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Method to Decompose Uncertainties in LCA Results into Contributing Factors

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ABSTRACT

Purpose

Understanding uncertainty is essential in using life cycle assessment (LCA) to support decisions. Monte Carlo simulation (MCS) is widely used to characterize the variability in LCA results, be them life cycle inventory (LCI), category indicator results, normalized results, or weighted results. In this study, we present a new method to decompose MCS results into underlying contributors using the logarithmic mean Divisia index (LMDI) decomposition method with a case study on natural gas focusing on two impact categories: global warming and USETox human health impacts.

Methods

First, after each run of MCS, the difference in simulated and deterministic results is calculated and the difference is decomposed using the LMDI decomposition method, which returns the contribution of each factor to the difference of the run. After repeating this for 1,000 MCS runs, the statistical properties of the contributions by each factor are analyzed. The method quantifies the contribution of underlying variables, such as characterization factors and LCI items, to the overall variability of the result, such as characterized results.

Results

The method presented can decompose the variabilities in LCI, characterized, normalized, or weighted results into LCI items, characterization factors, normalization references, weighting factors, or any subset of them. As an illustrative example, a case study on natural gas LCA was conducted, and the variabilities in characterized results were decomposed into underlying LCI items and characterization factors. The results show that LCI and characterization phases contribute 59% and 41%, respectively, to the uncertainty of the characterized result for global warming. For the human health impact category, LCIs and characterization factors contribute 32% and 68% to the overall uncertainty, respectively.

Conclusions and discussion
Using this approach, LCA practitioners can decompose the overall variability in the results to the underlying contributors under MCS setting, which can help prioritize the parameters that need further refinement to reduce overall uncertainty in the results. The method reliably estimates the uncertainty contributions of the variables with large variabilities without the need for large computational resources, and it can be applied to any stage of an LCA calculation including normalization and weighting, or to other fields than LCA such as material flow analysis and risk assessment.

Keywords: uncertainty analysis, uncertainty contribution, life cycle assessment, Monte Carlo simulation, LMDI method

1. INTRODUCTION

Life Cycle Assessment (LCA) is a method to quantify the environmental impacts of a product system (ISO 2006; Finnveden et al. 2009). Understanding uncertainty in LCA results is essential in supporting decisions that use them (Geisler et al. 2005; Basson and Petrie 2007; Lloyd and Ries 2008). Quantitative uncertainty analysis has been implemented in many LCA studies (Lo et al. 2005; Bojacá and Schrevens 2010; Clavreul et al. 2012). Two common forms of uncertainty propagation in LCA are (1) the sampling method and (2) the analytical method (Heijungs 1996; Björklund 2002; Heijungs and Huijbregts 2004). In general, the sampling approach can provide more statistics than the analytical approach while requiring much more computer time for large systems, such as the ecoinvent database (Heijungs and Lenzen 2014). Among them, Monte Carlo simulation (MCS), a sampling method, is one of the most widely used methods to characterize the variability in LCA (Huijbregts 2002; Sonnemann et al. 2003; Beltran et al. 2018). Increasing LCA software tools support MCS (SimaPro 2016; OpenLCA 2018). Recently, the distribution functions of the entire ecoinvent LCI database have been estimated using MCS (Qin and Suh 2017).

Typical MCS results show the distribution of the overall calculation, be them LCI, characterized result, normalized result, or weighted result. However, such distributions do not indicate which factor, for example, LCI item, characterization factor, normalization reference, or weighting factor, contributes the most to the overall uncertainty. Sensitivity analysis can be used to quantify the relative importance of the parameters to overall uncertainty. Local sensitivity analysis or one-at-a-time (OAT) technique varies one parameter for each run and measures the change in the result relative to the change in the parameter (Hamby 1994; Hughes et al. 2013). Global sensitivity analysis, on the other hand, simultaneously varies all uncertain parameters and considers parameter interactions to obtain the input-output mapping (Saltelli et al. 2008; Cucurachi et al. 2016). Global sensitivity analysis identifies the most influential parameters that contribute to the output uncertainty by measuring the relative importance of the model parameters, and the method has been utilized to estimate relative contributions of parameters to overall uncertainty (Geisler et al. 2005; de Koning et al. 2010; Mutel et al. 2013; Heijungs and Lenzen 2014; Wei et al. 2015; Groen et al. 2017; Igos et al. 2019; Patouillard et al. 2019). Parsing out overall distribution results to contributing factors becomes computationally intensive under an MCS setting (Ye and Hill 2017). Furthermore, although global sensitivity analysis provides the ranking and the sensitivity indices of contributing parameters, the index values cannot be interpreted as the measure of uncertainty contributed to the overall results (Xu and Gertner 2011). Attempts to avoid using rank orders and indices for uncertainty contributions have been made using regression or correlation analyses (Heijungs and Lenzen 2014; Groen et al. 2017; Igos et al. 2019), which require an even larger number of samples, exacerbating the problem of computational intensity.

In this paper, we present a new method to decompose the overall uncertainty of an LCA study derived from MCS. The method is then applied to a case study on a natural gas LCA. We compare our method against previously reported methods of analyzing uncertainty contributions.

In general, the change in the overall results of a model involving multiple variables can be allocated over contributing factors using decomposition analysis methods. Oaxaca (1973) and Blinder (1973) developed a decomposition method to analyze the wage differences by race and sex, which is now a standard method in applied economics (Jann 2008). The basic idea of the Oaxaca-Blinder decomposition has since been improved and expanded over the past three decades and evolved into various decomposition analysis approaches (Boyd et al. 1988; Fortin et al. 2011; Su and Ang 2012). Two main approaches of decomposition analysis are index decomposition analysis (IDA) and structural decomposition analysis (SDA) (Hoekstra and Van den Bergh 2003). IDA uses aggregate sector information, which only assesses the impact of direct effects, while SDA uses the economic input–output analysis framework allowing decomposition of both direct and indirect effects such as changes in economic structures, international sourcing, and changes in consumption patterns and volumes (Dietzenbacher and Hoekstra 2002; Hoekstra and Van Den Bergh 2002; Hoekstra et al. 2016). In our study, we chose IDA, as our objective here is to demonstrate the method to decompose the overall uncertainty into the four phases of LCA calculation without involving the analysis of structural effects. However, SDA can also be applied under the same framework that we are proposing here.

Index decomposition analysis was first developed to study the impact of structural changes on energy use by industry in the late 1970s (Kako 1978; Jenne and Cattell 1983; Marlay 1984). IDA has been used to quantify the impact of different factors on the change of energy intensity and extended to many regions and various application areas such as transportation, electricity generation and environmental study (Ang et al. 1998; Paul and Bhattacharya 2004; Malla 2009; Al-Ghandoor et al. 2010). For example, Zhang et al. (2009) used the IDA to decompose the influence of energy-related factors in CO_2 emission reduction in China.

Ang (2004) reviewed IDA studies and concluded that the logarithmic mean Divisia index (LMDI) method is the most preferable decomposition method. LMDI leaves no residuals in the analysis and performs well even with multiple variables and zeros in the dataset (Ang 2004; Ang and Liu 2007; Meng et al. 2018). The LMDI has been widely used in economy-wide studies and also in the energy field (Boyd et al. 1987; Ang and Liu 2001; Timilsina and Shrestha 2009; Baležentis et al. 2011; Jeong and Kim 2013; González et al. 2014).

The LMDI method in these applications was used as a method to decompose changes in the total results over time. We use the LMDI to decompose the variability of the results. The LMDI method was originally applied for the decomposition of variabilities in results over time. In our case, however, we apply the same decomposition method, while the variability in the results is not from the changes over time but from the perturbations in MCS. For example, the overall variability in a characterized result, say climate change impact measured by global warming potential (GWP) 100, of an electric vehicle can be decomposed into the variabilities in underlying factors such as the amount of cobalt or lithium needed to produce a unit of the electric vehicle.

This work aims to provide a methodology for quantifying the contribution of each variable in an LCA model to the overall variability of the model results using the LMDI method. To our best knowledge, this paper represents the first attempt to apply the technique of index decomposition analysis to uncertainty analysis.

This paper is organized as follows: a detailed methodology description of the proposed method is presented in the Methods section. We then apply the method using a case study in a subsection, Case study. The next section, Results, presents the findings of the case study. The Discussion and Conclusions section discusses the implications of the proposed method and concludes the paper.

2. METHODS

2.1 Basic Principle

Decomposing MCS results into contributing factors is challenging because the outcome of an MCS, which is a distribution, is a result of simultaneous sampling of all the variables involved in a model. Therefore, parsing out the contribution by each variable directly to the overall shape of the distribution is not feasible based on the MCS result alone. However, the outcome of each MCS run deviates from the outcome of the deterministic model generated from default values for all parameters. This difference between the deterministic and simulated results can be attributed to the differences between the default and sampled values of the underlying variables using a decomposition method. The result of decomposition can then be used as a measure of contribution by each variable to the variability of the overall result. The contribution by each variable will vary between model runs, as different values will be sampled for each run according to the stochastic properties of those variables. By sampling the variables, running the model, and decomposing the variability in the results for a sufficiently large number of times, it is possible to estimate the distribution of the contribution by each variable to the overall variability in the results. This basic idea is presented in more detail in steps from the following subsection.

2.2 Calculation steps for uncertainty contribution analysis

Six main steps are involved in the proposed method to calculate the uncertainty contributions of underlying factors in an LCA. Fig. 1 shows a summary of the procedure. For the sake of simplicity, we will use the characterized result, h_i as an example. Calculation steps for normalized and weighted results are presented later in this section.

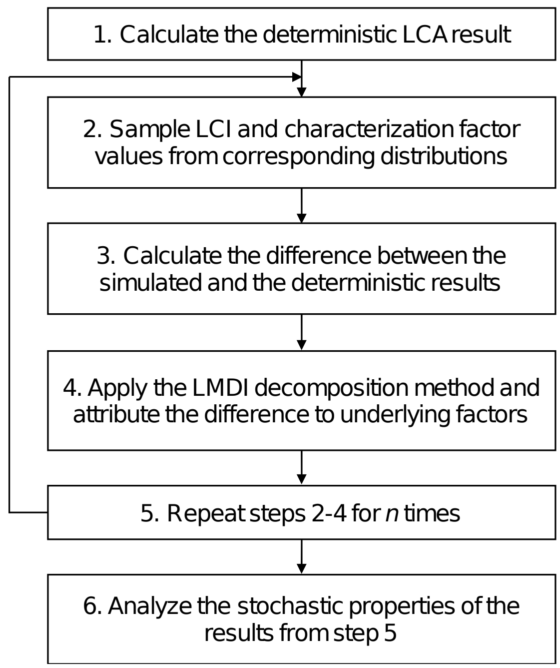

Fig. 1. Flow diagram of the use of the LMDI method in decomposing the uncertainty in the LCA results.

Fig. 2 (a) illustrates the procedure graphically. For each run from $k = 1$ to $k = n$, the overall difference in the deterministic and simulated results, Δh_i is decomposed into underlying factors that are denoted as m_1, m_2, … m_l (LCI items) and $c_{i,1}$, $c_{i,2}$, …$c_{i,l}$ (characterization factors). By running the decomposition for n times, the distribution of the contribution to Δh_i by each factor can be derived through the steps explained in the following section (Fig. 2 (b)). The average of the contribution can be illustrated in a pie chart (Fig. 2 (c)).

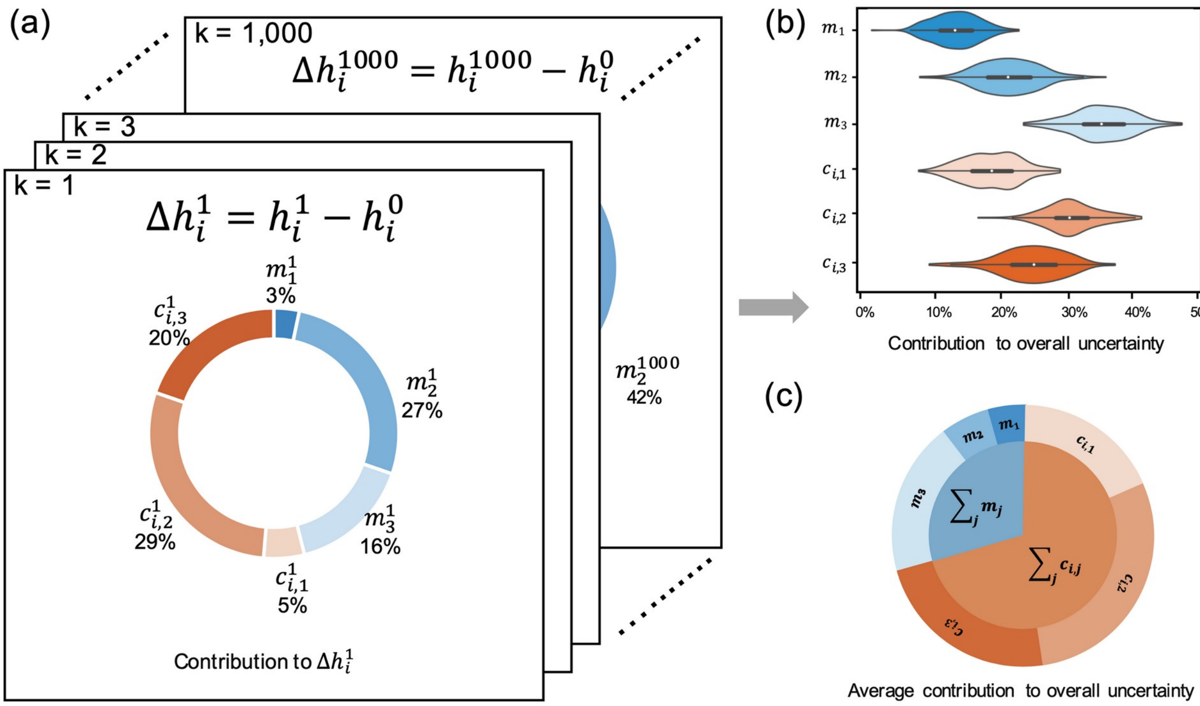

Fig. 2. Graphic presentation of the uncertainty decomposition method using the LMDI decomposition method combined with Monte Carlo samples.

Step 1. Deterministic result calculation

The first step is to calculate the deterministic characterized result. The characterized LCA result is calculated through

$$h_i = \sum_j c_{i,j} m_j \quad (1)$$

where, h_i is the characterized result for characterization model i;

$c_{i,j}$ is the characterization factor for the elementary flow j in impact category i;

m_j is the inventory for the elementary flow j.

Step 2. Simulated result calculation

The second step is to simulate LCI items and characterization factors by randomly selecting values from their specified distributions and store both simulated values and the characterized LCA result, h_i^k. In the study, k represents simulation runs. I.e., h_i^k is the kth simulation of the characterized result for impact category i. Deterministic value for ith characterized result is noted as h_i^0, where $k = 0$.

The equation for calculating the characterized result in impact category i in simulation k is provided as follows:

$$h_i^k = \sum_j h_{i,j}^k = \sum_j c_{i,j}^k m_j^k \qquad (2)$$

where h_i^k is the characterized result for impact category i in simulation k;

$h_{i,j}^k$ is the characterized result of elementary flow j for impact category i in simulation *k;*

$c_{i,j}^k$ is the characterization factor for the elementary flow j in impact category i in simulation k;

m_j^k is the life cycle inventory for the elementary flow j in simulation k.

Step 3. Difference calculation

The third step is to calculate the difference between the simulated LCA result and the deterministic LCA result for each simulation, and the difference is considered the change in the LCA results:

$$\Delta h_i^k = h_i^k - h_i^0 \qquad (3)$$

Step 4. Decomposition of the difference

The next step is to apply the LMDI decomposition method to find the contribution of each LCI item and characterization factor in the change of the LCA result for each simulation. The difference between the simulated and deterministic characterized results, $h_i^k - h_i^0$, can be decomposed into the influence of LCI items and characterization factors, $c_{i,j}$ and m_j, respectively.

The calculation of aggregate changes from h_i^0 in the deterministic result to h_i^k in simulation k followed the LMDI approach by Ang (2005, 2015). The additive decomposition suggests:

$$\Delta h_i^k = h_i^k - h_i^0 = \Delta h_{ic}^k + \Delta h_{\Im}^k \qquad (4)$$

where Δh_{ic}^k is the change in characterized result for impact category i in simulation k attributable to the variabilities in characterization factors;

$\Delta h_{\Im}^{k}$ the change in the characterized result for impact category *i* in simulation *k* attributable to the variabilities in LCI items.

In multiplicative decomposition method, the difference can be decomposed:

$$D_{h_i}^{k} = h_i^k / h_i^0 = D_{ic}^{k} D_{\Im}^{k} \quad (5)$$

where D_{ic}^{k} is the changes in characterized result for impact category *i* in simulation *k* attributable to the variabilities in characterization factors;

$D_{\Im}^{k}$ is the changes in characterized results for impact category *i* in simulation *k* attributable to the variabilities in LCI items.

Using the LMDI approach, Δh_{ic}^{k} and $\Delta h_{\Im}^{k}$ can be decomposed by additive decomposition:

$$\Delta h_{ic}^{k} = \sum_j L\left(h_{i,j}^k, h_{i,j}^0\right) \ln\left(\frac{c_{i,j}^k}{c_{i,j}^0}\right) = \sum_j \frac{h_{i,j}^k - h_{i,j}^0}{\ln h_{i,j}^k - \ln h_{i,j}^0} \ln\left(\frac{c_{i,j}^k}{c_{i,j}^0}\right)$$

(6)

$$\Delta h_{\Im}^{k} = \sum_j L\left(h_{i,j}^k, h_{i,j}^0\right) \ln\left(\frac{m_j^k}{m_j^0}\right) = \sum_j \frac{h_{i,j}^k - h_{i,j}^0}{\ln h_{i,j}^k - \ln h_{i,j}^0} \ln\left(\frac{m_j^k}{m_j^0}\right) \quad (7)$$

By multiplicative decomposition:

$D_{ic}^{k} = \exp$¿¿ (8)

$D_{\Im}^{k} = \exp$¿¿ (9)

where $L(a, b) = (a - b)$¿ is the logarithmic mean (Ang, 2004).

Step 5. Repeat steps 2-4

This step repeats steps 2 to 4 for *n*=1,000 times, and the results of each run are stored, so that, once completed, the statistical properties of the decomposition results are analyzed in the next step.

Step 6. Analysis of the distribution

The final step is to calculate the average contribution of each LCI item and characterization factor to the change in the LCA result.

For additive decomposition:

$$\Delta' h_{ic} = \frac{\sum_k \Delta h_{ic}^k}{n} \quad (10)$$

$$\overline{\Delta h_{\Im}} = \frac{\sum_k \Delta h_{\Im}^k}{n} \quad (11)$$

For multiplicative decomposition:

$$D'^{k}_{ic} = \frac{\sum_k D_{ic}^k}{n} \quad (12)$$

$$\overline{D^k_{\Im}} = \frac{\sum_k D_{\Im}^k}{n} \quad (13)$$

The LMDI decomposition method in Step 4 can be extended to find the uncertainty contribution in normalized and weighted results. The LMDI decomposition method for weighted results is presented in the following section.

2.3 The LMDI method for weighted results

Conceptually, the same steps described in the previous section can be applied to any stage of LCA calculation including LCI, characterized results, normalized results, and weighted results. Shown below is an application of the method to weighted results, where the contributions of the LCI items, characterization factors, normalization references, and weighting factors can be calculated.

Weighted results are calculated using Eq. 14 (Step 1):

$$W = \sum_i w_i (h \text{¿¿} i / n_i) = \sum_i w_i (h \text{¿¿} i \frac{1}{n_i}) = \sum_i w_i h_i q_i = \sum_{i,j} w_i c_{i,j} m_j q_i \text{¿¿} \quad (14)$$

where W is the normalized and weighted result;

w_i is the weighting factor for impact category *i*;

h_i is characterized result of impact category *i*;

n_i is the normalization reference for impact category *i*;

q_i is the inverse of the normalization reference, $n_{i,}$, for impact category *i*;

$c_{i,j}$ is the characterization factor for the elementary flow *j* in impact category *i*;

m_j is the LCI item for the elementary flow j.

Using Eq. 15, deterministic and simulated results are calculated (Step 2), and the difference between the two is derived (Step 3). Then the difference is decomposed into inventory items, characterization factors, normalization references, and weighting factors such that (Step 4):

$$\Delta W^k = W^k - W^0 = \sum_i \Delta W^k_{iw} + \Delta W^k_{ic} + \Delta W^k_{\Im} + \Delta W^k_{iq} \text{ (additive decomposition)} \qquad (15)$$

where ΔW is the change in the normalized and weighted result;

ΔW^k_{iw} is the change in normalized and weighted results for impact category i in simulation k attributable to the variability in weighting factors;

ΔW^k_{ic} is the change in normalized and weighted results for impact category i in simulation k attributable to the variabilities in characterization factors;

$\Delta W^k_{\Im}$ is the change in normalized and weighted results for impact category i in simulation k attributable to the variabilities in LCI items;

ΔW^k_{iq} is the effect of the variabilities in inversed normalization reference contributed to the change in normalized and weighted results for impact category i in simulation k.

$$D^k_W = W^k / W^0 = \sum_i D^k_{iw} D^k_{ic} D^k_{\Im} D^k_{iq} \text{ (multiplicative decomposition)} \qquad (16)$$

where D_W is the change in the normalized and weighted result;

D^k_{iw} is the change in normalized and weighted results for impact category i in simulation k attributable to the variability in weighting factor;

D^k_{ic} is the change in normalized and weighted results for impact category i in simulation k attributable to the variabilities in characterization factors;

$D^k_{\Im}$ is the change in normalized and weighted results for impact category i in simulation k attributable to the variabilities in LCI items;

D^k_{iq} is the change in normalized and weighted results for impact category i in simulation k attributable to the effect of the variabilities in inversed normalization references.

Under additive decomposition, the terms on the right-hand-side of Eq. 15 are calculated by:

$$\Delta W_w^k = \sum_{i,j} L\left(W_{i,j}^k, W_{i,j}^0\right) \ln\left(\frac{w_i^k}{w_i^0}\right) = \sum_{i,j} \frac{W_{i,j}^k - W_{i,j}^0}{\ln W_{i,j}^k - \ln W_{i,j}^0} \ln\left(\frac{w_i^k}{w_i^k}\right) \quad (17)$$

$$\Delta W_c^k = \sum_{i,j} L\left(W_{i,j}^k, W_{i,j}^0\right) \ln\left(\frac{c_{i,j}^k}{c_{i,j}^0}\right) = \sum_{i,j} \frac{W_{i,j}^k - W_{i,j}^0}{\ln W_{i,j}^k - \ln W_{i,j}^0} \ln\left(\frac{c_{i,j}^k}{c_{i,j}^0}\right)$$

(18)

$$\Delta W_m^k = \sum_{i,j} L\left(W_{i,j}^k, W_{i,j}^0\right) \ln\left(\frac{m_j^k}{m_j^0}\right) = \sum_{i,j} \frac{W_{i,j}^k - W_{i,j}^0}{\ln W_{i,j}^k - \ln W_{i,j}^0} \ln\left(\frac{m_j^k}{m_j^0}\right)$$

(19)

$$\Delta W_q^k = \sum_{i,j} L\left(W_{i,j}^k, W_{i,j}^0\right) \ln\left(\frac{q_i^k}{q_i^0}\right) = \sum_{i,j} \frac{W_{i,j}^k - W_{i,j}^0}{\ln W_{i,j}^k - \ln W_{i,j}^0} \ln\left(\frac{q_i^k}{q_i^0}\right) \quad (20)$$

Under multiplicative decomposition, the terms on the right-hand-side of Eq. 16 are calculated by:

$$D_w^k = \exp\left(\sum_{i,j} \frac{L\left(W_{i,j}^k, W_{i,j}^0\right)}{L\left(W^k, W^0\right)} \ln\left(\frac{w_i^k}{w_i^0}\right)\right) = \exp\text{¿¿} \quad (21)$$

$$D_c^k = \exp\left(\sum_{i,j} \frac{L\left(W_{i,j}^k, W_{i,j}^0\right)}{L\left(W^k, W^0\right)} \ln\left(\frac{c_{i,j}^k}{c_{i,j}^0}\right)\right) = \exp\text{¿¿} \quad (22)$$

$$D_m^k = \exp\left(\sum_{i,j} \frac{L\left(W_{i,j}^k, W_{i,j}^0\right)}{L\left(W^k, W^0\right)} \ln\left(\frac{m_j^k}{m_j^0}\right)\right) = \exp\text{¿¿} \quad (23)$$

$$D_q^k = \exp\left(\sum_{i,j} \frac{L\left(W_{i,j}^k, W_{i,j}^0\right)}{L\left(W^k, W^0\right)} \ln\left(\frac{q_i^k}{q_i^0}\right)\right) = \exp\text{¿¿} \quad (24)$$

2.4 Case study

The additive decomposition method presented in the previous section is applied to a natural gas LCA based on the ecoinvent database, version 3.1 (Allocation, default system model), (Wernet et al. 2016) to demonstrate the applicability of the method. Natural gas is the largest source (33%) of electricity generation in the U.S and will remain the primary energy source in the near future (EIA 2019). Characterization factors chosen for the comparison in the study are GWP 100 from IPCC 2013 (Stocker 2014) and carcinogenic human toxicity impact from

USEtox (Rosenbaum et al. 2008) because global warming impact is a time and space-insensitive model while the human health impact is time and space-sensitive.

The process flow diagram of natural gas production in the U.S. is presented in Fig. 3.

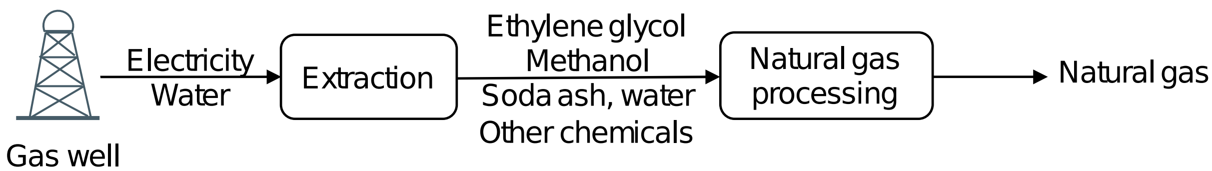

Fig. 3. Process flow diagram of natural gas production in the U.S.

The input data used for generating 1 m^3 of natural gas in the U.S. were extracted from ecoinvent v3.1. We applied the Pedigree method to estimate the uncertainty for 1,869 LCI items, 66 characterization factors of GWP 100, and 216 characterization factors of carcinogenic human toxicity impact in which the scores were obtained from the same group of experts through a survey (Qin and Suh 2017; Qin et al. 2020). The inputs follow lognormal distributions because the Pedigree method assumes the data follows a lognormal distribution (Qin and Suh 2017). The Pedigree score is determined based on the characteristics of the data according to the criteria from the Pedigree matrix. After 1,000 runs of MCS, we calculated the difference in the simulated and deterministic category indicator results and decomposed the difference using the LMDI decomposition method, which returns the contribution of each factor to the difference of the run. Then, we analyzed the statistical properties of the contributions by each factor after 1,000 MCS runs.

3. RESULTS

The deterministic values for life cycle greenhouse gas emissions (GHG) and carcinogenic human toxicity impacts of 1 m^3 of natural gas in the U.S. were, 0.45 kg of CO_2e and 1.27e-08 comparative toxic units (CTU_h), respectively. Fig. 4 shows the distribution of the simulated characterized results for the two impact categories. The average global warming impact of natural gas was 0.46 kg of CO_2e, and the corresponding standard deviation was 0.067 kg of

CO_2e. The average carcinogenic human toxicity impact was 1.39e-08 CTU_h, and the corresponding standard deviation was 4.46e-09 CTU_h.

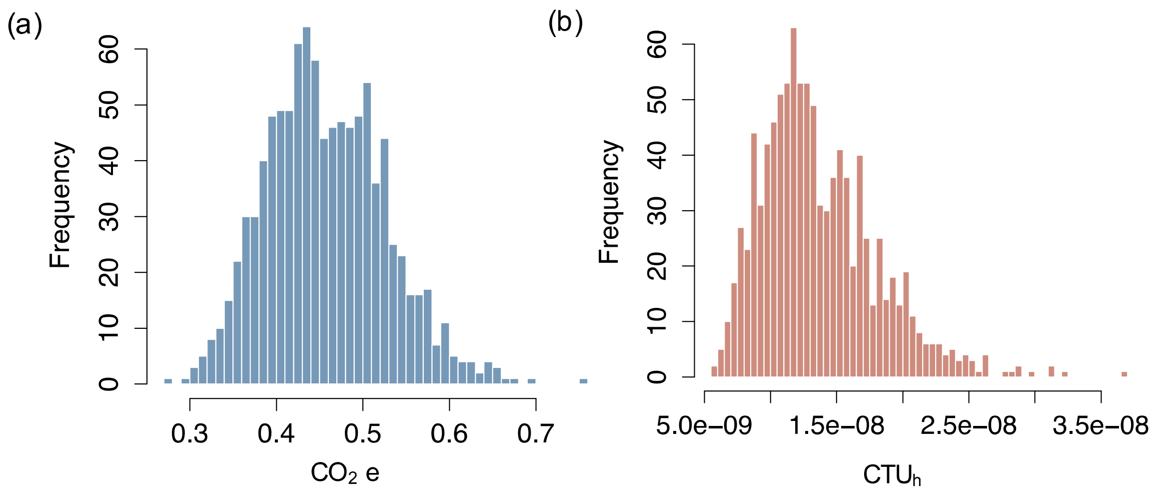

Fig. 4. Distributions of the characterized results of 1 m^3 of natural gas in the U.S. in (a) global warming impact and (b) carcinogenic human toxicity impact.

After running 1,000 MCS runs in conjunction with the LMDI decomposition analysis, the results showed that LCI and characterization factors contributed 65% and 35%, respectively, to the uncertainty in the characterized results for climate change (Fig. 5). Among the 65% of the uncertainty contribution from LCI, 51.2% of the total uncertainty came from methane emissions, and 8.2% from CO_2 emissions. The characterization factors of methane and the remaining characterization factors contributed to 33.7% and 1.7%, respectively, of the overall uncertainty in the characterized result.

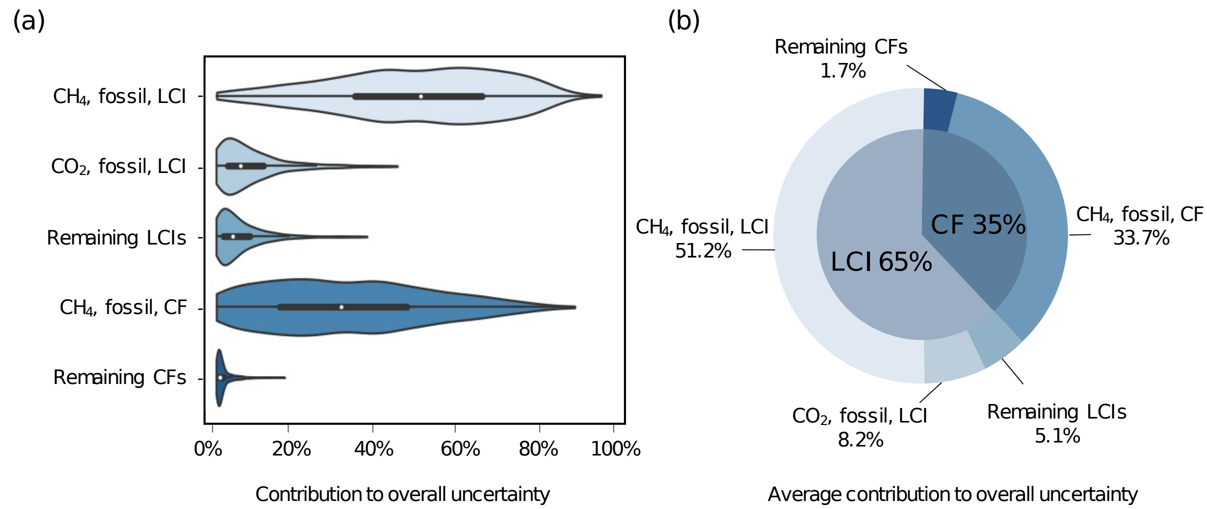

Fig. 5. (a) The distributions of the uncertainty contributions of the most influential factors in the climate change impact of natural gas production. (b) The average contribution of each factor to the overall uncertainty. The results are subject to change based on the selections of the Pedigree scores in the study.

The USEtox carcinogenic human health results indicated that 32% and 68% of the uncertainty can be attributed to LCI and characterization factors, respectively (Fig. 6). Among the LCI items, Chromium VI, Cr^{+}, contributed to 30.3% of the overall uncertainty. Arsenic, nickel, and the remainder of the LCI contributed to 1.2%, 0.4%, and 0.4%, respectively to the overall uncertainty in the characterized LCA result. Among the characterization factors, Chromium VI contributed 68% of the overall uncertainty. Arsenic, nickel, and the rest of the LCI contributed to 3.0%, 0.8%, and 1.1%, respectively to the uncertainty in the characterized LCA result.

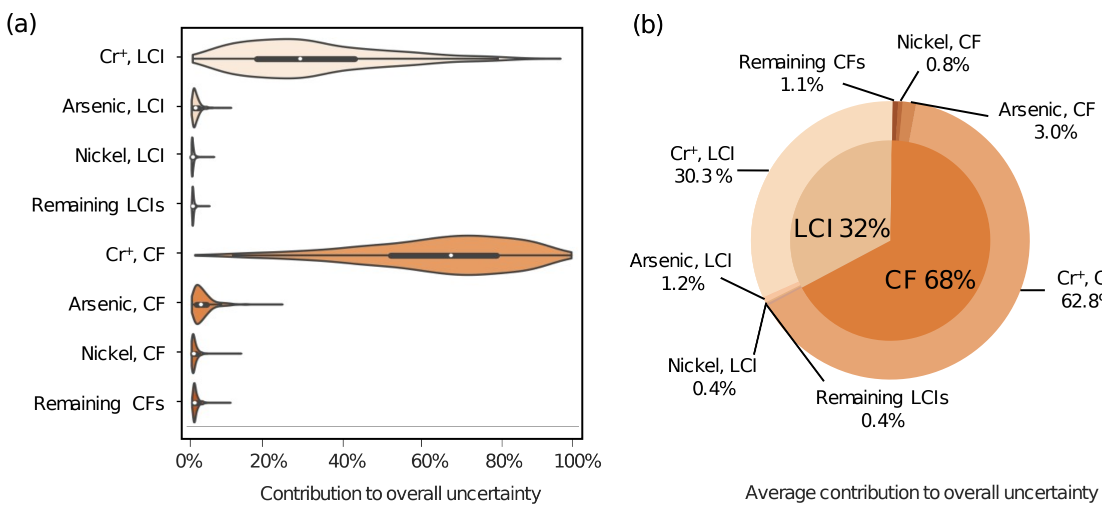

Fig. 6. (a) The distributions of the uncertainty contributions of the most influential factors in the carcinogenic human health impact of natural gas production. (b) The average contribution of each factor to the overall uncertainty. The results are subject to change based on the selections of the Pedigree scores in the study.

Both cases in climate change and human health carcinogen impacts suggested that the top 2 or 3 factors in LCI and characterization factors contributed to the majority (>90%) of the uncertainty, and the rest of LCI and characterization factors only had little (<10%) influence on the overall uncertainty of the characterized results. We have tested the multiplicative approach to the characterized results, and the relative contributions by underlying factors between additive and multiplicative approaches were identical. Improving the reliability of those top contributors, therefore, would reduce the uncertainty of the characterized results more effectively.

4. CONCLUSIONS AND DISCUSSION

This paper introduces a method to quantify the contributions of underlying variables in LCA to overall variability in the result. The proposed method uses the LMDI decomposition method combined with Monte Carlo simulation, with minimal additional needs of computational resources. To our knowledge, the method proposed in this paper is the first attempt to decompose the overall variability of an LCA derived from MCS into the variabilities of underlying parameters using an index decomposition approach.

Table 1 summarizes previously reported approaches and our method (LMDI decomposition) for analyzing uncertainty contributions drawing mainly from recent papers that reviewed multiple approaches (Groen et al., 2017; Igos et al. 2019). These approaches are compared against (1) the uncertainty propagation methods used, (2) the ability to explain small and larger input variabilities, (3) reliability in the results, and (4) computation time for sampling and calculation. According to Groen et al. (2017), global sensitivity methods require a sampling size (*N*) of 10^6 or larger for reliable results. Igos et al (2019) concluded that Sobol' indices method provides more reliable results than other methods, while it requires extensive computation time. Finally, as shown in Table 1, all but one (Sobol' total effect) of the existing approaches are not able to generate reliable uncertainty contributions for large input variability. The results from the LMDI decomposition method presented in this paper are close to those of the top contributors from Sobol' total effect approach, which is recognized as the most reliable approach in the literature, while substantially reducing the computation time. The results of the LMDI decomposition method, Sobol' total effect approach, and the OAT method are summarized in the Supplementary Information. Therefore, we believe that the LMDI decomposition method offers high reliability with reasonable computation time and is suitable for both small and large input variabilities.

Table 1. Key characteristics of common sensitivity methods.

Approach	Reference	Uncertainty propagation	Explain small input variability[a]	Explain large input variability[a]	Reliability[a]	Computation time[a]
Local sensitivity analysis						
One-at-a-time analysis	(Hamby 1994)	Sampling	Yes	Yes	Medium	Long
Perturbation analysis	(Heijungs and Kleijn 2001)	Analytical	Yes	No	Medium	Short
Global sensitivity analysis						
Key issue analysis	(Heijungs 2010)	Analytical	Yes	No	Low	Short
Standardized regression coefficient	(Huijbregts et al. 2001)	Sampling	Yes	No	Medium	Medium
Spearman correlation coefficient	(Sonnemann et al. 2003)	Sampling	Yes	No	Medium	Medium
Sobol' main effect	(Sobol 2001)	Sampling	Yes	No	High	Long
Sobol' total effect	(Saltelli et al. 2010)	Sampling	Yes	Yes	High	Long

Random balance design	(Tarantola et al. 2006)	Sampling	No	No	Low	Medium
LMDI decomposition	This paper	Sampling	Yes	Yes	High	Medium

[a] Drawn mostly from Groen et al (2017) and Igos et al (2019). The computation time is estimated from the calculation using the entire ecoinvent database.

Our case study showed a use case of the method proposed in this paper. A deterministic LCA result showed that 1 m^3 of natural gas generates 0.45 kg of CO_2e and 1.27e-08 CTU_h of characterized impacts for climate change and carcinogenic human toxicity categories throughout its life-cycle. The standard deviations of the distributions of climate change and carcinogenic human toxicity impacts were 0.067 kg of CO_2e and 4.46e-09 CTU_h, respectively. These distributions were then decomposed into underlying factors using the LMDI decomposition method as proposed in this paper. The results show that methane was the largest contributor to the overall variability of the characterized result of climate change, and Chromium VI was the largest contributor to the overall variability of the characterized result of carcinogenic human toxicity. Future data collection and refinement efforts can focus on these categories to more effectively reduce the overall variability of the results.

It is notable that our method and the case study only considered parametric uncertainty, which is the most commonly addressed uncertainty type in LCA studies (Lloyd and Ries 2008). These results are based on the uncertainty estimates from the Pedigree matrix for both LCI and characterization factors. Whether the Pedigree method is an appropriate approach to quantifying the variabilities of parameters in LCA is still debated (Qin et al. 2020). The method presented in this paper is agnostic about the method of variability estimation or the type of distribution functions used.

The method presented can be used in other fields of science, where quantifying the influence of underlying variables on the overall variability of the results is useful. For example, the proposed method can be used to quantify the uncertainty contribution of population, affluence, and technology to the impact of human activities on the environment using the IPAT equation (York et al. 2003; Ma et al. 2017). Likewise, the proposed method can be used to analyze uncertainty contributions in Kaya identity, where the total GHG emissions are expressed as a product of GHG emissions intensity of energy, energy intensity of fuels, fuel consumption intensity of products, final consumption per capita, and population (Jung et al. 2012; Pachauri et al. 2014). The results of the proposed method of uncertainty contribution analysis can help policy and decision makers better understand the uncertainty in the results and prioritize the research effort to reduce the overall uncertainty.

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