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Automating relative and absolute environmental sustainability assessments of bio-based products

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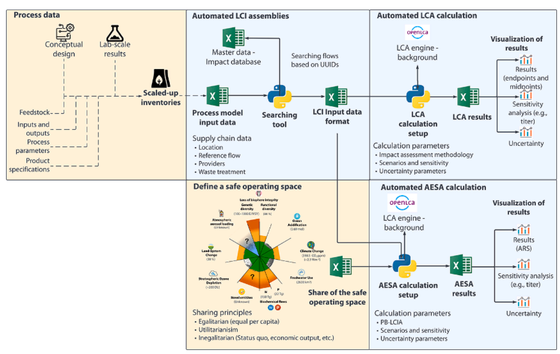
HIGHLIGHTS

- An automated sustainability assessment for bio-based products is presented.
- The protocol integrates relative and absolute sustainability assessments for agile calculations.
- GWP of 1 kg succinic acid corresponds to 5.46 kg CO_2 eq and 3.82 kg CO_2 eq for poly-lactic acid.
- Transgression of planetary boundaries (ASR > 1) is observed in both succinic acid and poly-lactic acid production.

GRAPHICAL ABSTRACT



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ABSTRACT

Awareness of long-term environmental challenges has motivated society toward a more sustainable future. Biotechnology is expected to contribute to the transition towards sustainability. Automation can play an important role in this transition, enabling faster decision-making at early stages. Therefore, an automated relative and absolute environmental sustainability assessment is presented to boost innovation in biotechnology. The automated calculation methodology uses computer-aided tools (dedicated software and Python codes) for the fast quantification of the environmental sustainability performance of bio-based products including scenario and uncertainty analysis. Two case studies (i) succinic acid (SA) and (ii) poly-lactic acid (PLA) are evaluated to test the capabilities of the automated assessment. The results show a carbon footprint and land use of 5.46 kg CO_2 eq and 1.26 m^2a crop eq for SA and 3.82 kg CO_2 eq and 0.74 m^2a crop eq for PLA. Transgression of planetary boundaries was found in both SA and PLA production.

Abbreviations: 1,3 PDO, 1,3-Propanediol; 3HP, 3-Hydroxypropionic acid; AESA, absolute environmental sustainability assessment; ASR, absolute sustainability ratio; BAU, business-as-usual; BF-N, Biogeochemical flow – N; BF-P, Biogeochemical flow – P; CC-CO2, Climate change – CO_2 concentration; CC-EI, Climate change – Energy imbalance; DE, Germany; EpC, equal per capita; FCE, Final consumption expenditure; FU, freshwater use; ILCD, International Reference Life Cycle Data System; IT, Italy; LCA, Life cycle assessment; LCI, Life Cycle Inventory; LCIA, Life cycle impact assessment; LSC, Land-system change; NL, the Netherlands; OA, Ocean acidification; PLA, poly-lactic acid; PB, planetary boundary; PB-LCIA, Planetary boundary-Life cycle impact assessment; R&D, research and development; SA, succinic acid; SDGs, Sustainable Development Goals; SQ, status quo; SHS, share of the safe operating space; SOD, stratospheric ozone depletion; SOS, safe operating space; TRL, Technology readiness level; UUIDs, unique universal identifier; US, United States.

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1. Introduction

The transition toward sustainability requires using renewable resources to meet the United Nations Sustainable Development Goals (SDGs) and the Paris Agreement to keep the temperature increase below 2 °C from the preindustrial value (Lokko et al., 2018). The planetary boundaries (PB) framework provides thresholds for humanity to avoid transgression of its safe operating space (Steffen et al., 2015) without compromising Earth's stability. Humanity has transgressed six out of nine PBs so it is urgent to take action to reduce the pressure on the Earth-system processes (Richardson et al., 2023). The interest in advancing disruptive biotechnology innovations has proliferated extensively and this field of science is expected to play a significant role in helping society reduce its environmental footprint globally (Dahiya et al., 2020). However, large-scale implementation of bio-based products could lead to environmental tradeoffs (Heck et al., 2018).

Product innovation in biotechnology faces the so-called "Valley of Death" which refers to the very low rate of innovations that reach product commercialization (Gatto and Re, 2021). Product development starts from academic and research institutes where the level of maturity defined by the Technology readiness levels (TRLs) (European Commission, 2014), locates the product between the basic science and proof of concept phases (TRLs 1–3). Industry involvement comes at later TRLs (7 to 9), while the in-between phases (TRL 4–6) are related to applied research and scaling-up activities. As depicted in Fig. 1 (top half), bridging the Valley of Death would require identifying challenges and building collaborations between academia and industry to bend the curve. The identification of the challenges and opportunities could be achieved by applying early-stage sustainability assessments (Mahmud et al., 2021).

This study proposes (Fig. 1, bottom half) that embracing the systemic perspective at low TRLs could enable tracking environmental sustainability impacts across a product's life cycle. Life cycle assessment (LCA) is the best-in-class system-based methodology to address the relative sustainability performance of product systems and has been applied to assess bio-based products (Aghbashlo et al., 2022). Even though the LCA is a powerful tool in decision-making, due to its relative nature it cannot answer the question if an alternative is sustainable enough considering nature's carrying capacity.

The absolute environmental sustainability assessment (AESA) is an emerging methodology with the advantage that provides impacts in terms of the PB. Even though AESA is a new methodology with its limitations, the number of studies applying this methodology is continuously increasing (González-Garay et al., 2019; Ryberg et al., 2018a). Data limitations and high uncertainties in early-stage assessment are often found at low TLRs, however, continued guidance of research and development (R&D) activities across TRLs could ensure advancing sustainable biotechnology innovations (Meramo et al., 2022a). As the number of biotechnology innovations is growing and the LCA (and AESA) could be time-consuming, automated relative and absolute environmental sustainability assessments are needed to speed up and simplify calculations of new bio-based products (Douziech et al., 2021).

Efforts have been made to develop sustainability assessment tools with applications in biotechnology. Integrated multi-scale and multi-sector models were performed on chemicals 3-Hydroxypropionic acid (3HP) and 1,3-Propanediol (1,3 PDO) by predicting economic and environmental impacts with varying metabolic and fermentation parameters (Zhuang and Herrgård, 2015). The work was expanded by the addition of upstream pathway predictors and a granular simulation of the petrochemical and bioprocess industry (Herrgard et al., 2015). Other efforts have focused on automating sustainability assessments in the form of an online calculator for fermentation-based processes under gate-to-gate boundaries (Lynch, 2021). BioSTEAM (Shi and Guest, 2020) is an emerging initiative that gives free access to such process modules that could also be tuned for fermentation and bioprocess developments. The contributions are often operated in a standalone manner but demonstrate the immense potential to generate and channel information if orchestrated in an automated workflow.

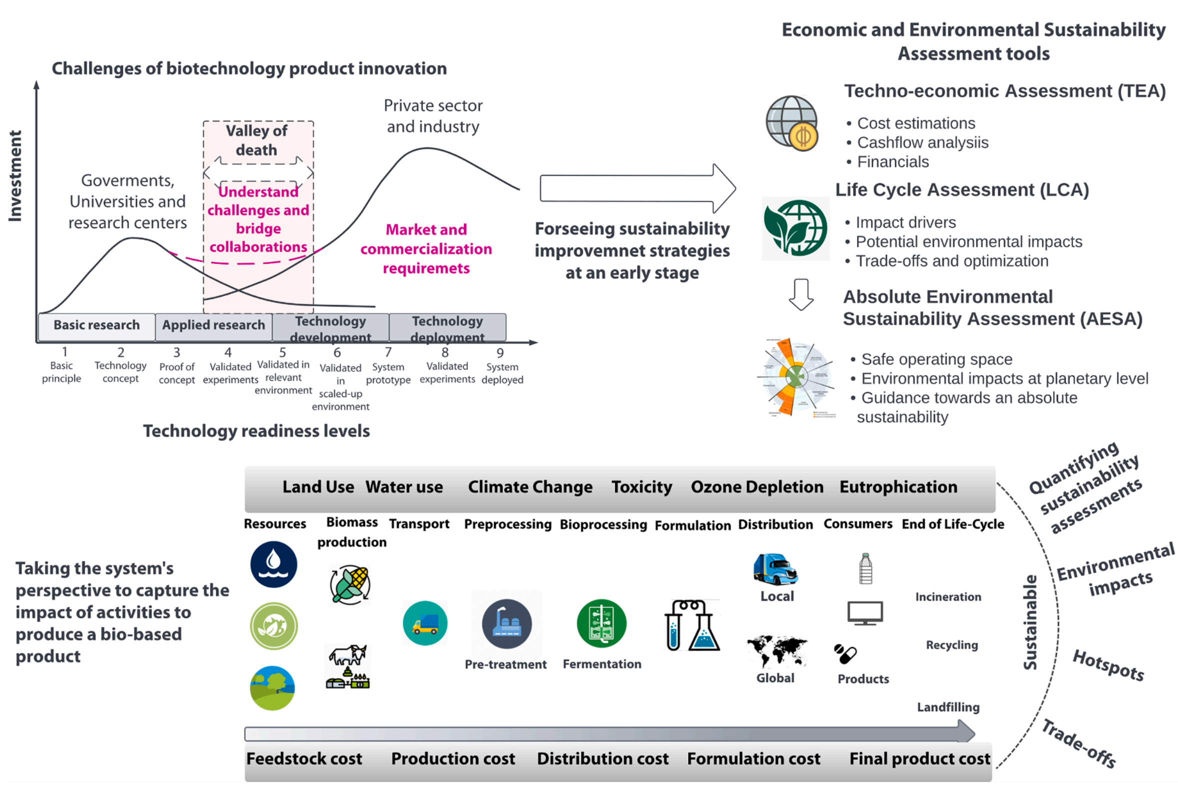


Fig. 1. Identifying the opportunities to improve the sustainability performance of biotechnology-based products at the early stages of innovation.

The scope and workflow automation needs to be performed using dedicated LCA engines. One such widely used infrastructure for LCA is the openLCA® modeling suite (Ciroth, 2007), which is open-source and offers code-based automation capabilities. OpenLCA's integration with Python® and ability to run this seamlessly by passing in external data is explored by the community to automate relative sustainability assessments. Apart from this, LCAs have been documented in the past to be sensitive to location, transformations, and the impact assessment method. To explore advanced evaluations and add-on to the possibilities offered by openLCA, Brightway®, an open-source software package (Mutel, 2017), offers added assessment capabilities for relative sustainability assessment. In addition, more developments are emerging in the open-source domain to facilitate integration and automation capabilities to LCA.

Performing AESA enables taking the planetary perspective to study the role of bio-based products in achieving SDGs and determining priorities to guide further R&D activities. The development of impact modeling and characterization factors in terms of the PBs (Ryberg et al., 2018b) enables the operationalization of PB impact assessment, but there could be some challenges in defining the safe operating space of the assessed bio-based product. A variety of allocation principles have been used to downscale PBs at different levels (Hjalsted et al., 2021), but this procedure is considered controversial (Bachmann et al., 2023). Safe operating spaces have been defined for safe and just Earth systems (Rockström et al., 2023), plastics (Bachmann et al., 2023), and the food sector in the United Kingdom (Lucas et al., 2021). Despite the remarkable development of LCA and the recent progress of AESA, there is still an opportunity to boost the R&D of bio-based products at an early stage through the integration of automated LCA and AESA workflows.

This work introduces a novel workflow to operationalize relative and absolute environmental sustainability assessments of bio-based products. While LCA and AESA rely on time-consuming calculation setups in software, automating relative and absolute sustainability assessment enables (i) speeding up calculations and feedback on low TRL products, (ii) identifying environmental hotspots that hinder the product's environmental performance, and (iii) quantifying the extent to which a bio-based product transgresses designated Earth's carrying capacity. This workflow will allow for the first time the integration of PB assessment into bio-based product R&D. To test the workflow, two representative case studies are used based on two broad biotechnology applications: (1) sustainable chemical, succinic acid (SA) and (2) material science, bio-poly-lactic acid (PLA).

2. Materials and methods

2.1. Automated relative and absolute sustainability assessments

The ISO 14040/44 standards (ISO, 2006) and the International Reference Life Cycle Data System (ILCD) guidelines (European Commission, 2010) provide recommendations regarding the LCA, describing four major stages: (i) goal and scope definition, (ii) life cycle inventory (LCI), (iii) life cycle impact assessment (LCIA), and (iv) interpretation of results (sensitivity and uncertainty analysis). A transition towards sustainability not only implies efforts to make things relatively better than the existing or current products/services but also should consider the Earth's capacity to sustain life as society knows (Lade et al., 2020). This rationale implies that although LCA is a powerful tool for improving processes and products, it cannot address transgression levels of Earth's carrying capacity (Hauschild et al., 2020). The AESA is conceived as an LCA-based methodology (follows ILCD and ISO guidelines) where environmental impacts are upscaled to PBs based on the control variables (Steffen et al., 2015).

Automating relative and absolute environmental sustainability assessment workflows requires using computer-aided tools for data management, impact calculations, and visualization of results. Different layers of information and steps are put together in the automated sustainability assessment workflow, as shown in Fig. 2. Data is related to the availability of process data (laboratory protocols, input–output flows, and process parameters) for upscaling the process model and generating inventory flows (Meramo et al., 2022b).

In addition, impact databases are required to provide supply chain and market data for performing LCA and AESA methodologies, LCI, and sensitivity analyses. It is worth noting that these databases can have commercial and/or free versions, but they often have data limitations that might require additional searches and steps to perform the assessments. For this work, the ecoinvent 3.8 database was selected as a source of background process.

In the case of AESA methodology, additional macro-level data might be required to define the share of the safe operating space (SOS) of the product system. For example, data on population, gross domestic product, environmental impact, and industry turnovers, among others, are used in different allocation principles (Lucas et al., 2020). The SOS relates to Earth's carrying capacity as metrics of environmental load limits, in this case, the PBs, and their recent updates (Richardson et al., 2023; Steffen et al., 2015) (Rockström et al., 2023), as illustrated in Table 1.

Different approaches have been proposed to share the SOS (Hjalsted et al., 2021); however, allocating safe operating space is still a controversial aspect of AESA methodology (Wheeler et al., 2021). Applied allocation principles include Status quo (SQ) or grandfathering, final consumption expenditure (FCE), and ability to pay (ATP), among others (Lucas et al., 2020). Considering the variety of the downscaling approaches and for simplicity, three of the most used principles (i) Equal per capita & FCE (EPC & FCE), (ii) SQ, and (iii) FCE only are applied in the calculation (see supplementary materials for more details on the downscaling principles). In the case of the Status quo (SQ) or grandfathering approach, knowledge about the economy's or industry sector's environmental impact on specific countries is needed to downscale/upscale the PBs to different stakeholder levels. Input-output models and EXIOBASE (Kucukvar et al., 2019) database could serve as the source for determining these environmental impacts.

Automating the calculation workflow makes integrating different computer-aided tools a priority. Assessing products at early-stage (TRL 1–3) implies that most of the data comes from laboratory experiments or estimations (Buchner et al., 2018). Process simulations are performed to generate mass and energy balances that make up an inventory of exchanges. There have been efforts to develop an open-software version of process simulation, however, these tools are not advanced enough for a full deployment. Connection to LCA and AESA is made through the LCI stage which is provided by the process simulation module.

Conventionally, performing LCA calculations in software is heavy on "clicks" and time-consuming as the flows and models are manually searched in the software. To operationalize this step, this workflow integrated a database model searching script (python-based) to fetch and select flow models in the database using the unique universal identifier (UUIDs). The searching tool uses a dictionary to translate process model data (flow name, amount, units, etc.) into database "language" (ecoinvent, in this case) so it sets up the LCI ready for performing the assessment, and the database file is used as master data. In addition, data on supply chain (providers), location, reference flow (functional unit), and waste treatment, among others, are defined as input in an Excel file and integrated into the searching tool based on the data availability of the database and user preferences. The code can be found as Mendeley Data and is readily accessible to anyone in (Meramo and Sukumara, 2023).

The formatted LCI works for both LCA and AESA modules. With the same purpose of reducing clicks and time, two scripts were developed (in Python) supported by the Python-OpenLCA API which allows running LCA calculations externally while Open-LCA software is running in the background. Aspects like impact assessment methodology, scenarios, or uncertainty input are defined at this stage. By default, the LCA module uses the ReCiPe 2016 (H) methodology as LCIA while the planetary boundary-life cycle impact assessment (PB-LCIA)

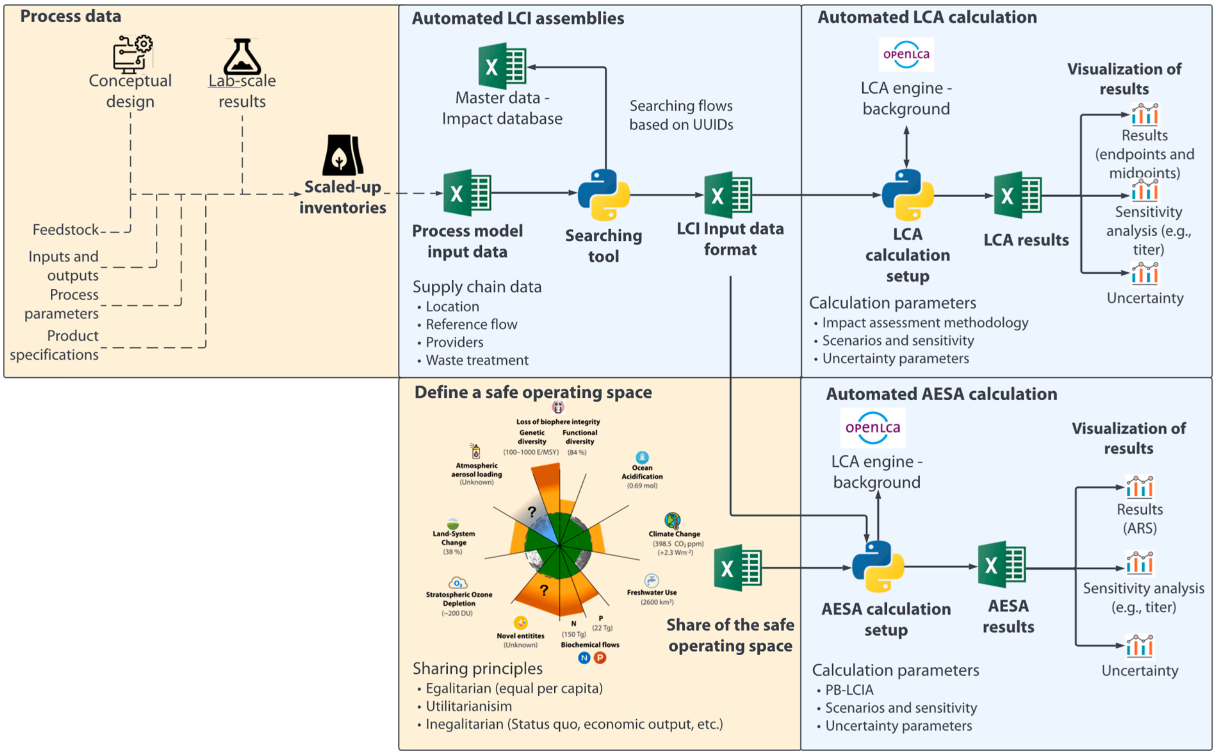


Fig. 2. Data generation, needs, and workflow of automated relative and absolute environmental sustainability assessment of bio-based products. Section 4 explains the integration methodology sequentially.

Table 1
Planetary boundaries, natural background, and full safe operating space values.

Impact category	Unit	Boundary	Natural background	Full SoS
Climate change – Energy imbalance (CC-EI)	Wm^{-2}	1	0	1
Climate change – CO_2 concentration (CC-CO_2)	ppm CO_2	350	278	72
Stratospheric ozone depletion	DU	275	290	15
Ocean acidification (SOD)	mol	2.75	3.44	0.58
Biogeochemical flow – P (BF-P)	Tg P/year	11	1.1	9.9
Biogeochemical flow – N (BF-N)	Tg N/year	92	0	92
Land-system change-Global (LSC)	%	75	100	25
Freshwater use – Global (FU)	km^3/year	4,000	0	4,000

methodology presented by (Ryberg et al., 2018b). Elementary flows are translated into variables defined by the PBs and the flows and functional unit should be adjusted on a yearly basis. As the PB-LCIA methodology is compatible with LCA calculation setups, these adjustments are quite smooth and do not compromise the automation of the calculation workflow.

The PB-LCIA includes many of the environmental categories addressed in the PBs; however, considering the limitations of modeling aspects and the absence of data, the presented workflow covers six categories: Climate change (energy imbalance and CO_2 concentration), Stratospheric ozone depletion, Ocean acidification, Biogeochemical flows N and P (phosphorus flow to freshwater systems and industrial nitrogen fixation), Land-system change (transformation of forest), and Freshwater use. The PB-LCIA does not cover impact modeling of novel entities, and biosphere integrity considering methodological limitations and knowledge gaps. However, this impact modeling has been applied by previous AESA studies (Bachmann et al., 2023; González-Garay et al., 2019).

Once the results of the planetary level impacts are available and the shares of the SOS assigned, the absolute environmental sustainability performance is measured based on the absolute sustainability ratio (ASR) of a PB i, relative to the estimated impact of the PB i ($Impact_{PB_i}$) and the assigned share of the safe operating space to this PB (SHS_{PB_i}), as given in equation (1).

$$ASR_{PB_i} = \frac{Impact_{PB_i}}{SHS_{PB_i}} \quad (1)$$

The criterion for an absolute sustainability performance corresponds to environmental sustainability for a specific PB if $ARS_{PB_i} \leq 1$, while the performance will indicate otherwise (not environmentally sustainable in absolute terms) if $ARS_{PB_i} > 1$.

Impact assessment results (including analysis of scenarios and uncertainty) are stored in Excel files and later visualized at midpoint and endpoint levels for the LCA, and as ARS for the AESA. Result data could be used for process optimization, identification of inefficiencies, and technology/product comparison, among others. The purpose and further use of results will depend on the stakeholders' goals and expectations. The successful implementation of this automated calculation workflow will require understanding between practitioners and stakeholders to define clear objectives. Due to the iterative nature of the LCA (and AESA), it is encouraged to follow the same iterative principle in this type of setup.

The automated relative and absolute sustainability assessments are being developed under the following limitations and assumptions:

- As automating LCA, the calculation follows the same calculation basis based on the guidelines (ILCD and ISO 14040/44).
- Ecoinvent is used as a source of background processes, and the names of ecoinvent processes are used in the search tool.
- The ReCiPe 2016 impact assessment methodology is used by default; however, the code can be updated to use other methodologies.
- Indirect land change impact was not considered in this calculation.
- For the AESA, the characterization factors are taken from (Ryberg et al., 2018b). Novel entities and atmospheric aerosol loading categories are not included.
- The AESA calculation was limited to three downscaling principles, but more can be included.
- Uncertainty analysis is performed using the pre-default distribution values given in the ecoinvent database (500 Monte Carlo simulations are defined by default).
- Regionality is considered based on the ecoinvent data, prioritizing country-level data first and market region models if country-specific models are not available.

2.2. Description of case studies

To test the developed tool, two case studies were used, (i) the bio-based production of succinic acid (SA) and (ii) poly-lactic acid (PLA) production. These products were selected considering their recent interest as bio-based alternatives with huge market size (or potential) and their representativeness of biomanufacturing processes. Process inventories and energy/mass flows were extracted from publications on LCA of bio-SA (Bello et al., 2022; Meramo et al., 2022a; Moussa et al., 2016) and PLA production (Ögmundarson et al., 2020).

2.2.1. Succinic acid production

SA is one of the most relevant chemicals with extensive applications in different fields and sectors. Additional bio-based production pathways have been assessed (Dickson et al., 2021; Nghiem et al., 2017); however, for this case study, the process reported by (Moussa et al., 2016) is used to test the automated workflow (see supplementary materials for details of process inventories and sources of background data).

A functional unit of 1 kg of SA with a concentration of 99.5 wt-% was set. The SA production is assessed in a cradle-to-gate boundary that includes biomass production and bioprocessing to produce SA and ammonium sulfate as a by-product. Subsequent after-gate stages are not included in the assessment since SA is mainly used as an intermediate for other supply chains. The production plant is assumed to be in Germany (DE), and transportation is negligible relative to the impacts of mass and energy flows (Cok et al., 2014). Uncertainty input data is taken from ecoinvent default distribution data for the background sources. A sensitivity analysis was performed to assess the variations in the environmental performance if the production plant operates in Italy (IT), considering its increasing SA production, and data availability.

The functional unit in the AESA is set as the total yearly SA production in DE, which is equivalent to 14,410 t/year of both petrochemical and bio-based SA. To apply SQ downscaling, the SHS was estimated based on the impacts of the business-as-usual (BAU) scenario, accounting for 90 % contribution of the petrochemical pathway over the bio-based alternative with 10 %. In addition to SQ, EPC-FCE, and FCE-only principles were applied (see supplementary materials for more details). Both uncertainty and sensitivity analysis are performed, where the last one evaluates: (i) changes in allocation principles and (ii) two different locations.

2.2.1.1. PLA production. PLA is selected as the second case study example, which has been previously assessed using LCA (Rezvani Ghomi et al., 2021) to test the automated workflow for the application of bio-products in the plastic industry. This study uses the process data reported by (Ögmundarson et al., 2020) for a first-generation PLA production from corn starch (see supplementary materials for details on the process flow diagram and details of process inventories).

A functional unit of 1 kg of PLA was set under a cradle-to-grave boundary that includes biomass production, bioprocessing to produce PLA, polymerization, and plastic recycling as end-of-life scenarios. In PLA production, the baseline location scenario is The Netherlands (NL), as this country is one of the major PLA producers in the world. The United States (US) is assessed as a secondary location for PLA production as this country is also a major producer. The functional unit in the AESA of PLA production is set as the total yearly production of PLA in NL, which is equivalent to 67,463 t/year. For the US scenario, the annual PLA production is equal to 98,920 t/year. The same system boundary of relative LCA was applied to the AESA. SHS for this case study was determined using the same approaches applied to the AS case study (see supplementary materials for more details).

3. Results and discussion

The automated environmental sustainability calculation protocol was run to assess the relative and absolute sustainability performance of case studies for SA and PLA production. Python codes, excel sheets, and OpenLCA software (triggered using the Python interface) were used to run the toolbox. The generated LCA and AESA results, sensitivity, and uncertainty analysis are documented and discussed in the subsequent sub-sections.

3.1. Relative environmental sustainability performance of case studies

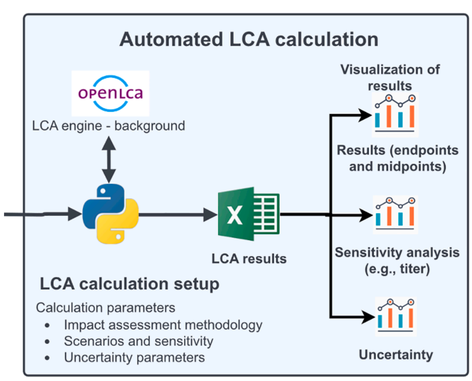
Relative environmental sustainability indicators for both case studies, including uncertainty values, were obtained at the midpoint level (see Table 2). Uncertainties were obtained by running 500 simulations by the built-in Monte Carlo algorithm of OpenLCA software. The values were obtained for a confidence interval of 5 % to 95 %, related to pre-defined distribution data of the background system given in the ecoinvent database. It is worth highlighting that in low-TRL technologies, uncertainties have a critical effect on interpreting the LCA results. Most of these uncertainty values are associated with assumptions, estimations, and other parameters necessary to assess at low maturity levels. Therefore, higher uncertainty levels are expected at an early stage, while progressing through the TRL's could potentially lead to lower levels (Meramo et al., 2022a). Results at the midpoint level are shown further to analyze the relevance of uncertainty levels in environmental performance (see Fig. 3).

In addition to the uncertainty of endpoints, sensitivity analysis was performed based on two different locations for both SA and PLA processes. Data presented in Fig. 3 show that there is room for optimization regarding the environmental sustainability performance, reflected as endpoints, considering the observed uncertainty ranges across categories and specifically for resource scarcity. The inclusion of a sensitivity analysis to foresee impacts by changing the plant's location is insightful as one can observe the tradeoffs between SA produced in DE compared to IT. The variations of impacts are mostly from a different electricity grid in these two countries; however, these differences are not significantly high. The SA production evaluated in (Moussa et al., 2016) showed a global warming potential of 0.87 kg CO_2 eq per kg of SA, while in the present work, this value corresponds to 5.46. The difference is related to the use allocation by system expansion in (Moussa et al., 2016), which allocates a lot of impacts to ammonium sulfate as a sub-product. If system expansion were not considered, the resulting global warming potential would be much closer to the value obtained by this work.

In the case of PLA, a similar sensitivity was performed by analyzing endpoints with uncertainties for the NL and US locations. Due to a more renewable and environmentally friendly electricity grid in NL, this location showed a higher performance compared to the US scenario. Relatively significant differences are observed in human health and

Table 2
Midpoint categories (with uncertainties) for based-case SA and PLA processes (baseline scenario in DE).

Impact category		SA production			PLA production		
	Reference unit	Mean	5 %th value	95 %th	Mean	5 %th	95 %th
Fine particulate matter formation	kg PM2.5 eq	7.41E-03	6.55E-03	8.29E-03	1.10E-02	9.10E-03	1.38E-02
Fossil resource scarcity	kg oil eq	1.47E	1.41	1.55	1.03	8.66E-01	1.16
Freshwater ecotoxicity	kg 1,4-DCB	3.21E-01	1.81E-01	5.28E-01	2.89E-01	1.33E-02	5.88E-01
Freshwater eutrophication	kg P eq	5.34E-03	3.06E-03	1.28E-02	5.13E-04	4.56E-05	9.44E-04
Global warming	kg CO2 eq	5.46	5.23	5.73	3.82	3.24	4.36
Human carcinogenic toxicity	kg 1,4-DCB	6.46E-01	1.93E-01	1.37	2.06E-01	9.35E-02	4.23E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	1.28E + 01	4.48	3.09E + 01	9.30	4.97	1.68E + 01
Ionizing radiation	kBq Co-60 eq	7.85E-01	1.20E-01	3.18	5.83E-02	5.68E-03	1.94E-01
Land use	m2a crop eq	1.26	8.94E-01	1.72	7.40E-01	5.86E-01	8.98E-01
Marine ecotoxicity	kg 1,4-DCB	4.37E-01	2.44E-01	7.24E-01	3.96E-01	1.38E-01	7.54E-01
Marine eutrophication	kg N eq	1.97E-03	1.48E-03	2.55E-03	3.23E-03	2.25E-03	4.79E-03
Mineral resource scarcity	kg Cu eq	1.05E-02	7.67E-03	1.43E-02	1.50E-02	1.09E-02	2.03E-02
Ozone formation, Human health	kg NOx eq	7.86E-03	6.82E-03	9.91E-03	1.20E-02	9.88E-03	1.45E-02
Ozone formation, Terrestrial ecosystems	kg NOx eq	8.05E-03	7.01E-03	1.01E-02	1.22E-02	1.01E-02	1.48E-02
Stratospheric ozone depletion	kg CFC11 eq	7.92E-06	6.07E-06	9.95E-06	1.27E-05	9.52E-06	1.67E-05
Terrestrial acidification	kg SO2 eq	2.28E-02	2.04E-02	2.54E-02	3.52E-02	2.82E-02	4.29E-02
Terrestrial ecotoxicity	kg 1,4-DCB	2.62E + 01	1.38E + 01	4.82E + 01	2.21E + 01	1.42E + 01	3.30E + 01
Water consumption	m3	1.31	−3.16E-01	2.47	1.11E-01	−1.17	1.15



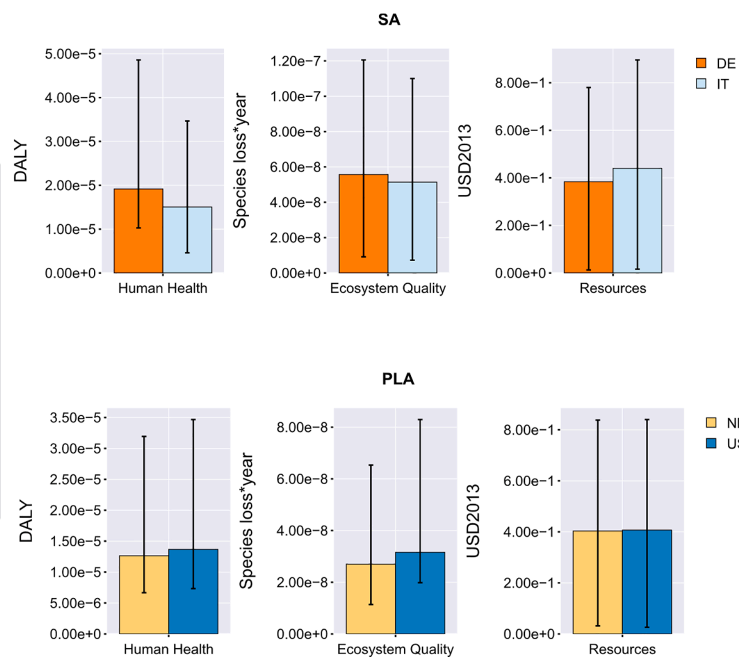


Fig. 3. Results endpoint impacts with uncertainties per functional unit of SA and PLA.

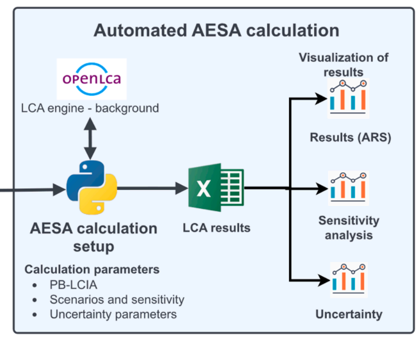
ecosystem quality impacts, while for resource scarcity both locations showed similar performance. Compared to the literature, the carbon footprint of the PLA assessed in this work was 3.82 kg CO_2 eq which is slightly lower than the value (4.19 kg CO_2 eq) obtained in (Ögmundarson et al., 2020). The difference between the two values might be due to the inclusion of the indirect land use change impact in (Ögmundarson et al., 2020) while this is not considered in the present calculation.

3.2. Absolute environmental sustainability performance of case studies

AESA was performed using the toolbox for both case studies to show the application of this tool to estimate the environmental sustainability performance at the planetary level. Results enable analyzing environmental performance in absolute terms and determining if SA and PLA production at selected locations transgress allocated ecological thresholds (FCE only) with respect to the PBs (see Fig. 4).

Results show that SA and PLA transgress their assigned safe operating space in many categories regardless of the evaluated location. Nevertheless, some locations (DE for SA and US for PLA) showed superior environmental performance in absolute terms. In the case of SA, mean values exhibit transgression of the phosphorus cycle, climate change (on both subcategories), and ocean acidification. However, uncertainties show that there is potential for optimization as in certain scenarios, the transgressed categories show environmental performance below the safe operating space with a high significance. High impacts on the described categories are expected as the bio-SA scenarios assessed in this work use first-generation biomass (sorghum grain) as the main feedstock which often leads to high impacts on climate change and eutrophication (Bello et al., 2021).

Regarding PLA production, high transgression levels are observed in almost all categories, excluding land system change and ozone depletion. Even if counting for uncertainties reaching their lower impact values, most categories transgressed their assigned safe operating space.



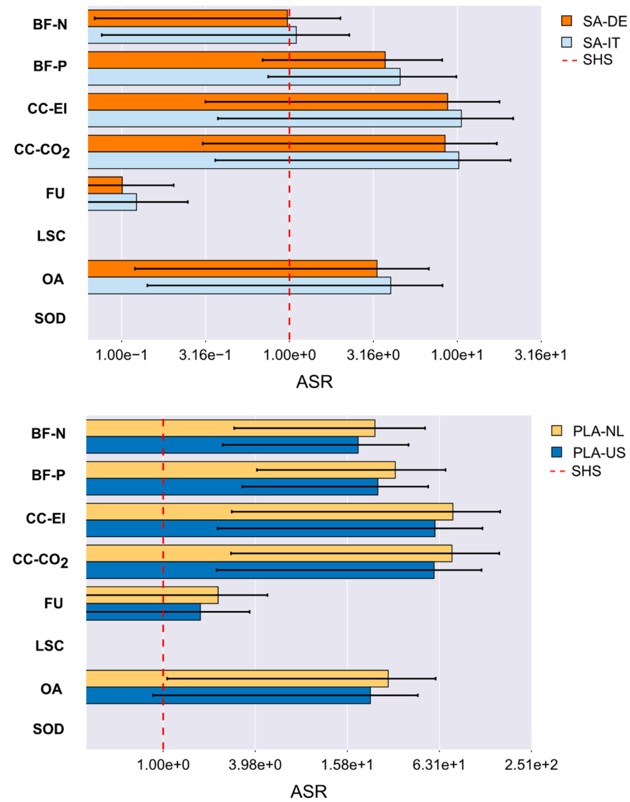


Fig. 4. AESA results including uncertainty values of SA and PLA scenarios for selected locations.

The results indicate that improvements are needed to achieve sustainable PLA production within the PB. However, a previous AESA study on circular plastics (Bachmann et al., 2023), showed that better performance can be reached for all plastic production (not exclusive to PLA) from more renewable energy sources and greener production pathways.

A sensitivity analysis was performed to assess different allocation principles and scenarios for production profiles of SA from petrochemical and bio-based pathways (see Fig. 5A). The BAU scenario is assessed along with a 100 % bio-SA scenario, and an equal 50 % petro- and bio-based scenario to show the shifting of impacts between the different cases. In addition to FCE-only allocation, SQ and EPC-FCE approaches were applied to SA production.

Previous studies applying AESA showed that the ASR values are highly sensitive to allocation principles (Ryberg et al., 2018a), leading to huge variations in the performance. It is worth mentioning that the purpose here is not to discuss the appropriateness of the used allocation principles to the case studies but to illustrate the variation of exceedance of planetary thresholds due to different shares of the safe operating space. LSC and SOD are the categories with no transgression in different allocation principles (except for the SQ approach in LSC). Under certain cases, FU and BF-P categories showed no exceedance of the SOS. Conversely, higher transgression levels are observed in many categories like nitrogen cycle, climate change, and ocean acidification. Overall, SQ and EPC-FCE show much higher transgression levels (in most categories) compared to FCE-only allocation.

These outcomes show that improvements are needed in the SA production towards a more sustainable production at the planetary level. No huge improvements are observed in climate change categories from changing a petrochemical-dominated supply chain to a full bio-based SA production. This is contradictory to previous relative LCA studies on bio-based SA production (Cok et al., 2014; Moussa et al., 2016) comparing petrochemical vs bioprocessing. However, higher impacts on SA were obtained in the present work as economic allocation was applied to assign impacts to AS instead of applying system expansion. Applying system expansion would give credit to avoid byproduct production, resulting in much lower impacts. As the AESA is not suited for consequential assessments (Ryberg et al., 2018b), system expansion is not applicable in the present work. This is confirmed by the fact that assuming byproduct production would not affect the supply chain of the avoided flow is not realistic from the planetary perspective.

Similarly, sensitivity analysis was performed for the PLA case study by assessing the ASRs under different allocation principles (see Fig. 5B). Only one case study was evaluated in the PLA scenario as there is no petrochemical PLA production and bio-based processing is the only route. The lowest transgression levels are shown in the SQ approach in most categories, except by SOD and FU. Results of the three allocation principles show a relatively high sustainability gap from the safe operating space to current transgression in BF-P, CC-EI, CC-CO_2, and AO, and this gap is increased in the EpC-FCE allocation. No transgression was observed under any allocation principle in LSC (SOS slightly transgressed in SQ scenario) and SOD. However, if the SOS is assigned based on SQ allocation, the sustainability gap is strongly reduced to values below the SHS in BF-N and FU. In addition, the performance of climate change categories and OA show ARSs slightly higher than the SHS in SQ allocation.

The case studies used in this work based on specialty chemical production (with a relatively small market) and bioplastic pollution (increasing demand) showed the applicability of AESA and its potential to boost production innovation in biotechnology. Furthermore, with the methodology and the presented framework researchers and practitioners could perform fast AESA calculations of bio-based products to generate insights at the planetary level not only to the evaluated product but also to other bio-based products and supply chains with higher market representativeness, like agriculture and food systems. The development of the microbial foods domain and other largely produced bio-based products will greatly benefit from applying the PB approach since the food sector is one of the major drivers of environmental impact globally (Campbell et al., 2017).

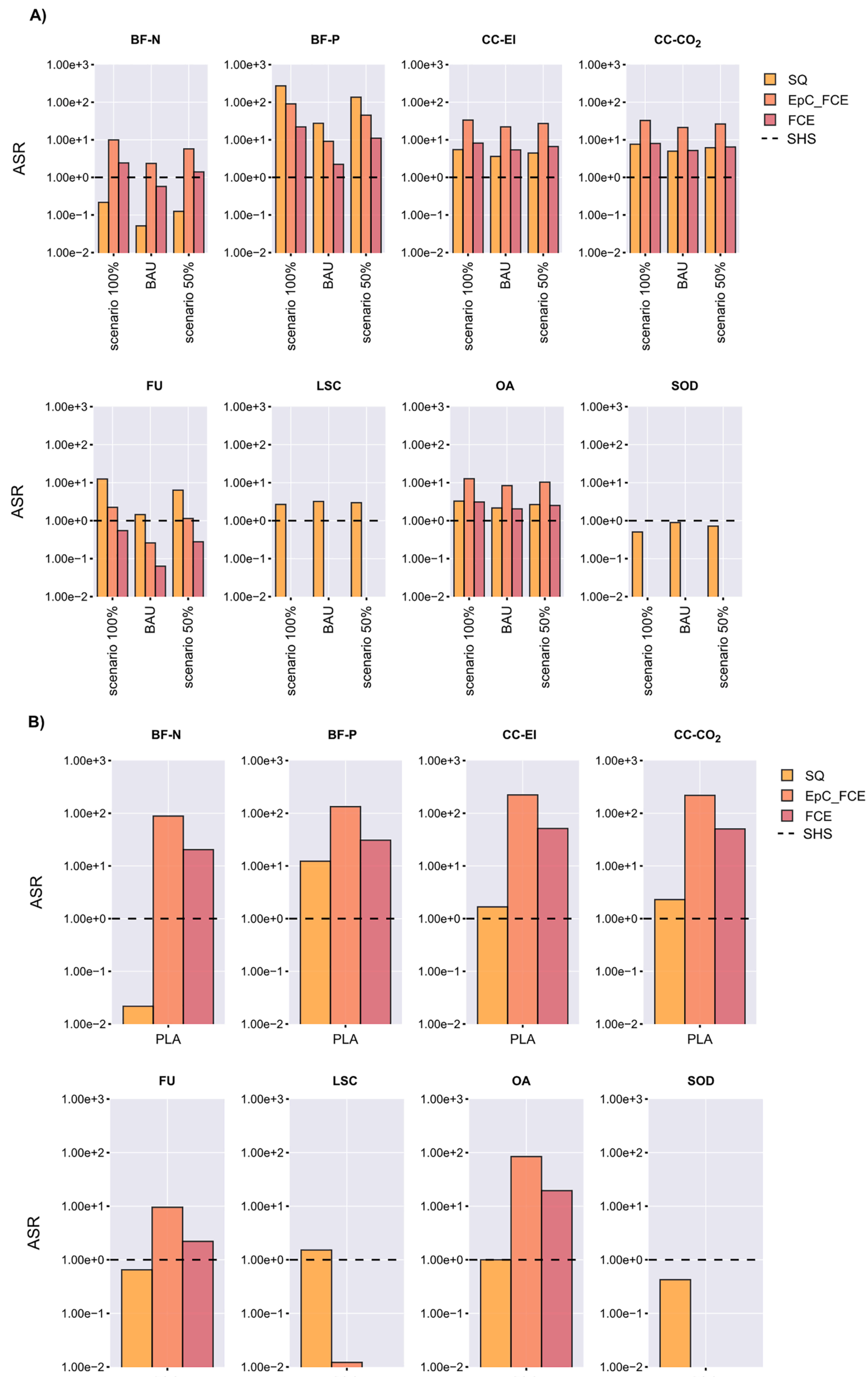


Fig. 5. Results of sensitivity analysis of different allocation principles for (A) SA, and (B) PLA case studies.

4. Conclusions

Achieving a holistic integration of computational models, generating parameters pertaining to fermentation performance, process configuration, supply chain orientation, and eventually planetary impacts would be a tremendous development in the field of bioprocess systems engineering. This manuscript's key outcome is defining the necessary parameters, access portals, and computational algorithms for the state-of-the-art automated calculation of LCA and AESA. While this integration has been the first of its kind in biotechnology, the field of sustainability assessment is progressing fast and pushing methodological developments. Hence, the proposed integration and algorithms would need to be updated frequently by the present contributors and the community.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at http://doi.org/10.1016/j.biortech.2023.130196.

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