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REVIEW

ENVIRONMENTAL PROGRESS & SUSTAINABLE ENERGY

Uncertainty in inventories for life cycle assessment: State-of-the-art, challenges, and new technologies

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Abstract

Uncertainty is a critical factor that can hinder the quality and potential applications of life cycle assessment (LCA) results. A prominent source of uncertainty stems from the life cycle inventory (LCI) data. Various methodologies exist to estimate the uncertainty associated with LCI data, primarily based on the widely used structured pedigree matrix approach or the computationally intensive Monte Carlo simulation. This perspective review explores how new technologies (e.g., computational algorithms and data collection methods) from data science and related fields can contribute to identifying, quantifying, and reducing uncertainty in LCI modeling. A brief overview of the sources of uncertainty in LCI modeling and how they are addressed in current LCA practice is provided. Additionally, several new technologies are identified, and the potential benefits of their implementation in reducing uncertainties in LCI modeling are discussed. This perspective review concludes by identifying potential areas that require further development for these technologies.

KEYWORDS

blockchain, life cycle assessment, life cycle inventory, machine learning, uncertainty

1 | INTRODUCTION

Life cycle assessment (LCA) is currently the most used methodology to holistically assess the environmental impacts of a product, process, or service within a well-defined boundary. The widely accepted LCA methodology is defined by two ISO standards, 14040[1] and 14044,[2] complemented by other ISO standards, for example, ISO 14071,[3] that define guidelines for performing a critical review of LCA studies and analyses. The aforementioned standards are the basis of other ISO standards, such as ISO 14064[4] and

14067,[5] that deal with the carbon footprint of products, processes, and services. Other assessments that consider these impacts, as well as risk evaluations, depend on environmental release information and its uncertainty.

Uncertainty in an LCA study can originate from various sources,[6] including the definition of allocation criteria/methodologies,[7] impact assessment methodologies,[8] and life cycle inventory (LCI) data.[9] The assessment of environmental impacts hinges on accurate LCI modeling, which requires an accurate accounting of elementary (e.g., emissions, minerals extracted from the Earth), energy, material, and waste flows within and across the system boundary. Consequently, the fidelity of an LCA study is directly tied to the uncertainty of the LCI data.[10]

Uncertainty in LCI data may still exist even when primary data measured directly from the system of interest is used. One example is the measurement error from sensors due to environmental interference, such as temperature fluctuations, humidity, or electromagnetic disturbances. When using inventory data from secondary sources (i.e., collected from literature or from dedicated LCI databases), the level of uncertainty in LCI modeling could be higher, for example, due to the need to rely on proxies[11] and approximations, or the utilization of data that is only partly suitable.

The issue of data uncertainty has been recognized since the inception of LCA. The ISO standard 14040 explicitly acknowledges the necessity of assessing uncertainty in an LCA study, but it does not provide specific suggestions or guidelines. Despite this, significant contributions were made in past decades to address the uncertainty in LCA studies.[12,13] While there are guidelines available for conducting uncertainty analyses,[14] their scope is limited, and many published LCA studies do not include uncertainty analyses. When conducting an uncertainty analysis, it is essential to begin with the definition of the goal and scope of the LCA, which is the first step in the standard LCA framework.[1,2] For example, the goal may be to identify hotspots within the life cycle of a product or to compare the life cycles of two different products. The intention could also be to make claims based on the life cycle results. Alongside defining the scope—what is included and excluded from the systems being studied—it is important to contextualize the uncertainty analysis. The various methods presented here should each be considered in light of how they inform the results and whether the uncertainty provides differentiated conclusions regarding whether the intentions of the goal have been achieved. Therefore, there is a clear need for further research to enhance existing methodologies or to develop new ones that can more appropriately address the uncertainty of LCA.

Over the years, there has been a significant increase in the availability of affordable computing power. With advancements in data science, machine learning, artificial intelligence, and related fields, there is a potential to improve existing methodologies (e.g., pedigree matrix and Monte Carlo simulation), or even develop new ones, to improve uncertainty assessment for LCI. This perspective article discusses the potential of several such new technologies in identifying and assessing uncertainty in LCI data.

2 | CURRENT METHODS FOR ASSESSING UNCERTAINTY IN LCA

Before discussing some current methods in assessing uncertainty (i.e., the lack of knowledge about the true value of a variable, parameter, or model output), it is worthwhile to distinguish it from variability (i.e., the changeable conditions describing instances of a system) and to briefly address the two categories of uncertainty: epistemic and aleatory. Epistemic (or systematic) uncertainty arises from a lack of knowledge related to underlying fundamentals and is characterized by alternative models and bounds on the parameters. It is directly linked to the choices one has to make when performing an LCA study, particularly when selecting inventory data sets and the associated vagueness, imprecision, and ambiguity. From a statistical point of view, this type of uncertainty can be described by Bayesian (subjectivist) probability perspectives that may involve subjective evaluations. In contrast, aleatory (also called random) uncertainty refers to inherent uncertainty due to probabilistic fluctuations of parameters and events, for example, the error associated with sensor measurements. From a statistical point of view, a classical (frequentist) framework can be used to characterize this type of uncertainty. Even though both types of uncertainties can be represented by probability density functions and treated similarly, different methodologies should be considered when assessing each type, as described in the following sections, explaining each method in detail, followed by an illustration of its application to addressing one or both types of uncertainties.

2.1 | Pedigree matrix

The pedigree matrix method is useful for describing data quality and can be used to define uncertainty distributions for inventory data.[15] The method involves practitioners using judgment to assign data quality scores between 1 (very good quality, e.g., site-specific data for the process of interest) and 5 (very poor quality, e.g., data does not represent the technology of interest) for five data quality characteristics: time coverage, geographic coverage, technological coverage, reliability, and completeness.[16] Thus, the pedigree matrix indirectly addresses epistemic uncertainty by evaluating these data quality indicators (DQIs). Similarly, the pedigree matrix does not explicitly account for aleatory uncertainty. Instead, it focuses on pointing practitioners to use available data of high quality.

The use of uncertainty distributions based on data quality scores is straightforward. One can evaluate the characteristics of inventory data and assign data quality scores accordingly. By default, the pedigree matrix method assumes that the uncertainty of a datum follows a log-normal distribution, although methods have been proposed to accommodate other distributions.[17] The uncertainty distributions are characterized by geometric standard deviations (GSD), which are factors that can be multiplied (or divided) by the mean value for a lognormal distribution. These GSD can be applied for each of the quality characteristics, multiplied (or divided) by the existing distribution so far developed. The GSD covers the 95% confidence interval; the lower limit and upper limit of the interval are the mean value divided by the GSD and the mean value times the GSD, respectively.[18] The importance of these distributions for describing uncertainty should not be overlooked, as the GSD is dimensionless and thus applicable to inventory values of various sizes.

The longstanding pedigree matrix method has recently been improved by incorporating uncertainty distributions that are defined for each characteristic and score, with larger uncertainty factors applied for larger data quality scores.[17] Nevertheless, using a dataset for analysis requires careful evaluation of its quality. If the dataset is deemed unsuitable due to inaccuracies or biases, it is best to avoid using it altogether. This topic has been examined in studies pertaining to both processes and flows.[19,20] These studies show that when data have wide distributions, they can still significantly differ from the target. It is crucial to consider overall technological development when identifying key factors[21] or evaluating the representativeness of data, particularly when adjustments to the pedigree matrix are needed.[22] Moreover, while the pedigree matrix does not directly characterize uncertainties, it plays an important role in ensuring reliable data for LCA. To fully account for uncertainties, additional modeling and analysis techniques are necessary. Techniques such as Monte Carlo simulation or sensitivity analysis help propagate uncertainties through the LCA model.

2.2 | Monte Carlo simulation

When uncertainties can be represented by a probability distribution function, the distribution of outcomes (i.e., dependent variables) can be obtained through a portfolio of probability combination methods, such as the combination of expected value and variances, moment-based methods, transformation methods, and Monte Carlo (MC) simulation.[23] The latter is more commonly used in practice,[12] and it is even implemented in existing LCA software, such as SimaPro.[24] The MC method allows repeated sampling from the probability distribution function of uncertain variables to calculate the probability distribution of dependent variables. Sampling often assumes independence between random variables, relies on classic probability theory, and continues until the variations in the average value of the dependent variables approach an asymptotic value suitable for the particular analysis. This type of uncertainty analysis is suited for aleatory uncertainty, which is usually associated with measurements. While MC simulation primarily focuses on aleatory uncertainties, it indirectly accounts for epistemic uncertainties by considering parameter variations. The impact of epistemic uncertainties can be assessed by comparing simulation results using different parameter values or models.[25]

The standard procedure for MC involves sampling the LCI data for the various products and processes included in a system and calculating the values of the environmental impacts for each case. This methodology can be very computationally demanding, as it requires extensive sampling of LCI databases and a large number of simulations to properly sample the LCI datasets, especially in a process system that includes hundreds or thousands of inputs and outputs.[26] This may limit the applicability of the MC methodology to small and medium-sized systems, making it beyond the reach of most practitioners as extensive computational resources would be necessary for large industrial processes or systems involving complex supply chains. This is due to the computational nature of an LCA study. Considering the matrix formulation,[26,27] each time a simulation is performed with the MC methodology, it is necessary to perform a matrix inverse, a very computationally intensive operation.

Pomponi et al.[28] examined the sample size such that additional MC calculations would not affect the results. Their calculations showed that for the LCA of construction materials, a sample of 10,000 points is sufficient regardless of the probability density function and size of the data sets. Similar conclusions were reached by Ross and Cheah,[29] who also analyzed the sample size necessary to adequately address the uncertainty of the utilization phase of electric appliances. The results show that larger samples lead to more statistically precise results, yet the marginal return in precision decreases with an increasing number of samples. Even though the form of the probability distribution function does not influence the sample size, the uncertainty values obtained depend on the selection made. Heijungs[23] also analyzed the required sample size to ensure meaningful results. Based on the study results, the author recommends using large samples from the input distributions (i.e., collected data), but restricting the number of MC simulation iterations to a number not greater than the input sampling. The issue created by using a large number of MC runs is that inaccurate inputs will be translated to the LCA results, but an MC simulation with too many runs will describe it as having excellent precision. Moreover, Heijungs[23] also concluded that if the parameters for the input distributions are obtained by a procedure (e.g., pedigree matrix) and not by sampling, then MC simulation should not be used. One can consider that the MC results are not statistically significant as the input distributions have been assumed rather than determined through data. A proposed conservative approach by Edelen and Ingwersen[16] would use the highest pedigree matrix score possible for each data quality characteristic, which can be combined with intentionally using few MC runs so as not to overly narrow the precision of the results.

While considering the points mentioned above, LCA practitioners who opt for MC simulation should be aware that guidelines for developing estimators of the mean, variance, and other statistical descriptors can be found in the literature.[30] However, in many cases, direct estimation of these parameters may not be feasible. As an alternative, practitioners often rely on standard probability density functions, such as the normal distribution. These distributions are often practical and adequate for modeling uncertainty, and their parameters can be estimated from inventory data or information obtained from the process or databases.[31] In many cases, it would be wise for practitioners to state the assumptions and methods used in their studies and warn readers not to overinterpret uncertainty results.

2.3 | Non-probabilistic methodologies

In LCA practice, data uncertainty is usually modeled using classical probability theory, on which MC and related methods are based.[12] When the uncertainty is due to the natural randomness (aleatory uncertainty) that occurs in measurement, the approach that considers MC and related methodologies is adequate. However, when the uncertainty arises from the inherent ambiguity linked to the choices made when doing an LCA study (epistemic uncertainty), different approaches are required. In this case, the uncertainty is not entirely random, as incomplete information is used to make choices.

Various forms to represent epistemic uncertainty have been proposed in the literature; for example, fuzzy set theory, Bayesian probability, or Dempster's theory of evidence.[6,32] Following Tan et al.,[33] this type of uncertainty corresponds to the imprecision associated with ambiguity due to subjective actions. In this context, possibility theory can be used to account for that fuzziness by assigning a possibility value that is proportional to the expectation of a particular outcome. The values assigned are not probabilities in the classical sense, as the information used to define them limits the possible values.

According to Tan et al.,[34] there are three main reasons to use possibility theory instead of methods based on classic probability theory. First, possibility theory allows a more rigorous description of certain types of uncertainty that are described as ambiguous or imprecise rather than random. Second, possibility theory is more compatible with subjective and/or heuristic information that may have a non-quantitative nature or have a decision aspect linked to its utilization. Examples include the utilization of expert judgment or surrogate data, in which subjective judgments are normally involved, as is the case when converting linguistic terms (e.g., good, bad) to numerical values.[35] The determination of adequate probability density functions to use in MC and related methodologies may be impossible when data appears to be contradictory, a situation that possibility theory alleviates by introducing subjective assumptions and/or decisions that allow the generation of adequate fuzzy numbers. Finally, for complex process systems, possibility theory can significantly reduce computational effort associated with the uncertainty evaluation. Even though it is less rigorous when compared with classic probability theory, possibility theory is simpler to apply for poorly described process systems where information is limited.

Some studies have analyzed and applied possibility theory principles, usually using fuzzy set theory to describe and make uncertainty calculations. Benetto and coworkers[36,37] have analyzed how possibility theory can be applied in LCA alone or coupled with decision-making methods. The authors concluded that possibility theory is an adequate form of dealing with uncertainty when the analysis involves human judgment and specialist perceptions and may be advantageous when analyzing LCA study results and decision-making based on them. André and Lopes[38] have analyzed the mathematical basis of implementing possibility theory and determined adequate conditions to use it when compared to other methodologies, in particular probabilistic ones. Heijungs and Tan[39] have analyzed the implementation of fuzzy methods in the LCA methodology using the matrix formulation to determine which conditions can be applied. Clavreul et al.[40] also reached similar conclusions; in particular, the authors determined that methods based on possibility theory focused more on the information available instead of on how one has to represent it. Thus, probability-based methods are easily used when information is abundant and adequate, but in other situations methods based on possibility theory are useful.

However, non-probabilistic methodologies should not only be used as a substitute for the lack of data. To fully reap its benefits, possibility theory should be considered when there are two or more distinct possible scenarios. Instead of evaluating them separately, the idea is to use all available information in a single combined analysis. Moreover, possibility theory can be used to assign weights to data, applying quality factors to scenarios rather than making a binary decision about whether to include or exclude certain data. Some examples of studies involving possibility theory, normally combined with fuzzy sets, can be found in the literature. Tan et al.[33,34,41] used this approach to compare the life cycle impacts of alternative fuels. A comparison of the possibility theory/fuzzy sets and MC to assess the life cycle impacts of biodiesel made from coconut oil concluded that similar results are obtained by both methodologies. The authors concluded that the uncertainty evaluation methodology based on possibility theory was faster than MC. Based on this fact, Meng et al.[42] have proposed an improved life cycle-based methodology to assess the environmental performance of products, in which fuzzy set theory is combined with MC for a quicker assessment. Li et al.[43] used fuzzy set theory to incorporate uncertainty in the assessment of distributed renewable energy systems, concluding that the methodology is fast.

Reza et al.[44] developed a methodology to assess the sustainability performance of a paved road system. Although not exactly an LCA study, as the energy was evaluated, the uncertainty due to the inventory was assessed and propagated using fuzzy-based methods, which were easier to implement than complex analytical expressions. Benetto et al.[36] have applied fuzzy sets to assess the environmental impacts of noise, which are notoriously hard to evaluate. The fuzzy nature of possibility theory lets one use data with a quality metric applied as a factor, instead of deciding in a binary fashion that the data is used or not.

The application of possibility theory, usually coupled with fuzzy sets,[45] requires information to perform the uncertainty analysis. In practice, this can be done either using data from the process system and the literature or by applying judgment or the consensus of specialists. For the former, the methodologies that can be used to define the probability density functions used in the MC methodology may be used, but without the need to calculate statistical parameters, as a qualitative analysis suffices many times. For the latter, one can utilize experts to define probability distributions, making the assessment based solely on their expertise and judgment rather than relying on data.[46] Some authors have obtained the required information in a more analytical way, for example, Gavankar and Suh[47] proposed a methodology to combine data from various sources, either qualitative or quantitative.

Despite the advantages of possibility theory for specific types of uncertainty, its application in LCA studies has been very limited when compared with probabilistic-based methodologies.[6,12] This may be due to the perceived lack of rigor in possibility theory as compared to MC and related methods, which may explain why no current commercial and open-source LCA software packages have implemented methodologies based on possibility theory[6,48] to the best of the authors' knowledge. Nevertheless, some works describe the implementation of possibility theory for uncertainty assessment. An example is the article of Tan et al.,[34,41] which implemented the methodology in spreadsheets aimed at the evaluation of transportation fuels. Another example is the work of Clavreul et al.,[40] in which possibility theory was implemented in MATLAB using fuzzy intervals and used in the analysis of willow cultivation for bioenergy production. They also compared the results using Monte Carlo sampling and a mixed methodology that combines random sampling with fuzzy intervals, concluding that this depends on the availability of information. If the information is abundant, a statistical representation is sufficient; however, when the information is limited, it is often more effectively conveyed through possibility distributions. Groen et al.[49] compared different uncertainty evaluation methods, particularly random sampling methods and fuzzy interval arithmetic, to define possibility functions with the latter. They considered three case studies: two regarding electricity generation, one more complex involving whitefish trawling fishery, and the LCA and uncertainty that were based on the matrix-based LCA calculation. The results show that the fuzzy interval arithmetic method requires less memory when compared to sampling methods, but the conclusions are less explicit.

3 | IMPROVED AND NEW METHODS

3.1 | Improving the Monte Carlo simulation method

As stated before, the current application of MC simulation in LCA is computationally intensive, in particular for large process systems with many inventory items for which many runs and sampling from many probability density functions must be performed. Various authors have analyzed MC to improve computational performance and speed up the effort, focusing on the nature of the calculations and the properties of the mathematical objects involved. Peters[50] has demonstrated that when the matrices involved in the computational evaluation of the environmental impacts are sparse (containing mostly zeros), a situation that occurs for large process systems and/or with many inventories and environmental releases, significant reductions in computational time are possible using algorithms designed specifically to invert sparse matrices, in particular iterative methods. The latter strategy was implemented in SimaPro Version 8 and subsequent versions.[24] Saab[26] also considered the question of memory allocation and how to invert matrices for large process systems with parallel programming methods. The author explored strategies to avoid inverting matrices by streamlining the calculations as much as possible.

Other researchers have focused on aspects related to sampling the probability distribution functions and their impact on the uncertainty calculations. Qin and Suh[51] conducted a thorough analysis of the most suitable probability density distributions to represent inventory data, an important aspect not only for simplifying MC simulation and reducing computational efforts but also for ensuring the credibility of the results. The authors concluded that log-normal distributions were appropriate for describing the datasets used from the Ecoinvent 3.1 LCI database,[52] employing a statistical method based on random sampling of the datasets. This methodology can be extended to other distribution-fitting algorithms, such as neural networks, thereby broadening its practical implications.

Qin and Suh[53] analyzed using pre-calculated distribution/uncertainty values calculated from random sampling of the LCI Ecoinvent 3.1 database instead of a full MC simulation. The results show that the utilization of pre-calculated values is adequate, particularly if the pre-calculated values were evaluated using a large enough sample. Lesage et al.[54] analyzed the utilization of aggregated datasets to reduce the computational effort and time in uncertainty evaluation in LCA studies. They concluded that independent sampling is not possible in most cases, as most datasets in LCI databases are interconnected. The study results show that the correlations between datasets should be taken into account and that no single correction factor exists to account for those effects.

Related methods are used to improve the performance of MC simulation. Many of these methods rely on sampling the probability distribution functions, taking into account the data and/or process system characteristics. When sampling from a large number of probability distribution functions (multidimensional), MC simulation can be too cumbersome and require too much computational effort,[55] and one may need to rely on variance reduction techniques.[56] Another option to minimize size and effort difficulties involves the application of Markov models. In particular, Markov Chain Monte Carlo (MCMC) sampling is a class of algorithms for systematic random sampling from high-dimensional probability distributions that allows for more optimal sampling when compared with standard MC simulation. Unlike MC sampling methods that draw independent samples from the independent distribution, in MCMC methods the samples are interdependent, forming a Markov chain.[55,57] This allows better sampling, in particular when a large number of random variables are involved, as is the case in LCA studies involving large systems. The methodology is used in other scientific and technical areas for uncertainty analysis, such as groundwater modeling,[58] geosciences,[59] and energy economics.[60] Yet, MCMC sampling is not extensively used in the practice of LCA. Existing examples include the work of Jin,[61] who analyzed the life cycle emissions in managing sewer pipelines; of Vázquez-Rowe et al.,[62] who considered the land use impacts of crop rotation in Luxembourg, in which a Markov chain was used to estimate future environmental impacts based on historical data; Paras and Pal,[63] who analyzed clothes reused in Nordic countries; Tian et al.,[64] who evaluated the environmental impacts of circular economy systems; and Yue et al.,[65] who analyzed the agricultural nitrogen emissions in China from a life cycle perspective, focusing on the influence of the crop trade. This represents an opportunity to further develop the application of this methodology in an LCA context. Moreover, there is potential to couple MCMC with other methodologies, for example, machine learning or using the expertise from other areas in applying the MCMC methodology for uncertainty evaluation, which will further streamline uncertainty analysis based on the sampling of the inventory probability distributions. Moreover, MCMC may better handle the interactions and/or interdependencies between variables.

3.2 | Other uncertainty assessment methods

Global sensitivity analysis (GSA) has been used in many LCA studies to address the uncertainty/variability of input parameters.[66] For emerging technologies, the descriptions of input parameters can be challenging, affecting the robustness of the GSA results. To address this challenge, Lacirignola et al.[67] developed a method that calculates several GSA to identify key parameters and understand how the descriptions of these parameters affect GSA results. The authors applied the method to an enhanced geothermal system and demonstrated how the description of each input affects its ranking and contributions to the variance of the outputs. The authors called for careful use of GSA in LCA and emphasized the need to investigate the stability and confidence of parameter assumptions. Piano and Benini[68] reviewed uncertainty in LCA and were proponents of Sobol sensitivity analyses to account for uncertainty.[69] While computationally expensive, this methodology can provide valuable information, in particular the contributions of the inputs to output variance. Cucurachi et al.[70] developed a moment-independent global sensitivity analysis method that can accommodate the presence of correlations in the input to LCA models and the multimodal output of LCA models. This new uncertainty evaluation method identifies and ranks the important contributors to the uncertainty of the model outcome, and it has been implemented in "The Activity Browser," an open-source LCA software based on the Brightway LCA framework.[71–74]

Machine learning (ML) methods have also been used to overcome incompleteness or uncertainty in data to deliver actionable recommendations for LCA.[75,76] Dai et al.[77] developed a streamlined inventory creation and uncertainty evaluation method that outputs the mean value and the corresponding uncertainty interval for the inventory data of interest. This method first quantifies the correlations among existing data across temporal, geographic, and taxonomic dimensions, followed by applying the Gaussian process regression, a machine learning algorithm, to predict the results for the LCI data of interest. No assumption of a pre-defined distribution (e.g., log-normal distribution) for the predicted LCI data is needed, as the uncertainty interval is generated by directly sampling the posterior distribution of the predicted LCI data. This new uncertainty evaluation method avoids the need for manually specifying the distribution (which is required by the Pedigree matrix method[15]), reducing the subjectivity in uncertainty analysis. This shift of uncertainty from the user input of data quality indicators (DQI) of the pedigree matrix method to that of the trained Gaussian process regression model is an example of converting input parameter uncertainty to model uncertainty.

Computationally intensive methods like Monte Carlo, commonly used in uncertainty analysis, can become impractical due to the associated computational burden, especially as the complexity of models and the number of variables increases. These complex models may be physics-based, modeled at different levels of granularity, and include several processing steps. Furthermore, these models are usually nonlinear functions of a large number of variables that have varying significance and interact with each other. In such complex, computationally burdensome, and intractable cases, along with variable reduction methods, surrogate models offer a practical and efficient solution. These models treat the mechanistic simulation model or plant data as a black box and develop an explicit lower-order meta-model from an implicit complex mechanistic model or noisy manufacturing or processing plant SCADA (Supervisory Control and Data Acquisition) system. For example, Huntington et al.[78] have developed surrogate models of bioproduction paths using flowsheet simulators. Material and energy balances, which are dependent on key process variables such as feedstocks, operating conditions, and properties, are thus empirically modeled. The results of those models correspond to the LCI inputs and outputs that are then used in LCA studies, reducing the computational burden and allowing the use of only the most significant variables along with much simpler explicit lumped models. The most sensitive parameters are used as decision variables for optimization of the objective function while formulating the surrogate model, which also accounts for the interactions between variables.[79]

In the development of surrogate models, ideally, complex models should be accurate and optimized. These models are most useful when design changes are not made. If plant data are available, these can be further used to tune the complex models prior to developing surrogate models. Naturally, digital twins can be used to develop surrogate models as well. Explicit surrogate modeling relations can be developed using data-driven machine learning techniques like symbolic regression.[80] Existing LCA modeling relations are, in part, high-level empirical relations and can serve as starting surrogate models. Similarly, lumped approximate physics-based modeling relations employed in optimization methods such as MINLP (Mixed Integer Non-Linear Programming) may serve as surrogate models.[81] Life cycle models, different libraries, or computational packages such as the MATLAB optimization toolbox can be very useful for solving these optimization problems and developing these models. Surrogate models are implementable using other computationally less demanding but more approximate probability combination techniques, such as variance combination as utilized by Ghosh.[82]

Other methods involve the combination of various tools. For example, a study combining process simulation and the Ecoinvent LCI database is the work of Calvo-Serrano and Guillén-Gosálbez.[83] The work focuses on the uncertainty characterization of life cycle inventories of chemicals used in the chemical industry, which are limited both in terms of chemicals included and data quality. This is a relevant problem due to the economic and environmental relevance of the chemical sector, in which a significant improvement in environmental performance is required. The authors developed a process network of the petrochemical sector, from which they obtained the information required to obtain the inventory data. By defining plausible scenarios and the statistical distributions of relevant inventory parameters, the authors could evaluate the uncertainty of producing a select set of chemicals.

4 | BLOCKCHAIN TECHNOLOGY TO REDUCE LCI UNCERTAINTY

Blockchain technology has the potential to decrease the uncertainty that arises from data collection. The availability of reliable supply chain data is fundamental to achieving high-quality LCA results. However, globalization and market expansion create supply chain inventory challenges due to the increasingly complex manufacturing of goods and product portfolios. Both data availability and uncertainty are associated with product origins, processing, and transportation, with traceability and data management systems remaining the main challenges. Blockchain technology is able to process data in real time and ensure traceability and transparency at different phases of the LCA framework, that is, inventory analysis and associated impact assessment.[84]

Nevertheless, implementing sensors and devices that generate a considerable amount of data in real time can enable this emerging technology for LCA. Moreover, blockchain technology can be decisive in creating a proper chain of custody for aggregated materials and energy, for which evidence exists of who generated the data and how the data was transferred through the various supply chains or life cycle parts maintained in a decentralized, secure digital system. This may provide the metadata necessary as evidence for a critical review of the data or the LCA study[12] and ensure that the information given by digital environmental labels, such as under development and implementation of the European Union Digital Product Passports.[85]

Blockchain technology is increasingly recognized as a viable solution for creating and developing efficient information exchange and traceability systems that can record reliable and up-to-date data across supply chains.[86] There are many benefits to using blockchain in LCA. It enables real-time data acquisition and processing, ensuring its traceability and transparency and promoting a more objective study. Additionally, it offers the potential to protect sensitive data, particularly intellectual property or business secrets, if necessary.

Even with the potential advantages of using blockchain technology in LCA practice, currently blockchain has not been widely adopted.[84,87,88] No specific standards or guidelines exist for implementing blockchain technology in the LCA domain.[89,90] Such standards and guidelines are essential to ensure the interoperability of blockchain systems between different LCA software and data systems. There are issues regarding how to collect data and the integration of blockchain with existing company information systems and across supply chains, in which there can exist a significant heterogeneity between the various parts, in particular, the different levels of operational digitalization between companies, even in the same sector.

Data availability is also a concern, not just in terms of obtaining the data, but also in ensuring its quality, representativeness, and suitability for the specific aims and nature of the intended application of the LCA study, as discussed by D'Eusanio and Petti in relation to social LCA.[91] Existing data quality frameworks, such as the one proposed by Henriksen et al., can be relevant in this regard.[22] Moreover, questions of intellectual property and/or business secrets may hinder the sharing of data, as blockchain is a transparent technology. To counter those issues, the possibility of data anonymization and/or smart contracts between different stakeholders of the supply chain may minimize the effect of the need for data protection.[92,93] Also, depending on the complexity of the product and the associated supply chain questions, the amount of data generated may be significant, and proper data management may be complex and expensive (even though it may create opportunities to extract knowledge from the data gathered).

Other questions concern the lack of incentives at the organizational level, mainly due to the novelty of blockchain technology, the lack of people with adequate expertise, and the potential costs involved, which can be significant for small-size companies. There is also a lack of incentives, guidelines, and regulations to frame and assist companies and other stakeholders in the implementation of blockchain and similar technologies in practice, an issue that may be very relevant, for example, in the development of Digital Product Passports in the European Union. Also, depending on how the blockchain technology is implemented, the significant environmental impacts may be substantial due to the energy-intensive nature of the technology. Hence, special care must be taken into account in the implementation of blockchain into the LCA framework, particularly the nature of the data being transferred and the various parts of the supply chain.[94,95]

Despite the current limitations, a few studies have explored the application of blockchain in LCA. For example, Lin et al.[92] proposed a blockchain-based LCA in which the blockchain technology is adapted to obtain inventory data from suppliers and other upstream supply chain partners, showing that the accuracy and automatic data update can be improved. Teh et al.[96] analyzed how blockchain can be combined with LCA to support the definition and adjustment of company strategies to promote their contribution to sustainable development, particularly to reach their goals regarding a more sustainable and environmentally friendly performance. Carrières et al. assessed the value of using blockchain for LCA studies of textile products, focusing on the potential for data traceability.[97] The results showed that using data traceability can significantly improve data quality, in particular by providing specific data to allow a more representative assessment.

5 | COMPUTATIONAL IMPLEMENTATION

A proper computational implementation may significantly reduce the resources and the time needed to perform an uncertainty analysis in an LCA study, increasing the size and complexity of the studies that can be done in practice. Moreover, it may allow a more accessible and straightforward automatization of LCA inventory analysis and/or calculations.[98] Most methods reviewed in this study handle uncertainty characterization in a standalone procedure (i.e., not part of LCI modeling). The implementation of these methods is not within the common LCA software (e.g., openLCA, SimaPro, and Gabi) yet, indicating a challenge for the wide adoption of these new methods by the LCA community. On the other hand, several of these methods are implemented mostly using the Python programming language, which shows their potential to be integrated with the LCA models. For example, Jolivet et al.[99] have developed and implemented a package to perform uncertainty analysis in the Brightway framework,[100] a Python-based, open-source LCA software package.[74] The package implements the MC simulation method using symbolic calculus to simplify the definition of parametric inventories and to accelerate the calculations required for the uncertainty analysis. The package includes post-application capabilities, particularly a factor contribution analysis used to generate simplified arithmetic models that can make a fast estimate of environmental impacts for the process system. Cucurachi et al.[70] have implemented their methodology in both the Activity Browser[71,72] and the Brightway framework.[74]

Despite the relevance of the new open-source packages, their utilization may be more complex than existing commercial software, as they require specific programming skills to be properly used. Moreover, the lack of manuals and/or case studies limits their utilization, making it harder and time-consuming to use. However, changing the code opens the possibility of using other methodologies in uncertainty analysis, including data science, machine learning, and artificial intelligence methods.

Another interesting future evolution that requires improvements in computational implementation is LCA automation, either standalone or combined with other software, in particular internal information systems of companies. The increase in the integration and networking between internal and external companies makes it possible to perform LCA calculations almost in real time by incorporating them into the information system of the organization. For example, it is now possible to combine process data obtained from sensors with data from suppliers or life cycle inventory databases, allowing the real-time calculation of the environmental impacts of products and processes, the immediate identification of the system aspects that need to be improved, and primary sources of variability and/or uncertainty.[101–104] This is also relevant for environmental reporting, either in a business-to-business or at a company level, fulfilling the future requirements of non-financial reporting and disclosure, for example, the European Union Directive on Corporate Sustainability Reporting.[105]

6 | SUMMARY AND RECOMMENDATIONS

Uncertainty is a significant factor in LCA. A major source of uncertainty in LCA is the life cycle inventory data. This study reviewed common uncertainty methods and recent methodological developments in uncertainty analysis for LCI modeling. Practitioners are urged to adequately describe input uncertainty and not calculate excessively precise output uncertainty. For quantifying the uncertainty associated with input data, efforts have been focused on improving the pedigree matrix method, non-probabilistic methods, GSA, interval analysis combined with MC simulation, machine learning, and scenario analysis. With respect to reducing the uncertainty associated with input data, blockchain can provide high-resolution inventory data (e.g., temporal, spatial). Some of the above-mentioned methods can be implemented using commercial (e.g., SimaPro, Gabi) and open-access software (e.g., OpenLCA, ActivityBrowser). Those applications often involve manually modifying the configuration of the software platform. Other implementations, although typically having the advantages of automation and higher flexibility in investigating different sources of uncertainty, need to be implemented as code scripts, which require LCA practitioners to possess a certain level of programming skills. Finally, potential areas that require further development include integrating blockchain technology with inventory modeling, standardizing uncertainty analysis methodologies, developing user-friendly software platforms, and integrating multiple uncertainty analysis approaches. These developments can enhance the reliability and credibility of LCA results and promote their wider adoption in decision-making processes.

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DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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