that

in Figure 5.5, by chance, the total sensitivity index for the correlated model ($\tilde{S}_T(B,1,1)$) for $\rho = 0.9$ and $CV = 25\%$ give the same result as the sensitivity index for the uncorrelated model ($S_{U;\rho=0}(B,1,1)$). This also happens for $\rho = 0.6$ and $CV = 5\%$ and is caused by overcoming the negative contribution to the correlated sensitivity index ($S_C(B,1,1)$). In case of positive correlation coefficients, the first term in Equation (5.23) will be negative and larger than the second and third term combined, leading to a negative contribution of the correlated sensitivity index.

5.5 Discussion and conclusion

Including correlations between input parameters for uncertainty propagation and global sensitivity analysis in LCA studies requires detailed knowledge about the correlation coefficients and the variances of the input parameters, which is often not available. Currently, correlations between input parameters are usually ignored, which can lead to under- or overestimation of the output variance. We described two approaches for including correlations between input parameters in LCA: an analytical approach and a sampling approach. It was shown that both approaches yielded approximately the same output variance and sensitivity indices for a specific case study. In addition, we demonstrated that the analytical approach can be used to predict an increase or decrease of the output variance when correlations between input parameters are included (Table 5.3). Ignoring correlations between input parameters in uncertainty propagation, can therefore lead to an under- or overestimation of the output variance, and affect the subsequent global sensitivity analysis. The risk of this under- or overestimation is described in Figure 5.6 for the case of a positive correlation coefficient ($\rho > 0$). Using the analytical approach we quantified the effect of ignoring correlations between input parameters on the output variance in Equation (5.14), and on the contribution to the output variance. The analytical expression of this approach required minimum knowledge of the input parameters, such as the mean and the variance of the input parameters and the correlations between the input parameters; but not about the type of distribution function. We decreased data requirement further, by describing analytical expression of this newly adapted approach as a function of the CV and the correlation coefficient between the studied parameters, which is the least possible amount of data required to predict the

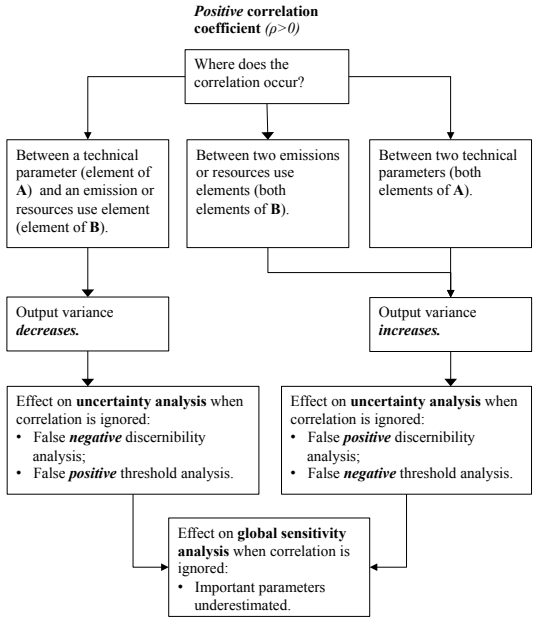

Figure 5.6: Decision tree describing the risk of ignoring correlations between input parameters on the output variance and the conclusion drawn from the subsequent uncertainty analysis, depending on the location of the correlation coefficient in the model. Results are described for a positive correlation coefficient, if the correlation coefficient is negative; the opposite of the ***bold italic*** words is true.

effect.

The matrix-based LCA model discussed in this paper, however, was only given up to the inventory phase (**g**). In the impact assessment phase that sums up emissions belonging to the same impact category, it is not included yet. For example, all greenhouse gas emissions are combined by multiplying the inventory vector **g** with the characterisation matrix **Q**. Furthermore, only normally distributed input parameters for the sampling approach were considered. As many studies in LCA considered normally distributed input parameters, this distribution type was selected over other type of distributions functions. Further research can focus on other type of distribution function. Moreover, approach as described in Equation (5.14) was only applied to a single case study. However, the method can be applied to any (matrix-based) LCA with correlated input parameters, to identify if including correlations will affect the output variance or the global sensitivity indices.

To quantify the risk of ignoring correlations between input parameters during uncertainty propagation in LCA, based on little data regarding the input parameters, we demonstrated that: (1) we can predict if including correlations among input parameters in uncertainty propagation will increase or decrease output variance; (2) we can quantify the risk of ignoring correlations on the output variance and the global sensitivity indices.

Supplementary material

This section is based on the work of Xu and Gertner [Xu and Gertner, 2008b], and is adjusted here to correspond with the terminology of the LCA model described in this paper. For the sampling approach, the total output variance was estimated by:

$$\hat{\sigma}^2(g,k) = \frac{1}{N-1}\sum_{r=1}^{N}(g_r - \bar{g})^2 \tag{5.26}$$

Where $\bar{g}$ is the mean: $\bar{g} = \frac{1}{N}\sum \hat{g}_r$, and N is the sample size. The total partial variance $\hat{\sigma}^2_T(g,k;p)$ of parameter p is estimated by [Xu and Gertner, 2008b]:

$$\hat{\sigma}^2_T(g,k;p) = \frac{1}{N-1}\sum_{r=1}^{N}(\hat{g}_r^p - \bar{g})^2 \tag{5.27}$$

and $\hat{g}_r^p$ is derived from simple linear regression. The uncorrelated partial variance $\hat{\sigma}^2_U(g,k;p)$ can be estimated by:

$$\hat{\sigma}^2_U(g,k;p) = \frac{1}{N-1}\sum_{r=1}^{N}(\hat{g}_r^{-p} - \bar{g})^2 \tag{5.28}$$

Where $\hat{g}^{-p}$ is derived from linear regression: it is based on the regression coefficients of the estimated residual g over all parameters but p.

The correlated partial variance is given by:

$$\hat{\sigma}^2_C(g,k;p) = \hat{\sigma}^2_T(g,k;p) - \hat{\sigma}^2_U(g,k;p) \tag{5.29}$$

The sensitivity indices are calculated by Equations (5.11) - (5.13), where the variance $\hat{\sigma}^2(g,k)$ is given by Equation (5.26).

CHAPTER 6

Assessing greenhouse gas emissions of milk production: which parameters are essential?

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Abstract

Life cycle assessment (LCA) studies of food products, such as dairy, require many input parameters that are often affected by variability and uncertainty. Moreover, correlations may be present between input parameters, e.g. between feed intake and milk yield. The purpose of this study was to identify which input parameters are essential to assess the greenhouse gas (GHG) emissions of milk production, while accounting for correlations between input parameters, and using a systemic approach. Three diets corresponding to three grazing systems (zero-, restricted and unrestricted grazing) were selected, which were defined to aim for a milk yield of 10,000 kg energy corrected milk (ECM) cow^{-1} $year^{-1}$. First, a local sensitivity analysis was used to identify which parameters influence GHG emissions most. Second, a global sensitivity analysis was used to identify which parameters are most important to the output variance. The global analysis included correlations between feed intake and milk yield and between N-fertiliser rates and crop yields. The local and global sensitivity analyses were combined to determine which parameters are essential. Finally, we analysed the effect of changing the most important correlation coefficient (between feed intake and milk yield) on the output variance and global sensitivity analysis. The total GHG emissions for 1 kg ECM ranged from 1.08 to 1.12 kg CO_2 e, depending on the grazing system. The local sensitivity analysis identified milk yield, feed intake, and the CH_4 emission factor of enteric fermentation of the cows as most influential parameters in the LCA model. The global sensitivity analysis identified the CH_4 emission factor of enteric fermentation, milk yield, feed intake and the direct N_2O emission factor of crop cultivation as most important parameters. For both grazing systems, N_2O emission factor for grazing also turned out to be important. In addition, the correlation coefficient between feed intake and milk yield turned out to be important. The systematic approach resulted in more parameters than previously found. By combining a local and a global sensitivity analysis, parameters were determined which are essential to assess GHG emissions of milk production. These parameters are the CH_4 emission factor of enteric fermentation, milk yield, feed intake, the direct N_2O emission factor of crop cultivation and the N_2O emission factor for grazing. Future research should focus on reducing uncertainty and improving data quality of these essential parameters.

6.1 Introduction

Due to a growing human population and changing consumption patterns, the environmental impact of food production is increasing [Gerber et al., 2013]. Dairy products, such as milk or cheese, are an important source of protein in human diets. Global protein consumption from dairy products increased

from 7 g capita^{-1} day^{-1} in 2001 to 8 g capita^{-1} day^{-1} in 2011 and is expected to increase further [FAO, 2015]. Dairy cattle across the world, however, are responsible for approximately 20% of the global greenhouse gas (GHG) emissions produced by the livestock sector, which is almost 3% (1.4 gigatonnes CO_2 e) of all anthropogenic emissions [Gerber et al., 2013]. In 2013, approximately one third of all global milk was produced in Europe [FAO, 2015]. Many studies, therefore, aimed to assess and monitor GHG emissions of European dairy production systems [Crosson et al., 2011; De Vries and De Boer, 2010; Yan et al., 2011].

At present, life cycle assessment (LCA) is a commonly accepted method to quantify GHG emissions of dairy production systems [De Vries and De Boer, 2010]. An LCA quantifies the use of resources and emissions to air, water and soil, of a product over the entire life cycle [ISO, 2006a,b]. Quantification of GHG emissions, therefore, is a single-issue LCA, also referred to as a carbon footprint analysis.

Performing an LCA of food products requires many input parameters, which are rarely easy to obtain and are often affected by natural variability and contain epistemic uncertainty [Walker et al., 2003]. Natural variability relates to observable variation, resulting from, for example, variation in weather conditions or differences in farm management, whereas epistemic uncertainty originates from a lack of knowledge about input parameters, including errors resulting from the instrument or those introduced by the observer [Walker et al., 2003]. To accurately assess and monitor GHG emissions from dairy production systems, we, therefore, need to identify sources of variability and uncertainty of input parameters and incorporate their impact in the GHG assessment.

Several studies examined the impact of natural variability [Henriksson et al., 2011; Lovett et al., 2008] or epistemic uncertainty on the GHG assessment of milk production [Flysjö et al., 2011; Gibbons et al., 2006], whereas others explored the combined impact of natural variability and epistemic uncertainties [Basset-Mens et al., 2009; Chen and Corson, 2014; Ross et al., 2014; Zehetmeier et al., 2014]. These studies, however, explored only a limited number of input parameters, and did not systematically explore all parameters, which might imply that potential essential parameters are overlooked. Moreover, abovementioned studies did not account for potential correlations between input parameters, which might result in an under- or overestimation of the output variance, and an underestimation of the most important parameters [Groen

and Heijungs, 2016].

The aim of this study is to use a systematic approach to identify which input parameters influence the GHG emissions of milk production most, and which parameters contribute most to the output uncertainty of GHG emissions while accounting for correlations between input parameters. To this end, we combined a local and global sensitivity analysis to analyse the influence of the input parameters and the effect of variability and uncertainty on the total GHG emissions of German milk production and a future milk production of 10,000 kg ECM (energy corrected milk) cow^{-1} $year^{-1}$. Flysjö et al. [2011] found that by comparing grazing systems of dairy production systems, a different set of essential parameters showed up for each grazing system. Therefore, we included three different grazing systems, based on the main grazing systems in Germany.

For these parameters, and for parameters that contained high uncertainties based on literature, we constructed distribution functions to be able to propagate uncertainties through the LCA model and apply the global sensitivity method. We combined the results of this local sensitivity analysis with a global sensitivity analysis, to determine which input parameters were essential in the LCA model of milk production.

6.2 Materials and methods

6.2.1 Milk production system

GHG emissions were analysed for model dairy production systems in Germany, from cradle-to-farm gate. A cradle-to-farm gate assessment implies that emissions are included for relevant processes up to the moment that milk left the farm gate (Figure 6.1). The production of diesel, seeds, fertiliser, lubricants, energy, feed and milk were included in the system, whereas the production of machinery, buildings, and water required for cleaning and as drinking water were excluded. We assumed a stable dairy herd, and fattening of surplus calves outside the farm.

The functional unit was 1 kg ECM (ECM: 4% fat and 3.4% protein, Spiekers et al. [2009]) leaving the farm gate. All GHG emissions were allocated to this functional unit. In case of a multifunctional production process of feed ingredients, such as production of rapeseed oil and meal, GHG emis-

sions were allocated to these multiple outputs based on their economic values (i.e. economic allocation). Economic allocation of feed ingredients is the most common method used in LCA studies for livestock products [De Vries and De Boer, 2010].

We modelled a typical German dairy system with 120 Holstein-Friesian cows. A 305-day milk production of 10,000 kg ECM was assumed, anticipating an increase in milk yield after abolition of milk quota [EC, 2009], with a dry period of 60 days. The replacement rate was 40% [Zehetmeier et al., 2012]; age at first calving was 25 months. Dairy cows and heifers were loosely housed in stables with cubicles and slatted floors, being most common in Germany, implying slurry-based manure management [Haenel et al., 2014]. During their first 60 days, calves were housed in groups, on a solid floor embedded with straw, as imposed by law [Haenel et al., 2014]. It was assumed that the slurry of all cattle is untreated and stored in a slurry tank with natural crust, which is most common in Germany [Haenel et al., 2014]. The manure produced by the cows and the replacement heifers was applied to the grassland used for the cultivation of silage, pasture and hay as well as to cropland for the cultivation of field grass silage, replacing artificial fertiliser based on N content. The share of manure applied to the grasses and crops depended on the grazing system (see below).

Emissions from crop cultivation, i.e. CO_2 emission from calcium ammonium nitrate (CAN) fertiliser and lime application, direct and indirect N_2O emissions from application of artificial fertiliser, manure and crop residues were included according to IPCC Tier 2 IPCC [2006c], using German (average) data for crop yields and N fertiliser rates and German emission factors [Haenel et al., 2014]. Approximately 23% of the CAN fertiliser is assumed to consist of CaCO3 which contributes to CO_2 emissions [Strogies and Gniffke, 2014]. The direct N_2O emissions from grazing, CH_4 and direct N_2O emissions from manure storage were included according to IPCC Tier 2, and CH_4 emissions from enteric fermentation of the cows were included according to IPCC Tier 3 [IPCC, 2006b,c], using German average data for feed content characteristics and German emission factors [Haenel et al., 2014]. CH_4 from enteric fermentation of the replacement heifers were included according to IPCC Tier 2 [IPCC, 2006b], adapted for Germany in 2014 [Haenel et al., 2014].

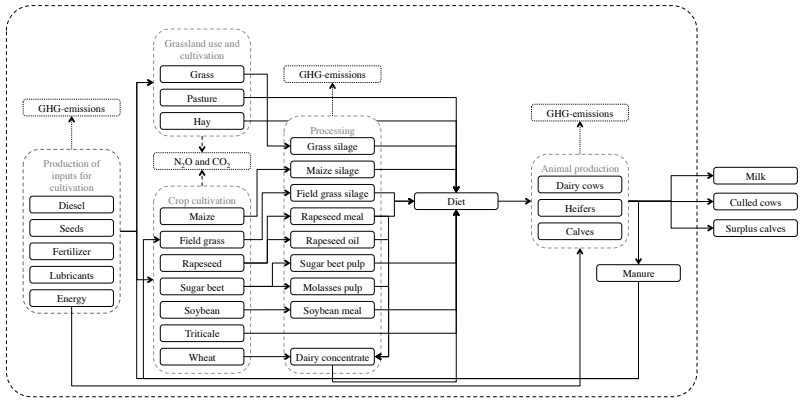

Figure 6.1: System boundaries and production processes involved in the production of 1 kg of energy corrected milk.

6.2.2 Diets

We compared three grazing systems, i.e. zero-grazing (i.e. 0 h day^{-1}; ZG), restricted grazing (i.e. 10 h day^{-1}; RG), and unrestricted grazing (i.e. 20.5 h day^{-1}; UG), grazing time from April till October (182 days year^{-1}), that reflected the most common pasture types in Germany, resulting in three distinct diets. All three diets were formulated to ensure a milk yield of 10,000 kg ECM. The diets consisted of grass-based feed ingredients, such as grass silage, pasture and hay, and crop-based feed ingredients, such as field grass silage, maize silage, beet pulp silage, soybean meal, rapeseed meal, triticale (*Triticosecale Wittm.*) and dairy concentrate (Table 6.1). The exact composition of the diets was formulated according to feed content characteristics, such as useable crude protein and net energy for lactation, based on Krauß et al. [2015].

The diets for the replacement heifers from birth to age of first calving (760 days) were calculated according to Kirchgessner et al. [2011]; Spiekers

[1]Feed intake replacement heifers: kg dry matter (760 days)$^{-1}$; dairy cows: kg dry matter year^{-1}.

[2]Rapeseed meal (32%), rapeseed oil (1%), sugar beet molasses (32%) and wheat (36%) [Spiekers et al., 2009] and is assumed to be equivalent to calf rearing fodder.

Table 6.1: Diets for dairy cows and replacement heifers in a zero-grazing (ZG), restricted grazing (RG) and unrestricted grazing (UG) system.

	Dairy cows			**Replacement heifers**	
	ZG	RG	UG	ZG	UG
Feed intake[1] (kg dry matter)	7,292	7,228	7,236	5,397	5,192
Grassland based feed, except pasture (%)	27	15	14	53	34
Pasture (%)	0	22	38	0	28
Field grass silage (%)	11	8	6	-	-
(High quality) maize silage (%)	26	21	13	43	34
Sugar beet pulp (%)	7	4	4	-	-
Soybean meal (%)	1	1	1	-	-
Rapeseed meal (%)	6	5	3	-	-
Triticale (%)	5	11	14	-	-
Dairy concentrate[2] (%)	16	13	8	4	4

et al. [2009]; Weiß et al. [2011]. They covered a daily gain of at least 700 g body weight per day. Based on a combination of dry matter intake, need for metabolised energy and raw protein, two diets were formulated for the replacement heifers. One diet was formulated for replacement heifers that are housed indoor the whole year around. These heifers are assumed to replace dairy cows in the ZG system. The second diet was formulated for replacement heifers having unrestricted pasture access in summer. These heifers are assumed to replace dairy cows in both the RG and UG system. The feed intake for replacement heifers until the first calving is presented in Table 6.1.

6.2.3 Use of matrix formulation to assess GHG emissions

To facilitate the local and global sensitivity analyses, we used a matrix-based approach commonly applied in LCA calculations (for more detail see Heijungs and Suh [2002]). In matrix notation, each individual production process (e.g. the production of 1 kg fertiliser) is represented as a column in the technology matrix **A**. Parameters that are given in **A** are referred to as technical parameters. The accompanying resource use and emissions, in this case the GHG emissions corresponding to the amount of fertiliser produced in the **A**-matrix, are found in the supporting matrix **B**. The production processes are linked to each other, e.g. production of seeds is used for the production of

one kg of sugar beets. The **A**-matrix is scaled to produce the amount defined as the functional unit (**f**); likewise the **B**-matrix is scaled to quantify the total resource use and emissions (**g**):

$$\mathbf{g} = \mathbf{B}\mathbf{A}^{-1}\mathbf{f} \tag{6.1}$$

Subsequently, the impact category totals are quantified by multiplying the **g**-vector with the characterisation factors:

$$\mathbf{h} = \mathbf{Q}\mathbf{g} \tag{6.2}$$

In our case, **Q** contains the characterisation factors of GHG emissions for global warming potential (GWP) on a 100-year time interval: carbon dioxide (CO_2), biogenic methane (CH_4, bio): 28 kg CO_2 e/kg methane, fossil methane (CH_4, fossil): 30 kg CO_2 e/kg methane; and nitrous oxide (N_2O): 265 kg CO_2 e/kg nitrous oxide [Myhre et al., 2013]. Because we only consider GHG emissions, as this is a single-issue LCA, **Q** is reduced to a row vector $\mathbf{q}'$ and the scalar gives the total amount of GHG emissions expressed in CO_2 e/kg ECM.

6.2.4 Quantifying the effect of uncertainty

Sensitivity analysis

In general, a distinction can be made between two types of sensitivity analysis: a local and a global sensitivity analysis [Saltelli et al., 2008]. A local sensitivity analysis looks at small changes around the original input values (or default values) and assesses the effect of those small changes on the output. Parameters that influence the output most are referred to as the most *influential* (Figure 6.2) input parameters. A local sensitivity analysis requires only information about the mean; information of the uncertainty around the input parameters is not needed. In LCA, a local sensitivity analysis can be quantified by means of the multiplier method (MPM). MPM was first introduced by Heijungs [1994] and is applied in LCA [Groen et al., 2015b; Jung et al., 2014; Wei et al., 2014]. A global sensitivity analysis decomposes the output variance to the individual input parameters. It can be used to assess which parameter contributes most to the output variance, which are referred to as the most *important* (Figure 6.2) input parameters. To apply a global sen-

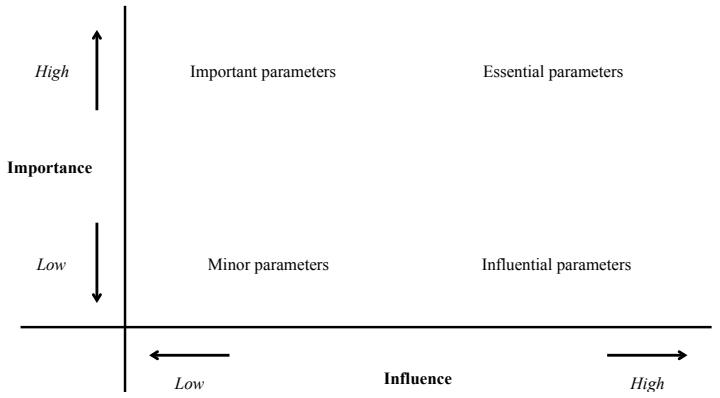

Figure 6.2: Framework for combining MPM and MEE. The horizontal axis shows the influence of input parameters, the vertical axis shows the importance of input parameters. Parameters that are both influential and important are shown in the top right corner (essential parameters) (Figure from Groen et al. [2015b]). Originally adapted from Heijungs [1996].

sitivity analysis, full knowledge of the input parameters is required, in the form of probability density functions. In LCA, the most common method for global sensitivity analysis is calculating the standardised regression coefficients [De Koning et al., 2010; Geisler et al., 2005; Mutel et al., 2013]. As we will consider correlated input parameter, we will use standardised regression coefficients for correlated parameters as described in general by Xu and Gertner [2008b] and applied in LCA by Wei et al. [2014] and Groen and Heijungs [2016]. Figure 6.2 illustrates influence and importance of input parameters and shows that parameters that influence the output most and contribute most to the output variance are the most *essential* input parameters.

Because we were unable to determine distribution functions for all input parameters, a local sensitivity analysis was performed first, to capture the most influential parameters in the model. For the parameters that were most influential, and for parameters that contained high uncertainties based on literature, we constructed distribution functions to be able to propagate uncertainties through the LCA model and apply the global sensitivity method.

Local sensitivity analysis

MPM quantifies the effect of a small change around the default value of each input parameter in **A** or **B** on h [Heijungs, 2010]. The partial derivatives $\frac{\partial(h,m)}{\partial(A,i,j)}$ and $\frac{\partial(h,m)}{\partial(B,i,j)}$ are normalised with respect to their original value A_{ij} and B_{kj}, where A_{ij} and B_{kj} are elements of **A** and **B** respectively. The normalised partial derivatives are called multipliers, and are used as estimators of local sensitivity around each input parameter. The multipliers equal:

$$\eta(h,m;A,i,j) = \frac{A_{ij}}{h_m}\frac{\partial(h,m)}{\partial(A,i,j)} \tag{6.3}$$

$$\eta(h,m;B,k,j) = \frac{B_{kj}}{h_m}\frac{\partial(h,m)}{\partial(B,k,j)} \tag{6.4}$$

The expression of the multipliers in Equation (6.3) and (6.4) can be found in Heijungs [2010]. The multipliers in these equations can be interpreted as the relative effect of a marginal increase (i.e. 1%) of each input parameter. For illustrational purposes, we will also use the absolute effect, given by: $|\eta|$.

Global sensitivity analysis

The global sensitivity analysis consists of five steps: (1) determine distribution function of input parameters, which is explained in Section 6.2.5; (2) determine correlations between input parameters, also explained in Section 6.2.5; (3) propagation of uncertainty through the LCA model using Monte Carlo simulation with a correlated sampling design; (4) determine the output variance; and (5) determine the contribution to the output variance (i.e. global sensitivity analysis) using standardised regression coefficients corrected for correlated input parameters. Step 3 to 5 are described in detail below.

Uncertainty propagation for correlated input parameters (step 3) We made use of a correlated sampling design that also allowed us to incorporate a covariance matrix. Based on the covariance matrix, the random values are drawn from the distribution functions described in Section 6.2.5, preserving the correlations between the input parameters. For each run, a random number is drawn for each input parameter and the output is calculated according to Equation (6.2).

Determine the output variance (step 4) Based on the uncertainty propagation, a distribution function of the output h is generated. The sampled output

h contains N response values, the sampling matrix contains $N \times k$ random values, where $i = 1$ to N is the sample size and $p = 1$ to k are the amount of input parameters. The output variance $\hat{\sigma}_h^2$ is calculated as:

$$\hat{\sigma}_h^2 = \frac{1}{N-1} \sum_{i=1}^{N} (h_i - \overline{h})^2 \tag{6.5}$$

Where $\overline{h}$ is the mean: $\overline{h} = \frac{1}{N} \sum_{i=1}^{N} h_i$.

Determine the contribution to the output variance (step 5) We calculated the standardised regression coefficients adjusted for correlated input parameters, based on the paper of Xu and Gertner [2008b]. The main idea behind this theory is that the total partial variance ($\hat{\sigma}_T^2(h;p)$) caused by parameter p can be split into an uncorrelated (U) and a correlated (C) part:

$$\hat{\sigma}_T^2(h;p) = \hat{\sigma}_U^2(h;p) + \hat{\sigma}_C^2(h;p) \tag{6.6}$$

Based on Equation (6.6), the total partial variance is estimated first; the correlated partial variance ($\hat{\sigma}_C^2(h;p)$) can be estimated by subtracting the uncorrelated partial variance from the total partial variance (see Groen and Heijungs [2016] for more detail). The total sensitivity index is given by:

$$\hat{S}_T(h;p) = \hat{\sigma}_T^2(h;p) / \hat{\sigma}_h^2 \tag{6.7}$$

Also, the correlated and the uncorrelated sensitivity index can be calculated, but they are not discussed in this paper.

6.2.5 Uncertainties in input data

Determine distribution functions of input parameters

Both the technical parameters in **A** and the GHG emissions in **B** contain uncertain input parameters. Based on the local sensitivity analysis, we implemented distribution functions for 33 input parameters. Distribution functions related to crop cultivation were constructed for:

- Artificial N-fertiliser rates for all feed ingredients (Table 6.2);
- Yield per ha of all feed ingredients (Table 6.2);

- Emission factors of direct and indirect N_2O emissions due to application of artificial N fertiliser (Table 6.3);
- Emission factors of direct and indirect N_2O emissions due to application of manure (Table 6.3);
- Emission factors of direct and indirect N_2O emissions from crop residues (Table 6.3);
- Emission factors of direct N_2O emissions due to application of manure during grazing (only for RG and UG).

Distribution functions related to animal production were constructed for:

- Dry matter feed intake cow^{-1} year^{-1} (Table 6.4);
- Milk production cow^{-1} year^{-1} (Table 6.4);
- Annual replacement rate (Table 6.4);
- Emission factor of CH_4 emissions from enteric fermentation of cows and replacement heifers (Table 6.3);
- Emission factor of CH_4 emissions from the storage of manure of cows and replacement heifers (Table 6.3).

The mean and standard deviation of the yields and N-fertiliser rates for all crops, except soybeans, were obtained from KTBL [2015]. Mean and standard deviation of soybean, which we assumed to originate from Brazil, were based on Garcia-Launay et al. [2014]. KTBL [2015] only provided data for low, medium and high yields for the feed ingredients as well as fertiliser rates; we interpreted the data for low and the high production of crops as the 95% confidence interval and assumed a normal distribution (Table 6.2).

The mean and the standard deviation from emission factors of crop cultivation (i.e. direct and indirect N_2O emissions from application of artificial fertiliser, manure and crop residues), direct N_2O emissions from grazing, CH_4 and direct N_2O emissions from manure storage and CH_4 emissions from enteric fermentation were included according to ranges given by IPCC Tier 3, adapted for Germany in 2014 [Haenel et al., 2014] (Table 6.4).

[3]Based on KTBL [2015] and Garcia-Launay et al. [2014], adapted for a normal distribution.
[4]Based on KTBL [2015] and Garcia-Launay et al. [2014], adapted for a normal distribution.

Table 6.2: Mean and standard deviation of crop yields, N from fertiliser. The distributions functions are assumed to be normal [Haenel et al., 2014]

	Yield (kg dry matter ha^{-1}) Mean[3] (std. dev)	**Artificial fertiliser** (kg N ha^{-1}) Mean[4] (std. dev)
Grassland:		
Grass silage	8,663 (1,455)	169 (34)
Pasture	10,170 (1,699)	162 (34)
Hay	7,756 (1,464)	109 (26)
Cropland:		
(High quality) maize silage	14,500 (1,276)	197 (17)
Field grass silage	14,632 (862)	201 (24)
Sugar beet	14,100 (1,199)	108 (11)
Triticale	5,146 (877)	89 (15)
Soybean	2,400 (112)	9 (2)
Rapeseed	3,159 (323)	119 (11)
Wheat	30,624 (3,906)	197 (26)

Variation of dry matter feed intake cow^{-1} $year^{-1}$ was assumed to be $\pm 5\%$, reflecting health issues among cows of one breed, housing and weather conditions [Gruber et al., 2004]. We assumed that the variation of the dry matter feed intake corresponded to a 2.5–97.5% interval of a normal distribution; hence the coefficient of variation ($CV = \sigma/\mu$) equalled approximately 2.5% for all grazing systems, and was used to calculate the standard deviation (Table 6.4). We assumed that the composition of the diets, however, remained fixed. The variation around milk yield was assumed to be $\pm 7\%$, due to genetic variations [Veerkamp et al., 2000]. We assumed the variation of milk cor-

[5]We used emission factors (EFs) according to Haenel et al. [2014], which mostly relies on IPCC [2006a], representing country specific data for Germany. However, the EF for leaching (0.025 kg N_2O-N (kg N)$^{-1}$ [IPCC, 2006a]) seems to be rather high compared to the new value of 0.0075 kg N_2O-N (kg N)$^{-1}$ [IPCC, 2006c]. IPCC [2006c] argues that EF has been changed because the EF for groundwater and surface drainage as well as the EF for rivers was too high. We decided to use the latter factor, as this EF is also used in the comparable studies of Chen and Corson [2014]; Flysjö et al. [2011]; Ross et al. [2014].

[6]ZG – zero-grazing system

[7]RG – restricted grazing system

[8]UG – unrestricted grazing system

[9]Based on Gruber et al. [2004].

Table 6.3: Mean and (standard deviation) of the emissions factors regarding crop cultivation, manure storage and enteric fermentation of the cows and replacement heifers; n.a: not applicable; DM: dry matter.

Emission factor	**Crop cultivation**	**Manure storage**	**Enteric fermentation**
	Mean (std. dev)	Mean (std. dev)	Mean (std. dev)
Direct N_2O (%)	0.0125 (0.0051)	0.005 (0.003)	n.a.
Indirect N_2O, leaching (%)	0.0075 (0.0088)[5]	n.a.	n.a.
Indirect N_2O, deposition (%)	0.01 (0.005)	n.a.	n.a.
Direct N_2O of N excreted (%)	0.02 (0.02)		
CH_4 (kg CH_4/ kg N excreted)	n.a.	ZG[6]: 0.18 (0.037)	
		RG[7]: 0.15 (0.031)	
		UG[8]: 0.12 (0.024)	
CH_4 (kg CH_4/ kg DM feed)	n.a.	n.a.	0.021 (0.0043)

Table 6.4: Mean and standard deviation of feed intake, milk yield and replacement rate of three grazing systems; ZG: zero-grazing, RG: restricted grazing; UG: unrestricted grazing; DM: dry matter; ECM: energy-corrected milk.

	Feed intake	**Milk yield**	**Replacement rate**
	(kg DM cow^{-1} $year^{-1}$)	(kg ECM cow^{-1} $year^{-1}$)	(%)
	Mean[9] (std. dev)	Mean (std. dev)	Mean (std. dev)
ZG	7,292 (186)	10,036 (345)	0.4 (0.051)
RG	7,228 (184)	10,068 (322)	0.4 (0.051)
UG	7,236 (185)	10,042 (322)	0.4 (0.051)

responded to a 2.5–97.5% interval of a normal distribution; the coefficient of variation equalled approximately 3.5% for all grazing systems (Table 6.4). The variation around the replacement rate was assumed to be $\pm$10% [Zehetmeier et al., 2012]. We assumed the variation of the replacement rate corresponded to a 2.5–97.5% interval of a normal distribution; the coefficient of variation

equalled approximately 13% (Table 6.4). Furthermore, a maximum replacement rate of 50% was assumed to be an unrealistic model output, because we assumed that raising of own replacement heifers imply a maximum of replacement rate of 50%. Random values drawn higher than 50% in the Monte Carlo simulation were therefore removed.

Determining dependencies and correlations

Before we can propagate the uncertainties through the LCA model, we first need to take into account that there might be dependencies between input parameters and correlations between the variances around the input parameters (step 2 of the global sensitivity analysis). In this study we made a distinction between three types of dependencies:

1. A proportional relation was assumed between feed intake and manure production [Haenel et al., 2014] because the diet composition remained fixed. For example, if feed intake increased by 5%, manure production of the dairy cow also increased by 5%. The feed intake of the replacement heifers was assumed fixed; therefore, no such relation was applied.

2. The equations for the emissions for crop cultivation of the IPCC, i.e. the direct and indirect N_2O emissions, were also implemented in the sample design. For example, the sampled values of the crop yields were used to calculate the direct N_2O emissions of the crops.

3. We included a correlation between the N-fertilisation rate and crop yield. We took data from KTBL [2015]; LEL [2014], and found a correlation of $\rho = 1$ between all crop yields and fertiliser applications. In addition, we assumed a correlation between feed intake and milk production, because the milk production depends on the intake of useable crude protein and net energy with feed. A correlation of $\rho = 0.5$ [Henriksson et al., 2011] between the dry matter feed intake and milk production was included. However, the emission factors of the N_2O emissions of crop cultivation and grazing are still assumed to vary independently from the N fertilisation and crop yield, because the emission factors also depend on other factors, such as the N content of crop residues, soil type and weather conditions. Also, the N_2O and CH_4 emission factors from manure management and enteric fermentation varied independently from

the amount of manure and the feed intake, because the emission factors did not only depend on the amount of manure, but also on other external factors such as climate conditions [IPCC, 2006b].

In theory, correlations may appear between all input parameters that vary, but we assumed that correlations only appear between parameters of the same part of the dairy production systems, so only between parameters belonging to crop cultivation (Table 6.2) and animal production (Table 6.4). The replacement rate and the milk yield were not correlated, because we already assumed a replacement rate that is related to the milk yield of 10,000 kg ECM cow^{-1} year^{-1} and the breed of Holstein Friesian. The variation of the milk yield was too small to find a valid correlation between milk yield and replacement rate in the literature.

The effect of correlation on uncertainty analysis and global sensitivity analysis

Data regarding the correlation coefficient between N-fertiliser rate and crop yield, and between dry matter feed intake and milk yield, came from different sources than the mean values of the parameters, and were therefore not considered adequate. Therefore, we determined the effect of changing the correlation coefficient between the most important parameters, on the uncertainty propagation and the sensitivity index. The effect of changing the correlation coefficient on the output variance and the global sensitivity index is described in Section 6.3.5. Details of this method are described by Groen and Heijungs [2016]. The measure of over- or underestimation of the correlation coefficient on the variance is given as:

$$\eta = \frac{\hat{\sigma}_U^2}{\hat{\sigma}_h^2} \tag{6.8}$$

Where $\hat{\sigma}_U^2$ is the variance from the LCA model that ignored correlations between input parameters and $\hat{\sigma}^2$ is the variance from the LCA model that included correlations between input parameters, as was given in equation (6.5). Furthermore, the sensitivity index from the LCA model that ignored correlations is equal to:

$$\hat{S}_{U;\rho=0}(h;p) = \hat{\sigma}^2_{U;\rho=0}(h;p)/\hat{\sigma}^2_U \tag{6.9}$$

Where $\hat{\sigma}^2_{U;\rho=0}(h;p)$ is the partial variance of parameter p, and $\rho = 0$ refers to an LCA model in which there is no correlation between any two pairs of input parameters [Groen and Heijungs, 2016].

6.3 Result and discussion

6.3.1 Greenhouse gas emissions of milk production

The total GHG emissions for 1 kg ECM for the ZG diet were 1.08 kg CO_2 e. For the RG system, 1.12 kg CO_2 e was emitted and for the UG system, 1.11 kg CO_2 e was emitted per kg ECM.

These results are in line with figures found in the literature for comparable milk yields and grazing systems in Germany. The GHG emissions per kg ECM found in our study, for example, are 15% higher than found by Zehetmeier et al. [2014] and 5% higher than found by Zehetmeier et al. [2012]. Compared to results from other European studies with similar milk yields and grazing systems, e.g. Ross et al. [2014], the results found in our study are similar when an average milk yield for one grazing system is assumed. The differences can be explained by several reasons. We for example used the new equivalency factors for the GWP as published by Myhre et al. [2013]. When equivalency factors from IPCC [2007] were used, the GHG emissions were reduced by 1-6%, depending on the grazing system (ZG 1.07 kg CO_2 e, RG 1.05 kg CO_2 e, 1.06 kg CO_2 e). In addition, our study is based on German average data for the crop yields and fertiliser rates, which include e.g. a wide range of soil types and efficiencies for the crop yields. Comparable studies are usually based on actual data from experimental farms, which can be assumed to be more efficient and developed than the average German farm.

The relative contribution of single parts of the production process to GHG emissions is shown in Figure 6.3. Enteric fermentation of cows and replacement heifers is responsible for approximately 50% of the total GHG emissions. This percentage is in line with results from other studies dealing with zero-grazing systems [Ross et al., 2014; Zehetmeier et al., 2014]. All processes belonging to the production of feed add up to 23% of the GHG emissions in our study. The auxiliary emissions mainly originated from the production of the crop inputs (production of CAN, P_2O_5 and K fertiliser) and on-farm electricity use.

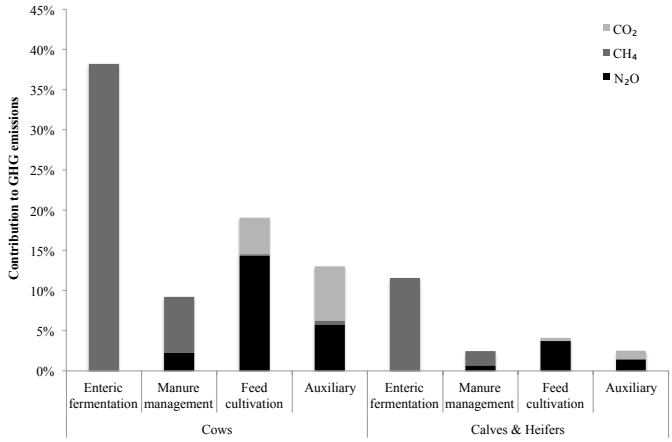

Figure 6.3: Relative contribution of GHG sources to GHG emissions of 1 kg energy corrected milk in a zero-grazing system.

Of the total GHG emissions, 59% consists of CH_4 emissions, 28% of N_2O emissions and 13% of CO_2 emissions. These results reflect the figures found in the literature, accordingly, the contribution of CH_4 emissions vary from 46%- 63% [Flysjö et al., 2011; Henriksson et al., 2011], the contribution of N_2O emissions vary from 19% - 35% [Henriksson et al., 2011; Ross et al., 2014] and the share of CO_2 emissions from 10% - 24% [Basset-Mens et al., 2009; Ross et al., 2014].

The relative contributions of the other two grazing systems (RG and UG) follow a similar pattern as the ZG system. Other studies also show relatively small differences between GHG emissions related to different grazing systems [Flysjö et al., 2011; Ross et al., 2014]. The reason for the resemblance between our results is that the emissions from crop cultivation (higher in a ZG system), are interchanged for the direct N_2O emissions from excreta during grazing in RG and UG grazing systems.

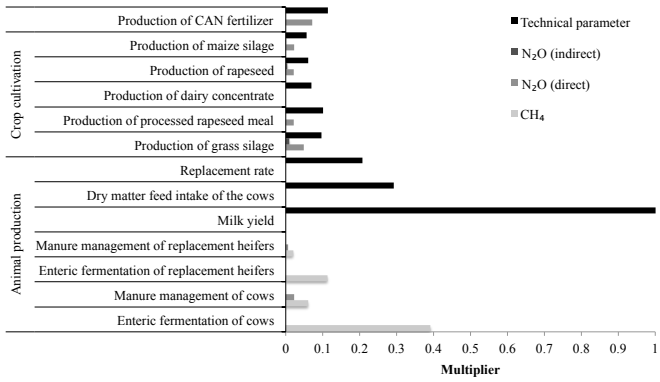

Figure 6.4: Multipliers of the most influential parameters ($|\eta| > 0.05$) and their corresponding emissions, for cows in a zero-grazing system

6.3.2 Local sensitivity analysis

Figure 6.4 shows the multipliers for the most influential parameters in the LCA model for a ZG system. Apart from milk yield, CH_4 emissions from enteric fermentation and dry matter feed intake of cows are the most influential parameter in the LCA model; increasing methane emissions due to enteric fermentation of the cows by 1% will increase the GHG emissions by 0.39%. The second most influential parameter is dry matter feed intake; increasing feed by 1% (while keeping the same milk production) will increase the GHG emissions by 0.29%. Crop yields also stand out as relative influential parameters. The N_2O emissions from crop cultivation, however, are less influential.

For the RG and UG system, the results were the same, apart from the components of the feed: especially for the UG system the yield and the N_2O emissions from the pasture became more important. The results are shown in the supplementary material, Figure 6.8 and 6.10.

The only study which is comparable to our approach of the local sensitivity analysis is the one-at-a-time approach of Flysjö et al. [2011].That study, however, only includes five technical parameters and four emission factors, which are varied within different ranges (e.g. an increase of 10%, 20% and 100%). To make their results comparable to ours, we recalculated their re-

sults to an increase of 10%, assuming a linear behaviour of the parameters. In Flysjö et al. [2011], the most influential parameter is dry matter feed intake, followed by the emission factor of the enteric fermentation, and the emission factor for direct N_2O emissions from N in excreta deposited during grazing. The system reflects a UG system and is in line with our results for a UG system. However, since our study included all parameters in the local sensitivity analysis, also replacement rate and crop yields turned out to be influential. The MPM method, therefore, facilitated ranking and comparing the influence of all input parameters.

Based on the results of the local sensitivity analysis, combined with knowledge from literature, 25 technical parameters and 8 emission factors were selected for the subsequent global sensitivity analysis. The technical parameters that were selected consisted of 11 N-fertiliser rates and 11 crop yields; replacement rate, feed intake and milk yield. The emission factors that were selected consisted of: the emission factor of direct and indirect N_2O emissions from cultivation, N_2O emissions from manure excretion during grazing, N_2O and CH_4 emissions of manure storage and CH_4 emission factor of enteric fermentation of the cows. Details on the uncertainty around these input parameters are described in Section 6.2.5. Although not all emission factors showed up as influential in Figure 6.4 (e.g. direct and indirect N_2O emissions from crop cultivation), based on literature [Basset-Mens et al., 2009; Chen and Corson, 2014; Flysjö et al., 2011] these parameters were found important and therefore included.

6.3.3 Global sensitivity analysis

Uncertainty propagation

The mean and standard deviation of the GHG emissions per kg of ECM for the three grazing systems resulting from the Monte Carlo simulation can be found in Table 6.5.

To compare our results of the uncertainty analysis with other studies, we calculated the relative variation by dividing the standard deviation by the mean value. We found a *CV* between 12% (RG) and 13% (ZG and UG). This is in line with relative variations found by Flysjö et al. [2011] with 16% (RG,

[10]The sample size was lower than 5000 because in 125 of the Monte Carlo runs, a value for the replacement rate higher than 0.5 was drawn and these runs were excluded from further analysis.

Table 6.5: Mean and standard deviation of the GHG emissions per kg ECM for zero-grazing (ZG), restricted grazing (RG) and unlimited grazing (UG).

	ZG (N=4875)[10]	**RG**	**UG**
Mean (kg CO_2 e/kg ECM)	1.08	1.12	1.11
Standard deviation (kg CO_2 e/kg ECM)	0.14	0.14	0.15

Sweden) and Lovett et al. [2008] with 15%-16% (RG and UG, Ireland). But rather high when compared to the 7% found by Basset-Mens et al. [2009], the 9% found by Henriksson et al. [2011] and the 4%-9% found by Zehetmeier et al. [2014]. However, as each study is based on a different set of parameters included in the uncertainty propagation the comparison should be treated with care.

Contribution to variance

Figure 6.5 shows the total sensitivity indices ($\hat{S}_T$), of the parameters that contribute most to the output variance. The variance of emission factor of CH_4 emissions from enteric fermentation, followed by direct N_2O emission factor of crop cultivation, milk yield, dry matter feed intake, yield and N fertilizer rate of grass silage, and indirect N_2O emission factor of leaching, contributed most to the output variance. The replacement rate, CH_4 and N_2O emission factor from manure the cows were less important. CH_4 from enteric fermentation of the replacement heifers were also less important.

For the RG and UG systems a similar result was found. Only the N_2O emissions from the pasture contributed more to the output uncertainty than the other feed components. The results are shown in the supplementary material (Figure 6.9 and 6.11).

That only a couple parameters show up as important is in line with earlier work [Heijungs et al., 2005]. We identified four studies that performed a (variant of a) global sensitivity analysis for dairy production systems. Basset-Mens et al. [2009] and Ross et al. [2014] calculated the (standardised) regression coefficients (not the squared standardised regression coefficients, which can be used to explain the output variance), so we could only compare their results based on the ranking of the parameters, and not on how much the parameters explained. Basset-Mens et al. [2009] concluded that dry matter feed intake, excreta during grazing and CH_4 emissions of enteric fermentation were most

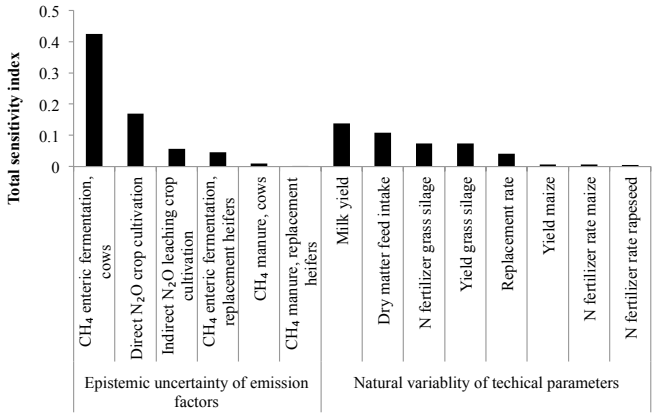

Figure 6.5: Parameters that explain most of the output variance, given by the total sensitivity index ($\hat{S}_T$, for cows in a zero-grazing system. Only parameters that explain more than 0.001 are shown, ($\hat{S}_T > 0.001$).

important, while Ross et al. [2014] concluded that N_2O animal manure (management and application), CH_4 enteric fermentation and CH_4 animal manure were most important. Chen and Corson [2014] used the squared correlation coefficient to quantify how much a parameter contributes to the output variance. The squared correlation coefficient is equal to the squared standardised regression coefficient [Groen et al., 2015a], and can also be used to explain the output variance. Chen and Corson [2014] only focused on the epistemic uncertainties of emission factors. For a conventional system (RG), they concluded that the emission factor of manure on pasture contributed approximately 70%, followed by cattle housing and manure storage (∼10%), manure spreading (∼10%), mineral fertilisation (∼5%), N_2O deposition and leaching (∼5%). The only study that used the same method for the global sensitivity analysis was Zehetmeier et al. [2014], but they considered only four parameters. They concluded that, N_2O from N input into soil contributed 75% to the output variance, followed by replacement rate (19%) and CH_4 from enteric fermentation of dairy cows (6%).

To summarise, our results were in line with the studies already performed,

but added insight by including more parameters (thirty-three, both technical parameters and emissions factors) and performing a global sensitivity analysis aiming at explaining the output variance, and not just the regression coefficients, which overestimate the importance of the parameters. In addition, this study showed the importance of the emission factor of direct N_2O emissions, replacement rate, and the importance of the yield and fertiliser rate of the main crops.

6.3.4 Combining local and global sensitivity analysis

Figure 6.6 combines the most influential parameters from the local sensitivity analysis with the most important parameters from the global sensitivity analysis for all three grazing systems. Parameters that were selected from the local sensitivity analysis changed the outcome with more than 0.1% when the input parameters were changed with 1% (i.e. $|\eta| > 0.1$). Parameters that were selected from the global sensitivity analysis contributed more than 1% to the output variance (i.e. $\hat{S}_T > 0.01$). The only difference between the systems is the EF for N_2O from grazing. As the ZG system did not include grazing, the EF did not show up in the results. In contrast, related to the EF in the UG system is the second most important parameter.

Figure 6.6 shows that when combining the two methods, the emission factor of CH_4 emissions from enteric fermentation, the emission factor of direct N_2O emission of crop, milk yield, and dry matter feed intake of the dairy cows are most essential. Also, N-fertiliser rate and yield of grass silage, the replacement rate of cows, the emissions factor of CH_4 emissions from enteric fermentation of the replacement heifers, and the indirect N_2O emission factor of leaching are an essential set of parameters. For parameters of which variability or uncertainty was not included due to a lack of data, but that did show up in the local sensitivity analysis (i.e. production of CAN fertiliser and rapeseed meal), we applied a default uncertainty of 10%. As can be seen in Figure 6.6, the importance of those two parameters remained minor. Depending on the grazing system, the emission factor of N_2O for grazing become more essential with increasing grazing time (given by the squares in Figure 6.6), while emissions from crop cultivation become less essential.

Both reducing uncertainty and increasing data quality can improve reliability. The epistemic uncertainty of parameters (given by the circles in Figure 6.6) can be reduced by gaining more knowledge of the parameters or

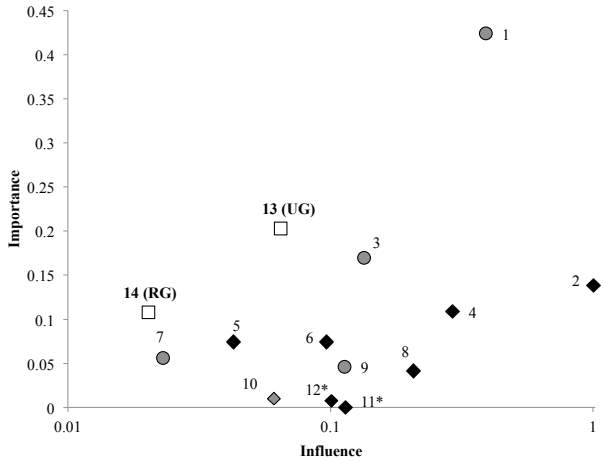

Figure 6.6: Combination of the most influential parameters parameters ($|\eta| > 0.1$) on the horizontal (log-) axis and the most important parameters ($\hat{S}_T > 0.01$) on the vertical axis. 1: Emission factor (EF) enteric fermentation cows, 2: EF direct N_2O, crop cultivation, 3: milk yield; 4: dry matter feed intake, 5: N-fertiliser rate grass silage, 6: yield grass silage; 7: EF indirect N_2O, leaching, 8: replacement rate, 9: EF enteric fermentation, replacement heifers, 10: EF CH_4 manure management cows, 11: production of CAN fertiliser; 12: production of processed rapeseed meal. 13: EF N_2O from grazing, unrestricted grazing system 14: EF N_2O for grazing, restricted grazing system The asterisk (*) indicates parameters that were varied with a default variation of 10%. ○: parameters containing epistemic uncertainties; ◇: parameters containing variability; □: do not exist in zero grazing system.

improve measurements. Parameters containing natural variability (given by the diamonds in Figure 6.6) that are essential should be of high quality before drawing conclusions. Parameters that were included in both the local and global sensitivity analysis, but do not show up in Figure 6.6, or appear in the left bottom corner can be of lower data quality. These parameters could be set to a fixed value in future studies, as both their influence and contribution to the output variance is low.

6.3.5 The effect of the correlation coefficient on the results

The effect of the correlation coefficient is more or less independent from the grazing system, because for each grazing system, dry matter feed intake and milk yield turned out to be important parameters. Therefore, the conclusions made on the following results are applicable for all three grazing systems.

The correlation coefficient between dry matter feed intake and milk yield is $\rho = 0.5$, based on Henriksson et al. [2011]. However, we were not sure of the value for this correlation coefficient because the data source did not match with the data source we used for the yields and the feed intake. Therefore, we tested what the effect was of varying the correlation between $\rho = 0$ and $\rho = 1$ on the output variance and the global sensitivity index.

The effect of ignoring correlation between dry matter feed intake and milk yield on the output variance is shown in Figure 6.7 by the grey dots. For example, if a correlation of 0.5 between dry matter feed intake and milk yield is ignored, the output variance is underestimated with approximately 8%, if a correlation of 1 is ignored, the output variance is underestimated with approximately 14%.

In Figure 6.7, also the results are given for the effect of changing the correlation coefficient on the global sensitivity index for milk yield. The grey bar on the left presents what happens if correlation between the two parameters was completely ignored (i.e. $\rho = 0$). The white bar represents the value that we have currently chosen (i.e. $\rho = 0.5$). Figure 6.7 shows that ignoring the correlation between dry matter feed intake and milk yield would lead to an underestimation of the importance of both parameters (dry matter feed intake and milk yield) and the output variance would be underestimated.

The effect of choosing the accurate correlation coefficient between dry matter feed intake and milk yield is clearly demonstrated to be important. And although the magnitude of the correlation between these two input param-

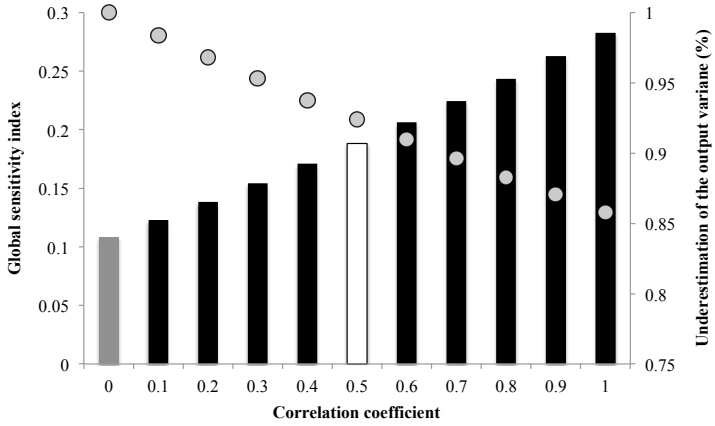

Figure 6.7: On the left vertical axis, the effect of varying the correlation coefficient between dry matter feed intake and milk yield between $\rho = 0$ (i.e. ignoring correlation; grey bar) and $\rho = 1$ on the global sensitivity index of *milk yield* are shown. The white bar represents our current assumption. The effects of ignoring the correlation coefficients on the output variance are represented by the grey dots on the right vertical axis.

eters is unknown, they remain one of the most important parameters in the LCA model. A reasonable assumption of variation of the correlation coefficients between milk yield and dry matter feed intake is found in Veerkamp et al. [2000], where the lower limit is given as 0.34 for a high diversity in breed and a large number of animals, and an upper limit is given as 0.66 for a lower diversity in breed or animals specific for a certain region.

6.4 Conclusion

Parameters that are essential to assess the GHG emission of milk production are: the emission factor of CH_4 emissions from enteric fermentation, milk yield, dry matter feed intake of the dairy cows and the emission factor of direct N_2O emission of crop cultivation. Depending on the grazing system, the emission factor of N_2O emissions from grazing become more important

with increasing grazing time. To improve reliability, the epistemic uncertainty of the emissions factors could be reduced by gaining more knowledge of the parameters or improve measurements. Also, parameters of minor importance, such as the emission factors of CO_2 emissions from liming or other parameters that turned out low in the local and the global sensitivity analysis could be set to a fixed value in future studies to reduce data collection efforts. In addition, data regarding variability of essential parameters should be of high quality before drawing conclusions, such as milk yield, dry matter feed intake, replacement rate and the N-fertiliser rate and crop yield of the most important crops.

The correlation coefficient between feed intake and milk yield seemed to be important, however, better data is needed to determine the strength of the correlation coefficient. Future research should focus on reducing uncertainty and improving data quality of the most essential parameters.

Supplementary material

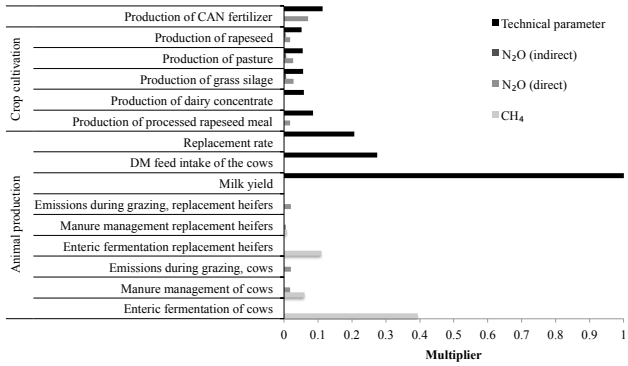

Figure 6.8: Multipliers of the most influential parameters ($|\eta| > 0.05$) and their corresponding emissions, for cows in a restricted grazing system.

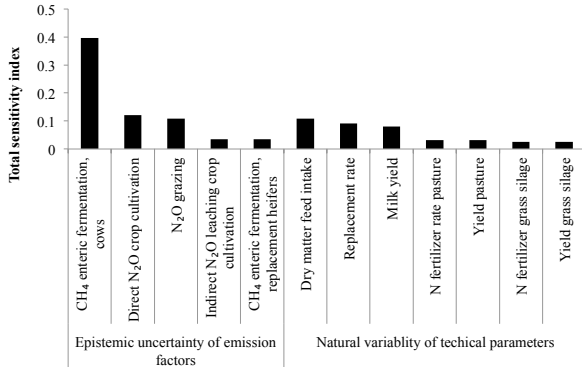

Figure 6.9: Parameters that explain most of the output variance, given by the total sensitivity index ($\hat{S}_T$), for cows in a restricted grazing system. Only parameters that explain more than 0.001 are shown, ($\hat{S}_T > 0.001$).

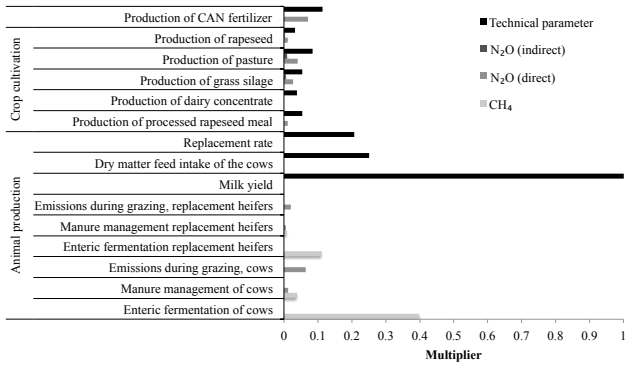

Figure 6.10: Multipliers of the most influential parameters ($|\eta| > 0.05$) and their corresponding emissions, for cows in an unrestricted grazing system.

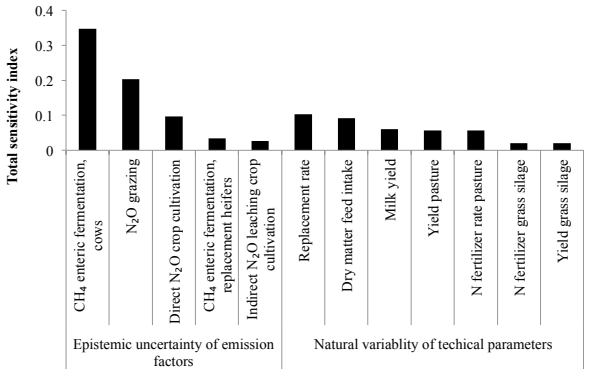

Figure 6.11: Parameters that explain most of the output variance, given by the total sensitivity index ($\hat{S}_T$), for cows in an unrestricted grazing system. Only parameters that explain more than 0.001 are shown, ($\hat{S}_T > 0.001$).

CHAPTER 7

Benchmarking nutrient losses of dairy farms: the effect of epistemic uncertainty

Joint work with:
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Abstract

A nutrient balance quantifies differences in nutrients entering and leaving the system, and can be used to determine nutrient losses. A nutrient balance, therefore, is commonly used as a tool to benchmark the environmental performance of dairy farms. Benchmarking nutrient losses of farms, however, may lead to biased conclusions because of differences in major decisive characteristics between farms, such as soil type and production intensity, and because of epistemic uncertainty of input parameters caused by errors in measurement devices or observations. This study aimed to benchmark nutrient losses by comparing nitrogen use efficiency (NUE_N; calculated as N output per unit of N input) of farm clusters with similar characteristics while including epistemic uncertainty, using Monte Carlo simulation. Subsequently, the uncertainty of the parameters explaining most of the output variance was reduced to examine if this would improve benchmarking results. Farms in cluster 1 (n=15) were located on sandy soils and farms in cluster 2 (n=17) on loamy soils. Cluster 1 farms were more intensive in terms of milk production per hectare and per cow, had less grazing hours, and fed more concentrates compared to farms in cluster 2. The mean $NUE_N$of farm in cluster 1 (43%) was higher than of farms in cluster 2 (26%). Input parameters that explained most of the output variance differed between clusters. For cluster 1, input of feed and output of roughage were most important, whereas for cluster 2, the input of mineral fertiliser (or fixation) was most important. For both clusters, the output of milk was relatively important as well. Including the epistemic uncertainty of input parameters showed that only 37% of the farms in cluster 1 (out of 105 mutual comparisons) differed significantly in terms of their NUE_N, whereas in cluster 2 this was 82% (out of 120 comparisons). Therefore, benchmarking $NUE_N$of farms in cluster 1 was no longer possible, whereas farms in cluster 2 could still be ranked when uncertainty was included. After reducing the uncertainties of the most important parameters, 72% of the farms in cluster 1 differed significantly in terms of their NUE_N, and in cluster 2 this was 87%. Results indicate that reducing epistemic uncertainty of input parameters can significantly improve benchmarking results. The method presented in this study, therefore, can be used to draw more reliable conclusions regarding benchmarking nutrient losses of farms.

7.1 Introduction

Nitrogen (N) is an important nutrient for milk production. The input of N into European milk production systems has increased in the past decades, mainly via purchase of fertiliser and feed, but also via atmospheric deposition and biological fixation [Powell et al., 2010]. These increased N inputs have also increased N losses to the environment, via leaching of nitrate (NO_3^-)

and emissions of N-gases, such as nitrous oxide (N_2O) and ammonia (NH_3). These N losses contribute to environmental problems, such as eutrophication, acidification and global warming [Whitehead, 1995; Smith et al., 1999]. To reduce N losses, the European Union introduced legislation, such as the Nitrates Directive [EU, 2011], which set limits on N application per hectare to reduce NO_3^- leaching.

There has been on-going studies and discussions on how to reduce N losses of dairy farms in Europe [Aarts et al., 1992; Schröder et al., 2003; Nevens et al., 2006; Phuong et al., 2013; Mihailescu et al., 2015]. Calculating the nutrient balance at farm level is the most commonly used approach to evaluate how efficient nutrient inputs have been used. In the Netherlands, for example, dairy farms are obliged to quantify their annual nitrogen and phosphorus balance from 2016 onwards [Veeteelt, 2015]. A nutrient balance reflects the difference in nutrients entering and leaving a system, and allows computation of environmental indicators, such as the nutrient use efficiency (NUE) or the nutrient surplus per ha of a farming system [Spears et al., 2003]. NUE generally is computed as the amount of nutrients in valuable outputs of a system over the amount of nutrients in all inputs of that system [Nevens et al., 2006].

Due to the simplicity of the method and relatively low data requirement, the nutrient balance has been used as a tool to benchmark the environmental performance of farms [Oenema et al., 2003; Schröder et al., 2003]. Benchmarking farms based on, for example, their NUE, however, may lead to biased conclusions because of two reasons. First, as pointed out by Schröder et al. [2003], comparing the NUE of farms is justified only if they have similar major decisive characteristics. These characteristics can be based on: (unmanageable) physical factors, such as soil type and climatic conditions [Roberts, 2008; Powell et al., 2010]; long term strategic decisions, such as the degree of self-sufficiency (e.g. grass-based versus concentrate-based), production intensity, or manure management system [Nevens et al., 2006]; and short term tactical decisions, such as choice of the feed crop, or grazing regime [Nevens et al., 2006]. In addition, operational decisions (i.e., day to day decisions), and other management skills of the farmer, such as the capacity to reduce losses (e.g. losses of feed, nutrients, milk or cows (culling)), can have an important influence on the NUE of a farm [Nevens et al., 2006]. Variation in NUE among dairy farms, therefore, does not only originates from physical factors but also from strategic and tactical decision-making. Second, comparing nutrient losses of farms may be affected by epistemic uncertainty of input data,

caused by errors in measurement devices or errors around observations. Epistemic uncertainty can arise from e.g. errors in practically determining the N fixation by clover, measurement errors around the feed intake of the cows or estimations around the N-content of the animals [Oenema et al., 2015]. Increasing knowledge or better measurements can reduce epistemic uncertainty [Walker et al., 2003; Groen et al., 2015a].

Previous studies focused on examining the epistemic uncertainties of nutrient flows by looking into e.g. quantity of nutrient inputs [Mulier et al., 2003; Gourley et al., 2012; Oenema et al., 2015]. However, they did not examine the impact of epistemic uncertainties on benchmarking results, nor did they benchmark farms with similar decisive farm characteristics.

The objectives of this study were to benchmark the nutrient losses by comparing nitrogen use efficiency (NUE_N) of farms with similar decisive characteristics while including epistemic uncertainty, and to examine which input parameters explain most uncertainty of NUE_N results. In addition, the epistemic uncertainties of input parameters that explain most of the output variance were reduced, to examine if this would significantly improve benchmarking results.

7.2 Materials and methods

7.2.1 Case study: European specialised dairy farms

We used data of specialised dairy farms from Dairyman. Dairyman was a project directed at improving regional prosperity through better resource utilisation on 113 dairy farms in different European countries [Dairyman, 2010]. From the 113 farms, 32 specialised dairy farms were selected. Specialised dairy farms were defined as farms that have less than 5% non-dairy purpose animals, and less than 10% of their agricultural area in use for non-dairy purpose activities. These 32 dairy farms were located in different countries and regions (i.e. Netherlands, Ireland, Belgium (Flanders, Wallonia), Germany and Luxembourg). Selected dairy farms differed in soil types (i.e. sandy soil, loam soil), milk production (i.e. milk production per cow and per ha), grazing hours per year, and feed import (i.e. kg concentrate usage per cow per year; Table 7.1). From these farms, farm data from the year 2010 were used as baseline values to determine all N-flows.

Table 7.1: Characteristics of the 32 European specialised dairy farms used in this study.

Characteristics	Unit	Mean	Min	Max
Agricultural area	ha	65	25	270
Herd size	number of dairy cows	90	37	384
Milk production	kg milk cow^{-1} $year^{-1}$	7689	5700	9853
Milk production	kg milk ha^{-1} $year^{-1}$	12598	3448	26300
Grazing hours	hour $year^{-1}$	2857	0	5146
Concentrate usage	kg cow^{-1} $year^{-1}$	1215	317	2459

7.2.2 Defining homogenous farm clusters

To enable benchmarking of NUE_N of farms with similar characteristics, farms were sorted into homogenous groups (i.e. typologies) based on their characteristics (Table 7.1). For this purpose, we used a two-step cluster analysis, because it allows using both continuous and categorical variables as clustering criteria [Chiu et al., 2001]. To perform a cluster analysis with n criteria, a sample size of 2^n farms is required [Formann, 1984]. Since our sample size included 32 farms, we selected 5 criteria for the cluster analysis, namely grazing hours, soil type, concentrate per cow per year, milk production per cow per year and milk production per ha [De Vries et al., 2015; Daatselaar et al., 2015]. The analysis was performed in the statistical software package IBM SPSS statistics 22 [SPSS, 2015].

7.2.3 System boundary and model assumptions of calculating NUE_N

The NUE_N was quantified at farm level, implying that only on-farm flows and losses were considered. The N-flows through a dairy farm included in this study are visualised in Figure 7.1. Inputs of N include N in mineral fertilisers, manure, animals, concentrates, roughages, biological N fixation and atmospheric N deposition. Outputs of N include N in animals, milk, manure and roughage. Stock changes (defined as final stock minus initial stock) of the mineral fertilisers, manure, animals, concentrates and roughages were taken into consideration during the computation processes. Manure output was subtracted from the total fertiliser inputs (i.e. through mineral fertiliser and

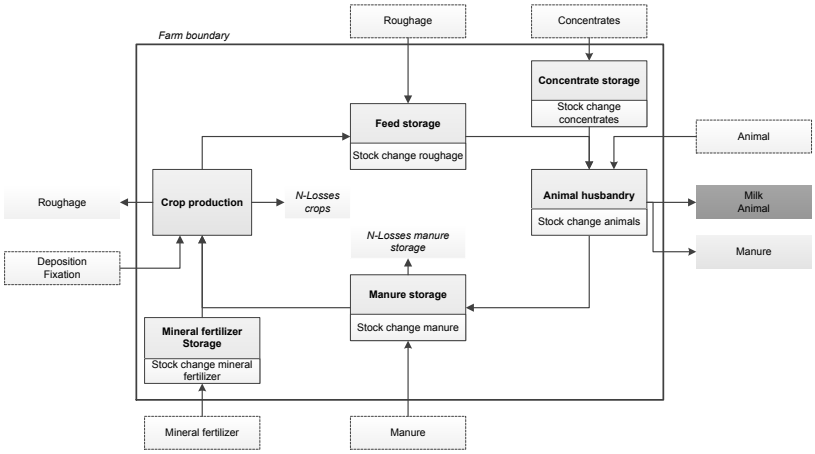

Figure 7.1: N-flows on a dairy farm to assess nutrient use efficiency; the production processes are given by the solid boxes, the N-flows are given by the arrows. A detailed description of the input parameters can be found in Table 7.2.

manure). If the total manure output of the farm exceeded its total fertiliser input, excessive manure was treated as a loss. The internal N-flow from crop production to feed storage was based on the energy requirements of the herd, minus feed input and stock changes of feed. Losses of N from manure storage were based on storage type and the baseline values of manure N and independent of the in- and output of production processes in further calculations [EEA, 2013].

7.2.4 Matrix based calculation for on-farm NUE_N

We used the matrix-based approach developed by Suh and Yee [2011] to quantify the N-efficiency of the 32 dairy farms. This approach was used to describe the herd and crop balance (Figure 7.1) in one equation, which facilitates the global sensitivity analysis to examine epistemic uncertainty. A matrix-based approach allows for the presence of loops and parallel components, as is often the case on dairy farms (e.g. manure is used for the production of feed

crops, which are consequently fed to the animals, producing manure). This approach requires a detailed insight into the nutrient flows within the farm.

The difference between the matrix-based approach to assess the farm N-balance and the more common nutrient balance is that in case of the matrix-based approach the internal flows are also given (e.g. the flows between manure storage and crop production, or crop production and feed storage), just as in a substance flow analysis. In the common nutrient balance, the farm is considered as a black box (e.g. Oenema et al. [2015] and Mu et al. [2016]). For more details, see the supplementary material.

In the matrix-based approach, the internal N-flows in Figure 7.1 are described by the **V** and **U** matrix, where the **V**-matrix describes how much kg N is supplied (rows) to each production process (columns). The **U**-matrix describes how much kg N is used (columns) by each production process (rows) [Suh and Yee, 2011]. The N-flows are corrected for the stock changes (**s**) on the farms. Combined, they are quantified in a matrix **A** for each (intermediate) process. The vector (**b**) gives the amount of nutrients extracted (**r**) to produce 1 unit of final product, which, in this case, is determined by the valuable outputs of the farm:

$$\mathbf{b} = \mathbf{r}\left(\mathbf{V}^T - \mathbf{U} + \hat{\mathbf{s}}\right)^{-1} = \mathbf{r}\mathbf{A}^{-1} \tag{7.1}$$

In our case, the four elements in **b** represent the production processes of Figure 7.1 (animal husbandry, manure storage, crop production, feed storage). The nitrogen use efficiency ($\mathrm{NUE_N}$) for the production process of the animal husbandry is quantified by:

$$\mathrm{NUE_N} = 1/b_{\mathrm{husbandry}} \tag{7.2}$$

A detailed example of this procedure can be found in the supplementary material of Suh and Yee [2011].

7.2.5 Quantifying the effect of epistemic uncertainty on benchmarking

To quantify the effect of epistemic uncertainties of the input parameters on the benchmarking, the distribution functions of the parameters need to be defined first. Subsequently, the input uncertainties are propagated through

the NUE_N model.

Defining distribution functions

Each parameter in the NUE_N model was considered as an uncertain parameter, only the N-flow from crop production to feed storage and the N losses during manure storage were fixed. The N-flow from crop production was fixed, because it was based on the energy requirements of the herd. The N losses during manure storage were fixed, because they were based on storage specific emission factors. All input parameters are assumed to be normally distributed. The coefficient of variation ($CV = \sigma/\mu$) described the epistemic uncertainty of the parameters and was based on Oenema et al. [2015] (Table 7.6). Based on the equation for the CV, the standard deviation was calculated per farm, because each farm had a different (i.e. farm specific) mean.

Quantifying the effect of epistemic uncertainty on benchmarking

The propagation of the uncertainties of the input parameters through the NUE_N model (Equation (7.1)) was done using Monte Carlo simulation and was performed for all farms in each cluster. From each distribution function (Table 7.1) a random value was drawn, and used to calculate the NUE_N. The output uncertainty was given by the variance:

$$\mathrm{var}(\mathrm{NUE_N}) = \frac{1}{N-1}\sum_{i=1}^{N}(\mathrm{NUE_{N_i}} - \overline{\mathrm{NUE_N}})^2 \tag{7.3}$$

Where the mean is given by: $\overline{\mathrm{NUE_N}} = \frac{1}{N}\sum_i \mathrm{NUE_{N_i}}$, for a sample size of $N = 5000$. We performed a discernibility analysis [Heijungs and Kleijn, 2001] to determine if the input uncertainties had an effect on benchmarking. To determine if there was a significant difference between farms the farms within a cluster were pairwise compared for the results for each Monte Carlo run. This means that we counted how many times the NUE_N of one farm was better than another farm, expressed as a frequency. A significance level of 5% was chosen [Heijungs and Kleijn, 2001; Henriksson et al., 2015]. This means, for example, that if farm A has a lower NUE_N than farm B in 630 out of 1000 runs, difference in NUE_N of the two farms was considered as not significant. But, if farm A had a lower NUE_N than farm C in 12 out of 1000 runs, than

farm C was considered as significantly better than farm A.

7.2.6 Explaining output uncertainty for different farm typologies

To identify which input parameter contributed most to the output uncertainty within a specific farm cluster, a global sensitivity analysis was performed by calculating the squared standardised regression coefficients (S_j) as a measure for the sensitivity index [Groen et al., 2015a; Saltelli et al., 2008]:

$$S_j = \frac{\text{var}(p_j)}{\text{var}(\text{NUE}_\text{N})}(b_j)^2 \tag{7.4}$$

Where var(p_j) gives the variance of each input parameter (p_j) based on Table 7.6 and b_j is equal to the regression coefficient.

7.3 Results

7.3.1 Farm clusters

Two homogeneous groups of farms, i.e. farm clusters, were derived from the cluster analysis. Farms in the first group, further referred to as farms in cluster 1, are located on sandy soils and relatively intensive in terms of milk production per cow and per hectare (Table 7.2). The number of grazing hours is low, whereas the amount of purchased concentrates per cow per year is high relative to the other farm cluster. Farms in cluster 2 are located on loam soils, and are less intensive when compared to farms in cluster 1. The number of grazing hours is higher, whereas the amount of concentrates per cow per year is lower than on farms in cluster 1. The average NUE_N of farms in cluster 1 is higher than of farms in cluster 2.

7.3.2 The effect of epistemic uncertainties on benchmarking

For each farm, the input uncertainties of Table 7.6 were propagated through the NUE_N model (Equations (7.1) and (7.2)). For each farm in both clusters, a

[1]Characteristics of these two clusters are significantly different (p<0.05)

Table 7.2: Results of the cluster analysis, showing the farm characteristics for 15 farms in cluster 1 and 17 farms in cluster 2, given by the mean (standard deviation) of each characteristic or a categorical characteristic per cluster.

Characteristics[1]	**Unit**	**Cluster 1**	**Cluster 2**
Soil type	n.a.	Sandy	Loam
Milk production	kg milk cow^{-1} $year^{-1}$	8519 (854)	6956 (878)
Milk production	kg milk cow^{-1} ha^{-1}	15970 (5108)	9623 (3792)
Grazing hours	hours cow^{-1} $year^{-1}$	1115 (1099)	4393 (1175)
Concentrate use	kg cow^{-1} $year^{-1}$	1719 (499)	770 (207)
NUE_N	%	43 (10)	26 (12)

mean and a variance were derived (Figure 7.2, cluster 1; Figure 7.3, cluster 2).

The results of the discernibility analysis for cluster 1 can be found in Table 7.3. For example, farm 5 had a lower NUE_N than farm 1, and a higher NUE_N than the other farms, except when compared to farm 8 and farm 14. In case of farm 6, only 53% of the Monte Carlo runs show a higher NUE_N than farm 3, meaning their performance is almost indistinguishable taking the epistemic uncertainties of the input parameters into account.

For farm 1, approximately 4% of the Monte Carlo runs resulted in a negative value for N losses of crop production, implying soil N depletion. This is explained by the importance of deposition as an N input on this farm, and the large uncertainty of this parameter ($CV = 17\%$; Table 7.6). The negative values, therefore, are more likely related to the uncertainty of deposition, than to display a realistic model outcome. The drawings including a negative value for deposition, therefore, were removed from the analysis.

Applying the 5% significance level, results show that farm 1 is most efficient when taking the epistemic uncertainty of the input parameters into account, followed by farm 5, which is only not significantly better than farm 8 and 14. The two least efficient farms are farm 3 and 6. The NUE_N of the other farms turned out to be very similar (Table 7.3).

The results of the discernibility analysis for cluster 2 are found in Table 7.4. For farm 2, approximately 46% of the Monte Carlo runs resulted in a negative value for N losses of crop production, implying soil N depletion. This is

[2]Approximately 4% of the Monte Carlo runs were excluded from the analysis due to unrealistic model outcomes.

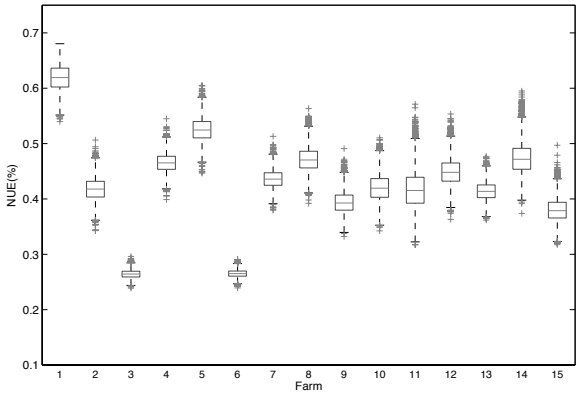

Figure 7.2: Box plot for the 15 farms in cluster 1. The horizontal line in each box gives the mean, the box gives the 75% interval, and the plusses are realisations that appear outside the 75% interval.

Table 7.3: Results of discernibility analysis for cluster 1 based on pairwise comparing Monte Carlo runs between farms. The column and row numbers 1 to 15 represent the 15 farms. The percentages show how often a farm (row) has a higher NUE_N than another farm (column). When α-value of 0.05 is applied, values between 2.5% and 97.5% indicate that the NUE_N of the farms are no longer considered as significantly different. The significant different farms are given by the bold-printed percentages.

%	1[2]	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1[2]		**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**	**100**
2	**0**		**100**	5	**0**	**100**	25	5	78	47	52	19	54	7	89
3	**0**	**0**		**0**	**0**	48	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
4	**0**	95	**100**		**2**	**100**	85	43	**99**	92	88	70	97	42	**100**
5	**0**	**100**	**100**	**98**		**100**	**100**	95	**100**	**100**	**99**	**98**	**100**	91	**100**
6	**0**	**0**	52	**0**	**0**		**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
7	**0**	75	**100**	15	**0**	**100**		13	93	69	71	37	79	16	97
8	**0**	95	**100**	57	5	**100**	87		**99**	93	90	73	97	49	**100**
9	**0**	22	**100**	**1**	**0**	**100**	7	**1**		22	31	6	24	**1**	67
10	**0**	53	**100**	8	**0**	**100**	31	7	78		55	23	57	9	88
11	**0**	48	**100**	12	**1**	**100**	29	10	69	45		23	50	11	81
12	**0**	81	**100**	30	**2**	**100**	63	27	94	77	77		84	28	97
13	**0**	46	**100**	3	**0**	**100**	21	3	76	43	50	16		5	88
14	**0**	93	**100**	58	9	**100**	84	51	**99**	91	89	72	95		**99**
15	**0**	11	**100**	**0**	**0**	**100**	3	**0**	33	12	19	3	12	**1**	

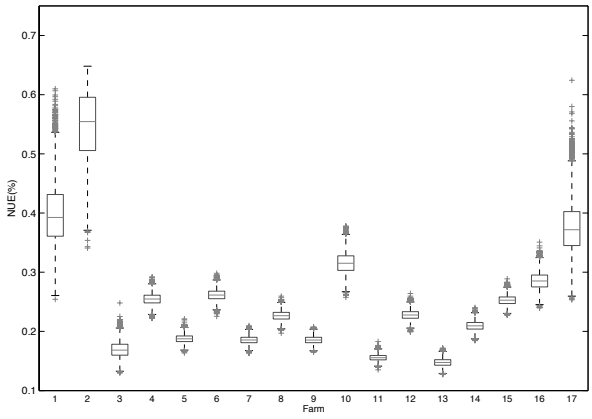

Figure 7.3: Box plot for the 17 farms in cluster 2. The horizontal line gives the mean, the box gives the 75% interval, and the plusses are realizations that appear outside the 75% interval.

explained by the importance of N fixation on this farm, in combination with a relatively large uncertainty of this parameter ($CV = 30\%$). Similar to farm 1 in cluster 1, negative values were assumed to display an unrealistic model outcome. Because of the high percentage of unrealistic model outcomes, it was decided to remove farm 2 from further analysis.

Applying the 5% significance level, results show that farm 1 is most efficient (only not significantly different from farm 10 and 17). Ranking the farms based on their NUE_N shows the following result: (1) farm 1; (2) farm 17 (only not significantly higher than farm 10); (3) farm 10 (only not significantly higher than farm 16); (4) farm 16 (only not significantly higher than farm 6); (5) farm 6 (only not significantly higher than farm 4 and 15); (6) farms 4 and 15; (7) farms 8 and 12 (only not significantly higher than farm 14); (8) farm 14; (9) farms 5, 7 and 9 (only not significantly higher than farm 3); (10) farm 3 (only not significantly higher than farms 11 and 13); (11) farms 11 and 13.

Contrary to the first cluster, including the epistemic uncertainties still allowed for some kind of ranking, although most farms overlapped with at least two other farms.

[4]Approximately 46% of the Monte Carlo runs were excluded from the analysis due to unreal-

Table 7.4: Results of discernibility analysis for cluster 2 based on pairwise comparing Monte Carlo runs between farms. The column and row numbers 1 to 17 represent the 16 farms[4]. The percentages show how often a farm (row) has a higher NUEN than another farm (column). When α-value of 0.05 is applied, values between 2.5% and 97.5% indicate that the NUEN of the farms are no longer considered as significantly different. The significant different farms are given by the bold-printed percentages.

%	1	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1		**100**	**100**	**100**	**100**	**100**	**100**	**100**	95	**100**	**100**	**100**	**100**	**100**	**99**	62
3	**0**		**0**	12	**0**	14	**0**	14	**0**	82	**0**	92	**1**	**0**	**0**	**0**
4	**0**	**100**		**100**	31	**100**	**99**	**100**	**0**	**100**	**98**	**100**	**100**	57	4	**0**
5	**0**	88	**0**		**0**	59	**0**	59	**0**	**100**	**0**	**100**	**2**	**0**	**0**	**0**
6	**0**	**100**	69	**100**		**100**	**100**	**100**	**0**	**100**	**100**	**100**	**100**	76	9	**0**
7	**0**	86	**0**	41	**0**		**0**	49	**0**	**100**	**0**	**100**	**1**	**0**	**0**	**0**
8	**0**	**100**	**1**	**100**	**0**	**100**		**100**	**0**	**100**	45	**100**	93	**2**	**0**	**0**
9	**0**	86	**0**	41	**0**	51	**0**		**0**	**100**	**0**	**100**	**1**	**0**	**0**	**0**
10	5	**100**	**100**	**100**	**100**	**100**	**100**	**100**		**100**	**100**	**100**	**100**	**100**	90	8
11	**0**	18	**0**	**0**	**0**	**0**	**0**	**0**	**0**		**0**	83	**0**	**0**	**0**	**0**
12	**0**	**100**	**2**	**100**	**0**	**100**	55	**100**	**0**	**100**		**100**	94	**2**	**0**	**0**
13	**0**	8	**0**	**0**	**0**	**0**	**0**	**0**	**0**	17	**0**		**0**	**0**	**0**	**0**
14	**0**	**99**	**0**	**98**	**0**	**99**	7	**99**	**0**	**100**	6	**100**		**0**	**0**	**0**
15	**0**	**100**	43	**100**	24	**100**	**99**	**100**	**0**	**100**	**98**	**100**	**100**		**2**	**0**
16	**1**	**100**	96	**100**	91	**100**	**100**	**100**	11	**100**	**100**	**100**	**100**	**98**		**1**
17	37	**100**	**100**	**100**	**100**	**100**	**100**	**100**	92	**100**	**100**	**100**	**100**	**100**	**99**	

7.3.3 Explaining the output variance

The global sensitivity analyses explained how much of the output variance can be explained by the variance of the individual input parameters. The results of the global sensitivity analysis can be found in Figure 7.4 (cluster 1) and Figure 7.5 (cluster 2).

Results show that in case of cluster 1, the input of concentrates, roughage, mineral fertiliser, and deposition, and the output of milk, roughage, and manure explain most of the output variance. Input of animals and manure, stock change of each of the inputs, and output of animals did not show up as important explanatory parameters in any of the farms, except for stock change of mineral fertiliser for farm 12. Further analysis showed that both the quantity as well as the N content of each parameter is approximately equally important in terms of their contribution to the output variance.

Figure 7.5 shows that in case of cluster 2, the input of mineral fertiliser, and, for some farms, deposition and fixation, and the output of milk and an-

istic model outcomes of farm 2, therefore, this farm was excluded from further analysis.

Parameter (%)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Input animals		0		0				0				0			0
Input concentrates	30	1	29	8	4	39	30	15	16	10	4	3	9	16	8
Input roughage	0		17	0	3		0	49	25	51	20	2	28	22	30
Input min. fertilizer	10	8	14	11	7	15	16		3	1	0	20	7	2	7
Input manure		2								1	0			1	
Deposition	21	4	4	7	3	6	7	15	7	9	13	16	30	9	7
Fixation									0		52			1	
SC animal	0	0	0	0	0	0	0		0	0	0	0	0	0	0
SC concentrates				0	0		0		0	0	0	0	0	0	0
SC roughage									0	1	2	1	1	4	2
SC min. fertilizer									0	1		31		0	
SC. manure									2	2	1		3	3	2
Output animal	1	0	5	1	0	4	1	1	2	1	1	1	2	1	1
Output milk	13	3	29	8	5	35	20	16	13	11	6	5	16	10	11
Output roughage	4	81	0	63	77							19	3		
Output manure	35	0	4				26		29	12	2		2	30	33

Figure 7.4: Sensitivity indices (S_j) for each input parameter, explaining how much each parameter contributes to the output variance for each farm in cluster 1. SC: stock change. An empty cell means that these parameters were equal to zero; 0% means that this parameter contributed 0% to the output variance.

Parameter (%)	1	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Input animals		0										12				0
Input concentrates	0	0	0	2	4	2	2	2	0	3	2	0	1	13	0	0
Input roughage		3	0	8	0	0	0	0	1	1		1	0	2		6
Input min. fertilizer		1	70	45	54	44	66	61	12	55	57	45	60	38	59	
Input manure	3	8														
Deposition	9	3	2	1	5	2	1	1	1	1	3	1	3	5	1	14
Fixation	82	78														68
SC animal	0	0	0	2	0	1	0	0	0	0	1	1	0	0	0	0
SC concentrates																0
SC roughage																1
SC min. fertilizer						13			10	0			0		15	
SC. manure																
Output animal	1	2	10	21	12	13	6	11	1	15	14	25	23	13	2	1
Output milk	2	5	17	21	25	27	25	24	2	22	21	15	14	28	8	1
Output roughage									73						11	8

Figure 7.5: Sensitivity indices (S_j) for each input parameter, explaining how much each parameter contributes to the output variance for each farm in cluster 2. SC: stock change. An empty cell means that these parameters were equal to zero. Output of manure is not included because none of the farms in cluster 2 exported manure. Farm 2 was excluded from the global sensitivity analysis.

Table 7.5: Effect of decreasing the input uncertainties of the most important parameters to 1%, for both clusters.

	Cluster 1	**Cluster 2**
Total number of pairwise comparisons	105	120
Significantly different farms before reducing input uncertainty	39 (37%)	99 (83%)
Significantly different farms after reducing input uncertainty	76 (72%)	104 (87%)

imals explain most of the output variance. Input of concentrates, roughage and manure and stock change of animals did not show up as important explanatory parameters in any of the farms in cluster 2.

7.3.4 Effect of decreasing uncertainty on benchmarking

To analyse if decreasing epistemic uncertainty can improve benchmarking, we reduced the uncertainty of the most important input parameters and reran the discernibility analysis. For cluster 1, the input uncertainty was reduced to 1% for: input of concentrates, roughage, mineral fertiliser, deposition and the output of milk, roughage, and manure (Figure 7.4). For cluster 2, the input uncertainty was reduced to 1% for: input of mineral fertiliser, and the output of milk and animals (Figure 7.5). Table 7.5 shows how many pairwise comparisons were made in both cluster, and how many were significantly different, before and after reducing input uncertainty. Results show that reducing the uncertainty of the most important input parameters based on the global sensitivity analysis, improved the ability to find significant differences between the NUE_N of the farms in both clusters. Benchmarking, therefore, can be improved when input uncertainties are reduced, especially for the farms in the first cluster.

7.4 Discussion

This study builds on, and extends the principles regarding epistemic uncertainty of nitrogen flows on dairy farms presented by [Oenema et al., 2015]. Although we used the same coefficients of variations of input parameters, re-

sults of our study and Oenema et al. [2015] show important differences. Based on our analysis, input of concentrates and roughage, and output of milk and roughage explain most of the output variance in cluster 1. Input of mineral fertiliser and fixation, and output of animals and milk explain most of the output variance in cluster 2. Oenema et al. [2015], however, concluded that N fixation, atmospheric deposition and stock changes of roughage and manure explain most of the output variance when determining the NUE_N of dairy farms. Differences between our study and Oenema et al. [2015] can be explained by two reasons. First, the characteristics of the farms were different. In general, Oenema et al. [2015] included farms with a lower input of feed, but a higher stock change of roughage, and a higher N input through fixation compared to the farms in our study. Uncertainties related to stock changes of feed are higher than uncertainties related to input of feed, whereas uncertainties related to N fixation is highest among all N flows. Second, Oenema et al. [2015] used a different approach to determine N intake during grazing. In our study, N intake from grazing and on-farm roughage production was fixed based on feed requirements and the baseline values of input of purchased feed. Oenema et al. [2015] changed the N-intake from grazing with a change in roughage and concentrate intake, which consequently influenced the importance of feed parameters. The contribution of the input of feed to the output variance was therefore found to be lower in Oenema et al. [2015] than in our study.

Dairy farms in Europe show different decisive characteristics. For example, most farms in the Netherlands are intensive farms because land resources are limited. The main N inputs on these farms are through purchased concentrates and roughages. In Ireland, however, most farms are grass-based extensive farms. The main N inputs on these farms are through purchased mineral fertiliser and N fixation. Comparing NUE of Dutch and Irish farms can lead to biased conclusions because of inherent differences between systems. Clustering of farms into groups with similar decisive characteristics, therefore, is a prerequisite for benchmarking the NUE of farms and facilitates the identification of major parameters. When comparing results of the global sensitivity analysis between the two farm clusters, for example, input of feed and output of roughage show up to be most important in case of cluster 1, whereas the input of mineral fertiliser (or fixation) is most important in case of cluster 2. Results show that the importance of parameters can vary between farm type (clusters). Methods to improve benchmarking of farms, therefore,

should account for differences in decisive characteristics. The method presented in this study, can contribute to more solid conclusions regarding the performance of farms in terms of their NUE.

Several methodological limitations could have affected the results of this study. A first limitation comprises the coefficients of variations that were used. Coefficients were based on Oenema et al. [2015], focussing on Dutch dairy farms only. Farms in our study are from different countries in Europe. Results of the uncertainty and global sensitivity analysis might have been different if country specific coefficients of variation were applied, but such information was not available. Second, changes in soil N-stock were not considered in this study due to data limitations. In practice, soil N-stock changes can have an important influence on the N balance of a farm. Assessing changes in soil N stock at the farm level is difficult but can significantly improve interpretation of nutrient balance results [Godinot et al., 2014]. Third, results of the discernibility analysis are influenced by the significance level that is chosen. In this study, a significance level of 5% was applied. Increasing the significance level facilitates benchmarking, but decreases the reliability of the results.

Reducing epistemic uncertainty and benchmarking NUE of farms with similar decisive characteristics can contribute to the identification of improvement options. Based on the variability between farms within a cluster, farm specific management options to reduce nutrient losses can be identified. Evaluating the (causes of) variability between farms within a farm cluster, therefore, can be a next step for further improving the NUE of farms.

7.5 Conclusion

Benchmarking the NUE of dairy farms requires an approach that accounts for differences in major decisive characteristics among farms, and for the impact of epistemic uncertainties of input parameters. The parameters that are most important in terms of epistemic uncertainty (i.e. explain most of the output variance), however, can vary among farm types. Clustering farms based on their main characteristics and understanding and reducing the impact of epistemic uncertainty of major parameters can significantly improve benchmarking results. The method presented in this study, therefore, can contribute to more solid conclusions regarding the performance of farms in terms of their nutrient use efficiency.

Acknowledgements

We gratefully acknowledge Jouke Oenema for his helpful explanation on his paper referred to in this study, and Reinout Heijungs for his suggestions on the statistical analysis.

Supplementary material

Input data

Table 7.6: Description of the parameters and their epistemic uncertainty given by the relative uncertainty (CV), which was taken from Oenema et al. [2015].

Process	**Type**	**Parameter** (kg N)	**Description**	CV (%)	**Remark**
Crop production	Resource input	N-fixation	Grassland area (ha)	5	
			Legume yield (kg/ha)	10	
			N-fixation (kg N/kg legume)	30	
		Deposition	Farm area (ha)	5	
			N-deposition (kg N/ha)	17	
		Mineral fertiliser	Mineral fertiliser (kg)	2.5	
			N-content mineral fertiliser (kg N/kg)	2.5	
		Stock change mineral fertiliser	Stock change mineral fertiliser (kg)	7.5	
			N-content stock change mineral fertiliser (kg N/kg)	2.5	
	Export	Roughage	Roughage (kg)	7.5	
			N-content roughage (kg N/kg)	7.5	
	Losses	N-losses crops	n.a.	n.a	Function
Feed storage	Resource input	Roughage	Roughage (kg)	7.5	
			N-content roughage (kg N/kg)	7.5	
		Stock change roughage	n.a.	17	GEP[5]
Fertiliser storage	Resource input	Manure	Manure (kg)	5	
			N-content manure (kg N/kg)	7.5	
		Stock change manure	n.a.	22	GEP
	Losses	N emissions from manure storage	n.a.		Fixed
Milk and animal production	Resource inputs	Animals	Number of animals (-)	2	
			Life-weight per animal (kg)		n.a.
			N-content per animal (kg N/kg)	5	
		Stock change animals	n.a.	5.68	GEP
		Concentrates	Concentrates (kg)	2.5	
			N-content concentrates (kg N/kg)	2.5	
		Stock change concentrates	n.a.	11	GEP
	Final use	Milk	Milk (kg)	1	
			N-content milk (kg N/kg)	2	
		Animals	Number of animals (-)	2	
			Life-weight per animal (kg)		n.a.
			N-content animal (kg N/kg)	5	
	Export	Manure	Manure (kg)	5	
			N-content manure (kg N/kg)	7.5	

[5]GEP: Gaussian error propagation is used to determine the CV of parameters when there is a lack of information to separate the N-content from the items in the stock change and therefore only the kg N of stock change is available (e.g., roughage can include different items with different N contents). Details on the method can be found in [Heijungs and Lenzen, 2014].

Matrix-based on-farm nutrient use efficiency

Figure 7.6 shows a nutrient balance of a dairy farm. The total input of N (in kg) is given by the dark grey boxes, the light grey boxes give the output. The uptake from the stock change of concentrates (C) is subtracted from the total input of concentrates, because it is considered as an input to the farm. The addition to the stock of animals (A) is considered as a useful output of the farm, and is therefore added to the output of animals. The amount of produced manure that is exported is subtracted from the input of fertilisers (i.e., mineral fertiliser and manure). Hence, manure export is considered to offset a farm's fertiliser input. However, if export of manure exceeded the input of fertiliser, it was considered as a loss. The nutrient use efficiency of nitrogen (NUE_N) on this farm is equal to 44%.

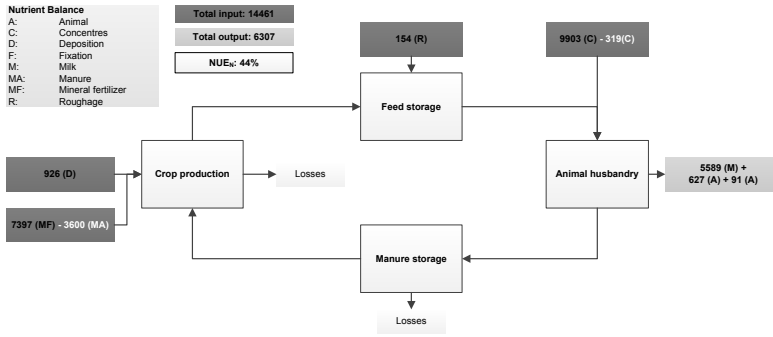

Figure 7.6: Nutrient balance of a dairy farm, in kg N. The total input of N (in kg) is given by the dark grey boxes, the output is given by the light grey boxes.

Figure 7.7 shows the same farm, with similar assumptions as described above, but then the NUE_N is quantified using a matrix-based approach as described by Suh and Yee [2011]. When the same assumptions are applied, the matrix-based approach results in the same efficiency of 44%. However, a difference is that the efficiency of the production processes (i.e. crop production, feed storage, animal husbandry and fertiliser storage), are given with respect to the whole farm, not of the individual processes, in case of the matrix-based approach. For example, the efficiencies of feed storage and animal husbandry are 100%, when looking at the individual processes, because there are no losses. The matrix-based NUE_N however, incorporates the losses that occurred elsewhere on the farm in the efficiency of the individual production processes. For example, the efficiency of feed storage equals 28%, which is determined by the efficiency of the previous processes, such as crop production, and input of

roughage. The efficiency of animal husbandry equals the efficiency of the farming system (44%), because it comprises the efficiency of all former processes.

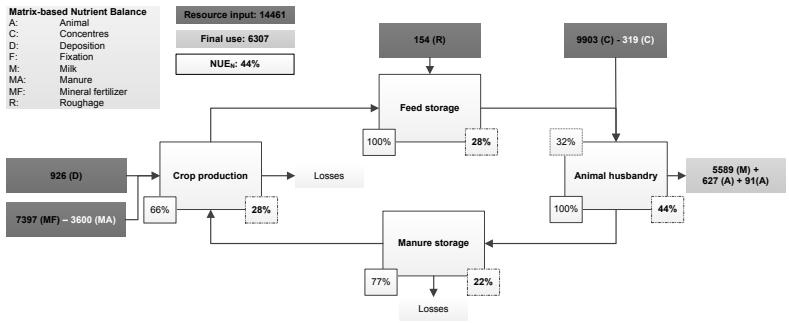

Figure 7.7: Nutrient balance of a dairy farm, in kg N. The total input of N (in kg) is given by the dark grey boxes, the output is given by the light grey boxes. The efficiencies in the bottom right corner display the efficiencies quantified with the matrix based nutrient balance, the efficiencies in the bottom left corner display the efficiencies quantified looking only at the in- and outputs of that specific production system. If an efficiency of 100% is give, it means that there are no losses at that process. The efficiency of 32% in the top left corner (animal husbandry) displays the efficiency when the export of manure is considered as a loss.

Figure 7.8 shows for the same farm, what happens if the export of manure is no longer subtracted from the input of fertiliser, but considered as an individual export of the farm. In that case, for the matrix based nutrient balance, there are now two efficiencies, one describing the useful output we considered earlier (milk and animal) and one describing the production of manure.

In this paper, we always subtracted manure from the input of fertiliser, including both mineral fertiliser and manure. However, some farms exported roughage. Based on the same principles as described above (i.e., considering the export of manure as an output), export of roughage was considered as an output. This resulted in a slightly different NUE_N than what would have been calculated using the normal nutrient balance approach, but differences were minor (1 – 2%).

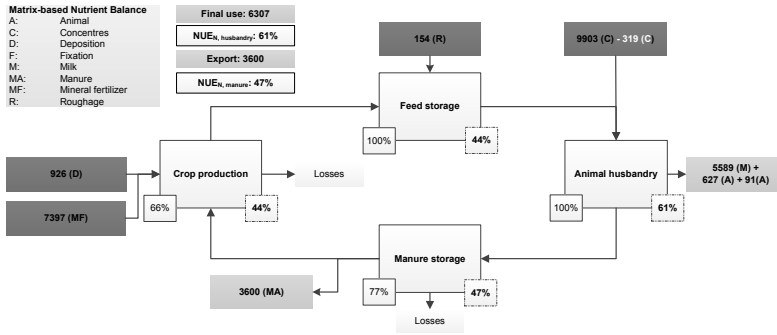

Figure 7.8: Nutrient balance of a dairy farm, in kg N, when export of manure is considered as an output. The total input of N (in kg) is given by the dark grey boxes, the output is given by the light grey boxes. The efficiencies in the bottom right corner display the efficiencies quantified with the matrix based nutrient balance, the efficiencies in the bottom left corner display the efficiencies quantified looking only at the in- and outputs of that specific production system. If an efficiency of 100% is given, it means that there are no losses at that process.

CHAPTER 8

General discussion

8.1 Introduction

The challenge to produce food in an environmentally friendly way has become urgent [Steinfeld et al., 2006; Gerber et al., 2013]. To develop strategies to produce food with a low environmental impact, environmental assessment models are developed that quantify the total environmental impact associated with food production, such as life cycle assessment or nutrient balance analysis. Input data required for these environmental impact assessment models, however, may vary due to seasonal changes, geographical conditions or socio-economic factors (natural variability). Moreover, input data may be uncertain, due to measurement errors and observational errors that exist around modelling of emissions and technical parameters (epistemic uncertainty). Although agricultural activities and food production are prone to natural variability and epistemic uncertainty, very few case studies made a thorough examination of the effects of variability and uncertainty on the result.

The aim of this thesis was to enhance the understanding of the effects of variability and uncertainty on the results. This was done by exploring how uncertainty analysis and sensitivity analysis can help to reduce the ef-

forts for data collection, support the development of mitigation strategies and improve overall reliability, leading to more informed decision making in environmental impact assessment models. To that end, methods for uncertainty analysis and sensitivity analysis were combined, and the effect of correlations in uncertainty propagation and global sensitivity analysis were explicitly accounted for. To be able to formulate case study specific suggestions that could improve reliability and point to potential mitigation strategies in food production, methods were applied to case studies of dairy and pork production.

This chapter starts with discussing the value of uncertainty analysis and sensitivity analysis in environmental impact assessment models, followed by the value of matrix notation (Section 8.2). Subsequently, recommendation of the use of methods for uncertainty and sensitivity analysis are given (Section 8.3). This chapter ends with an overview of the conclusions (Section 8.4).

8.2 The value of uncertainty analysis and sensitivity analysis in environmental impact assessment models

8.2.1 Local sensitivity analysis

Local sensitivity analysis in environmental impact assessment models, such as life cycle assessment (LCA) and nutrient balance (NB) analysis, are generally performed using a one-at-a-time (OAT) approach. An OAT approach takes a parameter, increases it e.g. 5% and quantifies the effect on the model output. OAT approaches in LCA or NB analysis usually consider a subset of all available parameters, based on expert judgment or perhaps a quantitative criterion, such as the contribution of the individual input parameter to the total environmental impact. However, when the selection of the input parameters considered for the local sensitivity analysis is based on such principles, influential (technical) parameters might be overlooked. For example, efficiency parameters (e.g. replacement rate or reproductive performance) are not directly related to emissions, only to their prior production processes. These subsets, therefore, might not contain all potential influential parameters. A systematic approach that considers the influence of all input parameters in LCA can only be done using the multiplier method.

In Chapter 6, for example, the multiplier method was used to identify the most influential parameters in an LCA that assessed greenhouse gas (GHG) emissions of milk production. Results showed that local sensitivity analysis identified milk yield, feed intake, and the emission factor of CH_4 from enteric fermentation of the cows, replacement rate and crop yields as most influential parameters in the LCA model. Moreover, previous studies performing a local sensitivity analysis using an OAT approach, overlooked influential parameters such as replacement rate and crop yields.

In contrast to LCA, no such a systematic method is yet available for matrix-based NB analysis. Currently, studies that did performed a local sensitivity analysis, performed followed an OAT approach [Suh and Yee, 2011]. Future research can focus on developing a similar approach for matrix-based NB analysis.

Some LCA and NB studies [Huang et al., 2013; Kim and Dale, 2002; Sayagh et al., 2010; Beltran et al., 2016], use a sensitivity analysis to refer to the effect of different modelling decisions on the model output, such as the effect of changing allocation techniques or characterisation factors. An explanation might be that ISO 14044 [2006] recommends performing a sensitivity analysis, which is defined as "systematic procedures for estimating the effects of the choices made regarding methods and data on the outcome of a study" [ISO, 2006b]. This definition not only refers to data, but also to methods used in a study, which indeed could refer to different allocation methods and characterisation factors. Although the effect of a methodological decision, such as the allocation method used, is very important to the model outcome and the subsequent interpretation, they should not be referred to as sensitivity analysis. Moreover, the ISO standard does not make a distinction between a local sensitivity analysis (which does not include information of the uncertainty or variability around input parameters) and a global sensitivity analysis (which does include uncertainty or variability).

The lack of distinction between local and global sensitivity analysis, has led in some studies [Flysjö et al., 2011; Basset-Mens et al., 2005] to include information about the uncertainty of the input parameters in, what is referred to as, a sensitivity analysis. For example, Basset-Mens et al. [2005] explored the effect of an increase of 1% for some parameters, that were assumed to vary only little, and 200% for other parameters, that were assumed to vary a lot. Results in Chapter 2, for example, showed that influential parameters in an LCA study of pork production were the feed conversion ratio, CH_4 emis-

sions from manure management and crop yields, especially maize. However, previous studies on this topic [Basset-Mens et al., 2005; Basset-Mens and Van Der Werf, 2005] included uncertainty ranges of the input parameters as well, and could therefore not be compared with the results presented in Chapter 2.

Referring to modelling decisions as a sensitivity analysis or including uncertainty information in a OAT approach leads to an ambiguous definition of the terminology of uncertainty and sensitivity analysis, because: (1) referring to a change in method or modelling structure has nothing to do with the intrinsic sensitivity of the model, and should therefore be given a different label, such as modelling decisions; (2) combining uncertainty information in an OAT approach belongs to the area of screening analysis, which is strictly speaking not a local sensitivity analysis [Saltelli et al., 2008; Mutel et al., 2013]. Also, if uncertainty information is included in an OAT approach, it becomes less evident what it means to mutually compare the parameters, because it does not give the influence of the input parameters to the model output, as the magnitude of the uncertainty is incorporated as well.

Developing a standardised definition and method for local sensitivity analysis in LCA and NB analysis, will increase comprehensibility between studies and will enhance comparability of results.

8.2.2 Uncertainty analysis

Uncertainty propagation refers to propagation of uncertainty and variability around input parameters through an environmental impact assessment model to generate output data. Uncertainty analysis refers the subsequent analysis of the generated output data, such as determining the output variance, determining a confidence interval etc.

Uncertainty propagation can be done using e.g. sampling approaches or analytical approaches. In Chapter 3, three sampling approaches (i.e. Monte Carlo sampling, Latin hypercube sampling, quasi Monte Carlo sampling), one analytical approach (i.e. on the basis of a Taylor series), and one fuzzy approach (i.e. fuzzy interval arithmetic) were compared, based on convergence rate and output statistics. The sampling methods led to more (directly) usable information, compared to fuzzy interval arithmetic or analytical uncertainty propagation. Latin hypercube and quasi Monte Carlo sampling provided more accuracy in determining the sample mean than Monte Carlo sampling. The Latin hypercube and quasi Monte Carlo sampling methods also

converged faster than Monte Carlo sampling for some of the case studies discussed in Chapter 3. The application of the more advanced sampling methods, therefore, might be less fruitful for applications in LCA, as the improvement mainly manifested itself in the number of runs generated. This seems less relevant in environmental impact assessment models, because the algorithm behind LCA and NB analysis does not require much run time. The latter depends on the specific software used and the capacity of the computer, nonetheless, classical Monte Carlo sampling seems a valuable sampling method to apply in LCA and NB studies.

The preference of a sampling approach versus an analytical for uncertainty propagation can depend on the amount of available information. A sampling approach requires a distribution function, including a parameter of dispersion such as the variance. Analytical uncertainty propagation as described in Chapter 3, does not require a distribution function, but only a parameter of dispersion. When less data is available about the uncertainty or variability of the input parameters, the analytical approach will become more suitable.

In Chapter 7, for example, we used an NB to benchmark nutrient losses on farms for two different farming systems. Our aim was to explore the impact of measurement errors (epistemic uncertainty) on the benchmarking of farms within two different farming systems. The first farming system contained intensive farms, in terms of e.g. milk production per hectare (ha) and purchased concentrates per cow, whereas the second system included grass-based farms, with a lower milk production per ha. The distribution function and the parameters of dispersions of parameters required to assess the NB were obtained from the literature. We assumed that the epistemic uncertainties around the N-flows were measured at different locations, using different measurement tools, and, therefore, could vary independently from each other. Uncertainty propagation could be performed using Monte Carlo sampling. The uncertainty analysis showed that benchmarking of concentrate-based farms was no longer possible when the epistemic uncertainty of input parameters was included, whereas including epistemic uncertainty did not affect benchmarking of grass-based farms.

In Chapter 6, where we assessed greenhouse gas (GHG) emissions of milk production, a correlation was assumed between N-fertiliser application and crop yield; and between feed intake and milk production. Again, uncertainty propagation was performed using a sampling approach. We showed that, in the uncertainty analysis, the correlation between feed intake and milk produc-

tion decreased the output variance.

To implement a correlation coefficient between input parameters during uncertainty propagation, as done in Chapter 6, information is needed not only on the distribution functions, but also on the correlation coefficients between input parameters. Using a sampling approach for uncertainty propagation with correlated input parameters, therefore, becomes even more data intensive. In Chapter 5, we demonstrated how to predict the effect of ignoring correlations in uncertainty analysis in LCA, using analytical uncertainty propagation. More detailed, in Chapter 5 we demonstrated that (1) we can predict if including correlations among input parameters in uncertainty propagation will increase or decrease output variance; (2) we can quantify the risk of ignoring correlations on the output variance and the global sensitivity indices. Moreover, this procedure requires only little data availability regarding the input parameters.

We conclude, therefore, that both sampling and analytical uncertainty propagation are indispensable in environmental impact assessment models. The analytical approach is especially useful when data is limited (e.g. only the variance of the input parameters is available). In contrast, the sampling approaches are more suitable when full knowledge is available (e.g. a distribution function, including a parameter of dispersion).

8.2.3 Global sensitivity analysis

A global sensitivity analysis quantifies the contribution of the variances of the individual input parameters to output variance. More specifically, a sensitivity index explains how much each input parameter contributes to the output variance. For example, the squared standardised regression coefficients can be interpreted as a sensitivity index. In Chapter 4, we compared rather common methods for global sensitivity analysis in LCA, namely methods based on regression or correlation approaches [Geisler et al., 2005] and key issue analysis [Heijungs, 1996], to less commonly applied methods in LCA, such as the Sobol' method and random balance design.

The comparison of the sensitivity methods was based on four aspects: (I) sampling design, (II) output variance, (III) explained variance, and (IV) contribution to output variance of individual input parameters, and illustrated for two hypothetical case studies. The evaluation of the sampling design (I) relates to the computational effort of a sensitivity method. Key issue analysis

does not make use of sampling (it is an analytical approach) and was fastest, whereas the Sobol' method had to generate two sampling matrices, and therefore, was slowest. The total output variance (II) resulted in approximately the same output variance for each method, except for key issue analysis, which underestimated the variance, especially for high input uncertainties. The explained variance (III) and contribution to variance (IV) for small input uncertainties, was optimally quantified by standardised regression coefficients and the main Sobol' index. For large input uncertainties, Spearman correlation coefficients and the Sobol' indices performed best. Therefore, it was concluded that these less commonly applied methods did not outperform the common methods. Moreover, they asked for more unconventional algorithms, and may be more cumbersome to implement compared to the more frequently used methods based on linear regression or correlation approaches. However, the use of the Sobol' method seemed better at explaining the output variance when input uncertainties are high. Also, other studies showed that the Sobol' method might be more useful in the impact assessment model [Cucurachi et al., 2014]. Also, when the impact on the environment is quantified such as for toxicity, which contains potential non-linear relations [Posthuma et al., 2002] the Sobol' method might become more useful. If future environmental impact assessment studies become more advanced in terms of including non-linear impact assessment, the Sobol' and random balance design methods as discussed in Chapter 4, may become more useful. Based on the results presented in Chapter 4, the squared standardised regressions coefficient (or the squared correlation coefficient), is considered as the most useful proxy for a sensitivity index.

For example, in Chapter 7, where we used an NB to benchmark nutrient losses on farms for two different farming systems, a global sensitivity analysis was applied using the squared standardised regression coefficients. We found that parameters that explained most of the output variance differed between systems. For the more concentrate-based system, input of feed and output of roughage were most important, whereas for the grass-based system, the input of mineral fertiliser (or fixation) was most important. Moreover, we showed that reducing epistemic uncertainty of the most important input parameters significantly improved benchmarking results.

In Chapter 6 we identified the most important input parameters to assess the greenhouse gas emissions of milk production, for three different grazing systems. We adapted the regression-based global sensitivity analysis to al-

low for correlated input parameters between feed intake and milk yield; and fertiliser rate and crop yield. We showed that the emissions factor of CH_4 emission from enteric fermentation of cows, milk yield, feed intake and the emission factor of direct N_2O emissions from crop cultivation, are the most important parameters for a zero grazing system. For restricted and unrestricted grazing systems, however, N_2O emission factor from manure excretion during grazing becomes increasingly more important.

When comparing the results of other studies to our results, we found that e.g. Ross et al. [2014] calculated the regression coefficients, so we could only compare their results based on the ranking of the parameters, and not on how much the parameters explained. Several studies implemented regression coefficients (not standardised and not squared) [Basset-Mens et al., 2009; Aktas and Bilec, 2012], or standardised regression coefficients (not squared) [Sugiyama et al., 2005; Vigne et al., 2012], or correlation coefficients (not squared) [Mattila et al., 2012; Mattinen et al., 2014; Wang and Shen, 2013] as a measure for a global sensitivity index. For example, regression or correlation coefficients that are not squared, cannot be mutually compared, and are therefore less suitable as a measure for a global sensitivity index. In Table 8.1, based on the case study represented in Chapter 4, the squared standardised regression coefficients and the squared (Pearson) correlation coefficients were compared to the standardised regression coefficients, the regression coefficients and the correlation coefficient.

For example, ranking the importance of the parameters in Table 8.1, in case of the (squared) standardised regression coefficients or the (squared) correlation parameter 1 is most important, but when looking at the regression coefficients, parameter 5 is most important. The squared standardised regression coefficient or the squared correlation coefficient are the most useful proxies for a global sensitivity index, because they can be added to each other.

Currently in the ISO standard for LCA, there is no method recommended for a global sensitivity analysis. Developing a standardised definition and method for global sensitivity analysis in LCA and NB studies, will increase comprehensibility between studies and will enhance the comparison of results between studies.

Table 8.1: Comparison of the regression and correlation coefficients, applied to the case study presented in Chapter 3 (in adapted form) containing six input parameters. In the last row, the total explained output variance is given. CV: coefficient of variation (σ/μ). Only the squared standardised regression and squared correlation coefficients can be added up, and are expressed in (%), the other coefficients cannot be added up, displayed by not applicable (n.a.) in the last row. (S(R))RC: (squared (standardised)) regression coefficients; (S)CC: (standardised) correlation coefficients.

Parameter (CV)	**Analysis of output variance by:**				
	SSRC	**SRC**	**RC**	**SCC**	**CC**
1 (15.0%)	58.1%	-0.762	-13.0	56.4%	-0.751
2 (11.5%)	1.08%	-0.104	-11.6	1.15%	-0.107
3 (–)	–	–	–	–	–
4 (20.0%)	3.53%	-0.188	-0.241	5.10%	-0.226
5 (15.0%)	34.7%	0.589	100	35.9%	0.599
6 (8.00%)	0.450%	0.0669	2.13	0.590%	0.0766
Output variance explained:	97.9%	n.a.	n.a.	99.1%	n.a.

8.2.4 The value of matrix notation in environmental impact assessment models

The environmental impact assessment models described in this thesis, LCA and NB analysis, both rely on matrix notation, to facilitate the application of uncertainty and sensitivity analysis. In matrix notation, the production processes are described by technical parameters given in the **A**-matrix. The corresponding emissions (and resource use) are given in the **B**-matrix. One may wonder, does matrix notation have any added value for sensitivity analysis? Uncertainty propagation using Monte Carlo simulation and global sensitivity analysis by means of standardised regression coefficients can also be performed for environmental impact models that do not make use of matrix notation. However, performing an analytical local sensitivity analysis that considers all input parameters, such as the multiplier method, applied in Chapter 2 and 6, requires a functional form of the impact assessment model, such as the matrix-based approach developed by [Heijungs and Suh, 2002]. Although other functional forms have been proposed [Ciroth et al., 2004; Clavreul et al., 2013] matrix notation seems to be the most straightforward approach.

When we also consider correlations between input parameters, the algebraic notation gives clear insight into the effect of the correlations on the uncertainty propagation (Chapter 5). Using matrix notation, it was possible to predict the effect of including correlations during uncertainty propagation on the output variance and the global sensitivity analysis. Without the matrix formulation, it would have been impossible to make a sweeping generalisation towards all different kind of case studies. To facilitate sensitivity analysis, matrix notation in LCA may not be eminent to implement uncertainty and sensitivity analysis, but it facilitates the algorithm implementation required to perform the methods, which otherwise would have been cumbersome to implement.

In Chapter 2 and 6, greenhouse gas emissions were calculated for pork production and milk production respectively. To quantify the greenhouse gasses for crop cultivation, manure management and enteric fermentation, equations were implemented between the technical parameters in the **A**-matrix (e.g. fertiliser applied, manure produced and feed intake) and the GHG emissions in the **B**-matrix. For example, for the emissions of crop cultivation, the CO_2 and indirect and direct N_2O emissions depended directly on the application of fertilisers and crop yield.

The aggregation level of the production process determined which parameters showed up in the local and global sensitivity analysis. For example, in Chapter 2, we showed that CH_4 emissions of manure turned out to be influential. However, the sensitivity analysis was modeled on the level of the total emissions, reflecting the parameters in the **A** and **B** matrix. Therefore, the influence of underlying factors determined by the type of manure storage system, such as the methane producing capacity, depending on temperature, wind speed etc., remains unknown. Further expanding crop and livestock models in LCA and NB analysis, can help to explain which underlying factors are important to make better estimations regarding environmental impacts. Future improvements can also be made regarding implementation of non-linear relationships. For example, it was assumed that N fertilisation and crop yield were correlated. At some stage, however, one additional input of N fertiliser will increase crop yield less than the previous unit of input, a phenomenon referred to as the law of diminishing returns. Therefore, a non-linear dependency, combined with a correlation factor (i.e. other circumstances, such as soil pH and humidity influence the dependency as well), might be a better representation of reality. Expanding knowledge on potential relationships

between input parameters, establish equations to implement these relations in environmental impact assessment models, and combine these equations with correlations between input parameters, can improve further assessments using environmental impact models. If the matrix notation might need to be adapted, or expanded to allow for the extensions of livestock models and underlying relations needs to be further developed.

8.3 Recommendations for future implementation of uncertainty and sensitivity analysis

8.3.1 Recommended analysis and methods

The uncertainty or sensitivity analysis to be applied depends on the question to be addressed and the available information. An overview of (generally) formulated research questions and the corresponding type of analysis and the recommended method (based on the results of this thesis), can be found in Table 8.2.

For example, in Chapter 2, very limited data were available and we were interested in determining which input parameters were most influential. Therefore a local sensitivity analysis, using the multiplier method was applied (question A.2, Table 8.2). In addition, a global sensitivity was applied (question D.2, Table 8.3), for those parameters, which either turned out to be influential, or were known to be uncertain, based on literature. In Chapter 6, full knowledge was available regarding the input parameters including correlations between some of the input parameters. We applied a global sensitivity analysis, to determine which parameters were most important to the output variance (question E.1 Table 8.3), which parameters could be set to a fixed value in improved data collections (question E.1, Table 8.3) and if correlations among parameters influenced the output variance (question C.3/E.3 Table 8.2 /Table 8.3). In Chapter 7, we studied benchmarking farms while accounting for epistemic uncertainties of input parameters (question B.6, Table 8.2) and identifying which input parameters explain most of the output variance (question C.3, Table 8.2).

Table 8.2: Methods for uncertainty analysis and sensitivity analysis corresponding to research questions addressed [continues in Table (8.3)].

Research questions corresponding to type of uncertainty or sensitivity analysis	**Preferred method in this thesis**	**Data requirements**
A. Local sensitivity analysis		
1. Which parameter changes the output value most? 2. Which parameters are most influential? 3. Of which parameters a high data quality is most urgent? 4. Which parameters are unlikely to influence the model output? 5. On which parameters should potential mitigation strategies be focused?	Multiplier method	Point values
B. Uncertainty analysis (neglecting correlation)		
1. Which product alternative is better when uncertainties are incorporated? 2. What is the likelihood that one product alternative performs better than the other? 3. Does the environmental impact of a product exceed the allowed boundary? 4. What is the confidence interval of the mean model output? 5. What happens to the output variance when input uncertainties are reduced?	Uncertainty propagation via e.g. Monte Carlo sampling	Distribution functions, including a parameter of dispersion (e.g. variance)
C. Uncertainty analysis (including correlations)		
1. Do correlations between parameters decrease the output variance? 2. What is the effect of ignoring correlations? 3. Will ignoring correlations affect decisions?	Uncertainty propagation adjusted for correlated parameters, *or:* analytical uncertainty propagation adjusted for correlated parameters	Distribution functions, covariance, *or:* covariance

Table 8.3: Methods for uncertainty analysis and sensitivity analysis corresponding to research questions addressed [continued from Table (8.2)].

Research questions corresponding to type of uncertainty or sensitivity analysis	**Preferred method in this thesis**	**Data requirements**
D. Global sensitivity analysis (neglecting correlations)		
1. On which parameters should improved data collection be focused?	Method of elementary effects, *or:*	Range, *or:*
2. Which parameters are most important for the output uncertainty?	Regression- (or correlation-) based method, *or:*	distribution functions, *or:*
3. Of which parameters should (epistemic) uncertainties be reduced to improve reliability of results?	key issue analysis	variance
4. Which parameters can be set to a fixed value to decrease data collection efforts of future studies?	Regression- (or correlation-) based method, *or:*	Distribution functions, *or:*
5. Which parameters contribute most to the output variance?	key issue analysis	variance
6. Can decreasing epistemic uncertainties of the most important input parameters reduce the output variance?		
E. Global sensitivity analysis (including correlations)		
1. Which parameters can be set to a fixed value to decrease data collection efforts of future studies?	Regression- (or correlation-) based method, *or:*	Distributions functions, covariance, *or:*
2. Which parameters contribute most to the output variance?	key issue analysis adjusted for correlated input parameters	covariance
3. Does correlation influence the importance of input parameters?		
4. Can correlations be ignored?		
5. On which correlation coefficients should data collection be focused?		

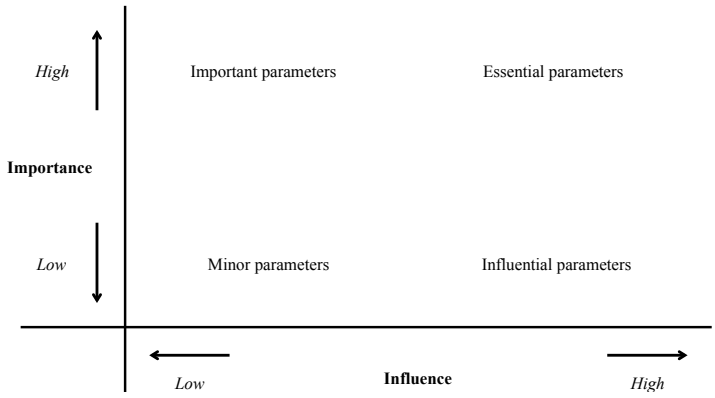

Figure 8.1: Parallel incorporation of local and global sensitivity analysis. Adapted from Heijungs [1996].

8.3.2 Combining local and global sensitivity analysis

Environmental impact assessment models, such as LCA, are based on many input parameters; therefore, it might be difficult to collect high quality data for all input parameters. A parallel implementation of local and global sensitivity analysis, such as in Chapter 2 and Chapter 6, gives a direct overview of the most influential (identified by a local sensitivity analysis) and important (identified by a global sensitivity analysis) model parameters. Parameters that are considered to be both influential and important, are considered to be the most essential parameters in the model, and can be used to further improve reliability or for development of mitigation strategies (Figure 8.1).

The importance of a parameter can originate from variability or epistemic uncertainty. A distinction between variability and uncertainty may in practice not be straightforward. However, it facilitates directions of mitigation strategies, which can be focused on essential parameters containing natural variability, and improvement of reliability, which can be focused on essential parameters that contain epistemic uncertainties (Figure 8.1).

Examples of parameters that are important, but not influential, are N-fertiliser rates of crop cultivation (as we showed in Chapter 6). The importance of these parameters is caused by, for example, variability in N-fertiliser rates

between years. An example of parameters that are influential, but not important are parameters that can be estimated very accurately, for example, the production of N fertilisers, and can for example be improved by innovations.

In Chapter 2, we focused on developing mitigation strategies and improving reliability of results. By combining local and global sensitivity analysis the most essential input parameters for environmental impact assessment in the pork production chain can be identified. Combining the results of these two analyses allowed to derive mitigation options, either based on innovations (e.g. novel feeding strategies) or on management strategies (e.g. reducing mortality rate), and to formulate options for improving reliability of results (e.g. decreasing epistemic uncertainties). Also reliability could be improved if data quality of the most essential parameters were improved.

In Chapter 6, we focused on improving reliability of results only. By combining a local and a global sensitivity analysis, parameters could be determined which are essential to assess GHG of milk production, focusing only on the reliability of the results. Essential parameters are the emission factor of CH_4 emissions from enteric fermentation, milk yield; DM feed intake of the dairy cows and the emission factor of direct N_2O emission of crop cultivation. Future research can focus on reducing uncertainty and improving data quality of the most essential parameters.

A local and global sensitivity analysis should, therefore, be seen as complementary. Moreover, in most environmental impact assessment models, data availability is limited and combining local and global sensitivity analysis makes sure that parameters are not overlooked.

8.4 Conclusions

This thesis shows that using a systematic approach for uncertainty analysis and sensitivity analysis improves overall reliability, reduces efforts for improved data collection and supports the development of potential mitigation strategies, especially for case studies of food production, where epistemic uncertainty and variability are ubiquitous.

Methods for uncertainty analysis and sensitivity analysis can be selected depending on the available data and the research question. By combining a local and global sensitivity analysis, we can identify the most essential input parameters for environmental impact assessment. This leads to more insight

in the influence and the uncertainty around the input parameters on the results, also when data availability is limited. This also allows deriving mitigation options in food production. Moreover, improving the value of uncertainty and sensitivity analysis in environmental impact assessment models, specifically in life cycle assessment (LCA) and nutrient balance (NB) studies, can be increased by standardising the use of definitions and methods.

More specifically:

- Uncertainty propagation in LCA using a sampling method leads to more (directly) usable information compared to analytical uncertainty propagation (Chapter 3).
- The choice for a method for global sensitivity analysis depends on the available data, the magnitude of the uncertainties in input data and aim of the study (Chapter 4).
- It can be predicted that including correlations among input parameters in uncertainty propagation in LCA can increase or decrease output variance. The effect of ignoring correlations on the output variance and the global sensitivity indices can be quantified, based on minimum data requirements (Chapter 5).
- Including uncertainty influences the outcome of decision-making tools. Reducing (epistemic) uncertainty of input parameters can significantly improve benchmarking of environmental performance. (Chapter 7).

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Summary

Production of food contributes to climate change. To develop strategies to produce food with a low environmental impact, environmental assessment models, such as life cycle assessment (LCA) or nutrient balance (NB) analysis are applied. Input data required for these models, may vary due to seasonal changes, geographical conditions or socio-economic factors. Moreover, input data may be uncertain, due to measurement errors and observational errors that exist around modelling of emissions and technical parameters. Although agricultural activities and food production are prone to natural variability and epistemic uncertainty, very few case studies made a thorough examination of the effects of variability and uncertainty on the result.

This thesis aimed to enhance understanding the effects of variability and uncertainty on the results. This was done by exploring how uncertainty analysis and sensitivity analysis can help to reduce the efforts for data collection, support the development of mitigation strategies and improve overall reliability, leading to more informed decision making in environmental impact assessment models. To that end, methods for uncertainty analysis and sensitivity analysis were combined, and the effect of correlations in uncertainty propagation and global sensitivity analysis were explicitly accounted for. To be able to formulate case study specific suggestions that could improve reliability and point to potential mitigation strategies in food production, methods

were applied to case studies of dairy and pork production.

To derive mitigation options and improve reliability in the assessment of greenhouse gas emissions (GHGs) along the pork production chain, two sensitivity methods were combined: the multiplier method and the method of elementary effects. The multiplier method showed how much the input parameter influences the assessment of GHGs, whereas the method of elementary effects showed the importance of input parameters on the output uncertainty. By combining the result of the multiplier method and the method of elementary effects, the essential parameters were identified. Results of this study showed that the most essential input parameter are the feed conversion ratio, the amount of manure, CH_4 emissions from manure management and crop yields, especially maize and barley. Combining the results of both methods allowed finding mitigation options, either based on innovations (e.g. novel feeding strategies) or on management strategies (e.g. reducing mortality rate). Furthermore, reliability could be improved by increasing data quality of the most essential parameters (Chapter 2).

Uncertainty propagation in environmental impact assessment models such as LCA, are usually performed using Monte Carlo sampling. However, other methods for uncertainty propagation are available, and it was unknown which method performed best. Monte Carlo sampling, Latin hypercube sampling, quasi Monte Carlo sampling, analytical uncertainty propagation and fuzzy interval arithmetic were compared based on convergence rate and output statistics. Each method was tested on three LCA case studies, which differed in size and behaviour. Results showed that uncertainty propagation in LCA using a sampling method leads to more (directly) usable information compared to fuzzy interval arithmetic or analytical uncertainty propagation. Latin hypercube and quasi Monte Carlo sampling provide more accuracy in determining the population mean than Monte Carlo sampling and can even converge faster than Monte Carlo sampling for some of the case studies discussed (Chapter 3).

Global sensitivity analysis in environmental impact assessment models, such as LCA, can be performed using several different methods. However, which method is most suitable was unknown. Five methods and coefficients that can be used for global sensitivity analysis were compared: standardised regression coefficient, Spearman correlation coefficient, key issue analysis, Sobol' method and random balance design. To be able to compare the performance of global sensitivity methods, two hypothetical case studies were constructed. The comparison of the sensitivity methods was based on four as-

pects: (I) sampling design, (II) output variance, (III) explained variance, and (IV) contribution to output variance of individual input parameters. Key issue analysis does not make use of sampling and was fastest, whereas the Sobol' method had to generate two sampling matrices, and therefore, was slowest (I). The total output variance (II) resulted in approximately the same output variance for each method, except for key issue analysis, which underestimated the variance especially for high input uncertainties. The explained variance (III) and contribution to variance (IV) for small input uncertainties, was optimally quantified by standardised regression coefficients and the main Sobol' index. For large input uncertainties, Spearman correlation coefficients and the Sobol' indices performed best. We concluded that the standardised regression coefficients, Spearman correlation coefficients or key issue analysis could be used for global sensitivity analysis in environmental impact assessment models (Chapter 4).

Incorporation of uncertainty propagation in LCA is nowadays widely acknowledged. Currently, most LCA studies that include uncertainty analysis ignore correlations between input parameters during uncertainty propagation, due to unfamiliarity with methods that include correlations or lack of data. The effect of ignoring these correlations on the output variance, however, remains unclear: it is not known if and under which conditions it can lead to erroneous conclusions. Two approaches to include correlations between input parameters during uncertainty propagation were studied: an analytical approach and a sampling approach. The use of both approaches is illustrated for an artificial case study of electricity production. Results demonstrated that that both approaches yield approximately the same output variance and sensitivity indices for this specific case study. Furthermore, we demonstrated that the analytical approach can be used to quantify the risk of ignoring correlations between input parameters during uncertainty propagation in LCA. We concluded that: (1) we can predict if including correlations among input parameters in uncertainty propagation will increase or decrease output variance; (2) we can quantify the risk of ignoring correlations on the output variance and the global sensitivity indices. Moreover, this procedure requires only little data regarding the input parameters (Chapter 5).

LCA of dairy products such as milk, require many input parameters that are often affected by variability and uncertainty. Moreover, correlations may be present between input parameters, e.g. between feed intake and milk yield. Three diets corresponding to three grazing systems (zero-, restricted and un-

restricted grazing) were selected, which were defined to aim for a given milk yield. First, a local sensitivity analysis was used to identify which parameters influence GHG emissions most. Second, a global sensitivity analysis was used to identify which parameters are most important to the output variance. The global sensitivity analysis included correlations between feed intake and milk yield and between nitrogen (N) fertiliser rates and crop yields. The local and global sensitivity analyses were combined to determine which parameters are essential. Finally, we analysed the effect of changing the most important correlation coefficient (between feed intake and milk yield) on the output variance and global sensitivity analysis. The mean GHG emissions for 1 kg energy corrected milk ranged from 1.08 to 1.12 kg CO_2 e, depending on the grazing system. The most essential parameters were the CH_4 emission factor of enteric fermentation, milk yield, feed intake, the direct N_2O emission factor of crop cultivation For both grazing systems, the N_2O emission factor for grazing also turned out to be important. In addition, the correlation coefficient between feed intake and milk yield turned out to be important. Moreover, systematically combining the local and global sensitivity analysis resulted in more parameters than previously found (Chapter 6).

A nutrient balance quantifies differences in nutrients entering and leaving the system and can be expressed in e.g. nutrient use efficiency (NUE). NUE is commonly used to benchmark the environmental performance of dairy farms. Benchmarking farms, however, may lead to biased conclusions because of differences in major decisive characteristics between farms, such as soil type and production intensity, and because of epistemic uncertainty of input parameters. To compare NUE of farms, farms were clustered based on similar characteristics, which resulted in farming systems. Farming system 1 was located on sandy soils and were more intensive in terms of milk production than farms in farming system 2. Farming system 2 was located on loamy soils. First, Monte Carlo sampling was used to propagate input uncertainties through the nutrient balance. Including the epistemic uncertainty of input parameters showed that benchmarking NUE of farms in farming system 1 was no longer possible, whereas farms in farming system 2 could still be ranked when uncertainty was included. Second, a global sensitivity analysis was performed to quantify how much the input parameters contributed to the output variance, using the squared standardised regression coefficients. Input parameters that explained most of the output variance differed between framing systems. For farming system 1, input of feed and output of roughage were most important. For

farming system 2, the input of mineral fertiliser was most important. Third, the uncertainty of the parameters explaining most of the output variance was reduced to examine if this would improve benchmarking results. After reducing the uncertainties of the most important parameters, benchmarking results significantly improved (Chapter 7).

Improving the value of uncertainty analysis and sensitivity analysis in environmental impact assessment models, specifically in LCA and NB analysis, would benefit from standardising the use of definitions and methods. Currently in the ISO standard for LCA, there is no method recommended for either a local nor global sensitivity analysis. Developing a standardised definition and method for global sensitivity analysis in LCA and NB studies, will increase comprehensibility between studies and will enhance the comparison of results between studies. The uncertainty analysis or sensitivity analysis to be applied depends on the question to be addressed and the available information. However, in most environmental impact assessment models, data availability is limited and combining local and global sensitivity analysis makes sure that parameters are not overlooked. A local and global sensitivity analysis should, therefore, be seen as complementary. Moreover, we concluded that both sampling approach for uncertainty propagation and analytical uncertainty propagation are indispensable in environmental impact assessment models. The analytical approach is especially useful when data is limited. In contrast, the sampling approaches are more suitable when full knowledge is available (Chapter 8).

This thesis showed that using a systematic approach to uncertainty and sensitivity analysis improves overall reliability, reduces efforts for improved data collection and supports the development of potential mitigation strategies, especially for case studies of food production, where epistemic uncertainty and variability are ubiquitous.

Populair-wetenschappelijke samenvatting (Summary in Dutch)

Achtergrond

De productie van voedsel kan nadelige gevolgen voor het milieu hebben, zoals een bijdrage aan klimaatverandering door de uitstoot van broeikasgassen. De belangrijkste broeikasgassen in de landbouw zijn CO_2 (koolstofdioxide), N_2O (lachgas) en CH_4 (methaan). De uitstoot van broeikasgassen tijdens voedselproductie vindt bijvoorbeeld plaats bij bemesting van landbouwgrond (in de vorm van CO_2 en N_2O), verbranding van fossiele brandstoffen bij transport van veevoer ingrediënten (in de vorm van CO_2) en tijdens de mestopslag (in de vorm van CH_4). Om deze vervuiling terug te dringen, moeten eerst de desbetreffende productieprocessen in kaart gebracht worden.

Echter, productieprocessen in de landbouw zijn onderhevig aan *natuurlijke variatie*: externe invloeden, zoals van het weer en klimaat. Daarnaast zijn alle cijfers ook nog onderhevig aan *epistemische onzekerheid*: ze kunnen meetfouten bevatten, of men weet niet zeker of de cijfers die worden gebruikt ook wel exact hetzelfde productieproces weerspiegelen. De cijfers die nodig zijn als invoer van een model om de milieu-impact van een product te berekenen, zijn dus onderhevig aan onzekerheden. Dit leidt tot onzekerheid rondom de uitkomst van een milieu-impact *model*. Daarmee lijkt het meenemen van

onzekerheid in eerste instantie alleen maar te leiden tot nog meer vragen: *hoe beïnvloedt natuurlijke variatie de modeluitkomst? Zijn de verschillen die ik vind in de modeluitkomst nog wel significant als ik onzekerheden meeneem van de input variabelen? Welke variabelen zijn verantwoordelijk voor de meeste spreiding rondom de uitkomst?* Over deze vragen, en nog vele anderen, gaat dit proefschrift.

Een uitleg van de *schuingedrukte* terminologie en methodes, die gebruikt worden in dit proefschrift, is terug te vinden in de kaders.

> ***Onzekerheid***: in de context van dit proefschrift is het een parapluterm voor zowel ***natuurlijke variatie*** (variatie door verschillen in klimaat, weersinvloeden, menselijk handelen) als ***epistemische onzekerheid*** (onzekerheid door gebrek aan kennis maar ook bijvoorbeeld meetfouten, of ontbrekende data). ***Spreiding***: de gekwantificeerde onzekerheid rondom een datapunt van een *input variabele* of een *output variabele*. ***Standaardafwijking***: spreiding van een dataset, bijvoorbeeld van de normale verdeling. ***Distributiefunctie***: de kansverdeling waarmee een variabele beschreven wordt, bijvoorbeeld bij een standaard normale verdeling vallen 99.7% van de waardes van de kansverdeling binnen $\pm$3x de *standaardafwijking* van de gemiddelde waarde van de verdeling. ***Correlatie***: (lineaire) samenhang tussen twee grootheden.

Doel van dit proefschrift

Het doel van mijn proefschrift is de betrouwbaarheid verbeteren van modellen die milieu-impacts kwantificeren, gebruik makend van methodes voor *onzekerheidsanalyse* en *gevoeligheidsanalyse*. Hiervoor heb ik verschillende methodes met elkaar vergeleken en expliciet gekeken naar het effect van *correlatie* op de *spreiding* rondom de uitkomst van milieu-impact modellen. Alle methodes gebruikt in dit proefschrift zijn toegepast op voedselproductiesystemen.

> ***Gevoeligheid***: hoe sterk een variabele doorwerkt op de modeluitkomst. Er bestaan drie soorten ***gevoeligheidsanalyses***: (1) ***lokale gevoeligsheidsanlyse***: kwantificeert wat er gebeurt met de modeluitkomst als de input variabelen één voor één een heel klein beetje worden veranderd; (2) ***screening analyse***: kwantificeert wat er gebeurt met de modeluitkomst als de input variabelen één voor één worden veranderd tussen hun daadwerkelijke minimum en maximum waardes; (3) ***globale gevoeligheidsanalyse***: kwantificeert hoeveel van de spreiding rondom de output variabele kan worden verklaard door de input variabelen, door middel van de ***gevoeligheidsindex***.

Enkele resultaten uitgelicht

In **Hoofdstuk 2** worden twee methodes voor gevoeligheidsanalyse gecombineerd: de “multiplier methode" (een *lokale gevoeligheidsanalyse*) en de “methode van elementaire effecten" (een *screening methode*). De methodes worden toegepast op een productie systeem in de varkenshouderij, inclusief de keten voorafgaand aan de houderij, zoals de productie van de veevoer ingrediënten. De resultaten van beide methodes worden met elkaar gecombineerd om tot suggesties tot reductie van milieu-impacts te komen en om betrouwbaarheid van de modeluitkomst te verhogen.

Variabele: een grootheid in het model, bijvoorbeeld brandstof (in liter), elektriciteit (in kWh) of broeikasgas (in kg CO_2). De variabelen die het model ingaan worden ***input variabelen*** genoemd, de modeluitkomst wordt ook wel de ***output variabele*** genoemd. Bijvoorbeeld, om de totale broeikasgassen van melk te bepalen is 10 liter diesel nodig. In dit geval is 10 de variabele (ook al varieert deze niet daadwerkelijk). Het kan ook zijn dat er gemiddeld 10 liter diesel nodig is, maar dat er een spreiding om dit gemiddelde ligt met een standaardafwijking van 0.5. In dat geval is de variabele gelijk aan de distributiefunctie, met een gemiddelde van 10 en een standaardafwijking van 0.5. ***Model***: in de context van dit proefschrift gaat het om modellen die de milieu-impact van een productiesysteem bepalen. Deze modellen bevatten meerdere input variabelen (meestal in de orde van enkele honderden) en meestal één output variabele, bijvoorbeeld het broeikasgas CO_2.

In **Hoofdstuk 3 en 4** worden verschillende methodes voor onzekerheids- en *globale gevoeligheidsanalyse* met elkaar vergeleken op verschillende aspecten: (1) type *onzekerheidspropagatie* (wel of geen gebruik makend van *sampling*), (2) hoe goed ze zijn in het bepalen van de spreiding rondom de uitkomst , en (3) hoe goed ze zijn in het verklaren van spreiding rondom de uitkomst. Methodes die het meest geschikt zijn (binnen milieu-impact modellen) zijn *Monte Carlo simulatie* voor onzekerheidspropagtie en op regressie gebaseerde methoden voor globale gevoeligheidsanalyse, de ‘kwadratisch gestandaardiseerde regressie coefficient’ fungeert dan als de *gevoeligheidsindex*.

Onzekerheidspropagatie: het voortplanten van onzekerheden rondom input variabelen door een model, wat resulteert in onzekerheid in de output variabele van dat model. ***Onzekerheidsanalyse***: analyseren van de onzekerheid van de uitkomst, bijvoorbeeld het bepalen van de spreiding, of het vergelijken van twee distributiefuncties. ***Sampling***: het trekken van random getallen uit een distributiefunctie. Bijvoorbeeld: uit een uniforme verdeling tussen 0 en 1, kunnen de eerste drie samples zijn: 0.1; 0.8; 0.2. ***Monte Carlo simulatie***: door middel van sampling de spreiding rondom de output variabele van een model schatten.

In sommige gevallen is er sprake van *correlatie* tussen de spreiding van twee (of meer) variabelen binnen een model. Binnen de landbouw kan men bijvoorbeeld denken aan een correlatie tussen voerinname en melkproductie van een koe. Als de voerinname en melkproductie beiden variëren zullen deze twee variabelen gelijk optrekken, maar niet helemaal: de temperatuur in de stal, de samenstelling van het voer, de gezondheid van de koe, kunnen ook allemaal invloed hebben op deze onderlinge afhankelijkheid. Het is echter vaak lastig om de waarde voor de correlatiecoëfficiënt boven tafel te krijgen, in sommige gevallen is deze waarde simpelweg niet aanwezig.

In **Hoofdstuk 5** wordt, zonder dat vooraf de waarde van de correlatiecoëfficiënt bekend is, bepaald in welke gevallen correlatie tussen variabelen genegeerd kan worden. Het blijkt dat, in sommige gevallen, het meenemen van correlatie geen tot weinig invloed heeft op de spreiding rondom de uitkomst, noch op de gevoeligheidsanalyse. In deze gevallen is het dus mogelijk om de correlatiecoëfficiënt te negeren, wat mogelijk veel tijd bespaart die beter besteed kan worden aan het verbeteren van de datakwaliteit van de andere variabelen. In sommige gevallen is heeft de correlatie wel een groot effect op de spreiding en de gevoeligheidsanalyse, dan is het dus wel noodzakelijk om de echte waarde van de correlatiecoëfficiënt te achterhalen. In **Hoofdstuk 6** wordt de in Hoofdstuk 5 beschreven procedure toegepast op een productiesysteem binnen de melkveehouderij. Hier blijkt dat de correlatiecoëfficiënt tussen voerinname en melkproductie wel degelijk van belang is, en dus niet zonder meer genegeerd kan worden.

In **Hoofdstuk 7** worden de milieu-impacts van verschillende boerenbedrijven met elkaar vergeleken op het gebied van efficient nutriënten gebruik. Vooraf waren de distributiefuncties van alle variabelen bekend. Vervolgens werden verschillende methodes voor onzekerheids- en gevoeligheidsanalyse toegepast. De onzekerheidsanalyse liet zien dat het meenemen van epistemi-

sche onzekerheden, er in sommige gevallen toe leidde dat de bedrijven geen significant verschillend nutrient gebruik hedden. Vervolgens wordt een globale gevoeligheidsanalyse toegepast, waardoor de variabelen konden worden bepaald die het meest bijdroegen aan de spreiding van de uitkomst. Vervolgens worden de standaardafwijkingen van de belangrijkste variabelen in het model verkleind, wat leidt tot meer onderling verschillende bedrijven.

In **Hoofdstuk 8** worden enkele aanbevelingen gedaan, die zich erop richten de betrouwbaarheid van toekomstige studies met behulp van milieu-impact modellen te vergroten. Ten eerste, het standaardiseren van methoden voor onzekerheids- en gevoeligheidsanalyse in wetenschappelijke literatuur leidt er toe dat de onderlinge vergelijkbaarheid tussen studies verbetert. Ten tweede, het in tandem uitvoeren van lokale en globale gevoeligheidsanalyse geeft beter inzicht in de meest essentiële variabelen dan het toepassen van slechts één methode, met name voor variabelen waarvoor het niet mogelijk is om een spreiding te vinden. Ten derde, door vooraf de grootte van het effect van correlaties tussen input variabelen op de modeluitkomst te bepalen (zoals beschreven in Hoofdstuk 5), kan het risico van het negeren op de spreiding rondom de modeluitkomst worden bepaald.

Deze drie punten dragen bij aan het vergroten van de betrouwbaarheid van milieu-impact modellen, en dragen daarmee bij aan het formuleren van strategieën om toekomstige milieu-impact van voedselproductie verder te reduceren.

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About the author

Curriculum Vitae

Evelyne Groen (1985) studied physics at the University of Amsterdam. In 2012 she started her PhD research at the University of Wageningen, which resulted in this thesis.

Please visit: http://evelynegroen.github.io, which contains an up-to-date list of publications and the MatLab code that was used for implementing sensitivity-analysis methods.

Publications and forthcoming publications

Journals

Groen, E.A., Bokkers, E.A.M., Heijungs, R., de Boer, I.J.M. Methods for uncertainty propagation in life cycle assessment, *Environmental Modelling & Software*, 62: 316 – 325, 2014.

Ziegler, F., Groen, E.A., Hornborg, S., Bokkers, E.A.M., Karlsen, K.M., de Boer, I.J.M. Assessing broad life cycle impacts of daily onboard decision-making, annual strategic planning, and fisheries management in a northeast Atlantic trawl fishery, *The International Journal of Life Cycle Assessment*, First online: 6 June 2015.

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Groen, E.A., Bokkers, E.A.M., Heijungs, R., de Boer, I.J.M.. Methods for global sensitivity analysis in life cycle assessment, *submitted*.

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Mu, W.*, Groen, E.A.*, van Middelaar, C., Bokkers, E.A.M., de Boer, I.J.M. Benchmarking European dairy Farms: the effect of epistemic uncertainty on nutrient use efficiency. *submitted*. **Both authors contributed equally (combined first-authorship).*

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Education Certificate

Conferences and seminars [4.5 ECTS]

SETAC Europe 21st LCA case study Symposium, Nisyros, Greece	2015
WIAS Science Day, Wageningen University	2012-2015
LCAFood conference, San Fransisco, USA and Rennes, France	2012 and 2014
LCA Discussion Forum, Zürich, Switzerland	2013

Presentations and talks [12.0 ECTS]

SETAC Europe 21st LCA case study Symposium, Nisyros, Greece	oral, 2015
Leibniz-Institut für Agrartechnik Potsdam-Bornin e.V., Germany	oral, 2015
WIAS Science Day, Wageningen University	poster 2013-2014 and oral, 2015
LCAFood conference, San Fransisco, USA	oral, 2014
WaCaSa meeting, Wageningen University	oral, 2014
LCA Discussion Forum, Zürich, Switzerland	oral, 2013
Centrum voor milieuwetenschappen (CML), Leiden University	oral, 2012
SP Technical Research Institute of Sweden, Göteburg, Sweden	oral, 2012
Life Cycle Management (LCM) conference, Göteburg, Sweden	poster, 2013
LCAFood conference, Rennes, France	poster, 2012

Courses and training [21.3 ECTS]

Environmental impact assessment of livestock systems, Wageningen University	2015
Linear and integer programming, Boulder University, USA (online)	2015
Efficient writing strategies, Wageningen University	2015
Writing grant proposals, Wageningen University	2015
WIAS introduction course, Wageningen University	2012
Ethics and philosophy, Wageningen University	2012
Statistics for the life sciences, Wageningen University	2012
Theoretical ecology, Groningen University	2012
Advanced LCA course, Aalborg University, Denmark	2012
Organising WhiteFish meeting, Wageningen University	2012
Preparing PhD research proposal, Wageningen University	2012

Supervision and lectures [7.7 ECTS]

Lecture, Environmental impact assessment of livestock systems	2015
Guest lecture, Humboldt University, Berlin, Germany	2015
Supervision BSc thesis: Flavia Casu, Lisanne de Goede, Vera van Bussel	2014-2015
Supervision IDW Praktijkproject, Wageningen University	2012-2013

Complied with the educational requirements set by the Graduate School of Wageningen Institute of Animal Sciences (WIAS). ECTS: European Credit Transfer and Accumulation System, equivalent to a study load of 28 hours.

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