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Ex-Ante Life Cycle Assessment of Emerging and Novel Technologies

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Abstract

Life cycle assessment (LCA) is a systematic approach to assess the environmental impacts of products, technologies, or service systems along their life cycle, most commonly applied to existing products with an established life cycle. Ex-ante LCA aims to assess the future impacts of novel technologies in research and development stages and compare them with incumbent technologies, dealing with uncertainty and data challenges. Strategies to address these challenges include scale-up modeling, scenario development, uncertainty analysis, and stakeholder engagement. LCA should be updated as technologies develop and more information becomes available; this way, ex-ante LCA shall support the development of low-footprint technologies.

Key Points

- Methodological advances for ex-ante LCA of novel and emerging technologies at early research and development stages.
- Technology development, readiness levels, and production scales.
- Challenges of conducting ex-ante LCA and strategies for overcoming them.
- Methods to scale up the life cycle inventory (e.g., simulation, process calculations, proxies).
- Scenario-building approaches for modeling future technology and external developments (e.g., electricity mix).

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- Types of uncertainty in ex-ante LCA and ways to analyze, model, and communicate uncertainty.

Introduction

The global societal issues of growing populations, increasing resource demand, and accelerating climate change require an urgent shift to a low-carbon and more sustainable production. To achieve this, we must rethink how to design, manufacture, and use products, reducing resource consumption, minimizing waste, and mitigating environmental impacts. In this context, early-stage environmental assessment of new technologies is needed to inform design, research, and development (R&D), policy, and investment decisions (Cooper and Gutowski, 2020; Cucurachi *et al.*, 2018). Life cycle assessment (LCA) is a systematic environmental assessment methodology that considers the product life cycle (Guinee, 2002; ISO, 2006a). LCA has been mainly applied to existing products and mature technologies with an established life cycle. *Ex-ante* LCA aims to assess the future impacts of novel and emerging technologies that are in an early stage of development. In addition, it allows to compare novel technologies with the incumbent technology mix and can help steer R&D in a more sustainable direction (Cucurachi *et al.*, 2018; Miller and Keoleian, 2015; Villares *et al.*, 2017).

This chapter discusses ex-ante LCA of emerging and novel technologies, outlining the challenges of conducting LCA in the R&D stages, discussing the methodological advances for addressing them and remaining gaps, and gathering recommendations from LCA research for improved practice.

Background

The ecodesign paradox

Technology environmental assessment is usually done when established in the market, relying on information from (past) data obtained from industrial facilities. Delaying such assessments until later stages guarantees that more information is available; however, the potential for environmental improvements diminishes. This is sometimes called the *ecodesign paradox* (**Fig. 1**) (Bhander *et al.*, 2003; Poudelet *et al.*, 2012; Villares *et al.*, 2017). Moreover, more significant impact reductions can be achieved by incorporating environmental considerations during technology R&D than in the product design stage (Moni *et al.*, 2020). Early R&D decisions significantly impact the future functionality, costs, and environmental performance of new technologies. Hence, conducting environmental assessments early on can help technology developers and stakeholders avoid unintended environmental consequences, prevent regrettable investments, and incorporate changes without major disruptions (Cucurachi *et al.*, 2018).

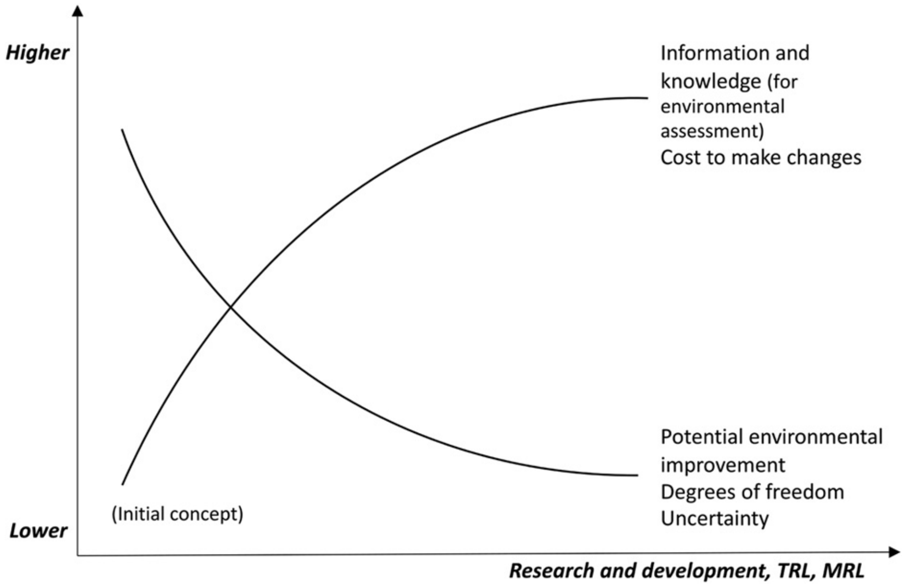


Fig. 1 Illustrating the ecodesign paradox (based on Bhander *et al.* (2003); Chebaeva *et al.* (2021); Poudelet *et al.* (2012)). TRL and MRL: Technology and manufacturing readiness levels, respectively.

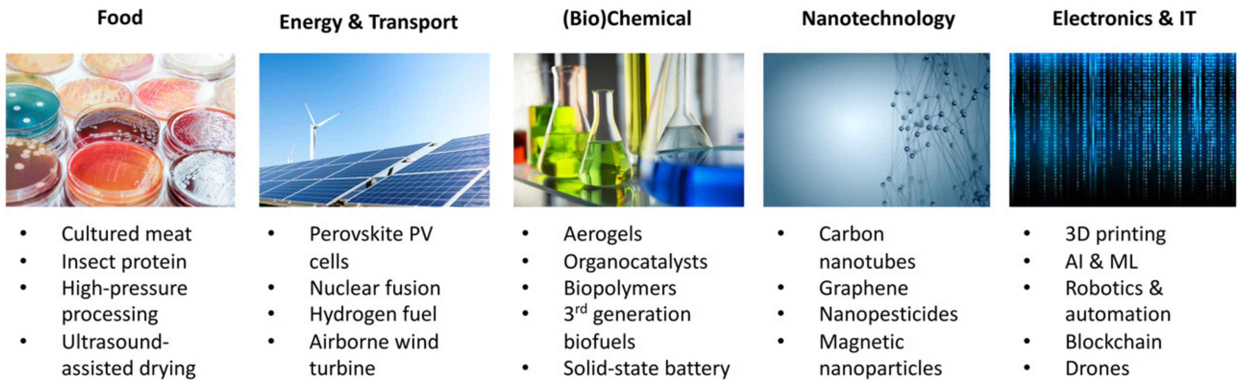


Fig. 2 Examples of emerging and novel technologies.

Stage	Technology readiness level	Manufacturing readiness level
Initial concept and research	**TRL1.** Basic principles observed	**MRL1.** Implications identified
	TRL2. Formulation of concept	**MRL2.** Basics identified
	TRL3. Proof of concept	**MRL3.** Proof of concept
	TRL4. Validation in laboratory	**MRL4.** Laboratory sample
Technology development	**TRL5.** Components in representative i.e., simulated environment	**MRL5.** Prototype components in simulated environment
	TRL6. Prototype in representative i.e., simulated environment	**MRL6.** Prototype system in simulated environment
Engineering development	**TRL7.** Prototype in operational environment	**MRL7.** Prototype system in production environment
Small-scale production	**TRL8.** System qualification	**MRL8.** Ready for small scale production
	TRL9. Technology ready	**MRL9.** Transition to full scale production
Mass production	–	**MRL10.** Lean mass production

Fig. 3 Technology development (based on DoD (2011); Gavankar *et al.* (2015b); NASA (2015)).

Technology development

Technology can be defined as "*the application of scientific knowledge for practical purposes, especially in industry*" (Oxford Dictionary). Emerging and novel technologies are observed in various sectors, e.g., materials, chemicals, processes, apparatus, and devices (**Fig. 2**). Novel technologies can be viewed as still in development and not yet commercially applied, while emerging technologies are also associated with a significant societal transformative nature, radical innovation, and/or rapid growth (Rotolo *et al.*, 2015). Though the terms "technology" and "product" are used interchangeably, they are not the same; a product is the realization of a technology to meet market demand (Pono, 2022; Wahab *et al.*, 2012). A product can incorporate incremental technological innovations or be created or adapted from the new technology. Hence, technology development precedes product development.

Technology development occurs in several stages, from the initial concept to research, technology development and prototyping, engineering development, small-scale production, and mass production (**Fig. 3**). Technology readiness levels (TRL) are used to track the technology progress from TRL 1: observation of basic principles to TRL 9: full commercial deployment (Humbird, 2018; NASA, 2015). However, technology readiness does not imply manufacturing readiness. Thus, a complementary scale, the Manufacturing Readiness Levels (MRL), was proposed to assess the maturity of technology components and subsystems from a manufacturing perspective (DoD, 2011; Gavankar *et al.*, 2015b).

Life cycle assessment

Life cycle assessment (LCA) is a methodological framework for assessing the environmental impacts of products or services throughout their life cycle stages, from raw materials production to manufacturing, distribution, use, and disposal. LCA is performed through four iterative phases: goal and scope definition, life cycle inventory analysis (LCI), life cycle impact assessment (LCIA), and interpretation (**Fig. 4**) (Guinee, 2002; ISO, 2006a).

LCA applications include product development, strategic planning, environmental labeling, and policy-making (ISO, 2006a, 2006b). Traditionally, LCA has been applied *ex-post* for mature technologies and products available in the market. LCA was adapted to assess low-TRL technologies in future-oriented, early-stage approaches.

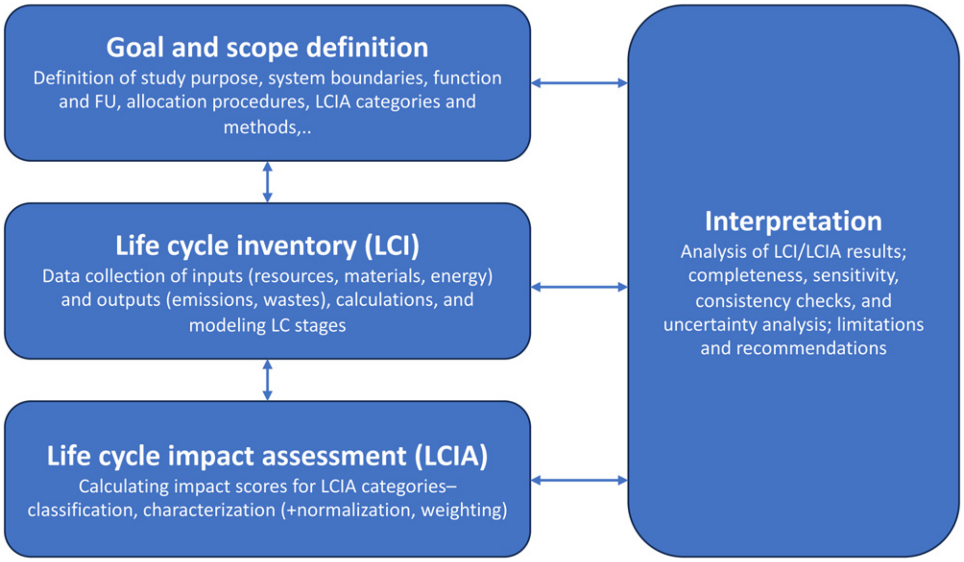


Fig. 4 Life cycle assessment steps (based on ISO, 2006a, 2006b).

Table 1 Future-oriented LCA approaches

Term	*Description*
Ex-ante	In general, studies that apply **scale-up modeling and scenarios** to assess technologies in development aiming to • **compare** them **with incumbent (existing) technologies** Ex-ante LCA are studies that *"scale-up an emerging technology using likely scenarios of future performance at full operational scale, and that compare the emerged technology at scale with a mature product serving the same (or similar) function"* (Cucurachi *et al.*, 2018) • **providing R&D decision support** *Ex-ante LCA refers to "performing an environmental life cycle assessment of a new technology before it is commercially implemented in order to guide R&D decisions to make this new technology environmentally competitive as compared to the incumbent technology mix"* (van der Giesen *et al.*, 2020)
Prospective	A broader scope of LCA studies that assess either a **novel** (low TRL) or **existing** technology **in the future** (e.g., Cucurachi *et al.*, 2022; Mendoza Beltran *et al.*, 2020)
Anticipatory	Combines **ex-ante LCA modeling and other approaches** such as risk assessment, stakeholder engagement, and multi-criteria decision analysis (MCDA): *"(a) forward-looking, non-predictive tool that increases model uncertainty through the inclusion of prospective modeling tools and multiple social perspectives"* (Wender *et al.*, 2014)

Future-oriented LCA

Different terms have been developed for future-oriented LCAs of novel technologies; examples are ex-ante, prospective, and anticipatory LCA, detailed in **Table 1**.

Ex-ante LCA and prospective LCA (pLCA) are often used to describe the same type of study (**Table 1**), i.e., focused on novel technologies in development. In this chapter, they are distinguished as follows: Ex-ante LCA refers to upscaled novel (low-TRL) technologies and pLCA to either novel or existing technologies assessed in the future (Cucurachi *et al.*, 2022; Mendoza Beltran *et al.*, 2020; Spielmann *et al.*, 2005). Anticipatory LCA was proposed by Wender *et al.* (2014) as an overarching framework for stakeholder engagement, risk assessment, and decision-making support, being particularly suitable for cutting-edge innovative technologies developed by interdisciplinary R&D consortia (Buyle *et al.*, 2019; Villares *et al.*, 2017).

Challenges of Conducting Ex-Ante LCA of Emerging and Novel Technologies

LCA practitioners face distinctive obstacles when assessing novel technologies, primarily because of the absence of reliable data at scale and inherent uncertainties in predicting technological advancement trajectories and the evolving socio-economic context

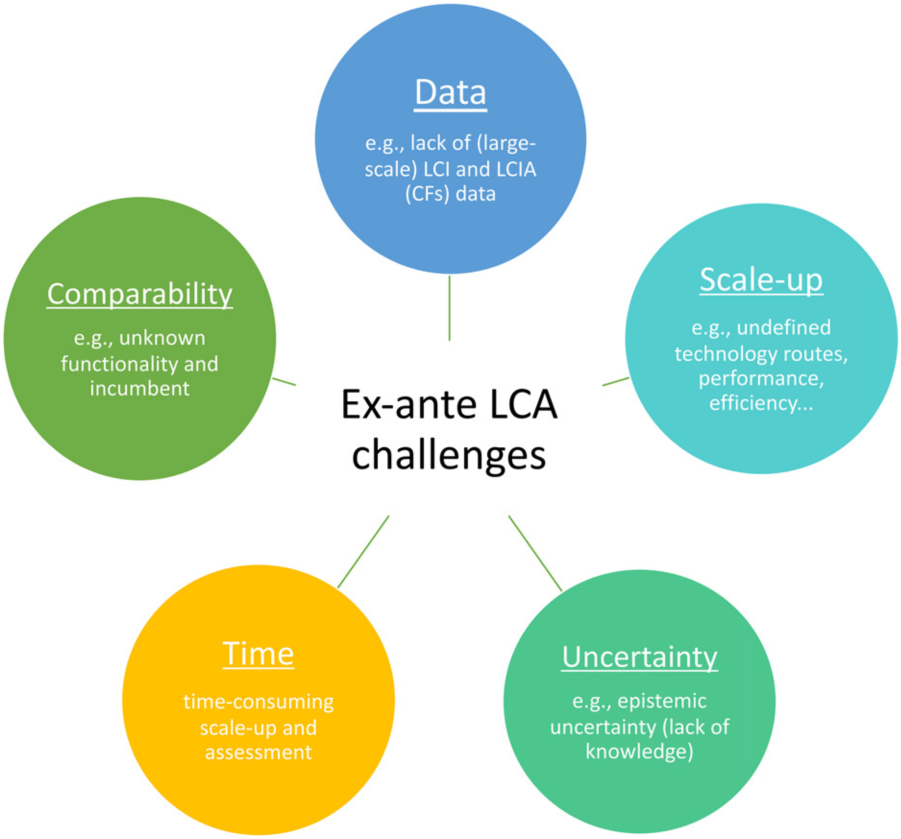


Fig. 5 Ex-ante LCA challenges (based on Hetherington *et al.* (2014); Moni *et al.* (2020); Thonemann *et al.* (2020).

(Arvidsson *et al.*, 2018; Cucurachi *et al.*, 2018; Miller and Keoleian, 2015). The challenges of ex-ante LCA can be aggregated into five clusters– data, scale-up, comparability, time, and uncertainty (**Fig. 5**).

Lack of Appropriate Data

R&D stages are characterized by scarce information, making it difficult to assess the life cycle impacts of a novel technology, as the data needed for the LCA may not yet exist. Data challenges include low data availability for new processes (often only at the lab scale), access to data (e.g., confidentiality), and data quality (Hetherington *et al.*, 2014).

The rapid pace of technological development hampers production data access (Cucurachi *et al.*, 2018) to build the LCI. The production, use, and disposal of novel products might lead to additional impacts unknown at present (Cucurachi *et al.*, 2018). Moreover, technology development outpaces characterization models, which may compromise the impact assessment since some substances and materials are not yet covered by LCIA methods (e.g., nanoparticles) (Hetherington *et al.*, 2014). Choosing impact categories for the novel technology can also be difficult, as the lack of experience (i.e., evidence from other LCA studies) prevents the identification of relevant impact categories (van der Giesen *et al.*, 2020).

Another related issue concerns the evolution of incumbent technologies and the background system. Background system refers to the components of a product system that lie beyond the direct influence of a specific decision maker, such as the developer of new technology (EC-JRC, 2010), and are usually modeled by using secondary data from LCI databases. As a new technology may take years or decades to reach industrial implementation, there will be background system changes (e.g., electricity mix), and this should be captured in the LCA (Hulst *et al.*, 2020; Mendoza Beltran *et al.*, 2020) to avoid a temporal mismatch between foreground (emerging, in development) and background systems (Arvidsson *et al.*, 2018; Thonemann *et al.*, 2020). This is significant as background processes typically account for approximately 99% of all unit processes within a product system (Wernet *et al.*, 2016). Likewise, the novel upscaled technology in the future should ideally be compared to the evolved incumbent technology (Cucurachi *et al.*, 2018), e.g., capturing potential incremental innovations (e.g., efficiency).

Scale-up Difficulties

Performing an ex-ante LCA requires modeling a large-scale (e.g., industrial) system from the small-scale information available at that stage, i.e., upscaling. **Table 2** characterizes different plant scales. The scale-up challenges lie in anticipating how unit processes,

Table 2 Characteristics of different plant scales from R&D to industrial production (based on Shibasaki *et al.*, 2006))

Scale	*Description*
Laboratory scale	Serves as a basis to determine chemical reaction behavior and detect the chemical magnitude of influence (e.g., molar ratio of the inputs, selectivity, yield), temperature, pressure, etc.
Mini plant	Serves as a replica of a future industrial plant approximately at the size of laboratory scale, including all process steps, inputs, and outputs based on the laboratory results to establish a technically transferable base (parameters).
Pilot plant	Serves as small chemical processing systems, operated to generate additional detailed information required to scale up to industrial plant and optimize process parameters.
Industrial plant	Economically viable and optimized commercial production is designed to maximize each machine's efficiency by utilizing its processing capacity, including process synergies.

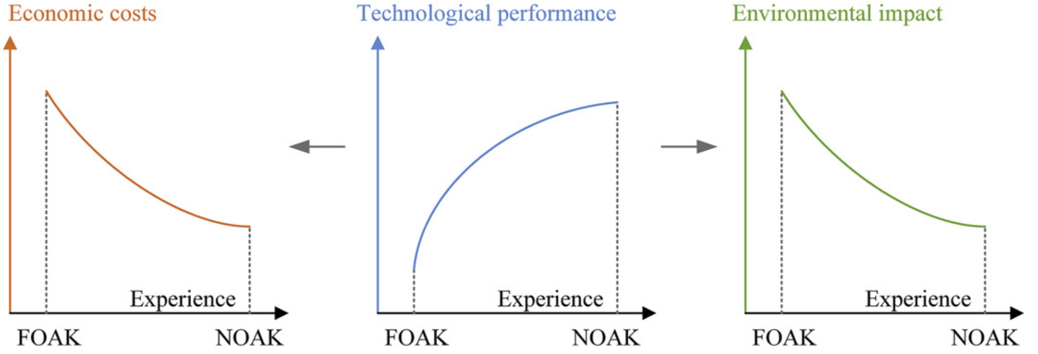


Fig. 6 Technology learning effects for technological performance, economic cost, and environmental impacts. From Thomassen *et al.* (2020). FOAK: First of a kind (new technology entering the market); NOAK: Nth of a kind (established technology).

material and energy consumption, and the performance of a novel technology will develop at a larger scale than what has been tested or produced (Blanco *et al.*, 2020; Maranghi and Brondi, 2020; Villares *et al.*, 2017).

Only laboratory- (lab) or pilot-scale information is often available for novel technologies. The main differences between pilot and industrial plants are capacity utilization and configuration. Contrarily to an industrial plant, the processing capacity may not be fully utilized in a pilot plant, resulting in a capacity utilization rate of less than 100 %. This underutilization can significantly impact the energy consumption of apparatus or plants with high energy requirements when they are in standby mode, starting up, shutting down, or idling (Shibasaki *et al.*, 2007). The differences between lab and industrial scales are even more diverse and significant (Maranghi *et al.*, 2020; Shibasaki *et al.*, 2007; Villares *et al.*, 2017):

- Employment of different materials and chemicals (e.g., reactants, solvents, etc.);
- Shift of energy source (e.g., from electricity to thermal energy);
- Change of processes, technologies, and equipment employed in the lab and industry;
- Lack of optimization and lower efficiency at lab equipment, contrarily to industry;
- Material and energy recovery (synergies) are little exploited in the lab but pursued in industrial facilities;
- Yield and productivity may increase from lab to industrial production;
- Batch processing is typical at lab scale, while continuous processing is common at industrial scale;
- Multiple outputs (e.g., co-products and by-products) are not well explored at initial lab experiments, but they are at the industrial level;
- With upscaling, emissions, waste, and wastewater may change qualitative and quantitatively;
- Plant design is simple at the lab scale but incorporates reuse, recycling, sanitary and other facilities at the industrial scale.

Although some used unmodified lab-scale LCI data (de Figueirêdo *et al.*, 2012; Leceta *et al.*, 2013), this has been found not to accurately represent a full-scale production (Hetherington *et al.*, 2014; Piccinno *et al.*, 2018a). Using lab or pilot data often overestimate the environmental burdens associated with the product, sometimes in the order of 90% (Gavankar *et al.*, 2015b; Müller-Carneiro *et al.*, 2023), and the relative contributions of inputs and processes can also change significantly (Pereira da Silva *et al.*, 2021; Piccinno *et al.*, 2016). The assumptions made in scale-up can greatly influence the environmental profile of a technology. It is crucial to have a comprehensive understanding of the technology and its materials and processes. Further, addressing multiple possible technological pathways may require applying scale-up scenarios (Blanco *et al.*, 2020).

Moreover, when the technology reaches TRL 9 and begins to be commercially implemented, there may be additional reductions to environmental impacts due to economies of scale and learning effects– i.e., the initial implementation of a production process tends to be less efficient compared to a well-established process that has been operational for several years (Thomassen *et al.*, 2020) (**Fig. 6**).

Box 1 Comparability of nano-enabled and existing technologies

Applying LCA to nano-enabled products is challenging because they may offer superior properties or performance not achievable by incumbent technologies for comparison (Pourzahedi and Eckelman, 2015) while potentially harming ecosystems and human health (Salieri *et al*., 2018).

For example, we may want to compare clothing (Walser *et al*., 2011) and food packaging (Motelica *et al*., 2020) incorporating silver nanoparticles (AgNP) with antimicrobial properties with existing products without AgNPs. In the case of clothing, the benefits of antimicrobial function could lead to a reduction in washing frequency, while in food packaging, this could lead to a decrease of food loss due to spoilage. However, these are difficult to estimate and uncertain without statistical data. While the toxicity effects associated with the use and end-of-life of AgNPs-enabled clothing appear to be only marginal (Walser *et al*., 2011), the health effects due to ingestion of AgNPs due to packaging migration are not fully known or accounted for in human toxicity LCIA categories (Bi *et al*., 2018; Istiqola and Syafiuddin, 2020).

Comparability Limitations

A possible goal for performing an LCA of a novel technology can be to benchmark its environmental performance against the incumbent technology. However, their comparison may be limited due to an inability to consider certain parts of the emerging system or to account for unknown or innovative functionalities (Cucurachi *et al*., 2018; Hetherington *et al*., 2014) (Box 1).

How a technology at low TRL will perform in a real application is unknown, and it may not be a one-to-one replacement of an existing one. Defining the function(s) and functional unit (FU) is not a trivial task– especially if dealing with a disruptive technology innovation (Cucurachi *et al*., 2018) or new functions. There may also not be an obvious incumbent technology to compare (van der Giesen *et al*., 2020). Further, the lack of information and uncertainty about life cycle stages (e.g., end-of-life) may hinder their inclusion in the model. However, excluding life cycle stages from comparative analyses can be misleading and give erroneous conclusions on which product to promote (Bergerson *et al*., 2020; Blanco *et al*., 2020; Hetherington *et al*., 2014; Thonemann *et al*., 2020).

Uncertainty

Uncertainty can be defined as "*any deviation from the unachievable ideal of completely deterministic knowledge of the relevant system*" (Walker *et al*., 2003). While all LCAs are under a certain degree of uncertainty, ex-ante LCA tends to be more uncertain than ex-post, as they rely on informed assumptions and qualified guesses about the future (Herrmann *et al*., 2014), making them subjected to a combination of uncertainties (Hetherington *et al*., 2014). While there are different classifications for uncertainty (Igos *et al*., 2019; Kwakkel *et al*., 2010; Walker *et al*., 2003), we will follow Cucurachi *et al*. (2022), who integrated the vast literature on this subject (**Fig. 7**).

Uncertainty can have two natures: Epistemic or ontic. Epistemic uncertainty arises from a lack of knowledge or understanding about a particular phenomenon or system, being particularly relevant for ex-ante and pLCA (Mendoza Beltran *et al*., 2020). It can be reduced through further investigation, research, or learning; however, this is only possible later in development. Ontic uncertainty is related to the natural variability of reality (e.g., biogenic cycles) and, therefore, cannot be reduced by additional research (Blanco *et al*., 2020; Igos *et al*., 2019; Spielmann *et al*., 2005). The location dimension of uncertainty relates to the LCA phase in which it manifests. Quantity uncertainty is quantifiable and related to parameters and inputs in LCI and LCIA (sometimes called parameter uncertainty). Model structure uncertainty corresponds to the mismatch between mathematical relationships and the reality of the system they describe (e.g., assumptions of linearity of consumption per reference flow, use of generic characterization factors not considering specific location, etc.). Context uncertainty (also called scenario uncertainty) relates to the methodological choices taken by the LCA analyst (e.g., functional unit, allocation, cut-off rules) (Igos *et al*., 2019; Lloyd and Ries, 2007). Moreover, the level dimension is related to the magnitude of the uncertainty – at best, shallow, and, at worst, recognized ignorance. **Table 3** shows examples of types of uncertainty for the four LCA phases, classified by the location and nature dimensions.

It is paramount to fully acknowledge and understand uncertainty and its sources in ex-ante LCA studies. If uncertainty is too great, results may become meaningless for product development, leading to poor environmental decisions and defeating the purpose of such studies. Moreover, it is imperative to be transparent and effective in communicating uncertainty to decision-makers to ensure the credibility of results and avoid biased interpretations from non-expert stakeholders (Gavankar *et al*., 2015a; Hetherington *et al*., 2014; Igos *et al*., 2019).

Time Required for Modeling and Assessment

Conducting an LCA is a time-consuming task, particularly ex-ante LCA, that requires additional modeling steps (e.g., scale-up and multiple scenarios). Building upscaled LCI models takes time, particularly when using process design and simulation software (e.g., Aspen Plus). It may require extensive research and expert engagement to understand all plausible scenarios (e.g., manufacturing processes and unit procedures to be implemented at future industrial facilities). This problem is exacerbated when applying LCA to support technology development decisions since timely decisions are required (Moni *et al*., 2020). A way to overcome this challenge is through streamlined LCA (Hung *et al*., 2020)– e.g., using a small number of impact categories, omitting

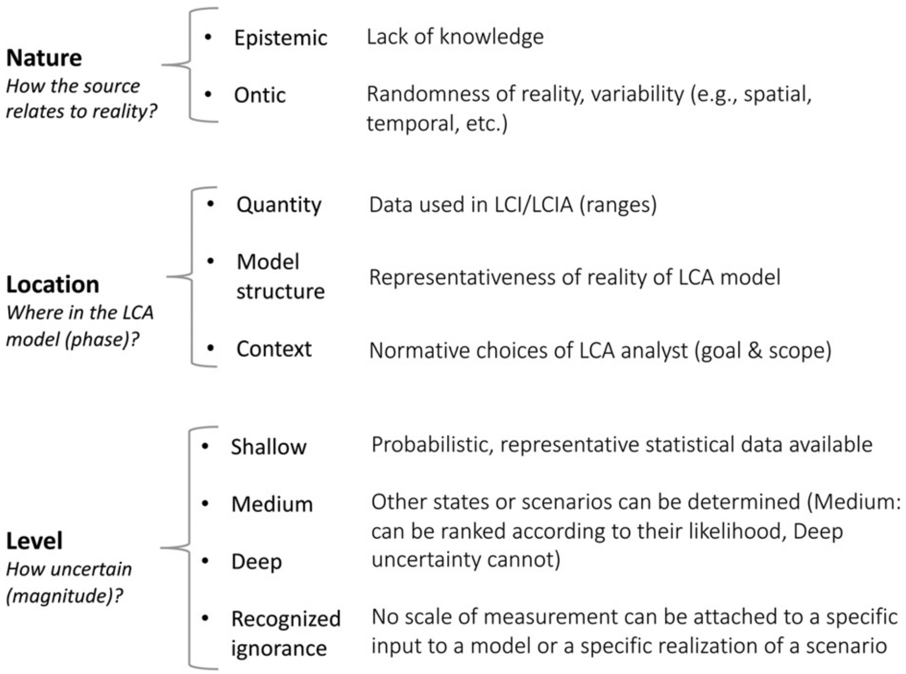


Fig. 7 Dimensions of uncertainty– nature, location, and level (based on Cucurachi *et al.* (2022); Kwakkel *et al.* (2010); Walker *et al.* (2003)).

Table 3 Examples of uncertainties in ex-ante LCA (modified from Blanco *et al.* (2020)).

LCA phase	*Uncertainty source*	*Location*	*Context in ex-ante LCA*
Goal & scope definition	Functional unit	Context	The technology may have a different purpose or application than initially projected, or it may offer additional functions
	System boundary; end-of-life	Context	End-of-life options (e.g., reuse, recycling) may develop after the technology has been deployed Waste management regulations may change over time
Life cycle inventory	Unit procedures	Context	Manufacturing techniques and processes routes may change as the technology moves from lab to industrial scale
	Flows	Quantity	Scale-up and process optimizations will likely lead to reduced or substituted material and energy input/output flows
	Allocation	Quantity	Parameters used for allocation might change (e.g., forecasted market prices for economic allocation)
Life cycle impact assessment	Characterization model	Model structure	New materials and substances may have unknown impact mechanisms and pathways
	Characterization model: fate	Quantity	Parameters that affect transport and fate of substances may change over time (e.g., temperature, rainfall)
	Characterization model: exposure	Quantity	Exposure-related parameters (e.g. population densities) may change along the assessment time horizon
	Characterization model: effect	Model structure	Marginal changes may result in exponentially larger effects as the baseline condition deteriorates (e.g., impact of increased radiative forcing on ecosystems)

parts of the system (e.g., downstream processes), using proxies, etc. However, it is necessary to balance time requirements and uncertainty caused by oversimplification (Moni *et al.*, 2020; Tsoy *et al.*, 2020).

Methodological Advances and Recommendations for Improved Practice

Several researchers have proposed methodological approaches and strategies for conducting ex-ante LCA of emerging technologies, arriving at some insights (Arvidsson *et al.*, 2018; Buyle *et al.*, 2019; Cucurachi *et al.*, 2022; van der Giesen *et al.*, 2020). These will be discussed in this section.

Goal and Scope Definition

In the goal and scope definition phase, several modeling aspects and assumptions are defined: the purpose of the study, data sources, system boundaries, functional unit, allocation procedures, scenarios, LCIA categories, and methods, among others (ISO, 2006b). Ex-ante LCA involves different goals and additional modeling elements to consider. Two general goals for conducting ex-ante LCA are: a) to compare the novel technology to an incumbent technology (established, usually at TRL 9/MRL 10), and b) to identify pathways for improving the new technology's environmental performance (Arvidsson *et al.*, 2018; Buyle *et al.*, 2019; Thonemann *et al.*, 2020; Cucurachi *et al.*, 2022). Concerning LCA scope, there are essential elements to consider, some of them familiar to standard LCA but vital in ex-ante studies (e.g., FU, allocation) and additional ones (e.g., TRL/MRL, reference year) (Arvidsson *et al.*, 2018; Gavankar *et al.*, 2015b; Thomassen *et al.*, 2019).

TRL, MRL, scale, temporal, and geographical considerations

When an ex-ante LCA aims to compare a novel technology to an incumbent, it is vital to consider the TRL, MRL, and production scale (e.g., annual production volume) and assumptions regarding the time horizon and geographical context (Gavankar *et al.*, 2015b; Hulst *et al.*, 2020). The TRL and MRL indicate how comparable the technologies are in maturity, efficiency, and optimization. Mature technologies benefit from economies of scale, energy and material efficiencies, and accumulated improvements due to years of experience (i.e., learning effects); hence, technologies are only fully comparable at TRL 9 and MRL 10 (Gavankar *et al.*, 2015b). Gavankar *et al.* (2015b) argued that ex-ante LCA results should be interpreted with their TRL/MRL, highlighting the need to standardize how the maturity level and (LCI) production scale are reported. Defining the assessment's time horizon (reference year) is also essential. The time horizon establishes a timeframe for when the technology is expected to achieve maturity, being crucial for background system modeling (Arvidsson *et al.*, 2018; Thonemann *et al.*, 2020). Further, for a future industrial system, where the production will take place may be unknown. Thus, explicit geographical boundaries should be defined (Cucurachi *et al.*, 2022; van der Giesen *et al.*, 2020) as they affect LCA results (e.g., regional and local impact categories).

Definition of the functional unit and system boundaries

Ensuring functional equivalence in LCA is paramount; hence, careful functional unit and system boundaries considerations must be taken. Hospido *et al.* (2010) recommended taking as a start the classification of product properties (Weidema, 2003) (Box 2) to define the FU and the incumbent technology to compare. The functional unit defined should include obligatory properties and, whenever feasible, positioning properties. Further, if positioning properties require additional specific functions, these should be treated as co-products using, for instance, system expansion.

Regarding the system boundary, it may be advisable to limit the scope of comparative analysis to the processes affected by changes in the production technique or innovation unless the product quality or material efficiency is affected (Hospido *et al.*, 2010). Some guidance is available for defining the FU and boundaries for bio-based technologies (Cucurachi *et al.*, 2022) and novel foods (Hospido *et al.*, 2010) that may inspire assumptions for other sectors. Further, testing various relevant FUs and boundaries is advised (Moni *et al.*, 2020).

Box 2 Product properties (based on Weidema, 2003)

- **Obligatory properties** are those that a product must have to be considered a relevant alternative.
- **Positioning properties** differentiate the product, making them more attractive to consumers than other products with the same obligatory properties.
- **Market-irrelevant properties** are the ones that do not influence consumer preferences.

Building the Life Cycle Model

Foreground system

In ex-ante studies, modeling the foreground system (parts of the system specific to the technology/products under investigation) consists of applying scale-up assumptions to better represent the future industrial system associated with a novel technology in order to assess its environmental performance.

The choice of scale-up approach should consider the time requirements, software availability, and uncertainty. Process-based methods (e.g., simulation) offer more accuracy of process data but are time-consuming and require process engineering expertise, while proxies are more agile and uncertain (Parvatker and Eckelman, 2019) (**Fig. 8**). Tsoy *et al.* (2020) discussed scale-up in ex-ante LCA in depth and proposed a decision tree for choosing a scale-up approach, considering the type of process/technology, data available, etc.

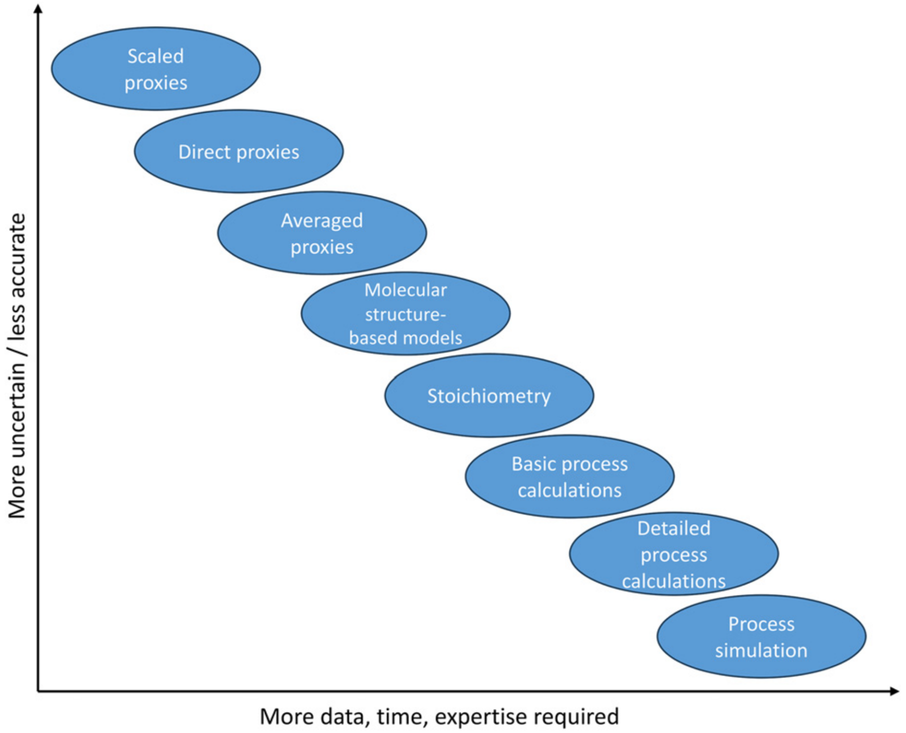


Fig. 8 Scale-up approaches for ex-ante LCA (based on (Milà i Canals *et al.*, 2011; Parvatker and Eckelman, 2019; Cucurachi *et al.*, 2022)).

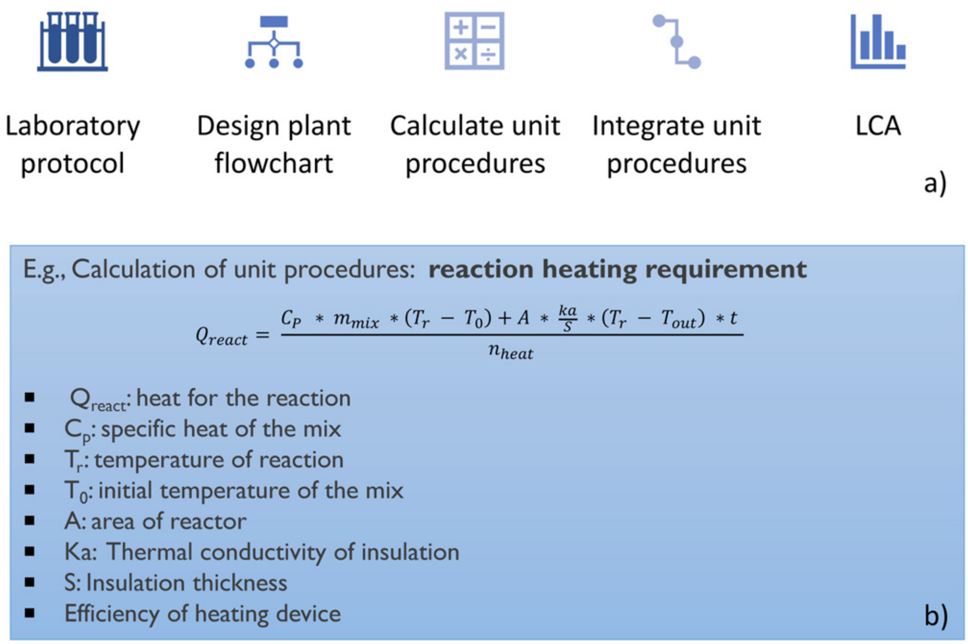


Fig. 9 Illustration of the scale-up method proposed by Piccinno *et al.* (2016); (a) Method steps; (b) Example of calculation of unit procedures (step 3).

Process calculation methods use engineering principles and thermodynamic equations to upscale unit procedures (Piccinno *et al.*, 2016; Sanjuán *et al.*, 2014). Piccinno *et al.* (2016) proposed a framework for upscaling chemical technologies at lab phases (**Fig. 9**), consisting mainly of calculating unit procedures and integrating them (e.g., including heat and solvent recovery, pumping, etc.).

Scaling and optimization factors have been applied as means of scale-up by estimating inputs and outputs reduction with increased production. A method for upscaling pilot-scale chemical processes was proposed (Shibasaki *et al.*, 2007, 2006) based on conducting a preliminary LCA at a pilot scale and applying optimization factors only to the unit processes with significant impacts.

Scaling laws have also been employed (Caduff *et al.*, 2011, 2014; Valsasina *et al.*, 2017), similar to conventional cost scaling (Baumann, 2018).

Other studies combined different upscaling approaches and mechanisms. Hulst *et al.* (2020) proposed a comprehensive framework covering several effects, such as process changes, size scaling, synergies, technology learning, and background system changes. Weyand *et al.* (2023) proposed a modular approach for building upscaling scenarios considering a range of upscaling mechanisms, such as equipment scaling and technology learning– which can be estimated by learning curves (Thomassen *et al.*, 2020). Simon *et al.* (2016) proposed a scale-up framework for novel technologies at a lab scale, by analyzing similarities, production conditions, and functions based on similar technologies. In addition, approaches have been proposed based on machine learning (Karka *et al.*, 2022), patent analysis techniques (Spreafico *et al.*, 2023), etc.

Multifunctionality and allocation procedures

Multifunctionality is a major LCA discussion topic (Ijassi *et al.*, 2021; Kyttä *et al.*, 2022; Schrijvers *et al.*, 2021). ISO 14044 (ISO, 2006b) defines that allocation should be avoided, if possible, by subdivision or system expansion. Otherwise, allocation by partition is necessary, using physical relationships (e.g., mass or energy) or other relationships (e.g., economic value). While economic value may better represent the causality of production and economic systems in some situations than mass (Kyttä *et al.*, 2022), prices do not yet exist for novel technologies. However, there are ways to circumvent this, such as using market estimates or minimum selling prices when available (de Assis *et al.*, 2017) or considering prices of similar products (Pereira da Silva *et al.*, 2021). Further, co-products often are not obtained or identified until later TRLs (Maranghi *et al.*, 2020). Assessing the influence of different allocation procedures using scenarios or sensitivity analysis is advised (Müller-Carneiro *et al.*, 2023; Saavedra del Oso *et al.*, 2023). Moreover, it is important to report and share information about the sensitivities that arise from allocation with the R&D team (Hetherington *et al.*, 2014).

Adapting the background model

The background system should be properly modified to avoid a temporal mismatch and consider changes outside the specific technology. This adaptation may be disregarded if these system components are believed to remain constant over the time horizon considered (e.g., shorter timeframes) or if time or computational limitations hamper modeling background systems in the future. It is recommended that ex-ante LCA outcomes are presented without the influence of background systems or that background and foreground systems impacts be reported separately to allow the results to be usable in different contexts. Further, it may be worth exploring multiple background scenarios, e.g., best- and worst-case scenarios (Arvidsson *et al.*, 2018; Thonemann *et al.*, 2020).

Tools based on Integrated Assessment Models (IAM) have been proposed to model future background developments by adapting LCI database processes to different future pathways. Mendoza Beltran *et al.* (2020) combined the Integrated Model to Assess the Global Environment (IMAGE) (Stehfest *et al.*, 2014) with the ecoinvent v3 database (Wernet *et al.*, 2016) by adapting activities in the electricity sectors based on the shared socio-economic pathways (SSPs). SSPs describe future societal and natural system trends globally and regionally through narrative storylines and quantified development measures (O'Neill *et al.*, 2017) (**Fig. 10**). Sacchi *et al.* (2022) presented a tool that streamlines the creation of prospective (background) inventory (pLCI) databases, enabling the integration of different IAMs into the LCI model. Further, Steubing and de Koning (2021) proposed the "superstructure approach" to facilitate the application of (background) scenarios in the Activity Browser software (Steubing *et al.*, 2020). IAM-based background scenarios have been used in prospective and ex-ante LCA (Ballal *et al.*, 2023;

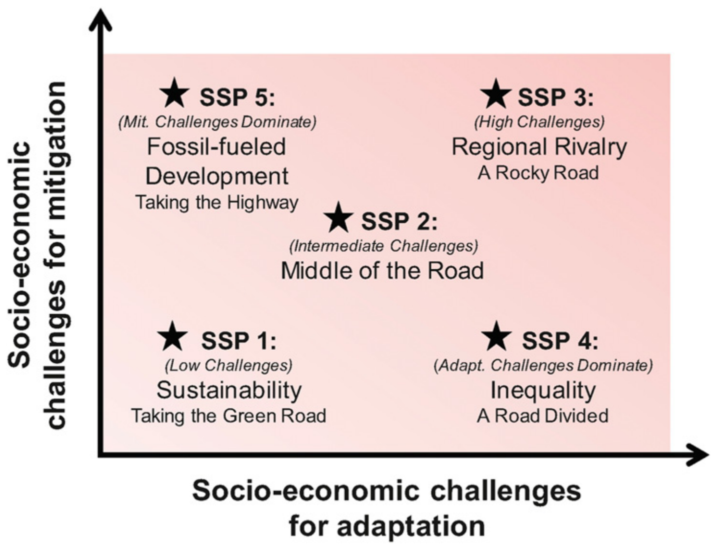


Fig. 10 Shared socio-economic pathways. From O'Neill *et al.* (2017).

Mendoza Beltran *et al.*, 2020; Saavedra del Oso *et al.*, 2023; Voglhuber-Slavinsky *et al.*, 2022). Furthermore, Steubing *et al.* (2023) discussed the obstacles and conditions for the broad adoption of pLCI databases by LCA practitioners (e.g., scientific integrity, usefulness, accessibility, usability).

Addressing external factors and market effects

There may also be relevant exogenous and indirect variables influencing future technology, which could significantly affect its environmental performance. Miller and Keoleian (2015) characterized intrinsic (e.g., resource criticality, functionality changes, infrastructure change), indirect (e.g., technology displacement, behavior change, rebound effects), and external (e.g., policy and regulatory changes, exogenous system effects) factors affecting emerging technologies. These authors qualitatively assessed the expected influence of the different factors in LCA results and the relative uncertainty surrounding these factors, which can help prioritize factors to include in scenario modeling. Cooper and Gutowski (2020) also addressed market factors at early commercialization, such as market diffusion, displacement of incumbent technologies, and rebound effects, proposing a modeling framework based on stakeholder engagement, learning curves, diffusion modeling, etc.

Scenario Building and Analysis

Definitions and scenario types

Scenarios have been widely used across many fields (e.g., policy development, planning, environmental impact assessment, climate science) (Börjeson *et al.*, 2006; Kosow and Gaßner, 2008; Spoerri *et al.*, 2009; Swart *et al.*, 2004). **Table 4** depicts some examples of scenario definitions.

Scenarios are built from visions of the future and specific questions. A classification of scenario types was introduced by Börjeson *et al.* (2006), associated with research questions closely related to ex-ante LCA (Cucurachi *et al.*, 2022):

- Predictive scenarios (how *will* the future develop?);
- Explorative scenarios (how *could* the future develop?);
- Normative scenarios (how *should* the future develop?).

Predictive scenarios deal with a likely future, explorative with plausible futures (scenarios funnel) and normative with a preferable future. Alternatively, Arvidsson *et al.* (2018) divided scenarios into predictive scenarios and scenario ranges, similar to explorative and the so-called cornerstone scenarios (Hospido *et al.*, 2010; Pesonen *et al.*, 2000), sometimes assessing best- and worst-case scenarios. Predictive scenarios are valid in cases where some developments are more likely than others; otherwise, explorative/scenario ranges are more appropriate (Arvidsson *et al.*, 2018; Langkau *et al.*, 2023).

Table 4 Examples of scenario analysis definitions

Scenario definitions
Scenarios are "hypothetical sequences of events constructed with the purpose of focusing attention on causal processes and decision points" (Kahn and Wiener, 1967)
"a narrative description of a consistent set of factors which define in a probabilistic sense alternative sets of future business conditions" (Huss, 1988)
"a description of a possible set of events that might reasonably take place. The main purpose of developing scenarios is to stimulate thinking about possible occurrences, assumptions relating these occurrences, possible opportunities and risks, and courses of action" (Jarke *et al.*, 1998)
"a description of a possible future situation, including the path of development leading to that situation. Scenarios are not intended to represent a full description of the future, but rather to highlight central elements of a possible future and to draw attention to the key factors that will drive future developments" (Kosow and Gaßner, 2008)

Fig. 11 Scenario creation steps (based on Börjeson *et al.* (2006)).

Scenario methodology and applications

Scenarios have been used in ex-ante LCA for different purposes, such as generating upscaling models (Weyand *et al.*, 2023), exploring future technology developments (Saavedra del Oso *et al.*, 2023), quantifying potential environmental improvement (Müller-Carneiro *et al.*, 2023), evaluating the (background) effects in different climate policies (Mendoza Beltran *et al.*, 2020), and so forth. Scenario analysis can also address model structure and context uncertainty (Cucurachi *et al.*, 2022; Igos *et al.*, 2019).

The majority of LCAs used scenarios in an intuitive, informal, and non-structured manner, with few exceptions, e.g., LCAs combined with formative scenario analysis (FSA) (Spielmann *et al.*, 2005) or general morphological analysis (GMA) (Delpierre *et al.*, 2021; Saavedra del Oso *et al.*, 2023). A generic scenario creation structure is illustrated in **Fig. 11**. Further, Bisinella *et al.* (2021) proposed a conceptual LCA scenario framework, incorporating previous scenario development methodology (Börjeson *et al.*, 2006; Ritchey, 2018).

Some general recommendations for using scenarios in ex-ante LCA are summarized as follows. Scenarios should be defined from the beginning of the ex-ante LCA study, in the goal and scope phase, considering the purpose of the study and research questions so that the models be structured accordingly (Cucurachi *et al.*, 2022; Langkau *et al.*, 2023). In addition, it is beneficial, when possible, to include probabilities of occurrence of each scenario to avoid misleading interpretations and limit the number of scenarios (Blanco *et al.*, 2020). Langkau *et al.* (2023) proposed a scenario-based modeling approach for pLCA focused on the goal and scope and LCI phases (**Fig. 12**). Additionally, an illustrative example of scenario building for a novel biopolymer is presented in Box 3.

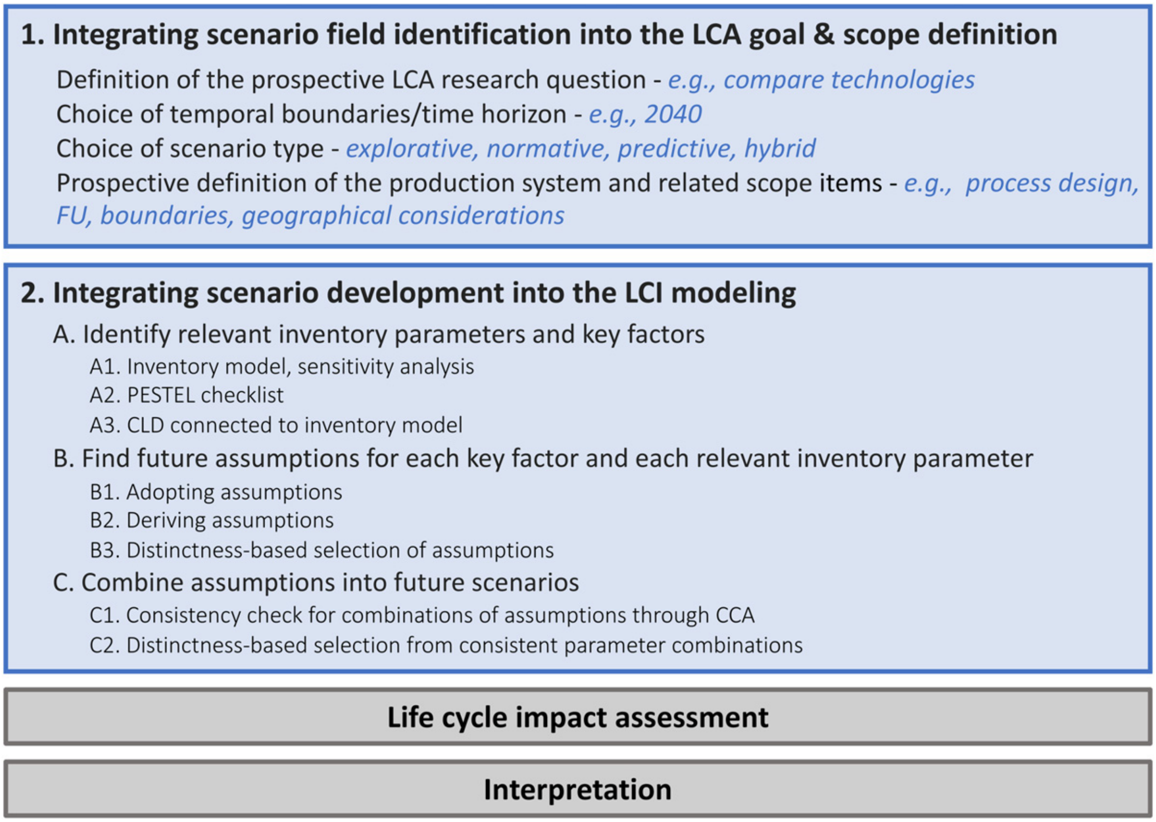


Fig. 12 SIMPL scenario approach for prospective LCA (based on Langkau *et al.* (2023)). PESTEL: Political, Economic, Sociological, Technological, Environmental, Legal; CLD: Causal loop diagram; CCA: Cross-consistency assessment.

Box 3 Scenario development for the case of nano-reinforced biopolymer based on mango processing waste

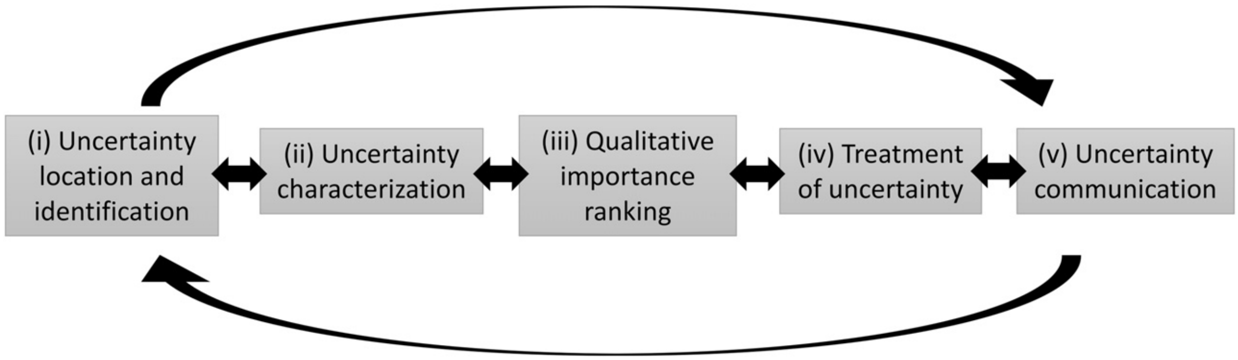
A pLCA scenario approach similar to Langkau *et al.* (2023) was proposed for bio-based technologies (Cucurachi *et al.*, 2022), and illustrated for a biopolymer film produced from mango seeds (waste) at a lab stage based on Müller-Carneiro *et al.* (2023). An ex-ante LCA was carried out to analyze the future impacts of producing the biopolymer, currently at **TRL 3** and expected to reach industrial production by **2040 (time horizon)**. An **initial LCI** was built at industrial scale using process calculations. PESTEL and Causal Loop Diagram tools were used to identify parameters influencing the product system. The following **parameters** were considered in the model, for which **sub-scenarios were built**: production scale (batch size), acid usage (with or without recovery), environmental policy (more or less ambitious), and share of renewables (lower or higher). The **background system** was adapted using the **Integrated Assessment Models** based on shared socio-economic pathways – **SSP2** (Middle of the road). Internally-consistent scenarios were built from the sub-scenarios by applying **CCA** and morphological fields. Finally, the LCI was refined, incorporating each scenario.

Life Cycle Impact Assessment

The impact assessment phase has received less attention in ex-ante and prospective LCA methodology. The development of impact assessment methodologies often falls behind the creation of new materials and emissions; thus, there may be a lack of characterization factors required for the LCIA (Moni *et al.*, 2020). Some works highlighted difficulties in assessing the impacts of nanomaterials and nanoparticles releases (Baumann and Arvidsson, 2021; Gavankar *et al.*, 2012), which are not yet fully covered by LCIA methods, although this has been investigated (Salieri *et al.*, 2019). Combining LCA with risk assessment (Arvidsson, 2015; Weyell *et al.*, 2020) or qualitative inferences (Gavankar *et al.*, 2012) was proposed to address this gap. Similarly, important impact categories to evaluate plastics (conventional and novel polymers) are missing in LCIA methods; for example, research is ongoing towards the development of marine litter impact categories (e.g., Lavoie *et al.*, 2021). Moreover, a framework for deciding on the inclusion of emerging impacts was proposed focusing on three impact categories (ecological light pollution, noise, and radiofrequency electromagnetic fields) (Cucurachi *et al.*, 2014).

Addressing Uncertainty

Addressing uncertainty is crucial in ex-ante LCA studies since novel technologies are subjected to increased uncertainty, particularly epistemic uncertainty (related to the lack of knowledge). A comprehensive stepwise approach was proposed by Cucurachi *et al.* (2022) (**Fig. 13**), suggesting a range of methods (e.g., global sensitivity analysis (GSA), correlation analysis, scenario analysis, etc.) for each uncertainty dimension (nature, location, quantity). Several studies addressed uncertainty in ex-ante and pLCA studies, e.g., applying GSA (Lacirignola *et al.*, 2017), probabilistic approaches (Cooper and Gutowski, 2020) combined with multi-criteria



(i) uncertainty location and indification by LCA phases		(ii) uncertainty characterization											(iii) ranking	(iv) method
		location			nature		level							
		quantity	model structure	context	ontic	epistemic	shallow uncertainty	medium uncertainty	deep uncertainty	recognized ignorance	→	uncertainty expression	high (1) to low (4)	
Goal & Scope:	technological representativness (CE, MAE1+2)			x		x		x			→	S	2	**Scenario analysis**
	representativeness of performance characteristics			x		x		x			→	S	3	Scenario analysis
	geographical representativeness (Sicily, IT)			x		x		x			→	S	1	**Scenario analysis**
LCI:	variability in orange juice production	x			x			x			→	V,S	1	**Scenario analysis**, Analytical resolution, **OAT**, KIA, MoEE
	representativeness of flows considered		x			x	x				→	S	4	Scenario analysis
	representativeness of BG processes used		x			x		x			→	S	3	Scenario analysis
	representativeness of data for FG processes used	x				x	x					P,F,V	1	**MCS**, advanced sampling, analytical resolution, fuzzy logic, hybrid approach, OAT, KIA, MoEE, **correlation analysis**, (e)FAST/Sobol
LCIA:	representativeness of CF	x				x	x				→	P,F,V	3	**MCS**, advanced sampling, analytical resolution, fuzzy logic, hybrid approach, OAT, KIA, MoEE, **correlation analysis**, (e)FAST/Sobol
	variability of each CF	x			x		x				→	P	3	**MCS**, advanced sampling, OAT, MoEE, **correlation analysis**, (e)FAST/Sobol

Fig. 13 Stepwise approach for uncertainty analysis illustrated for microwave-assisted extraction of pectin (based on Cucurachi *et al.* (2022)). P: probability distribution; V: variance; F: fuzzy sets; S: multiple scenarios; FG: foreground; BG: background; OAT: one-at-a-time; KIA: key issue analysis; MoEE: method of elementary effects; MCS: Monte Carlo sampling (MCS); (e)FAST: (extended) Fourier Amplitude Sensitivity.

decision (Ravikumar *et al.*, 2018) or scenario analysis (Blanco *et al.*, 2020). Moreover, a visual tool was proposed to support the communication of different types of uncertainties in LCA of emerging technologies to non-expert stakeholders, expressing uncertainty related to scenarios, modeling, variability, and lack of knowledge in an "uncertainty diamond" (Gavankar *et al.*, 2015a).

It should be noted that ex-ante LCA results should not be viewed as conclusive but exploratory (Villares *et al.*, 2017), especially at the earliest and more uncertain stages. LCA should be performed and adapted as technology develops and more information becomes available (Hetherington *et al.*, 2014). Further, dealing with uncertainty and building more robust models can be done by engaging with technology experts and stakeholders.

Stakeholder and Expert Engagement

Conducting ex-ante LCA may require knowledge and skills from different disciplines that an LCA analyst may lack. Hence, involving stakeholders and experts to guide model construction is crucial (van der Giesen *et al.*, 2020; Wender *et al.*, 2014) for the scale-up – which may require, e.g., process engineering expertise – and building plausible scenarios – e.g., informed by industrial and market experts. Responsive evaluation involves discussion and negotiation with different stakeholder groups to reach a consensus (Guba and Lincoln, 1989). Such practice can be challenging since it involves dealing with actors with contrasting views and biases. However, it can make ex-ante LCA more transparent and reliable and help deal with deep uncertainty (van der Giesen *et al.*, 2020). Moreover, LCA practitioners can provide insights to researchers, process design, and technology experts to guide the development of new technologies and processes (Maranghi *et al.*, 2020; Righi *et al.*, 2018); thus, a closer collaboration between different actors can be mutually beneficial.

Toward Ex-Ante Life Cycle Sustainability Assessment (LCSA)

Sustainability is characterized by three pillars: social, environmental, and economic (people, planet, and profit). Hence, LCA practitioners have sought to implement life cycle sustainability assessments (LCSA) combining (environmental) LCA, social LCA (sLCA), and life cycle costing (LCC) (Finkbeiner *et al.*, 2010; Kloepffer, 2008). Ex-ante analyses focused almost solely on the environmental and sometimes the economic dimension, with few exceptions (Keller *et al.*, 2015; Popien *et al.*, 2023). Environmental and economic evaluations were combined by integrating ex-ante LCA and techno-economic analysis (TEA) (Mahmud *et al.*, 2021; Thomassen *et al.*, 2019; Zimmermann *et al.*, 2020) or life cycle costing (LCC) (Röder *et al.*, 2022; Sauve *et al.*, 2023), or proposing eco-efficiency methods (Piccinno *et al.*, 2018b; Sauve *et al.*, 2023). The social dimension has received little attention and remains an untapped research opportunity.

Table 5 Summary of ex-ante LCA challenges and possible solutions

Challenges	*Insights*
How to define the functional unit?	Use the product properties classification (Weidema, 2003) to establish functional equivalence; Apply multiple FUs in sensitivity analyses
How to compare novel technology with the incumbent?	Make careful assumptions regarding the functional unit and system boundary, including sensitivity analyses; Interpret LCA results together with TRL/MRL and production scale
How to model a future industrial-scale system?	Apply scale-up approaches: simulation, process calculations, proxies, etc.; Use decision trees (Tsoy *et al.*, 2020; Cucurachi *et al.*, 2022) to decide on which approach to use; Use comprehensive approaches including different scaling mechanisms (e.g., Hulst *et al.*, 2020)
How to consider learning effects and market effects? (later stages/TRL)	Use learning curves based on similar technologies; Consider product substitution and cannibalization (Cooper and Gutowski, 2020); Prioritize effects to include in model using relevance/uncertainty quadrants (Miller and Keoleian, 2015)
How to build future scenarios?	Apply SIMPL approach (Langkau *et al.*, 2023) or other general (non-LCA) approaches (e.g., GMA); Use the Superstructure approach to facilitate computation in software (Steubing and de Koning, 2021)
How to adapt the background system?	Define assessment time horizon and apply integrated assessment methods (e.g., IMAGE, premise, etc.); Use the Superstructure approach (Steubing and de Koning, 2021)
How to include emerging impacts not covered by LCIA methods?	Apply Cucurachi *et al.* (2014) method to decide on the inclusion of emerging impacts; Combine LCA with other tools such as risk assessment or qualitative inferences (Gavankar *et al.*, 2012) for nano-impacts
How to deal with different types of uncertainty?	Identify uncertainty dimensions (location, quantity, nature) and apply the relevant method (e.g., probabilistic, multiple scenarios, GSA); Apply stepwise approach (Cucurachi *et al.*, 2022)
How to communicate uncertainty to study users and stakeholders?	Use visual tools such as the Uncertainty Diamond (Gavankar *et al.*, 2015a)
How to improve model robustness/representativeness?	Involve stakeholder/experts to guide assumptions and modeling (e.g., responsive evaluation technique)
How to include economic and/or social dimensions?	Integrate LCA with techno-economic assessment (TEA) or conduct eco-efficiency assessment; Include socio-economic indicators and/or health LCIA categories.

Summary

A summary of the challenges of conducting ex-ante LCA of novel and emerging technologies and the solutions proposed in the literature is depicted in Table 5.

Conclusions

Ex-ante LCA is crucial for anticipating hotspots from the early stages of R&D– when the potential for environmental improvement is maximized– and identifying sustainable pathways for developing emerging and novel technologies. However, ex-ante LCA encounters significant challenges related to data gaps, comparability with existing technologies, and uncertainty. The available tools to address these challenges increase the analyst workload, making LCA more time-consuming while requiring substantial and diverse technical expertise. While considerable progress has been made on process scale-up, scenario development, uncertainty analysis, and future LCI databases, little has been done regarding impact assessment methods for covering new substances and materials. Further, there is a lack of studies that systematically involve stakeholders to guide modeling, even though LCA researchers have strongly recommended it. LCA should be updated and improved iteratively as more information becomes available, involving different experts in this process. This way, ex-ante LCA shall support the development of low-footprint technologies.

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