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Contributors to output uncertainty in prospective Life Cycle Assessment of emerging artificial photosynthesis technologies

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Abstract
Despite the additional uncertainties inherent in assessing emerging technologies, key contributors to output uncertainty often remain unidentified because uncertainty and sensitivity analyses are not systematically applied in Life Cycle Assessment (LCA). To effectively guide the development of emerging technologies toward improved environmental sustainability performance, it is essential to integrate uncertainty and sensitivity analysis methods that enable the identification of input variables contributing to environmental impact uncertainty. In this study, prospective LCA tools were embedded within a flexible, transparent, and reproducible framework designed to incorporate epistemic uncertainties and support a large number of model runs. The approach is demonstrated using two exemplary CO_2-removing artificial photosynthesis product systems, representing an emerging technology at an early stage of development and associated with considerable uncertainties. The results show that, depending on the characteristics of the product system, either scenario- and process-related input variables or system design-related input variables can dominate the output uncertainty. The choice between various climate mitigation pathways exerts a relatively moderate influence on output uncertainty, whereas catalyst materials and their associated production processes have comparatively low influence. The resulting ranges of environmental impacts, when uncertainty is accounted for, can be substantial, challenging straightforward technology ranking. However, identifying the key contributors to output uncertainty provides insights for guiding environmentally oriented technology development. Future work should extend the analysis to additional product systems, broaden the representation of uncertainties, develop heuristics to enhance modeling and computational efficiency, and explore methods to mitigate and communicate uncertainties for decision-making.

Keywords Global sensitivity analysis, Uncertainty analysis, Uncertainty apportioning, Sobol' indices, Prospective life cycle assessment (LCA), Emerging technologies, Artificial photosynthesis

1 Introduction

Uncertainty and sensitivity analyses have been recognized as essential components of Life Cycle Assessment (LCA) since the early 1990s for assessing result reliability and identifying key influencing factors [1]. Uncertainty analysis or uncertainty quantification, as defined by [2], refers to the calculation of the combined effect of error and variability, whereas sensitivity analysis examines how changes or fluctuations in input data influence the results. However, no consistent terminology exists in the LCA field. Instead, multiple definitions and interpretations have been proposed [2].

While uncertainty and sensitivity analyses have been regularly mentioned and recommended since early LCA practice, practical methods and standardized procedures for their implementation have often been lacking. The first matrix-based calculation framework for uncertainty and sensitivity analysis was introduced in 1992. Since around 2000, more advanced concepts, such as Monte Carlo simulation, Sobol' indices, Morris' elementary effects, and standardized regression coefficients, have been presented in the context of LCA [2]. Heijungs [2] provides a comprehensive review of early developments, historical progress, applications, current practices, and future directions in this field. More recently, additional methods have been introduced. Villacis et al. [3] propose a structured and transparent approach for incorporating uncertainty directly into the Life Cycle Inventory (LCI) modeling process by introducing a decision-support flowchart. Regarding method development, Andrae [4] suggests incorporating rebound effects into LCA, which helps to clarify the extent of uncertainty tolerated before it undermines conclusions about whether the investigated technology is environmentally beneficial. To avoid misleading conclusions about key uncertainty drivers, Kim et al. [5] present an enhanced sensitivity analysis protocol for LCA that accounts for correlated uncertainties, demonstrating that neglecting such correlations can significantly alter input importance rankings. Nevertheless, the conclusions of former review studies remain consistent: the application of uncertainty and sensitivity analyses in LCA is infrequent [6] and remains limited [2]. Fewer than 20% of LCA studies report any uncertainty analysis [7, 8]. When applied, these analyses often focus on specific LCA stages (primarily the LCI) and are typically conducted independently rather than in an integrated manner [1]. Furthermore, "questionable practices" [1] persist, and calculation tools within LCA software remain limited [9], even though their direct integration into dedicated LCA software is essential to be workable for daily LCA practitioners [2].

The need to address uncertainty and sensitivity could become even more critical when evaluating emerging technologies using prospective LCA. While LCA focuses on existing technologies based on their current state, prospective LCA is forward-looking in nature [10], often considering the upscaling of emerging technologies to industrial levels and assessing their environmental impacts in future scenarios [11]. However, these modifications introduce additional uncertainty sources arising from assumptions about future developments, technology upscaling, and incomplete knowledge of the system design of the emerging technology. These input uncertainties can lead to wide result ranges, complicating interpretation and hindering conclusions about the product system's environmental performance [12], as also demonstrated in previous work by the author [13]. Disregarding such uncertainties may result in misleading recommendations [12]. Given that LCA has been identified as a key tool to strengthen and enable policies for achieving the Sustainable Development Goals (SDGs) within planetary boundaries

[14], such misleading recommendations could have a detrimental effect on sustainable development—particularly in relation to SDG 7 (Affordable and Clean Energy) and SDG 13 (Climate Action). For emerging technologies, which are expected to contribute to sustainable development [15], the risk of drawing misleading recommendations may be even more pronounced. Therefore, statistical and probabilistic methods, supported by appropriate software tools, are required to better quantify uncertainties and enhance the reliability of LCA and prospective LCA outcomes [2].

A tool addressing prospective LCA is the premise Python library [16], which systematically transforms the LCI database ecoinvent to align with climate mitigation pathways. By matching the outputs of an Integrated Assessment Model (IAM) with data from the LCI database, premise produces background databases representing different IAM scenarios. For emerging technologies with low Technology Readiness Levels (TRLs) expected to operate in the future, prospective background databases facilitate the representation of anticipated technosphere developments. Applications of premise have shown that results can vary by 18–80% [17]. When applied to an emerging technology, as observed in previous work by the author, climate change impacts may be underestimated by 65% [18]. A recent review study noted that "limited adoption of existing scenarios for upgrading background systems introduced inconsistencies and potential biases" [19]. While modified background databases have been analyzed in previous work by the author [13, 18], a systematic incorporation as an uncertainty contributor has, to the best of the author's knowledge, only been established in a single study for passenger car carbon footprints [20]. Such an approach enables the direct identification of the uncertainty contribution associated with IAM scenarios in comparison to other sources of uncertainty.

However, this gap is acknowledged in the research literature: regarding the application of prospective LCA to low-TRL or emerging technologies, a recent review study covering 79 articles in this field concludes that the management of epistemic and data uncertainties remains challenging, and a systemic approach was identified as necessary to standardize uncertainty handling [19]. Furthermore, in previous work, the author applied prospective LCA to the emerging technology of artificial photosynthesis [13]. This technology enables the production of chemicals or fuels by direct conversion of solar light energy into chemical energy and utilizing carbon dioxide. The outlook of that study indicated that, beyond the methods employed, enhanced modeling using more flexible software solutions could help identify critical input variables,[1] allow dynamic handling of these variables, and enable evaluation of multiple supply chain configurations to identify more environmentally favorable production routes. The input variables that were varied in the sensitivity analysis of this previous study were manually selected and not systematically analyzed regarding their contribution to output uncertainty. This approach could lead to the omission of important input variables and does not allow for the identification of each input variable's significance relative to all other input variables.

To analyze and measure the contribution of input variables to the results, several analytical approaches exist: Beyond local[2] and discrete[3] sensitivity analysis, global sensitivity

[1] In previous work, the author used "parameter" instead of "input variable". Although this usage is common in modeling and LCA contexts, the author adopts the less ambiguous definition proposed by Heijungs [2] to avoid confusion with its use in characterizing probability distributions.

[2] Local sensitivity analysis examines the sensitivity of results to small changes in the nominal value [2].

[3] Discrete sensitivity analysis is the non-systematic variation of a few choices and items [2].

analysis (GSA) studies the effects resulting from changes over the full domain or probability support of the input variables [2]. Complementarily, uncertainty apportioning[4] examines "the subdivision of output uncertainties in terms of contributions by input uncertainties" [2]. In contrast to Heijungs [2], other authors [21–23] consider the apportioning of the output uncertainty to different sources as part of GSA. Within uncertainty apportioning methods (in the following considered as distinct from GSA as defined in [2]), Sobol' indices are recommended for LCA applications [2, 21] due to their ability to capture both main and interaction effects. Sobol' indices are variance-based global sensitivity measures that decompose the total variance of a model output into contributions attributable to individual input variables and their interactions [2]. Several studies have directly applied Sobol' indices, recently to the complete LCA model [22], though more commonly to the LCI stage [22, 24, 25]. Jaxa-Rozen found that Sobol' indices "can potentially be unreliable when analyzing non-normal model outputs" and recommend adding PAWN distribution-based sensitivity analysis [26]. Regarding software, the open-source Python library lca_algebraic [27], built on the Brightway2 framework [28], facilitates the construction of inventories for running Monte Carlo simulations and subsequently calculating Sobol' indices. Several studies have demonstrated its applicability in parametric, prospective, and dynamic LCA contexts [27, 29–42].

A prerequisite for applying GSA and uncertainty apportioning—which are not standardized in LCI—is to formulate the LCI not as fixed numerical values, but as random variables or as formulas defined over named variables [5], which can be varied across their respective uncertainty ranges. Although such an LCI is commonly referred to as parametric or parameterized within the LCA context, this terminology overlaps with established meanings in probability theory [2]. Therefore, this work adopts the naming convention of SymPy[5] [43], originating from computer science [44], and refers to this approach as symbolic LCI. Symbolic LCI enables LCA practitioners to avoid subjective evaluations [45] or estimates during LCI construction by directly incorporating available numerical ranges or distributions. For example, system characteristics such as the efficiency of a product system need not be approximated as fixed values but can instead be represented as random variables or expressed through functional relationships. In this way, symbolic LCI facilitates the integration of more complex relationships that better reflect real-world behavior, including technological, geographical, and temporal variability, as well as dependencies among input variables [5]. Beyond its application in GSA and uncertainty apportioning, symbolic LCI also enables methodological extensions. For instance, when coupled with an optimization solver, it allows for exploration of optimization pathways or adaptation to different specifications" [46], thereby identifying input variable values that minimize environmental impacts.

To address the gaps identified in the literature, as well as those highlighted in the author's previous work, this paper proposes a systematic integration of symbolic LCI, GSA and uncertainty apportioning using Sobol' indices, coupled with uncertainty quantification, within a prospective LCA framework for the emerging technology of artificial photosynthesis. This integrated approach enables the quantitative identification and

[4] Uncertainty apportioning is often mentioned as feature or part of GSA. It is separated in Heijungs [2] for clearer distinction.

[5] SymPy Python library, used by lca_algebraic, enables the transformation of LCA computations into symbolic mathematics.

measurement of the contribution of individual input variables to overall output uncertainty. The integration and application aim to better understand and explain the contributors behind the output uncertainty observed in the author's prior work. By employing symbolic LCI, the system design of artificial photosynthesis can be directly and flexibly incorporated into the LCA model. Furthermore, the use of dedicated open-source LCA software facilitates the integration within existing modeling environments, addressing the currently limited application of uncertainty and sensitivity analyses in LCA practice. This approach extends uncertainty and sensitivity analysis in LCA beyond the analysis of a selected set of input variables to a global, flexible and transparent framework that can be adapted to other emerging technologies.

With the overall aim of supporting more robust decision-making at early stages of technology development, in alignment with sustainable development, the following objectives were defined:

(i) Development of a flexible, transparent and reproducible prospective LCA model for artificial photosynthesis that incorporates system design variables, methodological uncertainties, and climate mitigation pathways in a symbolic LCI.
(ii) Implementation of a computational workflow that integrates prospective modeling including background system modifications with uncertainty quantification, GSA and uncertainty apportioning.
(iii) Quantification of overall output uncertainties, identification and ranking of key contributors to output uncertainty.

2 Methods

The Methods section is structured into distinct parts to adhere to LCA standards while also reporting further methodological choices. First, the LCA subsection covers the Goal and Scope as well as the LCI, including the specific adaptations required for prospective LCA. This is followed by the section on uncertainty quantification and apportioning, which outlines the steps involved in implementing the proposed framework and coupling it with the prospective LCA model. This section includes the transformation of the LCI into a symbolic representation, the execution of Monte Carlo simulations, the calculation of Sobol' indices, and the documentation of the methodological choices made.

2.1 Life cycle assessment

2.1.1 Goal & Scope

This study builds upon data from a previous publication [13]. The Goal and Scope are largely consistent with the earlier work. Therefore, the following section presents a summary, along with modifications introduced in the present study.

Goal Definition. With the aim to improve decision-making under uncertainty, the primary goal of this LCA is to identify the key contributors to output uncertainty. Achieving this entails the formulation of a symbolic LCI, the development of a flexible prospective LCA model, and the implementation of a software workflow integrating GSA and uncertainty apportioning. The assessed technologies in the field of artificial photosynthesis are photocatalytic synthesis gas production (H_2+CO) and photoelectrochemical co-production of hydrogen peroxide and methane (H_2O_2&CH_4). A main limitation of this LCA is the assessment of technologies with a low TRL (2–3), as the underlying data are derived from idealized calculations and laboratory-scale experiments, with limited information available for individual process steps. Due to the focus on micro-level decision support, the modelling approach adopted is attributional.

Product System and Parameterization. The two artificial photosynthesis product systems (H_2+CO and H_2O_2&CH_4) both incorporate carbon dioxide in the upstream supply chain. In addition, H_2+CO includes biogas, while H_2O_2&CH_4 requires water as a second reactant. The product systems further comprise components such as solar collectors, photoreactors, and photocatalysts. In the case of H_2O_2&CH_4, photoelectrodes, and a photoelectrochemical cell are additionally included, along with the associated manufacturing processes. Compared to the author's previous work, gas compression has been excluded due to insufficiently validated data. Furthermore, scenarios previously modeled separately (e.g., variations in CO_2 source or photocatalyst choice) are directly integrated into the symbolic LCI rather than treated as distinct scenarios. The implementation is based on the Brightway2 framework [28] and the lca_algebraic library [27], enabling LCA modelling, uncertainty quantification, as well as the application of GSA and uncertainty apportioning. All calculations, including process and system design, LCI construction and modification, as well as software adaptations were implemented in two Jupyter notebooks [47], provided in the Supplementary Information (SI). These allow the reproducibility and analysis of the product systems.

Reference and Competing Product Systems. Given that the primary focus of this study is the identification of contributors to output uncertainty, reference and competing product systems are not presented in the Results section. However, for completeness, they are included in the underlying model and documented in the Jupyter notebooks provided as SI. For H_2+CO, steam methane reforming is used as the reference product system and for H_2O_2&CH_4, the anthraquinone process. In addition, non-fossil-based competing product systems are included to broaden the comparison basis, including systems with similarly low TRLs. To enhance comparability with the reference product systems, H_2+CO and H_2O_2&CH_4 were reduced to the main products: synthesis gas, and co-production of hydrogen peroxide and methane. Side-products are handled by avoided burden and cut-off approaches, differing from the implementation in previous work with system expansion. Given that avoided-burden credits are subject to uncertainty, a binary input variable determines whether side-products are treated as by-products receiving avoided burden credits or are assumed to be burden-free.

System Boundaries & Allocation Procedures. In the background database, economic allocation is applied in accordance with ecoinvent standards, alongside the ecoinvent cut-off system model for handling burdens and credits related to recycling. In the foreground system, allocation approaches via the avoided-burden method, the cut-off approach, and partly economic allocation are varied by two input variables.

Functional Units and Reference Flows. The functional unit and reference flow for H_2+CO are defined as 1 kg of synthesis gas with a molar ratio of 1:1. Differing from previous work, the molar ratio has been modified, and side products are no longer included in the functional unit in order to enhance comparability. The resulting hydrogen deficit, arising from the adjusted molar ratio, is compensated by other hydrogen production pathways (e.g., steam methane reforming or electrolysis), which are flexibly incorporated via an input variable. For H_2O_2&CH_4 the functional unit and reference flow were defined as 1 kg of hydrogen peroxide and ~0.12 kg of methane. To improve comparability of hydrogen peroxide, this definition was slightly modified compared to the author's previous work.

Life Cycle Impact Assessment (LCIA) Methods. Environmental Footprint (EF) v3.1 method [48] and the Global Warming Potential as defined by the Intergovernmental Panel on Climate Change (IPCC) [49], modified using the premise-gwp Python library [50], were applied to include biogenic carbon dioxide. Global Temperature Potential (GTP), Cumulative Energy Demand (CED) and land occupation are no longer reported.

Modeling Framework and Databases. The entire model was migrated to Brightway2 and lca_algebraic, incorporating additional libraries such as premise [16] and premise_gwp [50] for the generation of prospective background database IAM scenarios, as well as the thermo [51] and chemlib [52] Python libraries for handling chemical and thermodynamic calculations. Premise was configured using 16 IAM scenarios representing different climate mitigation pathways for the years 2030 and 2050, resulting in a total of 32 IAM scenarios. The specifications of these scenarios are provided in the SI. The background databases are based on the LCI database ecoinvent version 3.12 [53].

Data Sources, Quality, and Representativeness. The data underlying this study originate from the author's previous work [13], and are described in detail in the original publication. Furthermore, the data are accessible in the SI.

2.1.2 LCI

H_2+CO was estimated to be at TRL 2, while H_2O_2&CH_4 was at TRL 3. Thus, both product systems are at the level of basic technology research. This necessitates the application of prospective LCI generation methods, which involve additional calculations described in more detail in the author's previous work [13]. The initial LCI, prior to applying any calculations, is provided as a spreadsheet file in the SI (LCI_AP.xlsx), accompanied by a Jupyter Notebook (LCA_AP.ipynb) that implements the required calculations. The LCI is generated by reading and mapping the spreadsheet using a framework[6] developed in earlier work [54], followed by writing the databases with Brightway2. The final LCI includes process and system design calculations, which are then linked to the relevant processes or material and energy flows. For materials lacking data and requiring stoichiometric calculations, the chemlib library is applied. In addition, the thermo library is used to estimate the reaction enthalpies. If modifications to background database processes are required, the respective processes are copied into the foreground system and adjusted accordingly. Once all calculations and modifications have been completed, the input variables—referred to in the Jupyter Notebook under the term parameters—are defined. Subsequently, the processes that depend on these input variables are implemented with lca_algebraic. At this stage, lca_algebraic transforms the LCI into a symbolic representation. The input variables, as part of this symbolic LCI, are documented both in the Jupyter notebooks and in the SI document. The Jupyter Notebooks, along with the LCI files and an installation guide, are available on Zenodo [55] and in the actively maintained repository on Codeberg [56], as referenced in the SI.

[6] While the framework supports large language model (LLM)-based mapping, this study uses only the basic_mapping approach and does not employ LLMs.

2.2 Uncertainty quantification and apportioning

To identify influential input variables in the model, GSA according to Saltelli's definition [23] and uncertainty apportioning following Heijungs [2] were applied alongside uncertainty quantification. The analysis was implemented using Sobol' indices, as provided in the lca_algebraic library. This approach enables the construction of a fully symbolic LCI, allowing epistemic uncertainties to be incorporated as input variables.

A total of 26 input variables for H_2+CO and 12 for H_2O_2&CH_4 were defined using either triangular or uniform distributions, except for input variables representing discrete choices. These distributions were selected due to the lack of knowledge regarding their underlying probability distributions. For input variables for which a mode could be derived from the literature or defined inherently (e.g., solar irradiation for a designated location), a triangular distribution was preferred. Detailed information on all input variables is provided in the SI. As part of the Sobol' indices workflow, uncertainty quantification was also conducted to determine the full range of results generated by the model.

To incorporate prospective LCA with varying background databases resulting from the implementation of IAM scenarios, a two-layer approach was applied using the Papermill Python library [57]. This approach consists of: (i) the Jupyter Notebook LCA_AP.ipynb, which calculates the product system for each climate mitigation pathway as a separate database, and (ii) Jupyter Notebook LCA_AP_DBs.ipynb, which integrates these databases as additional input variables into the model.

To ensure the stability of the Sobol' indices, between 2^{16} and 2^{19} model runs were executed, depending on the product system, with the higher number applied to H_2O_2&CH_4. To manage the computational demand, the SALib [58] function, which is used internally by lca_algebraic, was modified to support batch processing, as performing the computation in a single run exceeded available memory. Furthermore, lca_algebraic Sobol' indices visualization was modified to display them sorted by the highest median contribution across all impact categories, allowing for faster identification and approximate ranking of input variables according to their influence on output uncertainty. As the results are skewed and include extreme values, the median was preferred over the mean, as it is more robust to outliers [59, 60].

Sobol' indices can be distinguished into first-order and total-order indices. In this study, both first-order and total-order Sobol' indices were calculated. First-order Sobol' indices quantify the fractional contribution of an individual input variable to the total output variance, excluding interaction effects with other variables. In contrast, total-order Sobol' indices measure the total contribution of an input variable to the output variance, including its first-order effect as well as all higher-order interaction effects [2, 23]. To account for interactions, the analysis primarily focuses on total-order Sobol' indices. Moreover, for the additional analysis in H_2O_2&CH_4, highly influential input variables were iteratively removed, and further calculations were performed to provide clearer insights into less influential input variables. The complete results of the first-order indices, as well as the additional analysis of less influential input variables, are provided in the Supplementary Information.

3 Results

3.1 Synthesis gas (H_2+CO)

Across all impact categories, results span a range of values (Fig. S1, Table S4). For example, in the climate change category, the 10th percentile is −0.10 kg CO_2-eq per kg of product (−2.45 kg CO_2-eq kg^{-1} when including biogenic CO_2), while the 90th percentile reaches 1.17 (−0.75) CO_2-eq kg^{-1}. The distribution is skewed toward lower values and becomes approximately symmetric when biogenic CO_2 is included, with an interquartile range (25th–75th percentiles) of 0.08 to 0.66 (−1.98 to -1.20) kg CO_2-eq kg^{-1}. The median is 0.28 (−1.6) kg CO_2-eq kg^{-1}, which is lower than the mean of 0.45 (−1.58) kg CO_2-eq kg^{-1}.

The calculated total-order Sobol' indices (Fig. 1) show that input variables related to both scenario choices (e.g. biogas, hydrogen and IAM scenarios) and the process design (conversion rate of the main reaction, weighting of side reactions) influence the results across the majority of impact categories. For climate change impacts, the most influential input variables are the reaction conversion rate (0.33), followed by the solving of multifunctionality regarding by-products (avoided burden = 0.23; biogas avoided burden switch = 0.24), reactant supply chains (biogas switch = 0.19; CO2 switch = 0.15), the influence of side reactions (0.14), the hydrogen source used to adjust the H_2:CO ratio (hydrogen switch = 0.13), the IAM scenario (0.11), and the heat source in the biogas production (0.10).

In other impact categories, Sobol' indices reach up to approximately 0.81 and 0.88 for marine and terrestrial eutrophication. Although uncertainty contributions are also observed in toxicity-related impact categories and land use, system design-related input variables (such as solar-to-chemical efficiency, parabolic collector concentration ratio, and system lifetime) exhibit comparatively lower influence. Photocatalyst-related input variables, including photocatalyst lifetime, material choice, uncertain properties (e.g., density), and uncertain manufacturing processes (e.g., heat and electricity demand and efficiencies), show low influence across most impact categories (< 0.04). Methodological input variables present a mixed picture: solving multifunctionality (avoided burden or cut-off) regarding by-products affects certain impact categories, whereas economic allocation and the scaling factor in supply-chain processes are nearly negligible.

A significant portion of the output uncertainty arises from interactions among input variables, as indicated by lower first-order Sobol' indices (Fig. S2) compared to total-order indices. In particular, solar-to-chemical efficiency, system lifetime, and parabolic collector concentration ratio become nearly negligible at first order, suggesting that their contribution to overall uncertainty is primarily driven by interactions with other variables.

3.2 Hydrogen peroxide and methane (H_2O_2&CH_4)

Results show a wide range across all impact categories (Fig. S3). In the climate change category, the 10th percentile is 39 kg CO_2-eq kg^{-1}, while the 90th percentile reaches 674 kg CO_2-eq kg^{-1}. The median is approximately 124 kg CO_2-eq kg^{-1}, whereas the mean is substantially higher at 312 kg CO_2-eq kg^{-1}, indicating a right-skewed distribution. The interquartile range (64 kg CO_2-eq kg^{-1} to 282 kg CO_2-eq kg^{-1}) shows that the central 50% of results remains widely distributed, although considerably narrower than the overall range.

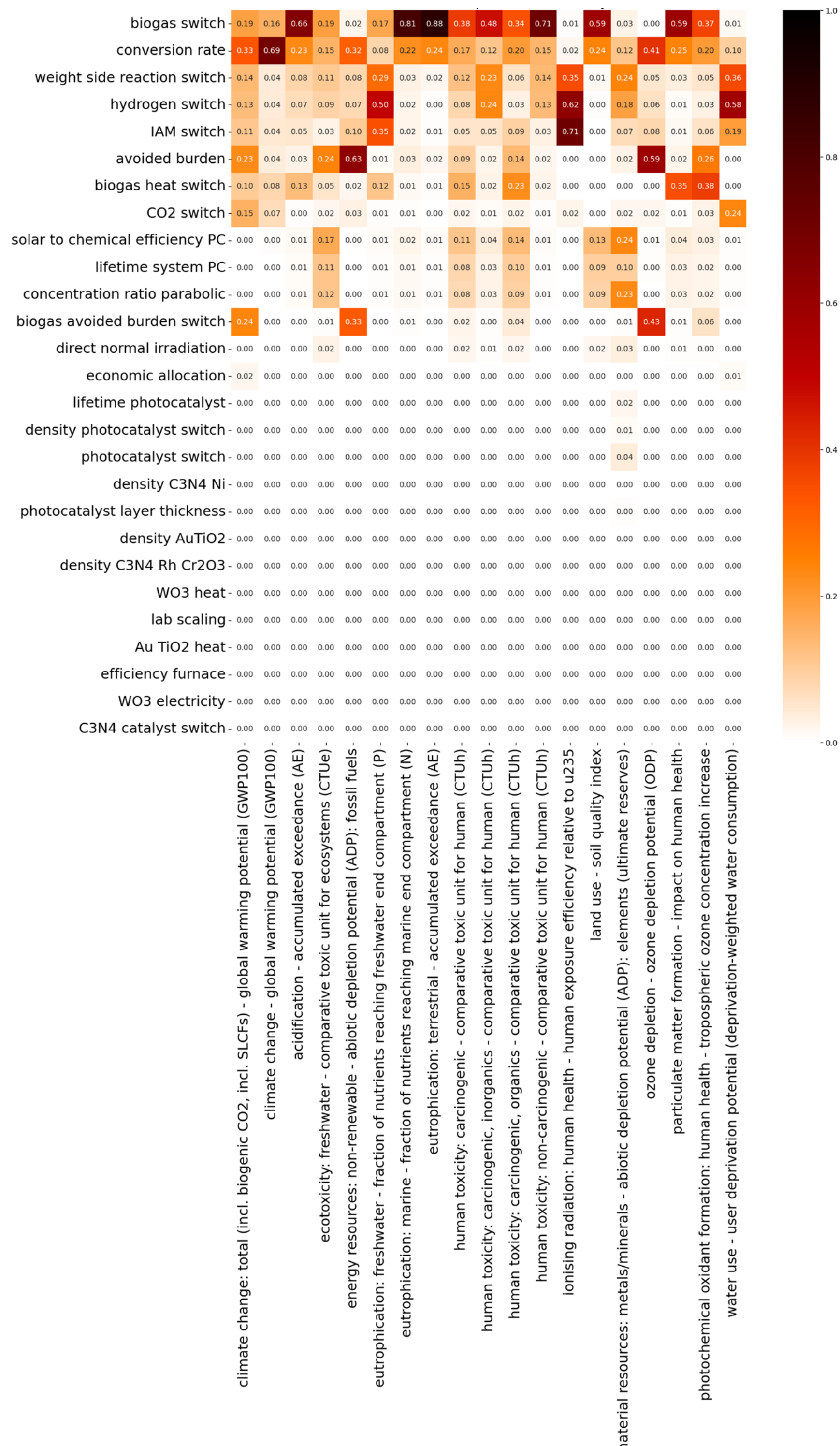

Fig. 1 Uncertainty apportioning showing the total-order Sobol' indices for the H_2+CO product system. Horizontal entries represent the input variables, while vertical entries correspond to the impact categories

Fig. 2 Uncertainty apportioning showing the total-order Sobol' indices for H_2O_2&CH_4. Horizontal entries represent the input variables, while vertical entries correspond to the impact categories

The calculated total-order Sobol' indices (Fig. 2) indicate that system design-related input variables, particularly solar-to-chemical efficiency and lifetime of the electrodes, contribute significantly to the model output uncertainty. Among these, solar-to-chemical efficiency shows a particularly high influence across all impact categories, with Sobol' indices ranging from 0.81 to 0.89. The lifetime of the electrodes is also influential (0.32–0.37), whereas the overall system lifetime has a negligible effect. The IAM scenario exhibits moderate influence overall but becomes significant in certain impact categories. In contrast, other scenario variables, such as mounting type (ground or roof installation), CO_2 source, and additional system components (e.g., methanation units), contribute negligibly to output uncertainty. Similarly, methodological assumptions, including projected material savings (photoreaction cell scaling) and uncertainties in furnace efficiency for catalyst and electrode production, have a minor effect.

Most of the output uncertainty arises from interactions among input variables, with the exception of solar-to-chemical efficiency. This is evident from first-order Sobol' indices (Fig. S4), where solar-to-chemical efficiency retains a high contribution, whereas other variables show lower first-order effects, indicating that their influence primarily stems from interactions.

When the most influential input variables (solar-to-chemical efficiency, lifetime of electrodes, global horizontal irradiation and IAM switch) are removed (Fig. S4), other factors become more influential. In particular, the system lifetime, the electricity demand for FTO glass production and assumptions related to storage increase in their contribution to output uncertainty.

4 Discussion

4.1 Interpretation of results

In H_2+CO, the results exhibit a comparatively moderate range in output uncertainty. However, the 25th and 75th percentiles indicate that the central 50% of simulated results falls within a relatively narrow range. In the author's previous work, point estimates (i.e., without integrated input uncertainty) ranged from −0.28 to −0.03 kg CO_2-eq per kg of synthesis gas [13]. When considering the interquartile range in the present study, the resulting values are higher, and the earlier point estimates are no longer reached. Including biogenic CO_2 reduces the lower bound of the results, as the methane reactant involves the uptake of biogenic CO_2. Consequently, the resulting values would fall below the earlier point estimates. According to the literature, climate change impacts for synthesis gas range from −3.3 to 5.4 kg CO_2-eq per kg [13, 53, 61–69], indicating that the findings of this study are consistent with previously reported values.

In contrast, for H_2O_2&CH_4, the results fall outside the range reported in both the literature and the author's previous work. The mean value in the climate change impact category is substantially higher than the median, indicating the presence of extreme values or outliers. Although the interquartile range is considerably narrower than the p10-p90 range, it remains relatively broad, reflecting significant variability within the results. A direct comparison is limited due to differences in the functional unit, however, the magnitude of the deviation suggests that the resulting range is substantially higher than that reported in the author's previous study [13], where point estimates ranged from 0.53 to 1.59 kg CO_2-eq per kg. It also exceeds values documented in the literature and databases, which report approximately 0.04 kg CO_2-eq per kg of hydrogen peroxide and between -0.04 and 0.3 kg CO_2-eq per kg of methane [13, 53, 65, 68, 70–73]. For both product systems, the systematic integration of uncertainties leads to a widening of the result range. Reliance on static input assumptions may result in an underestimation of environmental impacts. Consequently, conclusions regarding environmental performance and competitiveness may change, as demonstrated in the case of H_2O_2&CH_4.

The contribution analysis in the author's earlier work showed that reactants in the H_2+CO system, particularly biogas, contributed more significantly to environmental impacts than the device itself. This finding is supported by the uncertainty apportioning conducted in the present study, which indicates that biogas supply, along with process-related input variables, exerts the greatest influence on output uncertainty. In addition, a notable influence of the IAM scenario was identified. This is confirmed by the uncertainty apportioning results for both H_2+CO and H_2O_2&CH_4, and is consistent with findings from other studies, for example in the case of passenger cars [17, 20]. Moreover, increased output uncertainty in the impact categories freshwater eutrophication and ionizing radiation is observed for the IAM scenario input variable. This can be attributed to shifts in energy mixes, particularly changes in the shares of fossil and nuclear power. These results highlight that IAM scenarios influence not only the climate change impact category but also other environmental impact categories.

For H_2O_2&CH_4, removing the most influential input variables, thereby reducing the very large result range, reveals the importance of further component-related input variables. The system lifetime, the electricity demand for fluorine-doped tin oxide (FTO) glass production, and assumptions regarding material storage, become more influential. In contrast, these exert negligible influence, when analyzing H_2O_2&CH_4 with all input variables included, while solar-to-chemical efficiency, lifetime of electrodes, and global horizontal irradiation are the most influential input variables. These system design-related input variables exhibit a lower influence on output uncertainty in H_2+CO, however this system relies on light concentration through the assumed use of a parabolic trough collector. When considering the input variables solar-to-chemical efficiency, system lifetime, direct normal irradiation, and the parabolic collector concentration ratio together, their influence on impact categories such as material resources, land use, ecotoxicity, and human toxicity is substantial. However, their effect on other impact categories, such as climate change, remains negligible.

Due to the high output uncertainty associated with the identified input variables, generating point estimates at an early stage of technology development, when system design remains highly uncertain, is unlikely to enable robust comparisons with established reference technologies. The default input variable values used in the author's previous work appear to underestimate the environmental impacts. However, relying on current empirical values may also be unrealistic, as future technological improvements are expected. Nevertheless, the analysis provides guidance for technology development by identifying key contributors to environmental impacts and giving recommendations for action in alignment with the SDGs, particularly those related to affordable and clean energy, and climate action. For H_2+CO, optimization efforts should primarily focus on process-related input variables and the reactant supply chain. Furthermore, the strong influence of the IAM scenario on the LCIA results suggests that these technologies perform more favorably under ambitious climate mitigation pathways. For H_2O_2&CH_4, improvements in solar-to-chemical efficiency, and extending component lifetimes, particularly for electrodes, are essential to reduce environmental impacts.

Regarding other findings from the output uncertainty analysis, independent of the product system analyzed, the results are consistent with those reported in several previous case studies. The observation that point estimates, optionally combined with basic sensitivity analyses (e.g., varying selected input variables one at a time), can lead to differing results, interpretations, and conclusions is supported by Kim et al. [5], who demonstrated that neglecting uncertainties and correlations may result in misleading conclusions and misinterpretation of LCIA results. Concerning the contribution of individual uncertainty sources, the influential factors identified in this study vary depending on the product system. However, in line with Barahmand and Eikeland [6], the most significant sources of uncertainty generally include model and process input variables, data variability, as well as method and database choices. This corresponds to the findings for H_2+CO, where process-related input variables, such as the conversion rate, contribute substantially to output uncertainty. If model and process input variables are interpreted more broadly to include system design aspects, the findings for H_2O_2&CH_4 are also consistent: input variables, such as efficiency and component lifetime are identified as major contributors to uncertainty. More specifically, this is consistent with findings from a passenger vehicle footprint study [20], which identifies mileage and vehicle size as the most influential input variables.

Referring to data variability, the supply chain plays a dominant role for H_2+CO, particularly the biogas source. While different databases were not explicitly compared, variations in background data were implemented through IAM scenarios, which showed a significant influence on the output uncertainty. This finding is further supported by a study on passenger vehicle carbon footprints [20], demonstrating that future scenarios, which affect electricity and fuel carbon intensity, become increasingly important.

In contrast, Bamber et al. [7], in a review of uncertainty analysis in attributional and consequential LCA, identified data variability and data quality, quantified using the pedigree matrix, as primary sources of uncertainty. Although integrating the pedigree matrix could provide additional insights, its application introduces methodological challenges, such as the lack of a combination rule for its uncertainty factors, the absence of a methodological foundation for quantification, and its dependence on expert judgment [2]. Beyond the pedigree matrix, Bamber et al. [7] also highlighted the influence of modelling choices, including the definition of the functional unit, system boundaries, solving multifunctionality (e.g., by allocation methods), as well as characterization and emission factors [7]. In the present study, the functional unit and system boundaries were treated as fixed model definitions to ensure comparability with reference product systems and were therefore not varied. However, alternative approaches solving multifunctionality were partly examined and, depending on the product system and the definition of the respective input variable (e.g. avoided burden for by-products), showed a noticeable effect on the results.

Uncertainty associated with characterization and emission factors was not included in this study, although it may significantly influence outcomes. Nevertheless, Kim et al. [5] found that most uncertainty in LCIA scores for the climate change impact category originates from technosphere processes. Furthermore, when correlations are properly accounted for, as in their study, the importance and uncertainty in LCIA scores decrease, while uncertainties associated with combustion processes and electricity inputs become more dominant. This suggests that uncertainty contributions from the LCIA stage may, in some cases, be less significant. However, this assumption requires explicit testing for the specific product systems analyzed here, across multiple impact categories and LCIA methods, before definitive conclusions can be drawn.

4.2 Strengths and limitations

The computational framework presented in this study offers flexibility by integrating uncertainties, enabling not only the calculation of output uncertainty but also the identification of influential input variables through uncertainty apportioning. This creates direct opportunities to give recommendations to technology developers or decision-makers, as well as feedback to LCA modelers on where deeper investigation could be valuable. Instead of presenting a single point estimate for emerging technologies, the tool delivers the output uncertainty, along with the identification and ranking of key input variables that should be prioritized. This approach avoids misleading conclusions, as demonstrated in this study. The integration from LCI spreadsheet and system design (including the retrieval of chemical and physical substance properties), to LCA modelling, prospective LCA modifications, symbolic LCI generation, uncertainty quantification and apportioning allows for transparency, reproducibility, flexibility and facilitates updates, adaptations and incorporation of future advancements.

However, applying this approach requires substantial modeling effort, as all input variables must be constructed and integrated. While this methodology allows for the incorporation of epistemic uncertainties, full integration remains incomplete for certain aspects, including database uncertainties, characterization factor uncertainties, and other methodological sources of uncertainties within LCA. In addition to the modeling effort, computational demands are considerable, as achieving stable results requires a large number of model runs. For H_2O_2&CH_4, approximately 2^{19} runs were necessary, which was only feasible by implementing a batch-calculation modification. Despite this high number of runs, minor differences in the ranking of input variables could not be fully resolved. Further increasing the number of model runs would have substantially increased computation time or required access to cluster computing, which was avoided in this study to maintain applicability. The resulting output uncertainty remains very wide, limiting the ability to draw definitive decisions. Therefore, conducting an assessment at such an early stage of technology development requires careful consideration.

The uncertainty contributions of individual input variables, calculated using Sobol' indices, may be unreliable, as highlighted by Jaxa-Rozen et al. [26], particularly when analyzing non-normal model outputs. Alternative approaches, such as the PAWN distribution-based sensitivity indices in Jaxa-Rozen et al., as well as regression-based techniques described in [2], were not evaluated in this study and may yield different results.

With regard to the input variables, alternative distributions were not applied, representing a potential area for further research. However, commonly used alternatives in LCA, such as normal or lognormal distributions, do not demonstrate a clear advantage in all cases [2]. The selection of appropriate distributions remains an active area of discussion in LCA, as the choice of distribution (e.g., normal, lognormal, beta) could substantially influence the results.

Furthermore, the ranking of Sobol' indices across the multiple impact categories considered was based on the median. However, the median does not capture the magnitude of differences between input variables within individual impact categories, as it is insensitive to extreme values. While given the limited number of input variables in this study, individual extreme values can still be identified, more robust ranking approaches may be required for comprehensive analyses. For instance, the uncertainty treatment software OpenTURNS [74] recommends the use of a variance-weighted aggregation approach, based on Gamboa et al. [75] and applied in subsequent studies [76].

While this study addresses the limitation associated with the use of point estimates in many LCA applications, additional limitations inherent to LCA, prospective LCA and the underlying data remain. Previous work has discussed these limitations in greater detail, particularly in relation to the specific product systems analyzed in this study [13, 18].

4.3 Future research

Several epistemic uncertainties have not yet been fully integrated. For example, the incorporation of characterization factor uncertainties, as well as time-resolved emissions could be addressed using additional tools, such as the bw_timex Python library [77]. Furthermore, database-related uncertainties should be considered, including testing alternative databases to assess the sensitivity of results to data variability and database choice. In addition, different probability distributions for input variables should be applied and systematically compared. However, as already observed in this study, further integration of uncertainties is likely to increase output uncertainty. Therefore, additional methods for mitigating uncertainty should be explored to improve the interpretability of LCIA results and support more effective decision-making under uncertainty.

Further integration is also likely to increase computational effort. To reduce computational effort, a potential approach requiring further validation would be to determine the maximum deviation needed to match the environmental performance of the reference product system and then incrementally include input variables. While this approach does not capture the full range of possible outcomes, it may help reduce computational resources and support decisions on whether further modeling is justified. Additionally, a stepwise modeling strategy, for example, initially excluding catalyst material production, could further reduce resource use, as results from this study suggest that its influence is marginal. In terms of computational efficiency, further methods such as Morris' Elementary Effects may help reduce calculation time. Beyond efficiency considerations, applying multiple methods could enhance the robustness and reliability of the results. For example, in cases where Sobol' indices may be less reliable, as highlighted in [26], complementary approaches could provide additional validation. Therefore, integrating multiple methods in future work could offer both methodological benefits and insights on calculation efficiency.

From a software perspective, separating the functionalities currently implemented in the Jupyter notebook into a dedicated module would be beneficial. Such a module could automate library installation, improve usability for LCA practitioners, and facilitate the transfer and application of the approach to other technologies. This could help address the currently limited use of uncertainty analysis, sensitivity analysis, and uncertainty apportioning in LCA.

Moreover, it is important to assess whether the median can serve as a robust indicator, for example by applying this framework to a technology with known environmental impacts (e.g., photovoltaics). Comparing the median of simulated results with empirical outcomes could provide valuable insights into the reliability of median-based assessments under uncertainty.

5 Conclusions

A prospective LCA model was integrated into a tool that applies uncertainty quantification and apportioning to identify key contributors of uncertainty in a prospective LCA model for CO_2-removing artificial photosynthesis. Despite wide result ranges varying by product system, the main contributors to output uncertainty were identified and ranked, revealing key drivers for technology developers and decision-makers, as well as for LCA practitioners.

While process- and system design-related input variables are influential, the analysis indicates that external sources can exert substantial influence. For example, scenario-related input variables, such as reactant supply chains and the choice of climate mitigation pathways, suggest that new technologies should be developed in conjunction with environmentally sustainable supply chain and climate policy frameworks. For the product systems analyzed, catalyst materials and their manufacturing uncertainties were not among the most influential contributors to environmental impacts.

Finally, the findings raise new questions regarding the significance and interpretability of such results. Further research is needed to fully incorporate epistemic uncertainties, compare the effects of different input variable distributions, and optimize approaches to reduce both modeling effort and computational resource requirements. Additionally, the interpretation of probabilistic results requires further investigation to ensure both meaningful and implementable insights.

Supplementary Information

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Supplementary Material 1

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Author contributions
L.L. conceived and designed the study, conducted the modeling and analysis, prepared all figures, wrote the manuscript, and approved the final version.

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Data availability
The research datasets are provided in the Supplementary Information and through the linked repositories referenced therein.

Declarations

Ethics approval and consent to participate
Not applicable.

Consent for publication
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Competing interests
The authors declare no competing interests.

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