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Prospective LCA methodology for Novel and Emerging Technologies for BIO-based products

The PLANET BIO project

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Abstract

To make the transition to a more sustainable bio-based economy, new technologies and products will have to be developed. Nevertheless, it is essential to ensure- at an early stage of development- that emerging technologies and products present a genuine decrease of environmental burdens to guide investment and technology deployment towards a sustainable economy. Life Cycle Assessment (LCA) is a methodology that is well suited to assess the environmental performance of technologies. Prospective LCA is a type of LCA, which is forward-looking in nature, namely which specifically looks at the future environmental impacts related to technologies and their products. The Prospective LCA for Novel and Emerging Technologies for BIO-based products (PLANET BIO) JRC project assessed the state-of-the-art for a selection of relevant topics towards developing a prospective LCA methodology to tackle the challenges arising when dealing with emerging bio-based products (BbP).

This report focus on key aspects related to goal and scope definition (section 2) and inventory analysis (section 3), covering as well the topic on biogenic carbon (section 4) and providing guidance on how to conduct scenario analysis (section 5) and uncertainty and sensitivity analysis (section 6). These suggestions can be complemented with existing EC guidelines, i.e. the Product Environmental Footprint (PEF) method, which is the European Commission recommended method to assess the life cycle environmental performance of products on the market (EC, 2021), in particular for the Life Cycle Impact Assessment and Interpretation.

The suggestions presented in this report should be further tested with case-studies in order to further develop guidelines for prospective LCA of BbP aiming at integrating such guidance and harmonize it with existing literature, approaches and standards. Additionally, the report highlights the importance of designing and using scenario techniques as part of the prospective LCA exercise. All decisions and details of scenarios should be transparently reported by the LCA analyst, and further guidelines are needed to support the analyst. Part of the value and learnings of a study can come from the development of scenarios together with involved stakeholders rather than only from the final LCA results.

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Authors’ contribution

Stefano Cucurachi, Bernhard Steubing, Carla Caldeira, and Serenella Sala conceptualized the research and the report.
Stefano Cucurachi, Flora Siebler, and Nicolas Navarre lead the writing of sections 2 and 3.
Nicolas Navarre and Bernhard Steubing lead the writing of sections 4 and 5.
Stefano Cucurachi and Flora Siebler lead the writing of section 6.
Carla Caldeira supervised and coordinated the scientific work as input to the report.

Executive Summary

Bioeconomy related innovations might play a significant role towards a more circular and decarbonized economy. Nevertheless, it is essential to ensure- at an early stage of development- that emerging biobased technologies and products present a genuine decrease of environmental burdens to guide investment and technology deployment towards a sustainable economy.

To ensure this, it is **key that such innovations are assessed in a comprehensive, harmonized, and consistent manner, covering the entire life cycle and multiple environmental burdens and unveiling trade-offs**. Against this backdrop, in the context of the JRC exploratory project "**Prospective Life Cycle Assessment for Novel and Emerging Technologies for BIO-based products - PLANET BIO"** we assessed the state-of-the-art for a selection of relevant topics towards developing a prospective LCA methodology to tackle the challenges arising when dealing with emerging bio-based products (BbP).

This report presents **suggestions on how to perform prospective LCA for BbP**, providing analysts with the necessary background knowledge, practical tools, and suggestions on how to approach some of the challenges that arise when conducting a prospective LCA. The proposed framework was tested with case studies that are used in specific sections to illustrate the application of the framework. The report was reviewed by experts and presented and discussed in a Community of Practice Workshop of the Knowledge Centre for Bioeconomy.

This report focus on key aspects related to goal and scope definition (section 2) and inventory analysis (section 3), covering as well the topic on biogenic carbon (section 4) and providing guidance on how to conduct scenario analysis (section 5) and uncertainty and sensitivity analysis (section 6). These **suggestions can be complemented with existing EC guidelines, i.e. the Product Environmental Footprint (PEF) method** (EC, 2021), which is the European Commission recommended method to assess the life cycle environmental performance of products on the market, in particular for the Life Cycle Impact Assessment and Interpretation.

Goal and scope (section 2)

When evaluating a future product system, the number of possible outcomes can be overwhelming and it is challenging to evaluate them all. By defining the research question or the goal and scope of the study, the possible future scenarios can already be narrowed down. However, sometimes it can be difficult to define, for example, the functional unit, especially for technologies that are still at an early stage of development. Questions such as "When will the technology be mature? How can I compare it to the existing technology? Do I need to change my functional unit for BbP to be able to compare them?" are addressed in this section.

Life Cycle Inventory (section 3)

This section is dedicated to the life cycle inventory and how best to approach upscaling of unit processes in the foreground and background, which is one of the bigger challenges in prospective LCA. An important issue for BbP is also how to allocate processes with multiple product streams and how to appropriately define the system boundary. Both topics are covered in this chapter and guidance is given on how to find suitable solutions. This section is intended as a companion to the practitioner assessing emerging bio-based technologies. We refer the reader looking for a methodological discussion on specific aspects to the relevant expert literature. We also further refer the reader to section 4, in which methods of scenario development are described.

Biogenic carbon (section 4)

In this section, we first provide an overview on the key issues related to biogenic carbon accounting and then present how these issues are dealt with in scientific literature and in relevant standards. Finally, we briefly discuss the implications for accounting for biogenic carbon in the context of prospective LCA.

Scenario methodology (section 5)

The use of scenarios is essential in prospective. Prospective LCA is fundamentally about the potential development of product systems in the future. Since it is generally impossible to predict the future development of complex systems, such as those systems into which technologies are embedded, the only viable approach to assess anything in the future is to develop scenarios. In this section we propose a scenario methodology that applies to all prospective LCA studies, including ex-ante studies.

Uncertainty and sensitivity analysis (section 6)

In this section of the report, we zoom in onto the modelling of uncertainty analysis (UA) and sensitivity analysis (SA) for BbP at low Technology Readiness Levels, with a focus on how to model uncertainty and on how to characterize uncertain data in LCA models. While both UA and SA are recommended at the life cycle interpretation step, they are rooted in all other life cycle assessment phases. We propose a stepwise approach, which guides the analyst using prospective LCA to locate uncertain inputs across LCA phases, characterize uncertainty, qualitatively assess important sources of uncertainty, quantitative treat uncertainty with UA and SA, and finally communicate the qualified and quantified uncertainty in the results.

Outlook

This report presents inputs for the development of a prospective LCA methodology for BbP. These suggestions should be tested with case-studies in order to further develop guidelines for prospective LCA of BbP aiming at integrating such guidance and harmonize it with existing literature, approaches, and standards. Additionally, the report highlights the importance of designing and using scenario techniques as part of the prospective LCA exercise. All decisions and details of scenarios should be transparently reported by the LCA analyst, and further guidelines are needed to support the analyst. Part of the value and learnings of a study can come from the development of scenarios together with involved stakeholders rather than only from the final LCA results.

1 Introduction

The general procedure of life cycle assessment (LCA) is well known, standardized (ISO-14040, 2006; ISO-14044, 2006) and additionally supported by numerous handbooks and published guidelines. In most cases, the focus of LCA studies is on already existing products or services with an established life-cycle. We can broadly define as prospective LCA, on the other hand, all LCA studies that are forward-looking in nature. A subset of LCA studies and methodologies are further defined as ex-ante LCA, in particular when they aim to assess the impacts of product and service systems that are at an early development state, not commercialised yet, and are still emerging (Cucurachi et al., 2018). In this report, we use prospective LCA whenever we refer to any forward-looking LCA study, and use ex-ante LCA whenever we are specifically addressing the challenges of LCA applied to emerging technologies in evolution from the lab- to commercial scale.

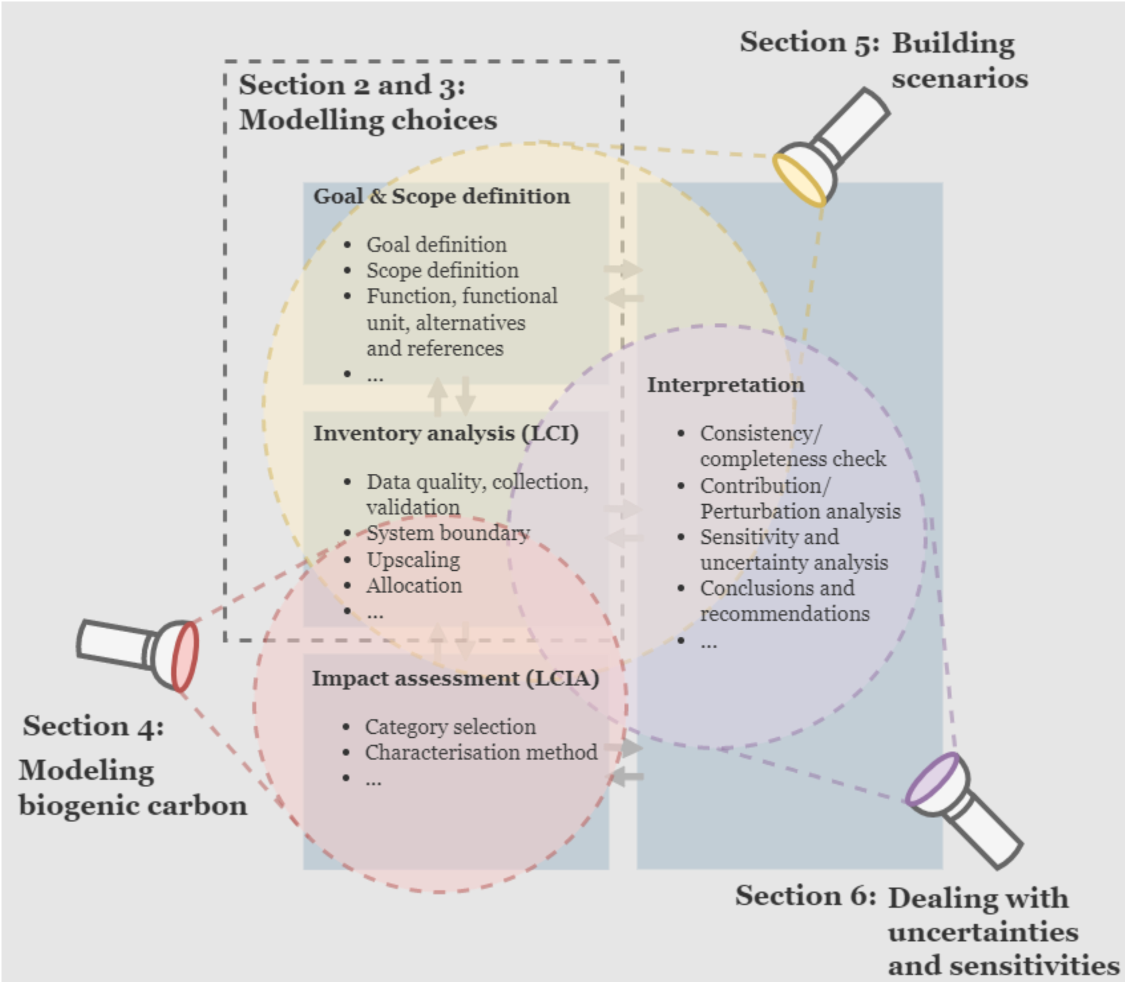
Recently, several comprehensive sets of guidelines and frameworks have been published to guide prospective and ex-ante LCA analysts (we further refer the reader to the work of Arvidsson et al., 2017; Cucurachi et al., 2018; van der Giesen et al., 2020; van der Hulst et al., 2020). Although such guidelines and frameworks have already been addressing some of the challenges of prospective LCA, some aspects are especially relevant when dealing with bio-based systems.

The aim of the report is to support decision-making for sustainability on bio-based systems, since the European Union is aiming for a strong bioeconomy with a shifted focus from fossil to bio-based resources. In spite of the increased attention and focus, the environmental impacts of bio-based emerging innovations have yet to be assessed. Such assessment should ideally happen pre-emptively to avoid costly lock-ins and unexpected environmental burdens. This report highlights some of the key challenges in the prospective and ex-ante LCA of bio-based products (BbP, hereafter; see Figure 1). The purpose of this report is not to provide a standardized recipe for pLCA of BBps. Instead, the purpose is to provide a compilation of selected state-of-the-art approaches from the scientific frontier, which may well be used in the future to discuss and derive more standardized ways to perform prospective LCA.

The report addresses specific aspects related to prospective LCA of BbPs for all 4 phases of an LCA, as shown in Figure 1. The highlighted sections complement existing standards, books and frameworks by filling their gaps, with a focus, when relevant, on the assessment of BbPs. In some sections, parts of the general LCA framework are repeated to increase overall readability. Figure 1 summarizes graphically how sections 2-6 of this document interact in relation to the general LCA phases. These sections are intended to shed light on gaps in latest prospective/ex-ante LCA frameworks and always include a state-of-the-art section and are concluded with an individual BbP case study to present new findings and explain possible courses of action.

In section 2 we focus on goal and scope definition and in section 3 on the LCI for BbP and how best to approach upscaling of unit processes in the foreground and background, which is one of the bigger challenges in prospective LCA.. The focus on these stages is intended to facilitate the approach to the first two LCA phases and to help define the overall modelling decisions. We than discuss in section 4, why it is important to handle biogenic carbon, what relevant standards and scientific papers recommend and how issues pertaining to biogenic carbon could be treated in the context of prospective LCA. Section 5 deals with scenario development, which is necessary step for prospective LCA studies. A comprehensive methodology for building transparent future scenarios is presented to encourage the analyst to think about all future possibilities, find the connection of all relevant parameters and link them to LCI. This methodology makes it possible to also include qualitative parameters in order to create complete scenario storylines for prospective LCAs. We focus in section 6 on performing uncertainty and sensitivity analysis to understand the reliability of the results of prospective/ex-ante LCA studies. This section highlights the different uncertainty and sensitivity semantics and definitions, which treatment methods have been developed so far and provides a framework to determine which type of treatment method is applicable for the identified uncertainties.

Figure 1. Important prospective/ex-ante LCA aspects and challenges for bio-based products. This graphic illustrates how the different sections of this document interact in relation to the general LCA phases and which part they mainly highlight



Scenario analysis is a good example to highlight the interconnectedness of different LCA phases. While it is an important method to approach goal and scope and LCI for prospective LCA, but it is also a method to treat uncertainties in the interpretation phase. If an analyst follows strictly LCA phases 1-4, the uncertainty treatment via scenario analysis in phase 4 can be seen as a refinement of the initial LCA set-up and calculations. Nevertheless, if an analyst is already aware of the sensitivity of certain parameters they can be included from the start. After all, LCA is an iterative process.

One aspect that is frequently discussed in the LCA community is that of attributional versus consequential LCA. Both modes of LCA differ fundamentally in the underlying research question. A typical attributional LCA question is: “what are the environmental impacts associated with product X”, while a typical consequential LCA question is: “what are the environmental impacts associated with a change in the consumption of product X”. Both types of questions can be asked in a future context, and therefore, prospective LCA can be conducted in either mode. In this report, we do not specifically provide recommendations for attributional or consequential LCA, but believe instead that the presented approaches could be applied to either type of study.

We hope to shed light with this document on important topics related to prospective LCA for BbP in order to provide analysts with the necessary background knowledge, practical tools, or at least and inspiration on how to approach some of the challenges that arise when conducting a prospective LCA.

2 Goal and Scope definition

When evaluating a future product system, the number of possible outcomes can be overwhelming and it is challenging to evaluate them all. By defining the research question or the goal and scope of the study, the possible future scenarios can already be narrowed down. However, sometimes it can be difficult to define, for example, the functional unit, especially for technologies that are still at an early stage of development. Questions such as" When will the technology be mature?, How can I compare it to the existing technology?, Do I need to change my functional unit for bio-based products to be able to compare them?" are addressed in this section.

2.1 Goal

Developing a clear research objective that defines the goal of the analysis is the first decision analysts need to make when attempting any LCA study. The objective of an ex-ante LCA is to quantify the future environmental impacts of an emerging technology (Moni et al., 2020), however, the analysis can be comparative or non-comparative and can be conducted with an output-, feedstock- or land-oriented perspective (Ahlgren et al., 2015). In comparative analyses, the emerging technology is frequently compared to an existing technology, defined as the system in the technology landscape that performs a similar function as the emerging technology (van der Giesen et al., 2020).

Depending on the technology readiness level (TRL) of the emerging technology, the expected delay to industrial production should be formulated within the goal (Moni et al., 2020). In the case of low TRL levels (1-4), the system is considered in the conceptual development phase and thus extensive process changes are expected due to furthered research developments (Gavankar, Suh, et al., 2015; Rivera-Tinoco et al., 2012). These so called lab-scale LCAs have the potential to identify hotspots in early phases of development (Pallas et al., 2020). At higher TRLs (TRL > 5), system synergies, such as waste recovery or energy recycling, can be included to further optimize the system (van der Hulst et al., 2020).

2.2 Geographic and temporal considerations

The impacts of incumbent industrial scale technologies are also expected to change over time (Cucurachi et al., 2019). Such technologies benefit from learning and are subject to changing systems, therefore accounting for the temporal developments of both the bio-innovation and its incumbent is paramount to providing a valid comparison (see also sub-section 5.2.1). These factors, such as advances in plant breeding and agronomic practices, have a large influence on the future availability and composition of the feedstocks and play a crucial role in developing a relevant life cycle inventory (Saxe et al., 2020). Future production volumes and conditions for crop growth may geographically shift over time, while growing seasons may be shortened or interrupted by more frequent natural hazards such as droughts or floods (Del Pilar Jiménez-Donaire et al., 2020; Jayarathna et al., 2020) or also extended (e.g. in Europe; Han et al., 2018; Menzel and Fabian, 1999). For example, in the past 50 years, over 300 million hectares of agricultural land have succumbed to desertification caused by changing rainfall patterns in northern China, significantly reducing the regions biomass output (Goudie, 2019). But not only the volume growth is affected by extended growing seasons and atmospheric fertilization by Nitrogen compounds and CO_2, but also material inherent characteristics, like wood density (Pretzsch et al., 2018). In addition to the **temporal context**, the **geographical context** affects the impacts associated with water demand and availability, electricity use, and land use (Cucurachi et al., 2019). Also the production process of the feedstock (e.g. conventional vs. regenerative agriculture) and whether the land or the biomass competes with other applications or products respectively (e.g. using crop for biopolymer instead of food) should be addressed. Sencan and Escriva-bou (2020) found that diverse climate conditions caused emissions to vary between farms producing similar products at different locations. The availability of different feedstock types also varies geographically, spatially limiting the relevance of certain feedstocks (Cherubini and Strømman, 2011). The relevance of certain raw materials, especially those that were previously waste or side streams, also depends on whether they can meet the necessary demand when the production process is scaled up.

Therefore, analysts must identify a geographical and temporal context, which is relevant for to the BbP assessed**.**

2.3 Functional unit

Once the objective of the study is clearly defined, a functional unit can be developed. For LCAs of bio-based products, the objective of the analysis and the characteristic of the biomass feedstock each play a key role in formulating a representative functional unit in order to report relevant LCA results of the system (Wiloso and Heijungs, 2013). In the case of LCAs of BbP, there are three main functional unit types: (1) output-based, (2) feedstock-based, (3) land-based summarized in Table 1. Feedstock- and land-based functional units are derivatives of input-based functional units, however we separate the input-based functional units as selecting the correct option is dependent on the feedstock characteristic.

Bio-based feedstocks can be categorized into four categories:

(1) dedicated biomass, sourced from agriculture, forestry and aquaculture, among others, and are grown with the intent of creating a predetermined product (Gabrielle et al., 2018)

(2) co-products, value-added products in addition to the primary product of a dedicated biomass (e.g. essential oils from citrus production).

(3) residues from dedicated biomass which have no current value-added or are sourced from non-edible biomasses, and

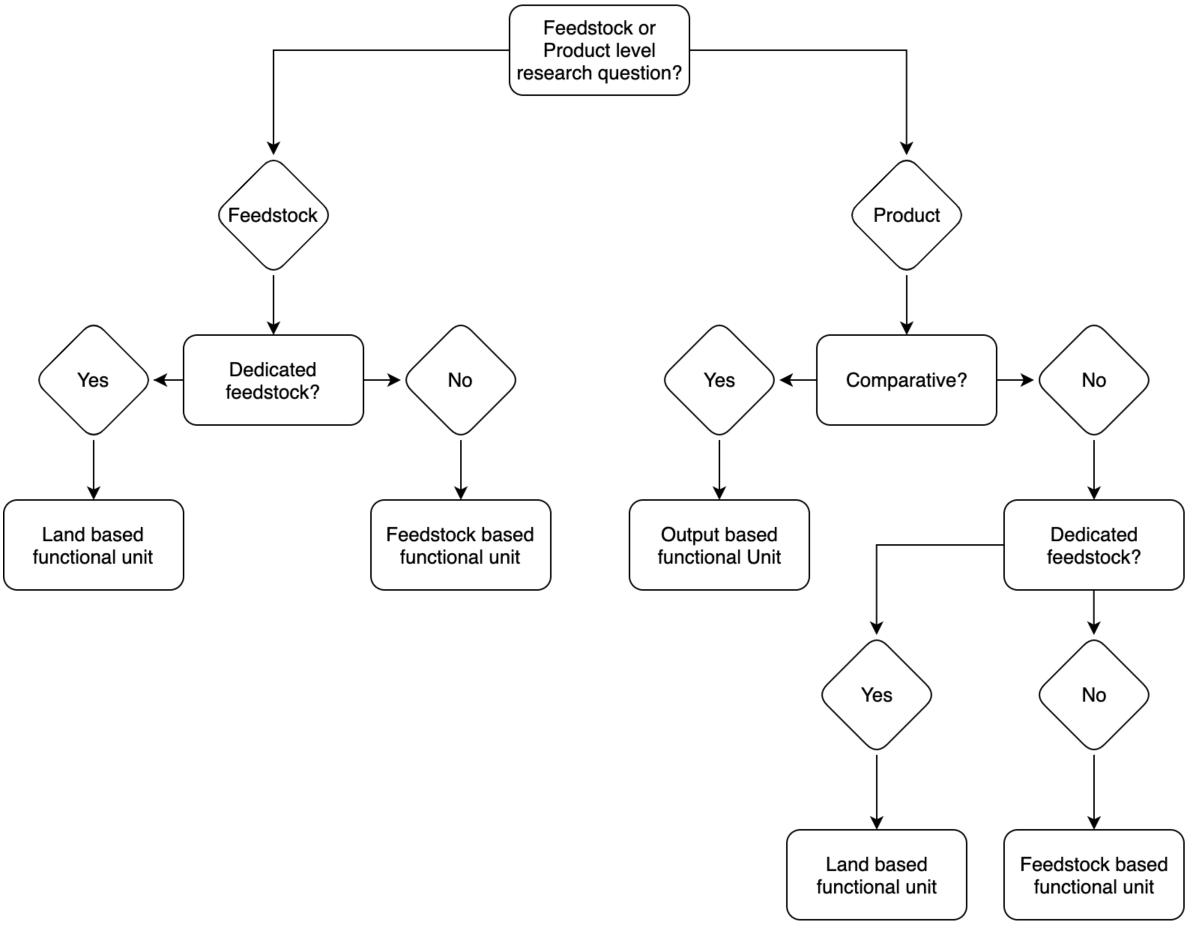
(4) wastes. have a disposal cost associated to their treatment (e.g. municipal solid waste).

Table 1. Functional unit types for bio-based systems (adapted from Ahlgren et al., 2015; Cherubini and Strømman, 2011)

Functional Unit Type	**Example of functional unit**	**Focus of Research**
output-based	1 kg product (e.g. 1 MJ electricity)	Novel technology, attempting to compare best feedstock to produce a product (useful for comparing incumbent vs novel technology) or to compare BbP with non-BbP to calculate substitution resp. climate mitigation effects
feedstock-based	1 ton biomass	Novel use of feedstock, attempting to compare best use of biomass feedstock
land-based	1 hectare	Novel use of land, attempting to compare best use of agricultural land

In the case of non-dedicated feedstocks (types 2, 3, and 4; e.g. citrus peels from juice production to produce pectin), future production volumes of the innovation may scale beyond the feedstock's availability as a co-product, residue or waste, and would thus require dedicated production to satisfy the remaining demand (e.g. adapt the citrus plant to maximize for peel production). It is therefore possible for an innovation's feedstock to be categorized as both a **dedicated and non-dedicated feedstock** depending on the temporal and geographic context previously established. A more detailed discussion about feedstock and co-product availability for LCAs of BbPs can be found in Hillman and Sandén (2008).

Figure 2. Decision tree to select the functional unit of bio-based products (see also Table 1)



For feedstock level analyses which aim to identify the best use of finite bio-based resources, feedstock-based functional units should be used (Figure 2 left path). In cases where a dedicated feedstock is required, land-based functional units should be used. By utilizing a functional unit derived from the inputs (feedstock or land), analysts can compare a broad range of applications of the feedstock (Ahlgren et al., 2015). **For example, to compare the greenhouse gas savings of using residual biomass for electricity production versus the production of biofuels for transportation, feedstock-based functional units provide the relevant insights into the impacts associated for each end product**. If the feedstock is dedicated biomass, the land used to grow the feedstock behaves as the de facto feedstock of the system while the biomass becomes the product. As land can be used for food, feed, and other crops, identifying the best use of the land is a crucial long term decision also in respect to the demand of the product which must be addressed to ensure an environmentally optimal use of dedicated feedstocks (Cherubini and Strømman, 2011).

If the analysis is oriented towards a product level assessment (Figure 2 right path), output based functional units are needed if the analysis is comparative. This functional unit allows for a direct comparison of the product or function of an emerging technology with an existing technology (or another emerging technology) based on their common output (Ahlgren et al., 2015). For example, evaluating the impacts of plastics sourced from bio-based sources compared to petrochemical sources. In such studies, the emerging technology has a clear conventional reference product it is attempting to replace, therefore focusing the analysis on a single output is reasonable. The output-based functional unit should be chosen in a way that guarantees that the performance in fulfilling the same functionality is the same. Let us consider the example of a bio-based application compared with a fossil one: 1 m^2 of PLA packaging film may have a different thickness of 1 m^2 of PP packaging film to have e.g. the same stiffness. Or even for the same thickness, the density of the two polymers is different, so we should not compare 1 kg of PP with 1 kg of PLA because to fulfil the same function (e.g. the same application - a cup or a bottle), the masses of the two products might be significantly different.

However, achieving the exactly same function in prospective LCAs is a good ambition and should always be aimed for, but can be quite difficult in practice (Hetherington et al., 2014). In assessments of emerging products with no clear incumbent, the final function of the technology may be difficult to narrow down to a single product. In such cases, feedstock-based functional units are most useful as they can be used to provide insights into the impacts of utilizing the feedstock regardless of the final product application. The flexibility of this approach is useful in the case of ex-ante analyses because the functions of technologies at low TRLs can change throughout the scaling process (Moni et al., 2020). Dedicated feedstocks of non-comparative analyses should again utilize land-based functional units to account for the fact that land is a limited resource and behaves as the system feedstock (Cherubini and Strømman, 2011). We refer the reader to Box 1 below for an illustrative example.

Box 1. Case study: Prospective LCA of waste-to-PHA biorefinery

Case study: Prospective LCA of waste-to-PHA biorefinery

Polyhydroxyalkanoates (PHA) are biobased and biodegradable polymers with multiple applications. PHA still have a reduced market share due to their high production cost. Previous LCA studies reported feedstock production, fermentation and downstream processing as the main hotspots within the PHA value chain. PHA production from carbon-rich waste streams by mixed microbial cultures (MMC) can diminish both environmental impacts and production costs. However, these processes are still at low technology readiness level (TRL 5-6). However, these processes are still at low technology readiness level (TRL 5-6). The goal of the study is to quantify the environmental impacts of the waste-to-PHA biorefinery in a future framework when its large-scale production is already implemented. Therefore, by evaluating its environmental performance, it is possible to identify the environmental hotspots and provide environmental guidance to the developers (Saavedra del Oso, et al., in prep).

As the system function is to produce PHA from complex organic wastes, the functional unit (FU) was defined as 1 kg of PHA powder. And, therefore, a cradle-to-gate approach covering all the unit processes within the waste-to-PHA biorefinery is defined (Figure 1), including within the system boundaries the PHA production (i.e. anerobic fermentation, VFA separation, PHA enrichment, accumulation and downstream processing) and the further energy valorization of the residual intermediate streams by anaerobic digestion (AD) and cogeneration unit plant (CHP).

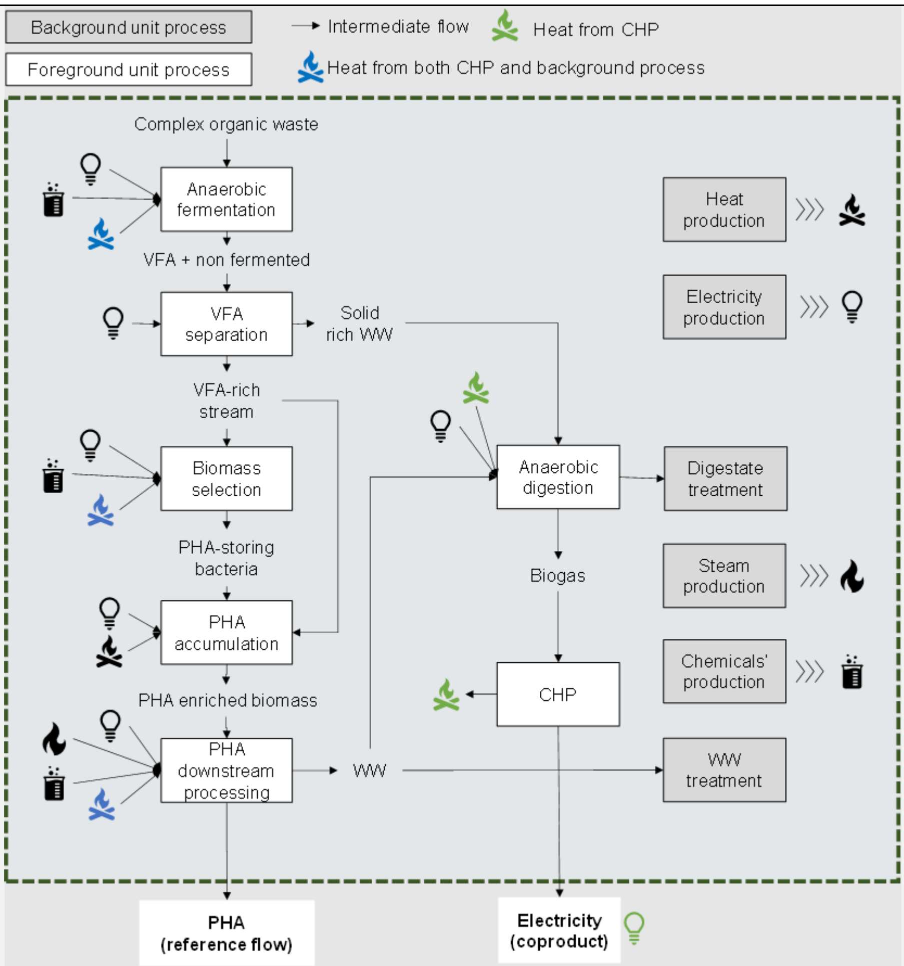


Figure 1. Waste-to-PHA biorefinery system boundaries.

The multifunctionality of the system was addressed by allocating the environmental burdens in VFA separation and in CHP to PHA and electricity production, respectively. This choice was made following the guidelines developed for the Joint Research Center on the LCA of alternative feedstock for plastics production.

Given the current technology readiness level (TRL), i.e., from 5 to 6, the temporal boundaries were established in 2030, when the market level maturity is expected to be reached. An explorative scenario approach was followed with the aim of envisioning how the PHA production by MMC could develop. The foreground system was modelled based on the technology analysis and using an upscaling framework for emerging technologies. For the background system, a futurized version of the ecoinvent 3.7.1 database was used, which includes scenario data derived from the IMAGE integrated assessment model. The latter model's global future scenarios are based on the Shared Socio-Economic Pathway (SSP) scenarios and representative concentration pathways. Two scenarios, the SSP2-base and the SSP2-RCP2.6 scenarios were derived here via the PREMISE framework. Both scenarios represent the SSP "middle of the road", however, they differ substantially in terms of climate change mitigation: in the SSP-base scenario a warming of 3.5 °C is modelled by 2100, while in the SSP2-RCP2.6 the temperature increase is limited to just below 2°C. The foreground scenarios were modelled against the background scenarios using the superstructure approach as implemented in the open source LCA software Activity Browser was employed.

The analysis of the environmental impacts followed a midpoint approach, being climate change (GWP), terrestrial acidification (TAP100), freshwater eutrophication (FEP), human toxicity (HTPinf), freshwater ecotoxicity (FETPinf) and fossil depletion (FDP) the selected impact categories, according to the latest reviewed LCAs on PHA production. The impacts categories were assessed using the Hierarchist ReCiPe (H) v1.13.

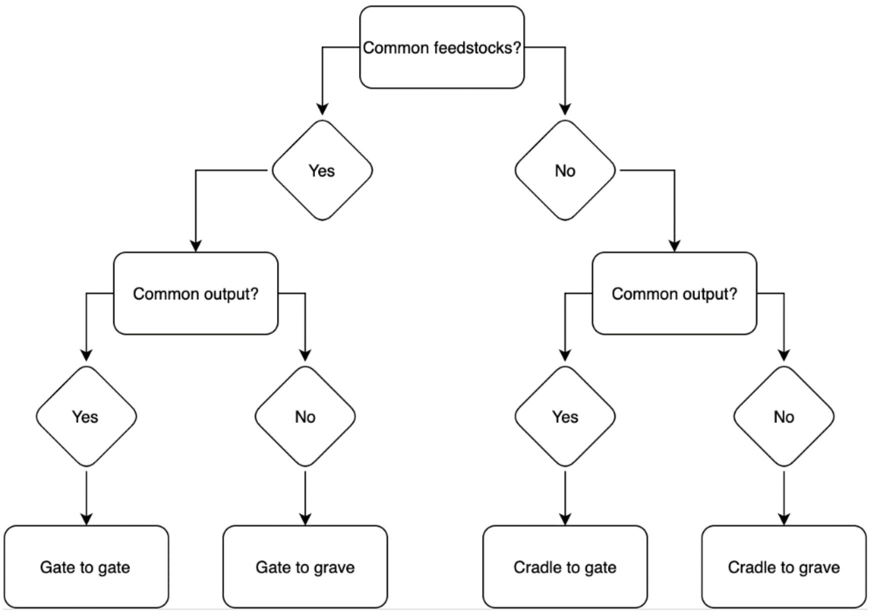
2.4 System boundary

The scope of the ex-ante LCA must then be established to avoid the omission of potential system hotspots (Katakojwala and Mohan, 2021). The system boundary and cut-off criteria are determined in this step (van der Giesen et al., 2020).

The nature of the system feedstock is a critical consideration when establishing the system boundary (Bernstad Saraiva Schott et al., 2016). In the case of dedicated biomass, the scope of the ex-ante LCA must include all activities pertaining to the production of the feedstock (Bernstad Saraiva, 2017). However, in the case of waste feedstocks, the system boundary is less clear. Historically, LCA analysts have adopted the 'zero-burden assumption' (Finnveden, 1999; Bernstad Saraiva, 2017; Olofsson and Börjesson, 2018). Under this assumption, the environmental impacts attributed to the production of the waste are excluded from the system boundary. The 'zero-burden assumption' argues that the innovation is generating new economic value from a stream that previously had none, thus the impacts associated with the production of the stream should not be reflected in the impacts of the innovation. Researchers have debated the merit of this assumption, as it disregards the environmental impacts associated with the current application of the feedstock (Ahlgren et al., 2015; Tonini et al., 2016). Furthermore, the zero-burden assumption is not applicable in the context of a circular economy, which inherently assigns an economic value to all flows (Olofsson and Börjesson, 2018). As such, waste feedstocks should be treated similarly to co-products and residues, for which an allocation method (see also sub-section 3.3) can be used to separate the environmental burdens of inputs and outputs (Bernstad Saraiva, 2017; Schrijvers et al., 2016b).

Following this, the analyst should consider to conduct all non-comparative bio-based ex-ante LCAs from cradle-to-grave (see also Guineé, 2002), regardless of the feedstock nature. Exceptions to this rule exist, for instance regarding feed and food products, for which the cradle-to-consumption approaches can be sufficient (even recommended by e.g. the PEF and other GHG accounting standards). However, exceptions to this rule must be clearly justifiable. In comparative assessments however, the system boundary can be adjusted according to the overlapping elements of the compared systems (Figure 3).

Figure 3. Decision tree to select the system boundary of bio-based ex-ante LCA for comparative assessments



For systems with identical outputs (product or service) to the incumbent technology (left side of the decision tree), a full cradle to grave analysis may not be necessary if the output used and end-of-life systems are identical. For example, when comparing the production of bio-based PET bottles versus petrochemical PET bottles, the factory output is chemically and functionally identical (Asgher et al., 2020). In such an instance, the two technologies do not have common feedstock but do have a common output, therefore a cradle to gate analysis (Figure 3) is sufficient (EC, 2010). Similarly, analyses of systems with identical feedstock sources can shift their upstream boundary to Gate. In systems which use both identical feedstocks and produce identical outputs, a gate to gate analysis is sufficient. For example, pectin from citrus peels has traditionally been extracted using chemical based extraction. A novel innovation using microwave energy provides a new pectin extraction pathway (Garcia-Garcia et al., 2019). In this scenario, the citrus peel feedstock and the produced pectin are identical in both systems, making a gate to gate analysis sufficient to compare the two systems (Figure 3, left path).

Besides the process system boundaries, temporal boundaries should also be considered. For example agricultural-based and forest-based biomass production can differ not only spatially but also temporally (e.g. annual harvest vs. several years of growth). Forest-based biomass production usually also comes with multifunctionality (e.g. stem wood, industrial wood, energy wood, wood residues) which should also be considered while defining the system boundaries (see also sub-section 3.3)

3. Life Cycle Inventory

This section is dedicated to life cycle inventory and how best to approach upscaling of unit processes in the foreground and background, which is one of the bigger challenges in prospective LCA. An important issue for bio-based products is also how to allocate processes with multiple product streams and how to appropriately define the system boundary.

To reduce the time and data intensity of their analysis, ex-ante LCA analysts can separate the system into foreground and background components. The foreground system describes the unique flows of the technology and its incumbent being evaluated, typically relying on primary data (van der Giesen et al., 2020). Background systems provide context to the analysis, modelling the upstream and downstream process in which the technology operates in. This data is often gathered from LCI databases which provides aggregated data (Wiloso and Heijungs, 2013).

A lack of representative life cycle inventory (LCI) data is a frequent bottleneck in the development of ex-ante LCAs (Moni et al., 2020). The emerging technology assessed has typically been realized at lab or pilot scale, however the data gathered at these scales is not directly applicable to the industrial scale version of the system (Piccinno et al., 2016). Therefore, ex-ante LCA analysts must often rely on secondary data which may also be scarce. The data shortage affects the development of both the foreground and background system modelling, each critical to achieve representative results (Arvidsson et al., 2017).

Furthermore, the implementation of optimized equipment, recovery systems, and monitoring systems at large scales all lead to efficiency improvements which are not possible at smaller scales which must be accounted for to properly inventory the material and energetic requirements of the system (Piccinno et al., 2016). Tools, in the form of upscaling approaches, have been developed to mitigate this problem and facilitate the development of representative LCI of the foreground system at a future time, however, selecting the proper upscaling approach for BbPs remains largely dependent on data availability and expert knowledge (Tsoy et al., 2020).

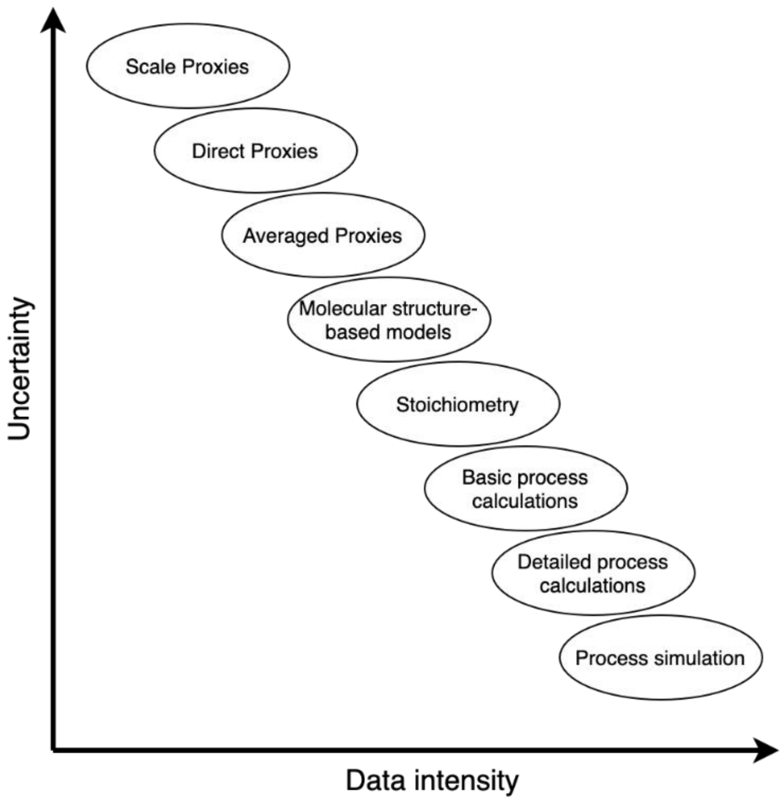
A more detailed discussion about up-scaling fore- and background data (e.g. outdated LCI data not suitable for prospective LCAs) can be found under sub-section 5.2.1.

3.1 Upscaling Foreground Systems

To estimate projected inventory data, an industrial scale project system diagram must be prepared (Tsoy et al., 2020). The unit processes and elementary flow relationships of the system are recorded to model a version of the system. Many lab scale processes are not transferable to industrial scale, and would therefore not be relevant in the case of ex-ante LCI. Therefore, the lab scale diagram must be adjusted to establish an industrial scale diagram, from which the processes can ultimately be upscaled (Piccinno et al., 2016).

Multiple upscaling approaches for unit processes have been proposed to model industrial scale inventory data from lab or pilot scale data. These upscaling approaches can broadly be distributed between two categories: (1) extrapolated data and (2) proxies (Milà i Canals et al., 2011; Parvatker and Eckelman, 2019). Parvatker and Eckelman (2019) summarized the extrapolated data methods for chemical processes and ranked them based on uncertainty of estimates. Although bio-chemical and conventional chemical processes might be quite different in their production route, the functionality of each is often the same, making existing upscaling knowledge of the chemical industry relevant to the bio-chemical industry (Clark et al., 2015). We have combined the work of Parvatker and Eckelman (2019) with the proxy definitions of Milà i Canals et al. (2011) to summarize the upscaling methods available to bio-based innovations based on data intensity and uncertainty of results in Figure 4.

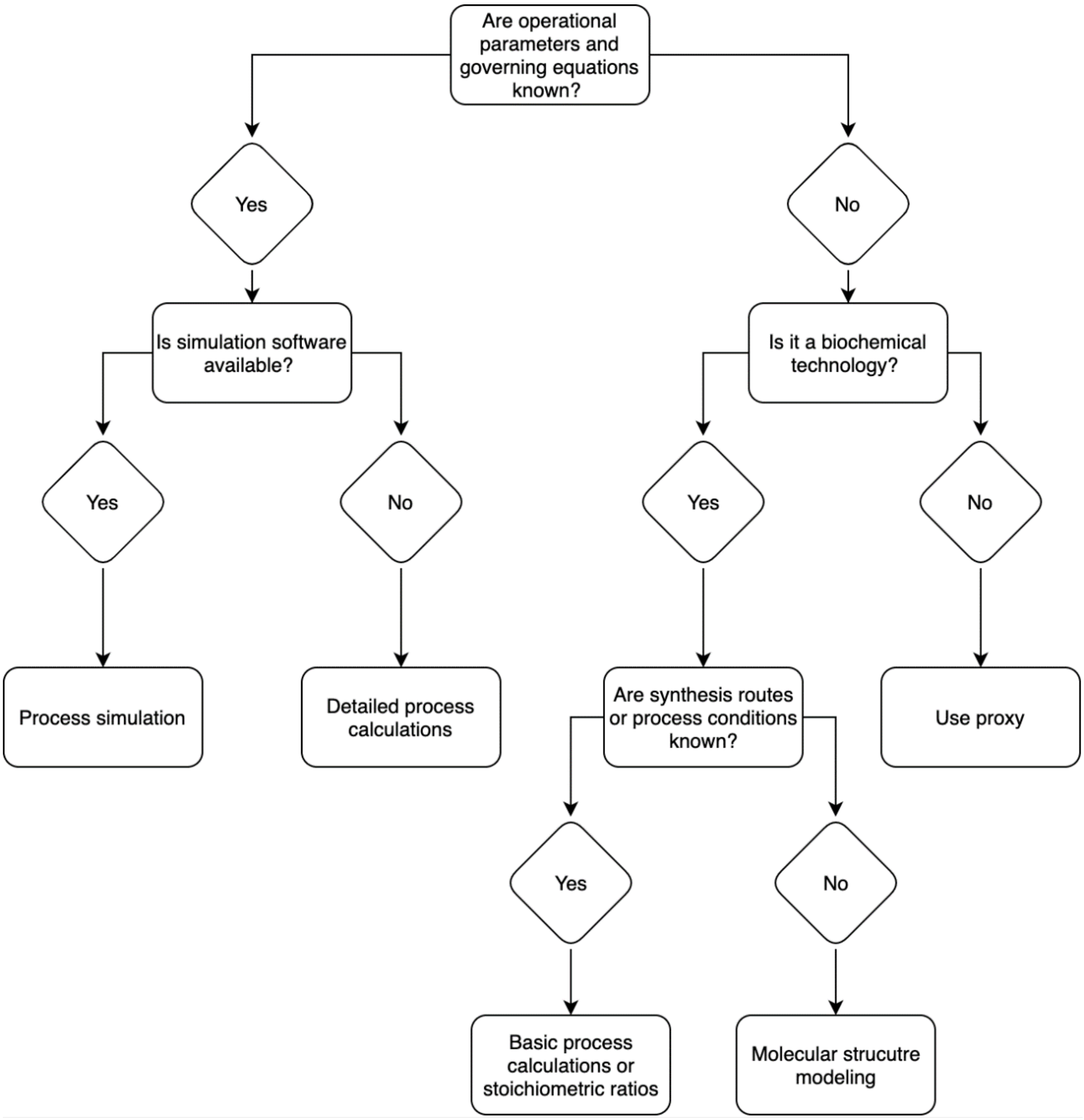
Figure 4. Upscaling methods ranked by uncertainty and data intensity (adapted from Milà i Canals et al., 2011; Parvatker and Eckelman, 2019; see also section 5 on Scenario methodology)



Among the eight upscaling approaches presented in Figure 4, the three proxy options are considered the most uncertain (Milà i Canals et al., 2011). Scaled proxies bridge data gaps through linear upscaling, while direct proxies use a similar existing process to resample the other (e.g. ethanol production from grass for ethanol production from pomegranate peals). If multiple comparable proxies are available, they can be averaged to result in an even more fitting approximation. Moving to extrapolation-based upscaling, molecular structure models take physical and chemical properties of the target chemical into account. The stoichiometric approach uses elemental ratios of the products to scale the system and detailed process calculations include mass and energy balance equations. Basic calculations do not include temporal and spatial changes unlike detailed process calculations. The least uncertain relies on software calculations where the whole process can be replicated in a virtual environment and the design be tested.

Although the highest ranked methods reduce uncertainty (Milà i Canals et al., 2011; Parvatker and Eckelman, 2019), they do provide additional challenges. Process simulation and process calculations each require a high degree of knowledge of process design, simulation software use, and technological expertise (Tsoy et al., 2020). Furthermore, the development of a technology often leads to efficiency gains, economies of scale, and industrial synergies which cause a non-linear progression of system inputs and outputs (Sacchi et al., 2019). The uncertainty of these non-linear factors can be mitigated by applying probabilistic methods (Blanco et al., 2020) or introducing scaling coefficients (Pizzol et al., 2021) providing a range of up-scaled inventories. The combination of these data and computational demands may render certain extrapolated upscaling methods inaccessible to ex-ante LCA analysts. In contrast, proxies are much less computationally demanding but present the highest levels of uncertainty. We refer the reader to Box 2 for an illustrative example.

Figure 5. Upscaling of bio-based technologies (adapted from Tsoy et al., 2020)



Previous research has directly ranked extrapolated and proxy based upscaling, however, Simon et al. (2016) argued that a direct comparison between the two may not be effective; particularly in the case of emerging technologies that are not closely aligned to existing infrastructures (Clark et al., 2015). In the case of non-comparative ex-ante LCAs, the lack of reference infrastructure and integration of multiple novel processes can make extrapolation-based upscaling strategies extremely complicated and time consuming (Simon et al., 2016), often limiting their practicability. Extrapolation-based upscaling approaches may be more effective for innovations that share the upstream and downstream infrastructure the incumbent technology, where industrial scale data is available (Clark et al., 2015). Accounting for the trade-offs between data intensity and uncertainty, Figure 5 presents the recommended upscaling approach depending on data availability and resources available to the LCA practitioner (adapted from Tsoy et al., 2020).

In cases where extrapolation-based upscaling methods are not effective due to data or time availability, Simon et al. (2016) proposed to identify proxies based on three criteria: (i) function, (ii) dimension, and (iii) similarities. When analysing for function, lab and pilot scale processes can be linked to mature industrial processes on the basis of their functionality (e.g. filtration, homogenization, drying). Secondly, processes can be evaluated based on (ii) dimension. These include reaction parameters (temperature and pressure, etc.), kinetics (reaction time, yield, etc.), and production quality. Finally, (iii) similarities are used to identify the working characteristics of industrial systems with similar functionality, for example power requirements, solvent demand, yield, and throughput of a comparable full-scale system.

Box 2. Exemplification of upcale for the case stduy of PHA biorefinery

Case study: Prospective LCA of waste-to-PHA biorefinery (continued)

The waste-to-PHA biorefinery current TRL is 5-6. As the operational parameters and governing equations are known, the foreground system was upscaled using detailed process calculations. The estimation procedure to be used as a calculation basis was the following:

1. PHA and biomass obtained in PHA on a tons per year and tons of chemical oxygen demand (COD) basis was calculated considering influencing parameters: scale, extraction yield and PHA content in biomass (Equations (1) and (2)).

$$m_{PHA,basis}\left[\frac{t\ COD}{year}\right] = \frac{Scale}{Y_{extraction}} \cdot COD_{PHA} \tag{1}$$

$$m_{X,basis}\left[\frac{t\ COD}{year}\right] = \frac{Scale}{Y_{extraction}} \cdot \left(\frac{1}{PHA_{content}} - 1\right) \cdot COD_{X} \tag{2}$$

2. Based on the amount of PHA produced in the accumulation and enrichment step and the amount of PHA storing biomass required, the amount of volatile fatty acids to fed in both enrichment and accumulation reactors was calculated based on influencing parameters: YX/VFA and YPHA/VFA (Equations (3) and (4)). The biomass productivity (XPR) and the organic loading rate (OLR) in the enrichment reactor are calculated in Equations (5) and (6)) considering the productivity.

$$m_{VFA,basis}\left[\frac{t\ COD}{year}\right] = \frac{m_{PHA,basis} \cdot (1 - PHA_{selector})}{Y_{PHA/VFA}} + \frac{m_{X,basis}}{Y_{X/VFA}} \tag{3}$$

$$f_{VFA,selector} = \frac{m_{X,basis}/Y_{X/VFA}}{m_{VFA,basis}} \tag{4}$$

$$XPR\ [g\ X \cdot L^{-1} \cdot d^{-1}] = Productivity \cdot \frac{m_{X,basis}/COD_X}{m_{PHA,basis}/COD_{PHA}} \tag{5}$$

$$OLR\ [g\ VFA \cdot L^{-1} \cdot d^{-1}] = \frac{XPR \cdot COD_X}{Y_{X/VFA}} \tag{6}$$

3. Finally, considering the efficiency on the VFA separation step and the acidification yield, the amount of feedstock required was estimated (Equation (7)).

$$m_{feed\ ,basis}\left[\frac{t\ COD}{year}\right] = \frac{m_{VFA,basis}}{Y_{VFA/feed} \cdot Y_{VFA,separation}} \tag{7}$$

Based on the mass balances, operational units were upscaled employing design parameters from pilot-scale, lab-scale, patents and heuristics. Regarding the utilities' consumption, heating, stirring, drying, high pressure homogenisation and filtration were estimated using the Piccino et al. 2016 framework. Reactants and solvent consumption were estimated base on pilot-scale data and patents. Electricity consumption in pumping was estimated considering 50 kWh per ton dry of material for the PHA production section and 0.155 kWh per cubic meter for the waste valorisation into electricity.

3.2 Developing Relevant Background Systems

In addition to upscaling the foreground system, it is necessary to model the background system to match the foreground and background systems temporally (Arvidsson et al., 2017). The background system refers to the processes and emissions of a product supply chain which are not directly modelled by an ex-ante LCA analyst and are not affected by the emerging technology (Mendoza Beltran et al., 2020). These background processes typically represent 99% of the unit processes in the total product system indicating the importance of developing a temporally relevant background system in case of ex-ante LCA (Wernet et al., 2016).

In the case of bio-based systems, background biosphere developments should be considered. As previously discussed (sub-section 3.1), the background system impacts of bio-based innovations vary geographically and temporally due to direct impacts of climate changes on the production of bio-based feedstocks and advances in for example plant breeding and agronomic practices (Sencan and Escriva-bou, 2020; Stavi and Lal, 2015). Furthermore, bio-based feedstocks frequently rely on the use of fertilizing products, pest protection products, water, and potentially other bio-based feedstocks (i.e. feed; Cucurachi et al., 2019) for which utilizing temporally and geographically relevant background systems is paramount to properly evaluate the impacts of the innovation.

Downstream waste processing systems also present a large variance in final impact assessment results (Bernstad Saraiva Schott et al., 2016). The background processes handling the bio-waste streams of the innovation must therefore also be properly adjusted to the future context in which the innovation will operate in. However, existing background process databases require future modelling to properly account for the impacts of an emerging technology.

Börjeson et al. (2006) presented three scenarios to model background systems: (1) *predictive*, (2) *explorative* and (3) *normative*. In the case of predictive scenarios, external databases such as input-output tables and integrated assessment models (IAMs) can be coupled to LCIs to develop forecasts based on likelihood of occurrence (Mendoza Beltran et al., 2020). Explorative and normative scenarios can be used to provide long-term ranges which present a distribution of results between extreme scenarios, such as comparing results between present energy mixes and 100% renewable energy mixes as background electricity systems (Pini et al., 2017). Using predictive scenarios is most valid when modelling key technological developments that are more likely to occur than others, for example an increasing renewable energy mix, while scenario ranges are most useful when information on future development trends is limited (Arvidsson et al., 2017). Please find more information on scenario development in section 5.

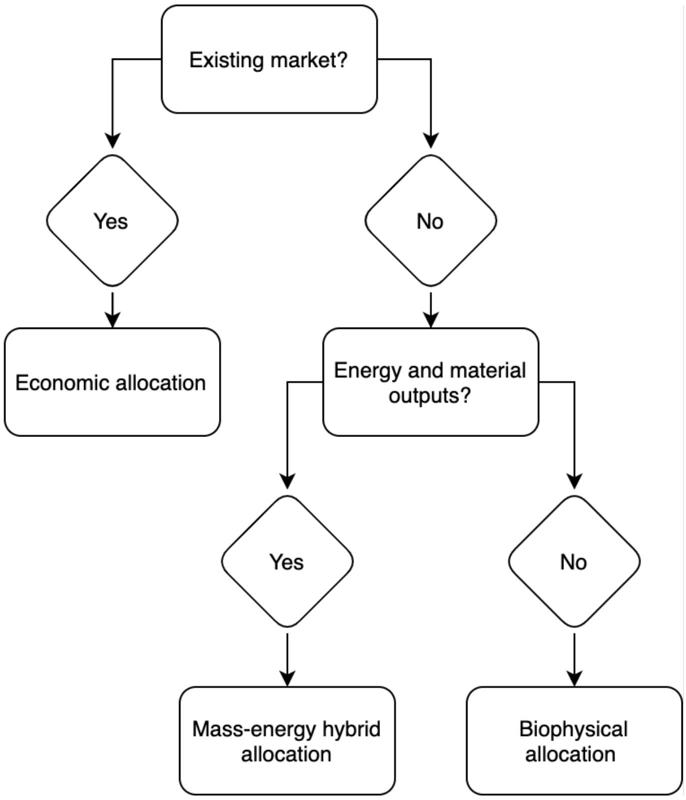
3.3 Handling multi-functional processes

If allocation cannot be avoided, either by increasing the level of process detail (sub-division) or through system expansion (preferred method) i.e. redefying the functional unit or system boundaries to include all functions, partitioning is necessary (ISO-14044, 2006). In the case of partitioning, an allocation based on a particular key e.g. mass, energy, exergy or economic value becomes necessary (ISO-14044, 2006). However due to the large variety of BbPs which can be produced and respective processes, none has emerged as suitable in all instances (Cherubini and Strømman, 2011; Fiorentino et al., 2014; Kami Delivand and Gnansounou, 2013; Singh et al., 2010). We further refer the reader to the work of Schrijvers and co-authors (Schrijvers et al., 2016b, 2016a, 2020) for guidelines on other specific aspects of allocation in LCA.

The second step of ISO-14044 (2006) recommends to partition the products “in a way that reflects the underlying physical relationships between them; i.e. they should reflect the way in which the inputs and outputs are changed by quantitative changes in the products or functions delivered by the system”. This type of allocation is referred to as “physical allocation” or physical causality allocation” but it has been also misinterpreted as a generic allocation based on a physical parameter (Mackenzie et al., 2017). To further clarify, ISO has released an amendment regarding multi-functionality in 2020 (amendment 2) reporting that ISO allocation by physical relationships means allocation by causal relationship and is applicable only “when: a) the relative production of co-products can be independently varied through process management, and b) this has causal implications for the inputs required, emissions released or waste produced".

Although the ISO-14044 (2006) standard suggests causal physical relationships should be favoured as an allocation method, modelling the nature of bio-based products limits the practicability of such an approach since it is rare that a biophysical parameter can reflect "ISO physical causality relationships". Moreover, many bio-based processes are constrained by stoichiometric or biological ratios which cannot be adjusted independently. Hence, allocation by other (causal) relationships is often necessary (Mackenzie et al., 2017). Hence, in bio-based systems, the causality of production may be better represented with economic allocation than with biophysical allocation methods (Ardente and Cellura, 2012; Mackenzie et al., 2017). Doing so, removes the need to prove the burden of physical causation between material flows (Finnveden et al., 2009; Mackenzie et al., 2017).

Figure 6. Decision tree for the allocation of multi-functional processes in bio-based ex-ante LCA. Only applies if system expansion is not possible



Although economic allocation can be effective, it raises many challenges. In the context of ex-ante LCA, the innovation may operate in an undeveloped market, where the outputs may not have a market value yet or be subject to large price fluctuations due to market development, technological progression, or government intervention (Ahlgren et al., 2015; Luo et al., 2009; Njakou Djomo et al., 2017). In such cases, economic allocation may be too uncertain to properly represent the future value of the outputs, thus allocation by a physical parameter reflecting other values (e.g. energetic) may be considered a more appropriate allocation method (Figure 6 right path; Njakou Djomo et al., 2017). In cases where the innovation is integrating an existing market, concerns regarding future price uncertainty can be mitigated by analysing the incumbent market, making economic allocation an effective method (Figure 6 left path; Mackenzie et al., 2017). Based on these principles, we suggest a decision tree logic which can provide the basis for practitioners to select an allocation method, if necessary (.

Figure 6).

Allocation by physical parameters reflecting other values for biomass products also present sometimes constraints. Multi-functional bio-based systems often produce a combination of outputs where contents either do not contain mass or energy (Ahlgren et al., 2015). In this case, multiple hybrid allocation methods have been proposed to address this issue including hybrid mass-energy and hybrid partitioning-substitution methods (Cherubini and Strømman, 2011; Njakou Djomo et al., 2017; Sandin et al., 2015). These methods can strongly mirror the benefits of economic allocation, simultaneously assigning environmental impacts to material and immaterial outputs despite only relying on physical properties. Such methods are most useful when the system analysed operate within uncertain future market conditions but they may still lead to misrepresentative results.

Special care has to be taken for biogenic carbon flows, which can be found in more detail in section. 4. For carbon balance via mass allocation, we would like to refer to the example given in sub-section 4.6.1.

4. Biogenic carbon flows

4.1 Background

The atmosphere does not distinguish whether greenhouse gases such as CO_2, CO[1], and CH_4, are of fossil or biogenic origin. Yet, from a climate change perspective, it makes a difference as carbon from fossil sources is additionally entering the atmosphere and thus leads to increased concentrations of GHG in the atmosphere, while for biogenic carbon there is a balance between carbon emissions and the uptake of carbon by plants, at least when supposing a sustainable management of biomass resources.

However, this by itself does not mean that there are by definition no climate effects from the use of biomass or that the carbon footprint (CF) of biogenic products is zero. A number of reasons why it is important to account for biogenic carbon include:

- Substantial CO_2 emissions from biomass combustion: For the same amount of useful energy generated, the quantity of CO_2 released from the combustion of wood is comparable to that of coal; biomass is used across the globe in large quantities for a large range of applications spanning from material to energy usages; sustainable management of forest and agricultural ecosystems is paramount to ensure the uptake of carbon from the atmosphere;
- Carbon neutrality does not imply climate neutrality: biogenic carbon emissions contribute to the greenhouse effect during their time in the atmosphere, i.e. before being re-absorbed by plants. This is especially the case when biogenic carbon is released in the form of greenhouse gases other than CO_2, e.g. methane, which is not directly taken up by plants and has a higher radiative forcing
- Temporary and permanent[2] carbon storage: contrary to the previous example, if biomass is harvested, but its emissions are temporarily delayed or permanently avoided, this may lead to a temporary or permanent reduction of GHGs in the atmosphere, and, therefore, reduce global warming, if CO_2 continues to be sequestered in the ecosystems where the biomass was produced (although this depends on the chosen time horizon, see also sub-section 4.2)
- Land use change: when biomass is used and biogenic carbon eventually released to the atmosphere (e.g. during combustion), but the biomass is not permitted to fully grow back, e.g. due to a land use change (conversion of a forest to a plantation or a road), there is a permanent addition of biogenic carbon to the atmosphere

For these, and possibly other reasons, it is important to understand the biogenic carbon flows related to products and services.

In this section, we first provide an overview on the key issues related to biogenic carbon accounting and then present how these issues are dealt with in scientific literature and in relevant standards. Finally, we briefly discuss the implications for accounting for biogenic carbon in the context of prospective LCA.

4.2 Key issues for biogenic carbon accounting

Key issues for biogenic carbon accounting involve:

Timing of carbon emissions. The points in time when biomass is emitted to the atmosphere and sequestered back (or the other way around) affects how carbon emissions from biomass (e.g., CO_2, CO, CH_4) contribute to global warming (Cherubini et al., 2011; Levasseur et al., 2012). For example, if a tree is harvested and used for energy in the same year, the level of atmospheric CO_2 will temporarily increase until the forest has sequestered back the same amount of carbon (Cherubini et al., 2011). Therefore, the timing of emissions matters even for sustainably managed biomass resources and as Cherubini et al. (2011) put it: carbon neutrality is not the same as climate neutrality. Additionally, many factors play into this accounting, such as tree species, stand age,

[1] Although CO is not given a characterization factor for climate change in the latest report of the IPCC (IPCC, 2021)
[2] Note that there is no universally accepted definition of "permanent storage" as different standards define it differently

growth phase, and other local conditions, such as the intensity of harvesting, set-aside forest areas, and in the longer perspective also climate change effects. Further, this is mostly an issue pertaining to long-rotation biomass, such as forests, and less of short-rotation crops and agricultural produce.

Temporary and permanent carbon storage. Strongly related to the previous issue is the question of how to account for the effects of temporary and permanent carbon storage. Storing carbon in BbP effectively delays the time of the emission and, therefore, temporarily or permanently reduces their global warming effect (Guest et al., 2013). This is why storing carbon in products has been seen as a way to buy time for climate change mitigation. The debate around this topic has been on how to account for carbon storage in a correct, but also practically feasible manner. A fundamental problem related to this is that at the time of accounting, usually at the beginning or before the actual carbon storage, the storage duration can only be an assumption, but not a fact yet, and it may turn out to be different than the assumption due to unforeseen events in the future. To complicate things, the benefit from temporary carbon storage depends on the chosen time horizon (a value choice) and would be zero when an infinity perspective would be adopted (Brandão et al., 2013).

Land use change. Land use change, e.g., the transformation of a forest into cropland or a road, is again related to the previous issues, however, in addition to the timing of emissions, it may lead to permanent carbon stock changes (Searchinger et al., 2009). For example, the clearing of a forest for a road will lead to permanent aboveground and soil carbon losses, and thus to a net addition of atmospheric CO_2 and other GHGs (afforestation would lead to the opposite; Levasseur et al., 2012). The question whether biomass comes from sustainably managed land resources, or from land that is transformed (i.e., undergoing a land use change) is an important one to consider for the LCA of BbPs. Further indirect land use changes may occur as a consequence of increased biomass demand in one country causing land use change somewhere else (e.g. an increased demand for biofuels could lead to the production of biofuels on land which was previously dedicated to food production, which in turn could shift food production to other land, such as tropical forests; see e.g. Melillo et al., 2009; Tonini et al., 2016).

4.3 Biogenic carbon accounting approaches used in the scientific literature

4.3.1 Conventional LCA

LCA, in its conventional form, is a static method, i.e., it does not have an explicit temporal dimension. This is a limitation whenever the temporal dimension plays an important role, which is the case of many bio-based systems. Nevertheless, this is still the most commonly used form of LCA and it is therefore important to understand the way biogenic carbon is typically treated at the inventory and the impact assessment levels.

Modelling biogenic carbon flows in the life cycle inventory. There are two common ways, in which biogenic carbon flows are typically included in the LCI (Arehart et al., 2021):

1. Not to account for biogenic carbon flows, relying instead on the assumption that biomass comes from sustainably managed sources and should thus not affect GHG emissions
2. To account for biogenic carbon flows through elementary flows, for both the uptake and the release

There seems to be a consensus that biogenic carbon flows shall be modelled separately to fossil carbon flows, e.g. “Carbon dioxide, biogenic” vs. “Carbon dioxide, fossil)”.

Modelling biogenic carbon flows in the impact assessment phase. Similarly, to the inventory phase, there are two main options for the characterization of biogenic CO_2 flows (Arehart et al., 2021):

1. <u>‘0/0’ approach</u>: To *not* characterize biogenic CO_2 flows, i.e., to ignore them during impact assessment
2. <u>‘-1/+1’ approach</u>: To characterize biogenic CO_2 flows in the same way as fossil CO_2 flows

Arehart et al. (2021) also report that a sizable fraction of LCA studies apply a ‘-1/0’ approach, in which the uptake of biogenic carbon is considered, but not its release, thus ignoring the EoL stage. This approach can help to showcase the potential benefits of BbPs compared to fossil-based products in 'cradle-to-gate' studies, i.e., when the EoL stage is not considered. Practically, this should lead to the same results as applying the '-1/+1' in 'cradle-to-gate' studies. Finally, the '0/-1' approach also exists (Christensen et al 2009, Tonini et al 2021) and it has been used especially in waste LCAs. In this case, the emissions of biogenic CO_2 are given a characterization factor equal to 0 (since uptakes/emissions are supposed to balance themselves) but biogenic carbon bound to soil, e.g. in landfills, is credited a saving (characterization factor equal to -1) since the CO_2 emissions did not happen in the studied time horizon.

Note that other GHG than CO_2, such as bio-based methane, should always be characterized as these are substances which are not by default part of the carbon cycle, but the result of conversion processes that lead to substances which have a higher radiative forcing than CO_2 (Fazio et al., 2018). However, the characterization factor of biogenic methane is equal to the one of fossil methane in case of the '-1/+1' approach and it is lower than the fossil methane in case of the '0/0' approach because a portion of the methane is oxidised to CO_2 in the atmosphere and the characterization of this CO_2 depends on the approach used.

4.3.2 Dynamic LCA

The concept of **dynamic LCA** proposed by Levasseur et al. (2010) has been developed to include the temporal dimension through time-differentiated life cycle inventories that are used together with dynamic characterization factors and a fixed time-horizon (Breton et al., 2018). The dynamic characterization factors reflect the amount of cumulative radiative forcing that an emission in year x would lead to until the time horizon and includes typically the atmospheric decay of the emission (Levasseur et al., 2010). The global warming impacts for a dynamic LCA are then calculated by multiplying the dynamic inventories (positive and negative emissions of GHG over time) with the dynamic characterization factors.

Another dynamic approach is the **GWPbio indicator** (Cherubini et al., 2011) a metric that relates the amount of radiative forcing from biogenic carbon emissions to that of an equivalent amount of fossil CO_2. It has been developed with the perspective to show that "carbon neutral" is not the same as "climate neutral". Like the implementation of dynamic LCA by Levasseur (e.g. Levasseur et al., 2012), it combines a dynamic inventory of positive and negative GHG emissions related to the use and the re-growth of the biomass with the atmospheric response to a pulse emission (Joos et al., 2013). The latter reflects the interaction of the atmosphere with land and ocean carbon sinks. The GWPbio indicator has been extended to include temporary (and permanent) carbon storage (Guest et al., 2013), as well as the albedo effect, which is usually not considered in LCA, but does have an important contribution to radiative forcing (Cherubini et al., 2012).

According to Arehart et al. (2021), these two approaches are the most widely used "dynamic LCA" approaches to account for biogenic carbon. The effect of biogenic carbon emissions depends in both approaches strongly on the biomass re-growth function (e.g., short vs. long-rotation crops) and the choice of the time horizon. For more comprehensive reviews of the state-of-the-art of biogenic carbon accounting the reader shall be referred to e.g. Arehart et al. (2021), Breton et al. (2018), Hoxha et al. (2020) and Tellnes et al. (2017).

4.4 Ability of conventional and dynamic LCA to address the key issues

Timing of emissions. The timing of emissions, including both emissions on the land where the biomass was sourced from (e.g., re-growth) and emissions from the handling of the BbP in the anthroposphere, cannot be addressed properly in conventional LCA (Hoxha et al., 2020). Dynamic LCA and the GWPbio method, on the other hand, are specifically designed to include temporal dynamics of emissions and their interaction with the atmosphere, however, they also require additional data and software (e.g., to temporally describe the expected biomass re-growth and the carbon decay in the atmosphere; for the latter, generally accepted models such as that of Joos et al. (2013) can be used). The magnitude of the effects of temporal dynamics depends strongly on the chosen time horizon.

Carbon storage. Permanent carbon storage can be included in conventional LCA as it corresponds essentially to a quantity of biogenic carbon that is not emitted over the life cycle of a BbP. A proper consideration of temporary carbon storage is not possible in conventional LCA due to the static nature of the assessment, although approaches have been developed to at least approximate the effect of carbon storage (Levasseur et al., 2012). Dynamic LCA and the GWPbio method are well suited to account for both temporary and permanent carbon storage.

Land use change. Direct land use changes can be included in conventional LCA. Challenges include quantifying the carbon emissions related to land use changes and additional assumptions are necessary, e.g., as to how to allocate emissions over time. Dynamic LCA and the GWPbio method are suitable approaches to account for the dynamic profile of emissions from land use change and their atmospheric decay. The same applies, in principle, to indirect land use changes, although these are more difficult to quantify in the first place.

Table 2 summarizes the ability of conventional and dynamic LCA approaches to model the key issues.

Table 2. Summary of the ability of conventional and dynamic LCA to deal with some of the key issues for biogenic carbon accounting as well as remaining challenges

Issue	Conventional LCA	Dynamic LCA	Remaining challenges
Timing of emissions	Difficult to include	Designed to be included	Choice of time horizon
Temporary and permanent carbon storage	Difficult to include, although certain simplified accounting methods have been proposed	Designed to be included	Choice of time horizon; verification of storage;
Land use change (LUC)	Can be included based on an allocation of LUC emissions over time	Can be included based on a dynamic model	Data to model LUC Allocation of LUC emissions over time Quantifying indirect land use change

4.5 Biogenic carbon accounting approaches adopted in relevant standards

Here we review the following standards for their approaches to deal with biogenic carbon flows:

- ISO-14044:2006: Environmental management - Life cycle assessment - Requirements and guidelines (ISO-14044, 2006)
- ISO-14067:2018: Greenhouse gases - Carbon footprint of products - Requirements and guidelines for quantification (ISO-14067, 2018)
- PAS 2050: Publicly Available Specification (PAS) 2050 (BSI, 2011)
- GHG Protocol (World Resources Institute and the World Business Council for Sustainable Development, 2011)
- ILCD handbook (EC, 2010)
- EN 16760:2015 (ISO, 2015)
- PEF: Product Environmental Footprint (EC, 2021)

Table 3 summarizes how the different standards deal with biogenic carbon. ISO-14044 is excluded as it offers no specific guidance on the topic.

For the basic modelling of biogenic carbon flows in the inventory, there seems to be a consensus in technical standards (TS) to include both biogenic carbon emissions and removals, thus implementing the '-1/+1' approach, with dedicated elementary flows, e.g., "carbon dioxide (biogenic)". Also, biogenic carbon flows are included in the climate change indicator at the impact assessment stage, however, impacts shall be reported separately, e.g., in a category "climate change – biogenic". Important details, such as allocation, are dealt with differently across standards and only the PEF prescribes mass allocation for biogenic carbon flows, presumably in order to keep the physical carbon flows in the LCA model correct.

Concerning the key issues outlined earlier in this section, the standards differ:

- **Temporary carbon storage** is generally not included in the CF, but can in some standards be reported separately, using weighting factors to account for the temporal delay in emission.
- **Permanent carbon storage** is not considered in the CF in the ISO-14067 and PEF standards, but can be reported separately. In PAS 2050 carbon storage beyond the time horizon of the study is considered permanent and included in the CF.
- **Direct land use changes** are included in all compared standards, yet they are to be separately reported except for PAS 2050.
- **Indirect land use changes** are not included in any of the standards, but can be separately reported at least in the GHG Protocol. ISO-14067 states that it "shall be considered [...] once an internationally agreed procedure exists".

Table 3. Comparison of approaches to biogenic carbon accounting in technical standards (CF = carbon footprint, LCI = life cycle inventory).

Issue / Standard	ISO-14067	PAS 2050	GHG Protocol	PEF	EN 16760:2015	ILCD Handbook
Biogenic carbon flows in the LCI	Required	Required; simplified approach for food/feed products	Required	Required; simplified approach for food/feed products (only methane) Carbon content shall be reported for intermediate products	Required	Required
Handling multi-functional processes	Not specific for biogenic carbon; following the ISO-14044 stepwise procedure	Not specific for biogenic carbon; supplementary requirements, then physical allocation	Not specific for biogenic carbon; physical allocation, then economic	Mass allocation (by which likely a carbon-content allocation is actually meant)	Not specific for biogenic carbon	Not specific for biogenic carbon
Biogenic carbon flows during impact assessment	Characterization factors for CO_2 uptake/release: -1/1 Included in the total climate change impact, but reported also separately.	Characterization factors for CO_2 uptake/release: -1/1 Included in the total climate change impact.	Characterization factors for CO_2 uptake/release: -1/1 Included in the total climate change impact.	Characterization factors for CO_2 uptake/release: 0/0 Other biogenic GHG emissions (e.g. CH_4) are included and impacts can be reported in the sub-categories 'Climate change –fossil', 'Climate change – biogenic' and 'Climate change - land use and land use change' shall be reported separately, if they show a contribution of more than 5% each to the total score of climate change."	Characterization factors for CO_2 uptake/release: Option 1: -1/1 Option 2: 0/0 Included in the total climate change impact and reported also separately (Annex B).	Characterization factors for CO_2 uptake/release: -1/1 Included in the total climate change impact
Temporary carbon storage[3]	Not included in CF, but can be reported separately[2]	Not included in CF, but can be reported separately[2] using weighting factors	Carbon stored in products to be reported for 'cradle-to-gate' studies; not included in CF, but can be reported separately[2]	Not included in LCI or CF	May be taken into account, but reported separately. Assessment may be carried out according to CEN ISO/TS 14067 or ILCD.	The effect of delayed emissions (within 100 years) may be calculated based on linear discounting – calculation method specified – if required in the goal of the study.
Permanent carbon storage[3]	Not included in CF, but can be	Considered in CF if stored > 100 years	Considered in CF if stored > 100 years; carbon not emitted	Generally not included in LCI or CF, yet soil carbon storage may be included as additional		Emissions beyond 100 years inventoried separately "Carbon

	reported separately[2]		during EoL treated as stored carbon and included in CF	environmental information and if a proof is provided.		dioxide, biogenic (long term)”. Emissions beyond 100,000 years not accounted (permanent carbon storage).
Direct land use change	Included in LCI and CF, but reported also separately[1]	Included in LCI and CF (not reported separately); type and timing of LUC must be reported; country-specific data partly provided;	Included in LCI and CF, but reported separately[1]	Included in LCI and CF, reported also separately in the sub-category ‘climate change – land use and land transformation’; Calculation based on PAS 2050	Included in LCI and CF.	Included in the assessment, considering land use change occurring not more than 20 years or a single harvest period prior to the assessment (following the IPCC guidelines).
Indirect land use change	Shall be considered once an internationally agreed procedure exists	Not considered	Can be reported separately[2]	May be included under additional environmental information	Not considered due to the lack of an agreed methodology. It may only be addressed during interpretation.	Not considered.

[1] it shall be reported separately, but accounted towards total climate change impacts

[2] it shall be reported separately, but *not* accounted towards total climate change impacts

[3] Note that there is no universally accepted definition of “temporary storage” or “permanent storage” as different standards define it differently.

4.6 Discussion

4.6.1 General discussion

The need for accounting for the "carbon stocks and fluxes associated with standing biomass and its harvest" to calculate the GHG emissions related to biomass fuels has been recognized already more than 25 years ago, e.g., by Marland and Schlamandinger (1995). However, despite the number of scientific methods and standards that have been developed in the meantime to account for biogenic carbon in LCA, there is still no full consensus on the right approach (Breton et al., 2018). Key issues for which there is currently a lack of consensus are:

- How to include temporary carbon storage
- How to include indirect land use changes
- Which time horizon to choose, especially for dynamic accounting approaches, where this has a large influence on the results

From a scientific perspective, a dynamic LCA approach seems to be more appropriate when the timing of emissions plays an important role, e.g., for long-rotation biomass and for product systems involving temporary and/or permanent carbon storage. From a consistency point of view, the application of dynamic LCA should include also other impact categories where the temporal dimension matters. While the presented approaches have focussed on biogenic carbon flows, it was outside the scope of this work to assess whether dynamic LCA is already sufficiently developed to be applicable in practice for other impact categories than climate change.

From the perspective of harmonization and standardization, different standards suggest different approaches. Some of the reasons for this may lie in the fact that the accounting of carbon storage relies on:

- **methodological choices**, e.g., the question of which (scientific) approach to choose for the consideration of delayed emissions, and
- **value choices**, e.g., that of the choice of time horizon may strongly affect the final results.

These are points on which all compared standards could be criticized. Obviously, there is a trade-off between not including certain phenomena (e.g., carbon storage) due to the lack of consensus (safe but incomplete) and including such potentially important information (less safe, but more complete). This is why most standards provide the possibility of including separately reported information to still enable a discussion on these issues.

There are also a number of additional issues and considerations that concern the implementation of biogenic carbon accounting across technical standards and scientific approaches:

- **Counter-factuality and verification**: typically, an LCA is conducted relatively close to the beginning of the time horizon considered for a product. This means that values for the temporary or permanent carbon storage and other related effects are fundamentally *assumptions about the future and not yet fact*. That is, for the LCA to be correct, these assumptions would still have to be verified over time. For example, timber used in a building may not actually be stored for 100 years even though this might have been the initial assumption. Similarly, a forest may not fully sequester back all the carbon if a forest fire, a war, or any other event happens that leads to its premature destruction.
- **Multi-functionality**: Unit processes, as modelled in LCA, may have more than a single purpose (e.g. co-production, combined waste processing, or recycling processes), and this is when they are called multi-functional. Multi-functionality needs to be resolved, if possible by further disaggregation, or by system expansion, or else by allocation (ISO-14044, 2006). It is important to realize that allocation can distort the physical reality of mass flows and thus introduce problems for the accounting of biogenic carbon flows. Therefore, some of the solutions to dealing with multi-functionality may be incompatible with a physically correct biogenic carbon accounting. For example, let's assume a process has two BbP with equal mass and

carbon content (e.g. roundwood and wood residues from felling a tree), but different revenues from each product (e.g. 90% revenue from roundwood and 10% from wood residues). If revenue allocation is applied to this co-production process, 90% of the CO_2 that the tree has taken up from the atmosphere would be allocated to the roundwood. At the EoL of these two products (let's assume incineration), this would mean that the roundwood would have a net negative and the wood residues a net positive elementary flow of "CO_2, biogenic". The only way to avoid such a non-sensical result is to apply an allocation based on the carbon content of the products to the carbon flows (while the rest of the process may be allocated in another way). To our knowledge this is already implemented in such a way in certain LCI databases, such as ecoinvent.

- **System boundaries (cradle to gate vs. cradle to grave)**: As explained in sub-section 4.3.1, two main approaches are commonly used to evaluate the climate effects of biogenic CO_2 flows: the "0/0" and the "-1/+1" approach. When performing comparative 'cradle-to-gate' LCAs according to the PEF, the carbon footprint of fossil and bio-based products may be equal if the processing stages are otherwise comparable since biogenic uptake and releases are not considered ("0/0 approach") (Thielen et al., 2021). Therefore, the potential climate advantage that a bio-based product may have over a fossil-based product does not become visible in a 'cradle-to-gate' study using the "0/0 approach". Other standards deal with this via the "-1/+1 approach", i.e., by including the CO_2 uptake by plants as a negative emission and the release of biogenic CO_2 as a positive emission. This helps to showcase possible climate advantages of bio-based products since using the "-1/+1 approach" in a 'cradle-to-gate' study, will likely yield a climate advantage of bio-based over fossil-based products. A potentially misleading issue is, however, that when only considering the uptake of biogenic CO_2 and not the release – as the EoL stage is by definition excluded in a 'cradle-to-gate' study – the overall carbon footprint of the bio-based product may turn out to be negative, while it would most likely be positive if a 'cradle-to-grave' perspective was adopted and the EoL emissions considered. This may be a reason why the PEF with its "0/0 approach" suggests to report the biogenic carbon content of products in 'cradle-to-gate' studies.
- **LCI data for biogenic carbon uptake and release**: the inclusion of biogenic carbon flows into the CF requires a correct modelling (and allocation) of biogenic carbon flows by the analyst and within background LCI databases. Especially inputs from background databases are hard to correct by LCI analysts and if these do not contain correct carbon balances, or if the carbon balances refer to, e.g., slightly different biomass properties and supply chains, then there will likely be a mismatch of carbon uptake to release for systems where both should sum up to net zero emission. Thus, the correct modelling of biogenic carbon flows remains a practical challenge for the LCA of BbP.
- **Software**: Finally, mainstream LCA software does not provide specific support for modelling carbon storage (perhaps also due to the plurality of approaches that have been suggested). This is a practical hurdle for LCA analysts.

4.6.2 Implications for biogenic carbon accounting in the context of prospective LCA

The issues discussed here are certainly also relevant in the context of prospective LCAs for BbP. If a prospective LCA study aims at being compliant with a formal standard for LCA, if that is even possible, the rules of that standard should be applied. Else, it might make sense for the LCA analyst to use one of the state-of-the-art scientific methods, e.g., dynamic LCA, as discussed above.

Fundamentally, one could also argue that issues such as timing of emissions, carbon storage, and land use changes fall, almost by definition, into the realm of prospective LCA, since all rely on assumptions about the future. The LCA analyst may thus be well-advised to consider including any of these assumptions in scenario or sensitivity analyses. Some examples for scenario or sensitivity analyses could include:

- alternative biomass feedstocks and in relation to that

- different scenarios for the sequestration of CO_2 over time
- different possible emission profiles related to a land use change
- alternative assumptions on the time period for which biogenic carbon is stored in products
- different EoL options leading to different quantities of biogenic carbon re-used, recycled, or otherwise released and/or permanently stored
- different climate change indicators, such as the global warming potential (GWP) or global temperature potential (GTP)
- different time horizons chosen (e.g. 20, 100, or 500 years)

Further, sensitivity analysis could include variables that are value choices rather than classical model parameters, such as the time horizon of the assessment, the solutions applied to resolve multi-functionality, or to assess the influence of different biogenic carbon accounting methods applied.

5. Scenario methodology

5.1 Background

In this section, we propose a scenario methodology that applies to all prospective LCA studies, including ex-ante studies. Prospective LCA is fundamentally about the potential development of product systems in the future. Since it is generally impossible to predict the future development of complex systems, such as those systems into which technologies are embedded, the only viable approach to assess anything in the future is to develop scenarios. This is why relevant prospective LCA literature (e.g. Arvidsson et al., 2017; Bergerson et al., 2020; Cooper and Gutowski, 2020; Thomassen et al., 2019; Thonemann et al., 2020) all refer to the use of scenarios.

The use of scenarios is practiced in many fields and the range of available methods for developing scenarios is broad, ranging from qualitative methods, such as approaches to organize mental models, to fully quantitative approaches. Well-known methods include Influence Diagrams, System Dynamics, or General Morphological Analysis (Ritchey, 2018). The use and development of scenarios has also been discussed in the LCA literature (see e.g. Börjeson et al., 2006; Fukushima and Hirao, 2002; Pesonen et al., 2000 and others). However, precise procedures that support the LCA analysts in developing scenarios are largely missing and the application of formal scenario methods appears to be rare in LCA studies. This means that most prospective LCA studies develop scenarios without a formal methodology and often without a detailed description of how scenario data was derived. Although exceptions exist, e.g. Spielmann et al. (2005), who adapt the 9-step procedure of Formative Scenario Analysis (FSA) for the specific purpose of developing scenario-based life cycle inventories, we believe that prospective LCA in general would benefit from an increase application of a more rigorous scenario methodology.

Here, we propose a relatively simple methodology, consisting only of 4 steps, to support LCA analysts in developing scenarios for prospective LCA.

5.2 A practical scenario methodology for prospective LCA of BbP

Here we describe a practical scenario methodology for prospective LCA that can be applied to BbP. The methodology has been developed as part of the MIN-TEA project that was funded by the EIT Raw Materials and tested in a number of PhD and professional courses. The work developed with the PLANET BIO project made it possible to further develop, test and write down the methodology.

The methodology is focused on the goal and scope definition and inventory analysis phases, as these are in our view the two LCA phases where LCA analysts would benefit most from a scenario methodology: During the goal and scope definition, important decisions need to be taken concerning, amongst others, the consideration of technology-readiness level (TRL) and scale/capacity of the technology to be assessed, the definition of temporal and geographical system boundaries, foreground and background data, and the type of scenario analysis to be conducted. During the inventory analysis phase, scenarios need to be constructed and implemented in the LCI model.

The impact assessment phase is not covered in this report, although scenario techniques could certainly also be applied there to assess, e.g., the impacts of new substances, or to include scenarios in the models behind impact assessment methods. The fourth phase of an LCA, interpretation, deserves coverage when performing prospective LCA, and guidance for this phase can be found in section. 6 (Uncertainty and Sensitivity Analysis for bio-based product system).

In the following sections, we present the implementation of our scenario methodology across the goal and scope definition and inventory analysis phases of LCA. We focus on aspects that pertain to the modelling of scenarios, as general guidance for these two phases of LCA is provided elsewhere in the literature (e.g. Guineé, 2002; ISO-14044, 2006).

5.2.1 Goal and scope definition

During the goal and scope definition phase, important choices are made and boundary conditions defined for conducting an LCA. This is also true for prospective LCA, however, there are a number of additional considerations that need to be made. Here, we highlight important aspects to be defined, which will influence in the following how scenarios need to be constructed.

Technology-readiness level (TRL) and scale/capacity. Unlike in conventional LCAs, where typically mature technologies (TRL 9) are assessed, prospective LCA often deals with emerging technologies (<TRL 9). When an emerging technology is the subject of an LCA, additional data estimation (inventory analysis) may be required to close data gaps. Further, when conducting a comparative prospective LCA it is crucial to either compare technologies at the same TRL or to clearly discuss the limitations of a comparison if that is not the case. We advise to be very careful in cases where TRLs are not equal as this may result in unfair comparisons, where, e.g., the emerging technology is not yet optimized and may appear to perform worse than alternatives for this reason. For technologies at very early TRLs (e.g. <4), a fully quantitative LCA may not yet be possible and the analyst may be better advised to proceed with semi-quantitative approaches (Moni et al., 2020), such as described in the LiSET (Hung et al., 2018) or the ETEA framework (Thomassen et al., 2019). Along with the technology-readiness level, the scale/capacity of the technology to be investigated shall be defined as a basis for further data collection and modelling in the inventory phase.

Temporal and geographical system boundaries. Another aspect to consider is the definition of the temporal system boundaries as prospective LCA, by definition, looks at systems in the future. Therefore, we recommend defining a reference year for the LCA. This will not only help to define the technological development state for both the specific technologies under investigation, but also that of the technological context. In addition to that, as in conventional LCA, the geographical system boundaries shall be defined as this may define the technology context and operating conditions.

Foreground and background data. The specific technologies under investigation, shall be defined here as the *foreground system*, i.e. the part of the system that the analyst models him/herself, while the technological context shall be defined as the *background system*, i.e. the part of the system for which LCA analysts typically use LCI databases. During goal and scope definition, analysts need to think about available data sources to model foreground and background systems.

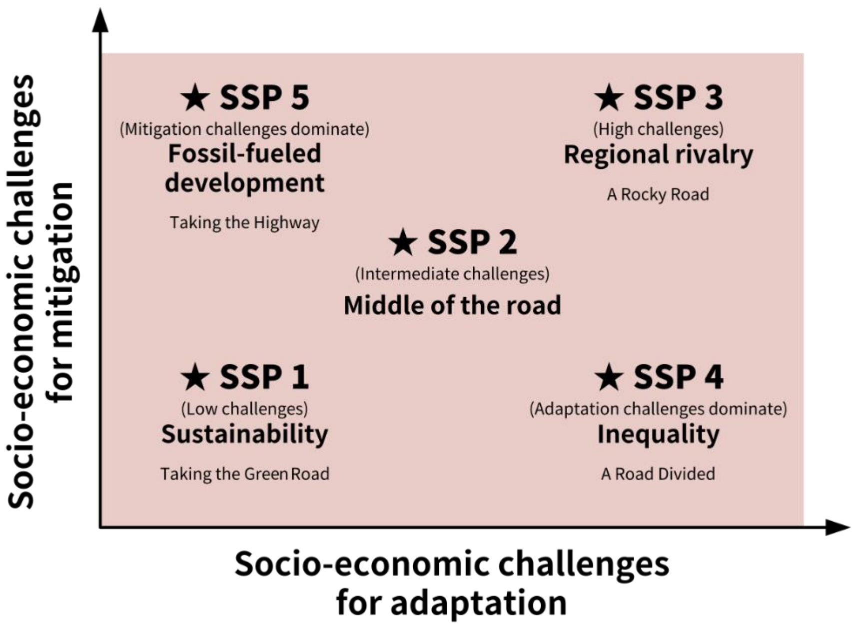
A *temporal mismatch* in the foreground and background systems, e.g. in the specific technology modelled and in the background database used, should be avoided (Arvidsson et al., 2017; Mendoza Beltran et al., 2020; Thonemann et al., 2020; van der Giesen et al., 2020). Therefore, especially for pLCA studies that look further into the future, initial choices need to be made as to how data for the foreground and background systems may be obtained.

Important progress has recently been made concerning the development of *LCI databases that represent future scenarios*, e.g. by integrating scenario data from Integrated Assessment Models (IAMs) with data from the ecoinvent database (see e.g. Gibon et al., 2015; Mendoza Beltran et al., 2020). Moreover, tools have been developed for the generation (Cox et al., 2020; Mutel, 2020; Sacchi et al., 2021) and use of future background databases in LCA software (Steubing and de Koning, 2021). For pLCAs that look further into the future, analysts are advised to use such databases to represent the background system in order to avoid a temporal mismatch, and therefore, important developments in key sectors such as energy supply, raw material supply, and market shares of important technologies, including the increased penetration of BbP.

However, while the use of future background scenarios is advisable, the LCA analyst should have a decent understanding of what scenario LCI databases represent and be aware of the fundamental assumptions and narratives of these scenarios in order to avoid a *narrative mismatch* between the foreground and the background system. For example, future background data, e.g. as developed by Mendoza Beltran et al. (2020), relies on IAMs, which are based on broader narratives, e.g. the Shared Socio-economic Pathways (SSPs; see Figure 7; O'Neill et al., 2014). This means that background scenarios should be chosen in a way that their narrative roughly fits the narrative(s) of the foreground scenario(s) developed by the LCA analyst. The development of foreground scenarios is discussed extensively in the section

Inventory analysis.

Figure 7. Shared Socio-Economic Pathway (SSP) scenarios (figure from (Brian C. O'Neill et al., 2017))



Scenario types. An important aspect to consider is the type of scenarios to be used. We base our classification here on (Börjeson et al., 2006), who divide scenarios into:

- *Predictive* scenarios: to assess how the future *will* be
- *Explorative* scenarios: to assess how the future *could* develop
- *Normative* scenarios: to assess how the future *should* develop in order to reach specific targets

The choice of scenario type thus affects how scenario analysis will be performed in general and what kind of scenarios need to be generated. For example, in a predictive analysis, there only needs to be one scenario, while in the explorative and normative cases there can be several scenarios. Predictive scenarios may also be more realistic for the near future than the far future, while explorative scenarios are more suitable for distant futures. Further, the tools for generating data are likely to differ, e.g. in a predictive scenario, extrapolations from the present to the future could be made, while in an explorative scenario possible future developments could be assessed by developing alternative narratives or by assessing "what-if" type of questions. In the case of normative scenarios, backcasting is often applied (Guinée et al., 2018), which starts by modelling the future at a specific reference year for which targets have been defined and then goes back in time to see which trajectory would lead to this desired future.

The implications of the type of scenario analysis to be conducted are summarized in sub-section 5.2.2.5 after the individual steps of the scenario methodology have been presented.

Identification of alternatives. Finally, while in conventional LCA, the alternative product systems (short "alternatives") are typically well-defined, the alternatives sometimes only become clear during scenario analysis in prospective LCA, since it is often the case that a technology that is currently at early design stages could be implemented in very different ways at a commercial scale. For example, as shown in Table 4, an early stage technology to produce bio-based ethanol could be implemented using two distinct designs, "Fermentation X" and "Fermentation Y", which have different process setups and, therefore, different flowcharts. Whether the steps A-D need to be performed for each alternative (2 in total) or each alternative-technology design combination (3 in total) will depend on how similar the technology designs are. For example, if a technology has an optional "acid recovery" stage, but is otherwise identical (as it the case in our example in), scenarios with and without acid recovery can probably be derived in the same causal loop diagram (CLD), consistency check, etc., as illustrated in the inventory analysis section. If, however, technology designs are fundamentally different, which typically also means that the important parameters are different, it may become too complicated to study these designs within the same diagrams and tables used during steps A-D. In that case, it is recommended to perform the steps A-D *separately* for each technology design.

Table 4. Alternative technology designs at present and in the future. If different future designs for the same technology are possible, it may be preferable to develop scenarios for each future alternative rather than for just "the incumbent" vs. "the novel" technology

#	Alternatives at ***present***	Alternatives in the ***future***	Flowchart	Scenarios
1	Bio-based ethanol (novel)	Bio-based ethanol (novel) – **design "X"**	A → B → Ethanol	For each row, scenarios should be developed
2		Bio-based ethanol (novel) – **design "Y"**	C → D → E → Ethanol	
3	Fossil based ethanol (incumbent)	Fossil based ethanol (incumbent)	F → G → Ethanol	

5.2.2 Inventory analysis

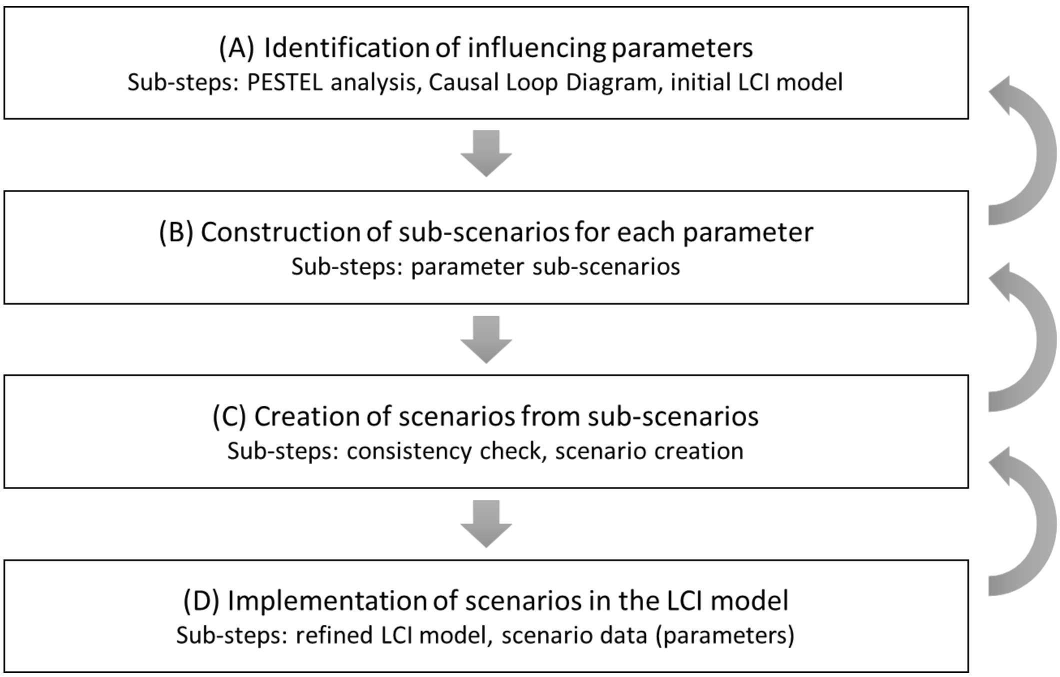
The core part of our methodology relates to scenario construction during the inventory analysis phase. It consists of a 4-step procedure that is to be carried out for each analysed alternative, as illustrated in Figure 8:

- In step (A), the relevant parameters that may influence the analysed technologies in the future are identified. For this we propose to approach the problem from two perspectives simultaneously: from the broader perspective of the real world (big picture) and from the perspective of the specific technology under investigation and its representation with in an LCI model.

- In step (B), sub-scenarios are constructed for each identified parameter, which means that potential developments and values for each parameter are recorded.
- In step (C), scenarios are created from the sub-scenarios constructed earlier.
- In step (D), the scenarios are implemented in an LCI model using, e.g., parameterization or other tools that LCA software may provide for modelling scenarios.

Please note the iterative nature of the 4 steps. The steps are discussed in the following sections.

Figure 8. A 4-step procedure for scenario development that is to be carried out for each studied alternative. Note the iterative nature of the 4 steps



5.2.2.1 Step (A) Identification of influencing parameters

Important influencing parameters can be identified in different ways, e.g.:

- By critically thinking about the product system
- By talking to technology developers or other stakeholders involved
- From the literature

PESTEL analysis. In addition to that there are structured approaches originating from market research to scan for macro-environmental factors. While several such approaches exist (and largely overlap in scope[3]), we pick out and recommend to use **PESTEL analysis**, which stands for:

- **P**olitical
- **E**conomic
- **S**ociological

[3] https://en.wikipedia.org/wiki/PEST_analysis

- **T**echnological
- **E**nvironmental
- **L**egal

In essence, the approach then consists of listing relevant parameters in each of these domains that may have an influence on the product system(s) under analysis. Depending on the scope and depth of the techniques applied during the PESTEL analysis can range from a simple brainstorming to including stakeholders and a systematic literature analysis as proposed just before.

Causal loop diagrams (CLD). As a next step, influences and correlations between identified parameters can be depicted as a causal loop diagram. CLDs are a powerful tool for scenario development as they help to:

- identify correlations between parameters that are not straightforward
- deal with the complexity of parameter interrelations
- reveal discrepancies and biases that might otherwise be overlooked
- add to transparency of the research, which is essential in LCA studies

CLDs may have the following **purposes** during a prospective LCA:

- <u>model development</u>: to support the development of the LCA model and scenarios by mapping relevant parameters and their interrelations, especially since CLDs can be developed "on paper", for which the burden is much smaller than implementing models in LCA software
- <u>communication</u>: to present to stakeholders how key parameters and their interrelations with the LCA model have (or have not) been included in the study

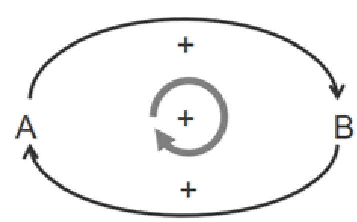
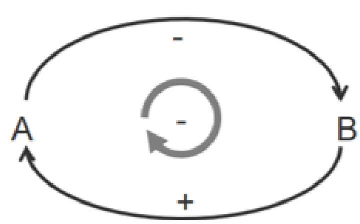
We propose to use the following conventions for CLDs (Table 5):

While a CLD may already yield useful information for a prospective LCA, one of the key challenges for the analyst may be to bring together the broader perspective that can be developed in a CLD with the specific implementation of an LCI model. Therefore, we propose to **combine a CLD with the flow diagram of an LCI model**, as illustrated in . We believe that this is a key element in constructing scenarios as it encourages the analyst to think from several perspectives simultaneously – the big picture, the technology under investigation, and its representation in an LCI model.

In the presented CLD we distinguish between surrounding parameters that are external to the LCI model (i.e. not quantitatively included) and technology parameters that quantitatively link to the LCI model and thus determine the values of inputs and outputs of foreground and background unit processes. Further, we believe that the distinction of parameters into foreground and background may be helpful when analysts use future background databases to represent the background system. The analyst has in that case the possibility to accept the future background databases as they are or to additionally modify certain processes in the background system – either approach should be clearly communicated.

Also partial or alternative representations of the content of this figure may be helpful to analysts. Ideally, the CLD helps to explain (a) which kind of parameters are considered qualitatively and quantitatively, and (b) how the parameters influence the LCI model. Our recommendation would be that one CLD diagram is developed for each studied product system.

Table 5. Proposed conventions for causal loop diagrams (CLD)

Aspect	Convention	Additional explanation
Interactions between parameters		
How parameters influence each other	$A \xrightarrow{+} B$	Positive influence (if A increases, B increases, and vice versa)
	$A \xrightarrow{-} B$	Negative influence (if A increases, B decreases, and vice versa)
	$A \xrightarrow{0/1} B$	Binary influence (A may enable the existence of B)
Feedback loops		Positive (reinforcing) feedback loop. If A increases, B increases, and in turn A increases, etc.
		Negative (mitigating) feedback loop. If A decreases, B increases, which in turn increases A, etc.

The **guiding questions** for developing the CLD diagram should be:

- **How could the surrounding parameters influence the technology?** To address this question, analysts may at first ignore the specific LCI model and think about the bigger picture, e.g. using PESTEL analysis, to come up with potentially important parameters (quantitative or qualitative) that could influence the specific technologies under study in the future.
- **Which are the important technology parameters?** To address this question, LCA analysts can use their own intuition, discuss with technology developers, and screen the literature.
- **How can these parameters be represented in the LCI model?** LCA analysts are typically not only working with constrained resources (time, money), but also with limited LCI models at hand. This means that while any LCI model can theoretically be developed, analysts often build their own models based on whatever data is available in the project or from existing databases. This means that not all important parameters that have been identified with the previous questions, may be included practically. For example, adapting the market shares of an electricity mix is relatively straightforward, while adding a

new future power generation technology may be not be feasible due to time and knowledge limitations. Further, LCI models are typically technology-focussed models that do not include socio-economic factors. The question is thus how the influence of possible developments in the surrounding parameters can be quantitatively included in the best way.

Initial LCI model. As outlined above, building scenarios based on a parameterized LCI model relies on a good understanding of the bigger picture as well as the specific LCI model. LCA analysts are therefore encouraged to develop CLDs and their scenarios “from both sides” (the bigger picture and the specific LCI model) as early as possible to understand on the one hand which parameters should be considered due to their importance and which parameters can be considered on the practical modelling level. Sometimes it may not be feasible to quantify the influence of surrounding parameters adequately in an LCI model. The CLD may also be used to communicate to stakeholders which surrounding parameters have *not* been considered in the study, although they may have an influence in the future (see dashed arrow in).

Finally, LCA is a fundamentally iterative process and there are various interconnections between different phases and steps when conducting LCA. For example, there is a connection between sensitivity analysis as part of the interpretation of LCA results and scenario generation: sensitivity analysis can inform the practitioner on the relevance of individual parameters and it can, therefore, also be used to identify important (or less important) model parameters. On the other hand, scenarios can be used as a method to further shed light onto uncertainties and sensitivities, see also sub-section 6.4.2.

In order to better illustrate the scenario methodology we use a case study on biopolymers from mango processing wastes (see Box 3) as an example.

Box 3. Description of case study for prospective LCA of biopolymer from mango wastes

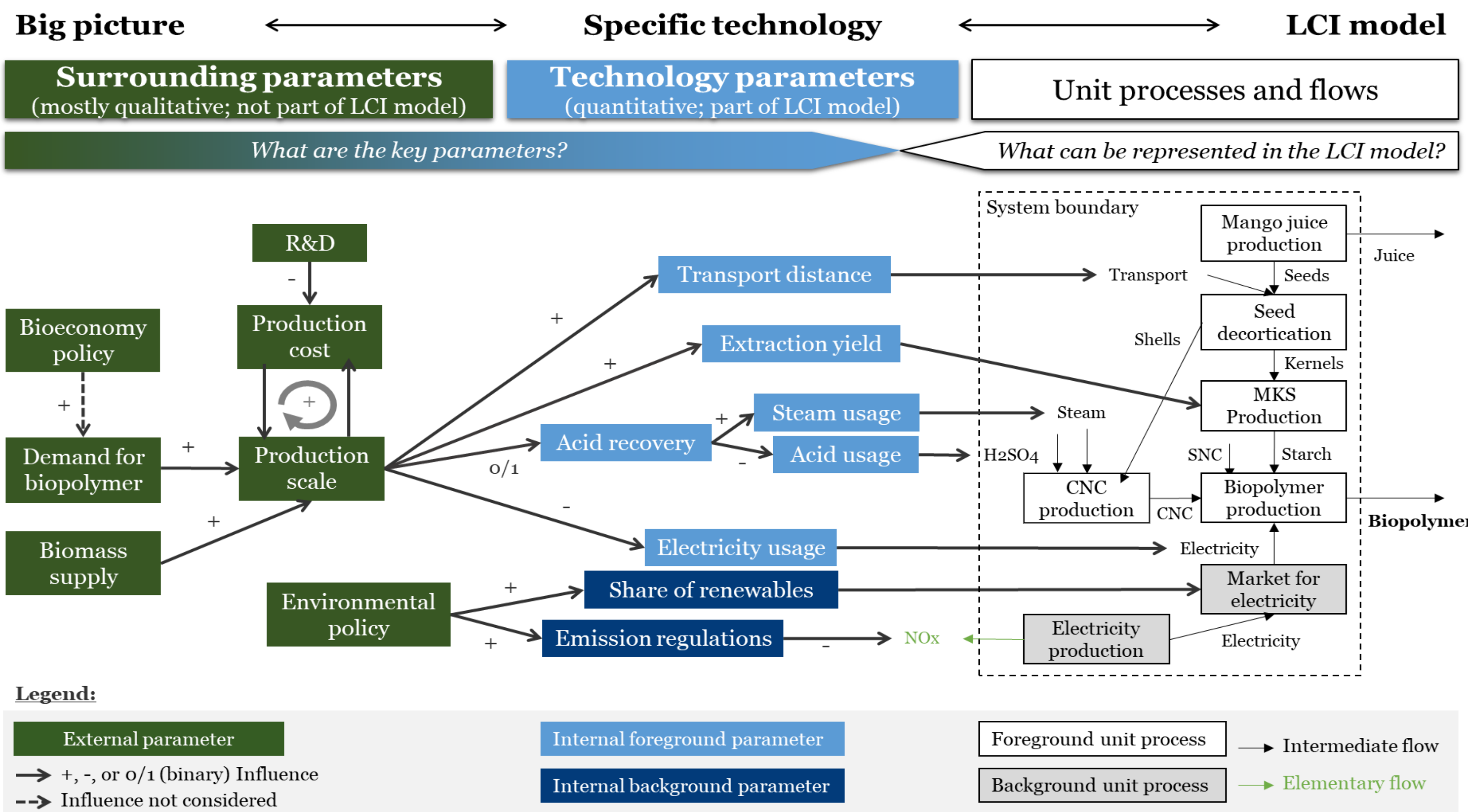
Case study: Biopolymer from mango processing wastes

Biopolymer films have been produced in experiments from several biological sources to find alternatives to fossil-based polymers for applications such as packaging, coatings, and agricultural mulch films; this includes innovative nano-reinforced materials with enhanced technical performance.

A biodegradable starch film was developed in the laboratory from the transformation of mango seeds– a waste from juice production– for food packaging. First, seeds were decorticated, i.e., separated into shells and kernels. Starch was extracted from kernels, and a small part was further processed into starch nanocrystals (SNC). Cellulose fibres were extracted from shells and then converted to cellulose nanocrystals (CNC) by acid hydrolysis. Finally, starch, plasticiser, CNC, and SNC were mixed to form the film by casting.

A prospective LCA was carried out to analyse the environmental impacts of the biopolymer film, currently at TRL 3 and expected to reach industrial production (TRL 9) by 2040. An initial LCI was built at industrial scale using process calculations based on the lab procedure; this model was the starting point for the scenario building and analysis.

Figure 9. Illustration of a Causal Loop Diagram (CLD) shown in conjunction with an LCI model. A core challenge for the analyst is to think big (left side), while at the same time understanding how important parameters can be modelled within the LCI model (right side)



Note that this diagram can include qualitative parameters for the bigger picture, quantitative parameters, as well as unit processes and intermediate and elementary flows for the LCI model. Additionally, a distinction between parameters influencing the foreground and background systems may be useful, especially when working with future background databases. The "0/1" means this is a binary choice. Alternative representations may be chosen if this is more effective for model development and) communication. (Other abbreviations: CNC = cellulose nanocrystals, SNC = starch nanocrystals, MKS = mango kernel starch).

5.2.2.2 Step (B) Construction of sub-scenarios for each parameter

Sub-scenarios for a parameter are specific manifestations of parameters under different narratives. Table 6 provides a few examples of how sub-scenarios could be defined for parameters for the case study described in Box 3 and .

Table 6. Examples of sub-scenarios for different parameter types used in (see also Box 3 for a description of the case study)

Parameter	**Type**	**Sub-scenario 1**	**Sub-scenario 2**	**Sub-scenario 3**	**Additional explanation**
Production scale	Qualitative/ Categorical	Small	Medium	Large	The number of sub-scenarios is specific for each parameter
Environmental policy	Qualitative/ Categorical	Liberal	Strict	-	
Acid usage	Qualitative / Categorical	Low	High	-	
Acid usage	Quantitative/ Numerical	0.1 kg / kg CNC	0.5 kg / kg CNC	-	Alternatively, if it can be easily quantified at this stage already
Share of renewables	Quantitative/ Numerical	20% wind 10% solar	30% wind 20% solar	-	
Share of renewables	Qualitative/ Categorical	Low	High	-	This could be a sufficient classification, when working with background scenarios

Note that, depending on the nature of the parameter, it may make sense to derive sub-scenarios as categorical data, e.g. for qualitative parameters, or as numerical data, e.g. for quantitative parameters. However, the analyst may also choose to define all parameter sub-scenarios as categorical data in a first iteration if a quantification would require additional work. Note also that it is not necessary to derive the same number of sub-scenarios for all parameters.

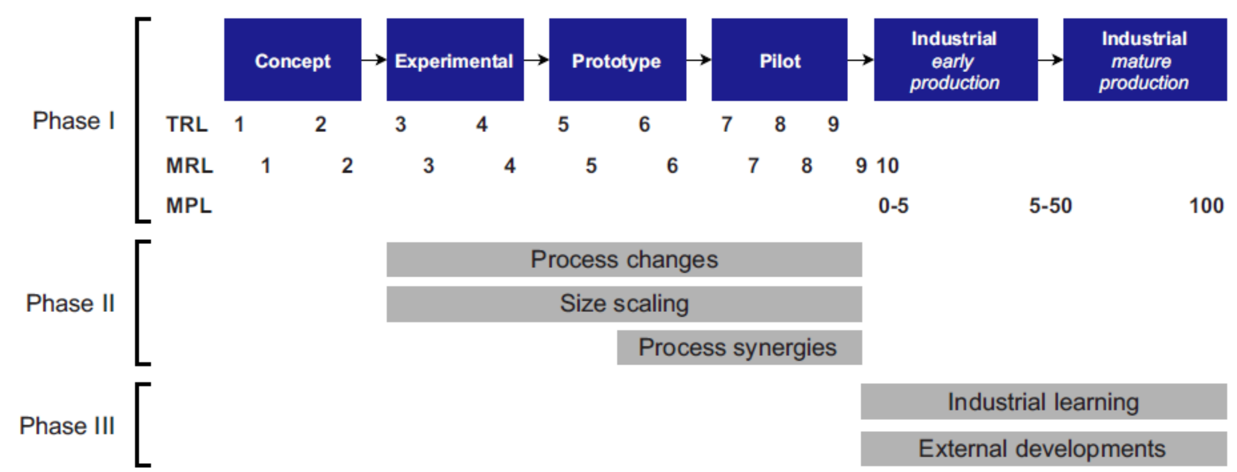
We have previously split the parameters into “surrounding parameters” that mostly qualitatively describe the bigger picture and “technology parameters” that quantitatively describe the technical parameters of the parameterized LCI model. Typically, the surrounding parameters are likely to influence the technology parameters rather than the other way around. For this reason, we recommend to start the construction of sub-scenarios for the surrounding parameters.

Sub-scenarios for surrounding parameters. Scenarios for surrounding parameters, such as GDP development or the development of the energy system are relevant for many studies and will most likely already exist, e.g. in so called 'framework scenarios'. Therefore, we recommend to first check the availability of framework scenarios that could be used to determine surrounding parameters. This will be advantageous for several reasons:

- Efficiency and effectivity: time can be saved by not repeating research that has been done before. Moreover, resources like time, knowledge and expertise might be higher in a study focusing on those scenarios specifically than when deriving them additionally in the context of a specific pLCA study.
- Transparency, credibility and reliability: framework scenarios are typically transparently documented and well defined, which gives them a certain credibility and reliability.
- Connectivity: it will be easier to use the results of a specific pLCA study in other studies or broader discussions if they are based on generally accepted assumptions or embedded into well-known framework scenarios.

Commonly used framework scenarios are, e.g., the Shared Socio-economic Pathways (SSPs; B C O'Neill et al., 2014), or projections by the International Energy Agency (e.g. IEA, 2021) the Intergovernmental Panel on Climate Change (e.g. IPCC, 2021) and other well-known institutions such as the Joint Research Centre (JRC) and the European Commission (EC). Ideally, such scenarios can provide data for all surrounding parameters. If this is not the case, data from different scenarios may be combined if they are deemed sufficiently consistent in terms of underlying narrative and assumptions. For parameters of the technology surroundings that are not covered by any previous studies or framework scenarios, new sub-scenarios have to be constructed for a pLCA study. Constructing a scenario usually starts with a narrative that later-on will have to be quantified. Though future scenarios themselves consist of assumptions, the best option to ensure their quality is to base them on all available knowledge. Gathering this knowledge should include reviewing literature as well as collecting expert opinions, e.g. by interviews, workshops or Delphi surveys.

Figure 10. Factors to consider when up-scaling (from van der Hulst et al., 2020). TRL = Technology Readiness Level. MRL = Manufacturing Readiness Level. MPL = Market Penetration Level

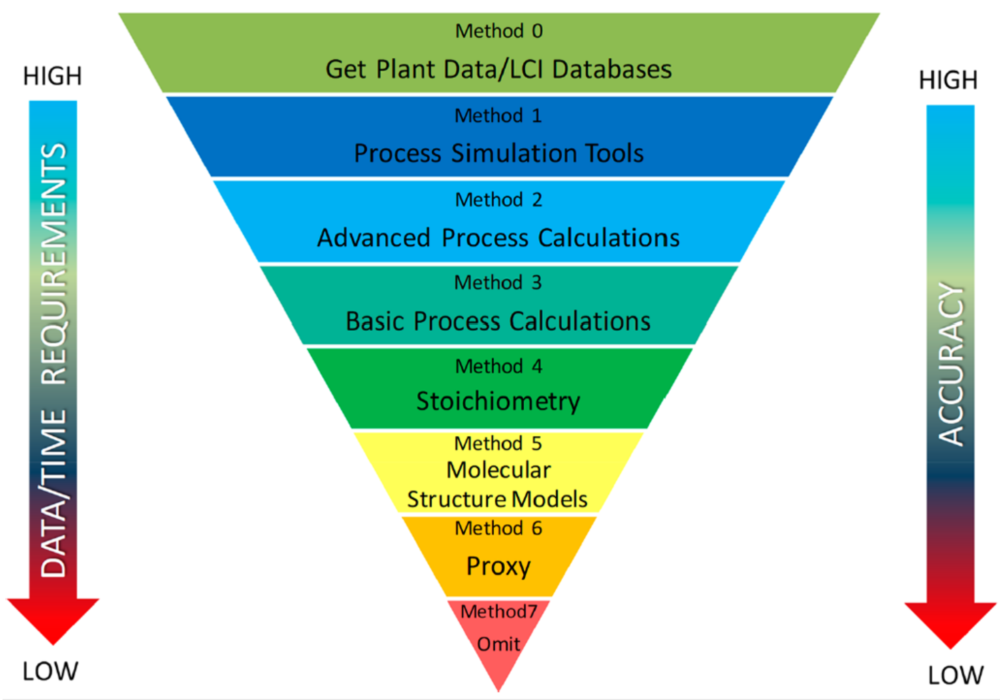


Sub-scenarios for technology parameters. Sub-scenarios for certain technology parameters may also be available from already existing framework scenarios. However, it should be kept in mind that the technology parameters should describe the potential development of the specific technology under study, which means that this data should primarily be developed within the pLCA study itself and best in collaboration with the technology developers (Tsoy et al., 2020). While it is difficult to give specific advice on how to do this, principal steps are likely to involve up-scaling and data estimation. Some (non-exhaustive) guidance for these two steps shall be given in the following.

Up-scaling. Prospective LCA looks at possible developments of a technology in the future. This typically involves the development of a technology from a lower to a higher TRL. The estimation of how the technology will look like at a more mature and usually also larger scale is referred to as up-scaling. Significant environmental improvements have been reported for up-scaled technologies (Gavankar, Suh, et al., 2015). Scaling relationships are sometimes used for this purpose (see e.g. Caduff et al., 2011, 2012, 2014). However, these are highly technology-specific and thus different up-scaling protocols may be required for different types of technologies, e.g. as proposed by Piccinno et al. (2016) for chemical technologies. Further, van der Hulst et al. (2020) provide additional guidance as to what to consider when performing upscaling (see Figure 10), including process changes, size scaling and synergies at earlier TRLs and learning at higher TRLs. Technological learning has been shown to be a relevant factor, especially over larger time scales and with large increases of cumulative production (see e.g. Louwen et al., 2016), however, it is still difficult to include this practically with in prospective LCA, especially for radically new technologies. A more comprehensive review of applied up-scaling approaches in different technological contexts has recently been published by Tsoy et al. (2020).

Data estimation. By data estimation, we mean approaches to derive unit process data for LCA, although we acknowledge that this is partially overlapping with (or complementary to) the purpose of up-scaling. Parvatker and Eckelman (2019) present a hierarchy of data estimation methods for LCA in general (Figure 11), which is, in principle, applicable to prospective LCA as well, although typically the method 0, i.e. "Get plant data" is not possible as plant data may not yet exist. The applicable methods thus range from process simulation and other kinds of process models (advanced/basic calculations) to using fundamental stoichiometric or thermodynamic data.

Figure 11. Data estimation methods for LCA (from Parvatker and Eckelman, 2019)



If that is not possible, data may be inferred from similar products/technologies directly or using molecular structure models (neural networks). If no approach for estimating data can be identified, it will not be possible to develop sub-scenarios for this specific parameter and it may have to be omitted.

5.2.2.3 Step (C) Creation of scenarios from sub-scenarios

Scenarios can be derived by choosing a set of parameter sub-scenarios (i.e. one specific value for each parameter). However, the analyst may face two problems at this stage:

a) The formal number of possible combinations of the different parameter sub-scenarios may be very high
b) Not all sub-scenarios may be consistent with each other (e.g. an ambitious environmental policy and a low share of renewables in Table 6)

While, technically, it may be feasible to screen a large number of scenarios, for analysis and communication reasons it may often be more desirable to work with a small set of diverse scenarios rather than a large set of similar scenarios. Performing consistency analysis can help to eliminate inconsistent parameter combinations and, thereby, already reduce the number of possible scenarios. At the latest at this stage, narratives should be developed to support the creation of scenarios.

Table 7. Cross-consistency matrix example for 4 parameters: Production scale, Environmental policy, Acid usage, and Share of renewables

	Parameter	**Production scale**			**Environmental policy**		**Acid usage**	
Parameter	*Sub-scenario*	*Small*	*Medium*	*Large*	*Liberal*	*Strict*	*Low*	*High*
Environmental policy	*Liberal*	3	3	3				
	Strict	3	3	3				
Acid usage	*Low*	3	2	1	3	3		
	High	1	2	3	3	3		
Share of renewables	*Low*	3	3	3	3	1	3	3
	High	3	3	3	1	3	3	3

<u>**Legend:**</u>

Inconsistent	1
Maybe consistent	2
Fully consistent	3

Consistency check. One way to check the consistency of scenarios is to critically evaluate whether a chosen set of parameter values makes sense when assessed against the previously developed CLD. A more formal way to check for consistency is to perform a cross-consistency assessment (CCA; Ritchey, 2015, 2013). In CCA a cross-consistency matrix is constructed to assess the pair-wise consistency between conditions, as shown in Table 7. Each coloured cell represents a pair-wise comparison of two parameter values. For example, with liberal environmental policy achieving a high share of renewables is evaluated here as "inconsistent", while a low share of renewables is "consistent". For a strict environmental policy, a high share of renewables is "consistent". For "production scale", an acid recovery is fully consistent only at large scale, but it may be consistent also at medium scale. Note that in principle a "consistent/not consistent" scale is sufficient to perform CCA, however any semi-quantitative scale (e.g. as defined here) is allowed. Our three-step scale here allows us to identify very likely vs. potential vs. unlikely parameter combinations and this information can be used during scenario construction.

Note also that "*if a particular pair of conditions is incompatible, or indeed in blatant contradiction, then all those configurations containing this pair of conditions would also be internally inconsistent*" (Ritchey, 2013). For example, if "share of renewables" and "emission regulations" were assessed against each other, all combinations could be assessed as "consistent". However, a *strict* "environmental policy" would lead to a *high* "share of renewables" and to *strict* “emission regulations” and vice versa. This means that even though there is no direct inconsistency between “share of renewables” and “emission regulations”, only specific combinations of these variables could co-exist in a scenario.

When assessing consistency, one may wish to distinguish different reasons for inconsistencies. Ritchey (2013) distinguishes three types of inconsistencies: logical contradictions (nature of concepts don’t fit), empirical inconsistencies (highly improbably or implausible on empirical grounds), and normative constraints (ethically or politically not possible). Ritchey emphasizes that normative judgements should not be included initially in the CCA in order to “*first investigate what is possible, before making judgements about what is, and what is not, desirable”* (Ritchey, 2013). Obviously, if the starting point of scenario creation is a normative one, normative inconsistencies must be included in the CCA.

Finally, it should be noted that while the previously developed CLD contains information on causality (which parameter affects which other parameter in which way), CCA is solely based on consistency and does not include any information on causality.

Scenario creation. Technically, analysts could stop after the consistency analysis and screen all internally consistent scenarios. Practically, most analysts probably aim to develop – also depending on the scenario type (predictive, explorative, and normative) – a small set of scenarios. Scenarios in turn are typically based on **narratives**, which describe the main features of a scenario and identify, e.g., the principal driving forces within a scenario. If narratives have not yet been developed, this is the step to define them. In order to facilitate comparative prospective LCA, the narratives should be general enough so that fitting parameter sub-scenarios can be created for each alternative that is to be compared. Once the analyst has defined parameter sub-scenarios for each alternative within each scenario, the scenario creation step is finished.

We do not provide a specific procedure of how analysts should develop narratives and scenarios, and select parameter sub-scenarios. Often analysts will already intuitively know which scenarios would be interesting to assess. However, the following additional considerations may be useful to the analyst in this process:

- It is recommended to write down the narratives as accurately as possible in order to support the choice of parameter sub-scenarios for each alternative
- It is also recommended to involve stakeholders (e.g. technology developers) during relevant steps of scenario development, e.g. when key parameters are identified, sub-scenario values determined, and the narratives and final scenarios selected, e.g. through workshops
- While the development of narratives may include technology-specific considerations, it is advised to develop narratives that are consistent with broader framework scenarios, or, e.g., the narratives behind future background LCI databases; this may not only strengthen the narrative, but also facilitate comparisons with other pLCA studies
- Cornerstone scenarios may help in the case of an explorative assessment to assess scenarios at the edge of the solution space (e.g. a best or worst-case scenario)
- The development and analysis of scenarios, thus steps A-D, should be seen as an iterative process rather than a linear one
- The use of morphological fields, as described by Ritchey (2013) may be a useful approach to select consistent parameter sub-scenarios for a given scenario, see example in Table 8

Table 8. The use of morphological fields may facilitate the creation of scenarios from a selection of parameter sub-scenarios. Morphological fields list all sub-scenarios for each parameter, which breaks down even highly multi-dimensional problems into a simple table (Ritchey, 2013). A colour coding can be used to specify drivers (here in red) and remaining consistent sub-scenarios (here in blue), which may help the scenario creation process. Here the scenarios are driven by the environmental policy (red cells identify the driver(s); blue cells indicate consistent parameter sub-scenarios). A) shows the case where only production scale is defined as driver, permitting all other parameter sub-scenarios except for low acid usage. B) shows a "worst case" scenario of small production scale and liberal environmental policy and c) a "best case" scenario.

a)

Production scale	**Environmental policy**	**Acid usage**	**Share of renewables**
Small	Liberal	Low	Low
Medium	Strict	High	High
Large	-	-	-

b)

Production scale	**Environmental policy**	**Acid usage**	**Share of renewables**
Small	Liberal	Low	Low
Medium	Strict	High	High
Large	-	-	-

c)

Production scale	**Environmental policy**	**Acid usage**	**Share of renewables**
Small	Liberal	Low	Low
Medium	Strict	High	High
Large	-	-	-

The final result of scenario creation could be a table as shown in Table 9, which lists the specific parameter sub-scenarios for each scenario.

Table 9. Description of selected parameter sub-scenarios for all scenarios

Parameter	*Sub-scenario*	Scenario 1 "worst case"	Scenario 2	Scenario 3	Scenario 4 "best case"	...
Production scale	Small	x		x		
	Medium					
	Large		x		x	
Environmental policy	Liberal	x	x			
	Strict			x	x	
Acid usage	Low		x		x	
	High	x		x		
Share of renewables	Low	x	x			
	High			x	x	

5.2.2.4 Step (D) Implementation of scenarios in the LCI model

Once the scenarios have been fully defined, they can be operationalized within an LCI model. This requires that the LCI model has been constructed in a way that it can represent the relevant parameters and that the scenario data is provided in a way that it can efficiently be included in the LCA software.

Refined LCI model. Any LCI model fundamentally consists of unit processes and flows. Flows are typically further distinguished into elementary and intermediate flows, describing interactions of processes with the environment and with other economic activities, respectively (ISO-14044, 2006). In addition, LCA software often allows for parametrization by providing the possibility to use variables and formulas instead of numbers only to describe the inputs and outputs of processes. For the implementation of scenarios in LCA software, we thus dispose of the following means:

- The use of alternative values for flows (elementary and intermediate)
- The use of alternative values for parameters that have been set up to represent specific relationships between flow values

Both approaches to model scenarios can be realized with existing LCA software in one or the other way. Here, we refrain from explaining how this can be done within a specific LCA software.

Scenario data. Although there are, as outlined above, different ways of including scenario data into an LCI model, we believe that it is very useful to gather and represent all scenario data within a single, or possibly a set of, tables. Essentially, it requires a full quantification of all parameter sub-scenario values that are part of the LCI model. For the case shown previously (see), this means a quantification of all parameters that are part of the LCI model for each scenario, as shown in Table 10. The surrounding parameters are *not* included in this table as they are not quantitatively included in the LCI model. Instead, they serve the purpose of scenario creation and definition of meaningful parameter sub-scenarios for the technology parameters (see for a disambiguation of both types of parameters).

Table 10. Quantified parameter sub-scenarios ready to be included in LCA software. Note that we have only quantified selected parameters here, but the full set of parameters needs to be quantified to conduct scenario analysis

Parameter	**Unit**	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 4**	**...**
Acid usage	kg / kg CNC	0.5	0.1	0.5	0.1	...
Wind power share	%	20%	20%	50%	50%	...
Solar power share	%	10%	10%	40%	40%	...
Electricity use	kWh	...	...	...	...	...
Transport distance	km	...	...	...	...	...
Extraction yield	%	...	...	...	...	...
Steam usage	MJ	...	...	...	...	...
Electricity use	kWh	...	...	...	...	...
NOx emissions	kg	...	...	...	...	...

Future background scenarios. When the analyst works with LCI databases that represent future background scenarios (see also sub-section 5.2.1) it may be, as illustrated in , that certain parameters are already included in these scenarios. In this case, certain parameters may not need to be explicitly modelled within the foreground LCI model and in those cases it is sufficient to describe the background parameters qualitatively and potentially list them in a separate table. For example, future background databases as generated from a combination of ecoinvent and the IMAGE model (Mendoza Beltran et al., 2020) could be used, e.g. making use of the superstructure approach (Steubing and de Koning, 2021), in LCA software to represent scenarios of future energy generation. In this case, the analyst should select the scenarios that best correspond to the previously determined parameter sub-scenarios "low/medium/high" for the "share of renewables" as shown in Table 11. Obviously, in this case "wind power share" and "solar power share" should not be included in Table 10. Sensitivity analysis could be performed to further analyse the role of the background data on the final LCA results, e.g. by using no future background scenario or conservative vs. optimistic ones against the same foreground data.

Table 11. A separate table for the description of parameters that are covered through the use of future background scenarios (examples here)

Parameter	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 4**	**...**
Share of renewables	*SSP2-base*	*SSP2-base*	*SSP2-2.6*	*SSP2-2.6*	...

5.2.2.5 Differences in the execution of the 4-step methodology depending on the scenario type

This section reflects on the different types of scenario analysis that can be performed (predictive, explorative, and normative) based on the steps A-D of the scenario development as described above. Table 12 provides a summary.

In a **predictive** scenario analysis, the question is "how *will* the future develop?" This means that, normally, only a single scenario is to be developed. Important parameters (step A) will be identified as for all other types of scenario analysis. However, only one set of parameter sub-scenario values will be determined for the single scenario. These values will be determined based on best-available knowledge about the future development of the specific technology and the wider technological context. Methods like forecasting and time series extrapolation may be applied, as well as other up-scaling and data estimation methods described in step (B). Finally, only one LCI model needs to be developed and parametrization is likely not necessary as the parameter sub-scenario values could directly be entered.

Table 12. Differences in the execution of the 4-step methodology depending on the scenario type

Scenario type	**Predictive**	**Explorative**	**Normative**
Perspective on scenario development	How ***will*** the future develop?	How ***could*** the future develop?	How ***should*** the future develop?
Steps for scenario construction			
(A) Identification of influencing parameters	Which parameters are relevant for answering the research question?		
(B) Construction of sub-scenarios for each parameter	One expected scenario for each parameter; methods may involve forecasting and extrapolation	Several sub-scenarios for each parameter to explore the solution space; methods may involve "what-if" analyses	One scenario is sufficient, but several are possible; backcasting methods: how each parameter needs to develop to reach the vision
(C) Creation of scenarios from sub-scenarios	Steps (B) and (C) are essentially a single step as only one scenario is developed; however a consistency check is recommended to avoid inconsistent parameter sub-scenarios	Many formally possible combinations of sub-scenarios. Consistency check reduces number, but further scenario creation, including narratives, is necessary if a small set of diverse scenarios is to be created; cornerstones may help	Consistent combinations of normative sub-scenarios that describe plausible pathways to the vision
(D) Implementation of scenarios in the LCI model	One LCI model; values could be entered directly	One or several LCI models (likely parameterized)	

In an **explorative** scenario analysis, the question is "how *could* the future develop?". This means almost by definition that several scenarios will be developed to explore possible future developments of the technology and its surroundings. The nature of explorative scenario may be quite different and range from an assessment of very extreme scenarios (e.g. best case and worst case) and "what-if" type of analyses to more likely developments that follow plausible narratives. Parameter sub-scenario values will have to be derived using methods, such as described in step (B). This may lead to a potentially very large number of scenarios, which has subsequently to be reduced, unless the approach is to brute force calculate LCA results for all scenarios. Consistency checks and the use of narratives are excellent tools to derive a small set of diverse scenarios. Parametrization of the LCI model is generally recommended to include the scenario data efficiently into the LCA software. Multiple LCI models may be required.

In a **normative** scenarios analysis, the question is "how *should* the future develop?". Here, the perspective is that of a manifested vision in the future and the question is which scenario(s) can lead in a plausible way to the realization of the vision. Therefore, the method of backcasting may be applied to define parameter sub-scenarios backwards from the desired future state to the present. It is conceivable that several scenarios lead to the future vision. Consistency checks are recommended, including normative constraints (e.g. of ethical or political nature). If several scenarios are assessed, a parametrization of the LCI model may be advantageous. Multiple LCI models may be required.

Finally, **hybrid scenario analyses** are also possible. A well-known example are "best / likely / worst" case scenarios, which include both explorative elements (best and worst cases) and predictive elements (likely case). Another example could be the evaluation of an up-scaled technology (thus a single foreground scenario) against multiple general futures (background scenarios), which combine aspects of predictive (foreground technology development) and exploratory (background system) scenario analyses. Also, practitioners may of course also develop several scenarios in a predictive setting, in which case the differences between the scenarios would probably be smaller than in an explorative context.

5.3 Discussion

The presented scenario approach should be seen as a suggestion for LCA analysts presenting a toolbox rather than a methodology that needs to be meticulously followed. For example, depending on the exact case and the preferences of the analyst, it may be helpful to change the order of the steps A-D (especially since this should be seen as an iterative process). It may make perfect sense if analysts prefer to start with the development of narratives and scenarios before developing parameter sub-scenarios. Further, analysts may choose to skip the consistency check, if, for example, the problem is small enough to avoid potential inconsistencies intuitively in the development of narratives and parameter sub-scenarios.

Beyond the field of LCA, a large variety of scenario development approaches are practiced, including approaches to organize mental models, such as General Morphological Analysis (GMA; Ritchey, 2013), from which we have also borrowed, System Dynamics, Influence Diagrams and Delphi methods to more quantitative approaches to build scenarios, such as Formative Scenario Analysis (FSA; Scholz and Tietje, 2002). Both GMA (Delpierre et al., 2021) and FSA (Spielmann et al., 2005) have been applied in the LCA context previously, although in general LCA studies tend not to strongly rely on specific scenario approaches. We encourage LCA analysts to look into this literature and borrow, if it supports their work, from other scenario approaches as well. Regardless of the approach, it will strengthen the scientific foundation of a prospective LCA study if the scenario generation approach is sufficiently and transparently described. This is also where the methodology presented here can make a contribution to future prospective LCAs, i.e. both for developing scenarios as well as for communicating and transparently reporting the underlying data and assumptions.

For further inspiration on scenario construction and scenario approaches, readers shall be referred, e.g., to Kosow and Gaßner (2008), who describe five basic steps of scenario construction as follows: 1) identification of the scenario field, 2) identification of key factors, 3) analysis of key factors, 4) scenario generation, and, if necessary, 5) scenario transfer. When related to the scenario methodology as presented here, step 1 would relate to the goal and scope definition phase of LCA, while steps 2-5 could be related to the inventory analysis phase.

6. Uncertainty and Sensitivity Analysis for bio-based product systems

6.1 Background

The importance of considering uncertainty and sensitivity of model results when making decisions is widely acknowledged (Funtowicz and Ravetz, 1990). Lipshitz and Strauss (1997) describe uncertainty as an indispensable ingredient of decision-making. In the context of LCA, the treatment of uncertainty increases the reliability and credibility of results (Igos et al., 2018), and this is especially the case when using LCA prospectively, thus when future states of the product system are under scrutiny. In this section of the report, we zoom in onto the modelling of uncertainty analysis (UA) and sensitivity analysis (SA) for bio-based products at low TRLs, with a focus on how to model uncertainty and on how to characterize uncertain data in LCA models. While both UA and SA are recommended at the life cycle interpretation step, they are rooted in all other life cycle assessment phases (Guineé, 2002). ISO-14044 prescribes that the interpretation of LCA studies "shall include an assessment and a sensitivity check of the significant inputs, outputs, and methodological choices to understand the uncertainty of the results" (see clause 4.5.1.1; ISO-14044, 2006). In this section, after reviewing and condensing recent updates in the relevant literature on the classification of uncertainty and sensitivity, we propose a stepwise approach, which guides the analyst using prospective LCA to locate uncertain inputs across LCA phases, characterize uncertainty, qualitatively assess important sources of uncertainty, quantitative treat uncertainty with UA and SA, and finally communicate the qualified and quantified uncertainty in the results.

The remainder of this section of the report is organized as follows. We provide a general introduction to the state-of-the-art on the classification of uncertainties, and conclude with a step-by-step approach to locating, identifying, characterizing, ranking and finally addressing uncertainties in the LCA of bio-based products. We conduct a case study to illustrate the approach.

6.2 Classification of uncertainties in LCA models: integration of the state-of-the-art

In this sub-section, we provide a brief overview of the state-of-the-art on the classification of uncertainties, which we combine in

Figure 12 following proposals from the relevant literature and adapt to the needs of the LCA analyst assessing bio-based products.

While a variety of definitions are available in the literature (see also Lloyd and Ries, 2008), in this report we follow Cucurachi et al. (2021) and Igos et al. (2018) and define UA as the quantification and propagation of input uncertainties to output uncertainties. Considering this definition, UA is concerned with the collection of uncertainty data (e.g., probability distributions) of the input variables, as well as the propagation into uncertain model results (Morgan et al., 1992). In LCA, uncertainty can be related to input data that are uncertain (for instance, the effects of a herbicide, such as paraquat, on biodiversity are not fully known), to input data that are variable (for instance, the yield of two identical fermentation processes is not exactly equal), and to choices that must be made by the analyst (for instance, related to the choice of mass-based or economic allocation; see also Heijungs, 2020). Besides, data may be missing and therefore estimated, introducing new uncertainties. To adequately propagate and treat uncertainty, one should understand the individual contributions to uncertainty, what defines an uncertain input to an LCA model, and how uncertainties can be classified.

We start with three main dimensions of uncertainty: the **nature**, **location,** and **level** of uncertainty (Walker et al., 2003). The **nature** of uncertainty refers to how the source relates to reality and is either *epistemic* (e.g. lack of knowledge) or *ontic* (e.g. randomness of reality, or variability). Epistemic uncertainty includes the lack of data, which is a major issue especially for emerging (bio-based) technologies, where data might not yet exist, or might be proprietary and unavailable (we further refer the reader to Baustert, 2021; Huijbregts, 1998; Huijbregts et al., 2001, 2004). Additional uncertainties that are also epistemic in nature and can play a major role for bio-based products are those added by the analyst that models the system. Mistakes and inaccuracies can, for instance, regard the selection of an indicator towards an area of protection, the use of a wrong background substance, or the use of a wrong unit (Baustert, 2021; Björklund, 2002). In this context, ambiguity is also seen as subset of epistemic uncertainty (Baustert, 2021; Warmink et al., 2010). Ontic uncertainties describe the randomness or the inherent variability of the real world, which can be spatial, temporal or between sources and objects. Population-density, water- availability or regional-variability are examples of spatial variabilities. Seasonal, weekly and daily variability in e.g., emission profiles and the corresponding environmental burdens are examples for temporal variabilities (Baustert, 2021; Igos et al., 2018). Variability between sources and objects can be, for example, various technologies having the same function (Huijbregts, 1998).

The **location** dimension describes where the uncertainty is found in the LCA model. We do not refer here to any spatial/geographic feature of the model, but rather to the phase of the LCA model, in which uncertainty can be found. To this end, we can refer to the proposed three aspects of Igos et al. (2018): quantity, model structure and context. Quantity refers to the uncertainty of data used for LCI or LCIA. It should be stated that current LCIA methods are typically not provided with uncertainty ranges (Igos et al., 2018). The model structure, model inputs or model variables account for the uncertainty in the representativeness of the reality of the LCA model. While a higher complexity of the model reduces the structural uncertainty of the model, the implementation in the model of specific realistic conditions can increase the quantity uncertainty (van Zelm and Huijbregts, 2013). The last subcategory, context, applies only to the goal and scope phase and describes the uncertainty caused by the normative choices of LCA analysts. These decisions or assumptions need to be stated in the LCA report (ISO-14044, 2006).

The last dimension is the **level** of uncertainty. Here, we can refer to the adapted classification of Walker et al. (2003), and reported in Kwakkel et al. (2010): *shallow*, *medium* and *deep uncertainty* and lastly *recognized ignorance*.

The first level can be described using probabilities, which means that representative statistical data are available. Medium uncertainty, on the other hand, describes the uncertainty where other states or scenarios can be determined and also ranked according to their likelihood. The same applies to deep uncertainty, except that in this case the alternatives cannot be ranked, i.e. no likelihood can be determined. The last level describes the highest uncertainty and is called recognized ignorance, which describes the uncertainty of not knowing, also known as the sample space ignorance (Giang, 2015). Thus, no scale of measurement can be attached to a specific input to a model or a specific realization of a scenario. In general, the level of uncertainty relates to the information and data available to describe the location subcategories quantity, model structure and context (Igos et al., 2018).

Figure 12. Classification of uncertainty. Uncertainty dimensions are chosen according to Walker et al. (2003) and level subcategories adapted after Kwakkel et al. (2010). Location subcategories are according to Igos et al. (2018). For the uncertainty nature ambiguity (Warmink et al., 2010) is seen as subset of epistemic uncertainty (Baustert, 2021).

DIMENSION			Uncertainty examples	Goal & Scope	LCI	LCIA
	Nature	**epistemic** (knowledge uncertainty/ uncertainty)	• accuracy or representativeness of an indicator towards an area of protection			X
			• data availability/ representativeness of background processes used		X	
		ontic (variability uncertainty/ aleatory uncertainty/ variability)	• variability of performance characteristics (are the functional units comparable?)	X		
			• variability of characterization factors (CF)			X
	Location	**quantity** (inputs and parameters)	• representativeness of data used for each flow		X	
		model structure (structure, parameters and variables)	• variability of LCIA indicator relationships			X
		context (modelling context and experimental frame)	• technological representativeness	X		
	Level	**shallow uncertainty** (probability distributions)	• representative statistical data available			
		medium uncertainty (rank ordered scenarios)	• multiple possible futures or alternative model structures (perceived likelihood)			
		deep uncertainty (probability measure ignorance)	• multiple alternatives without being able to rank order the alternatives			
		recognized ignorance (sample space ignorance)	• uncertainty where no alternative states can be determined			

6.3 Classification of sensitivity analysis

The most commonly used classification available in the literature for SA distinguishes two type of analyses: local and global (Razavi et al., 2021). Local approaches to sensitivity (LSA) refer to the variation of one input of an uncertain model around its reference point, keeping the others at their nominal values (Igos et al., 2018). Conversely, Saltelli et al. (2008) define global sensitivity analysis (GSA) as the study of how the uncertainty in the output of a mathematical model can be apportioned to different sources of uncertainty of its inputs. Further classifications and segmentation of SA can be identified by focusing on the size of the change (i.e. small change around the nominal value of an uncertain input, or change along the full range of an uncertain input) and the type of change (i.e. involving all input parameters simultaneously or only one parameter at a time).

We further refer the reader to the work of Razavi et al. (2021) on SA in general, and to the work of Cucurachi et al. (2021), Igos et al. (2018), and Groen et al. (2017) for the application of SA and GSA in LCA.

6.4 Definition of a stepwise approach

On the basis of the identified classifications, we propose here a stepwise approach (Baustert, 2021; Heijungs et al., 2019; Henriksson et al., 2015):

(i) uncertainty location and identification by LCA phases,
(ii) uncertainty characterization,
(iii) qualitative importance ranking,
(iv) treatment of uncertainty,
(v) uncertainty communication.

We remind the reader and analyst that the above steps are iterative in nature, as additional intuitions after performing the analyses can require the analyst to revise some modelling choices. We describe next the steps of the approach.

6.4.1 Step (i): Location and identification

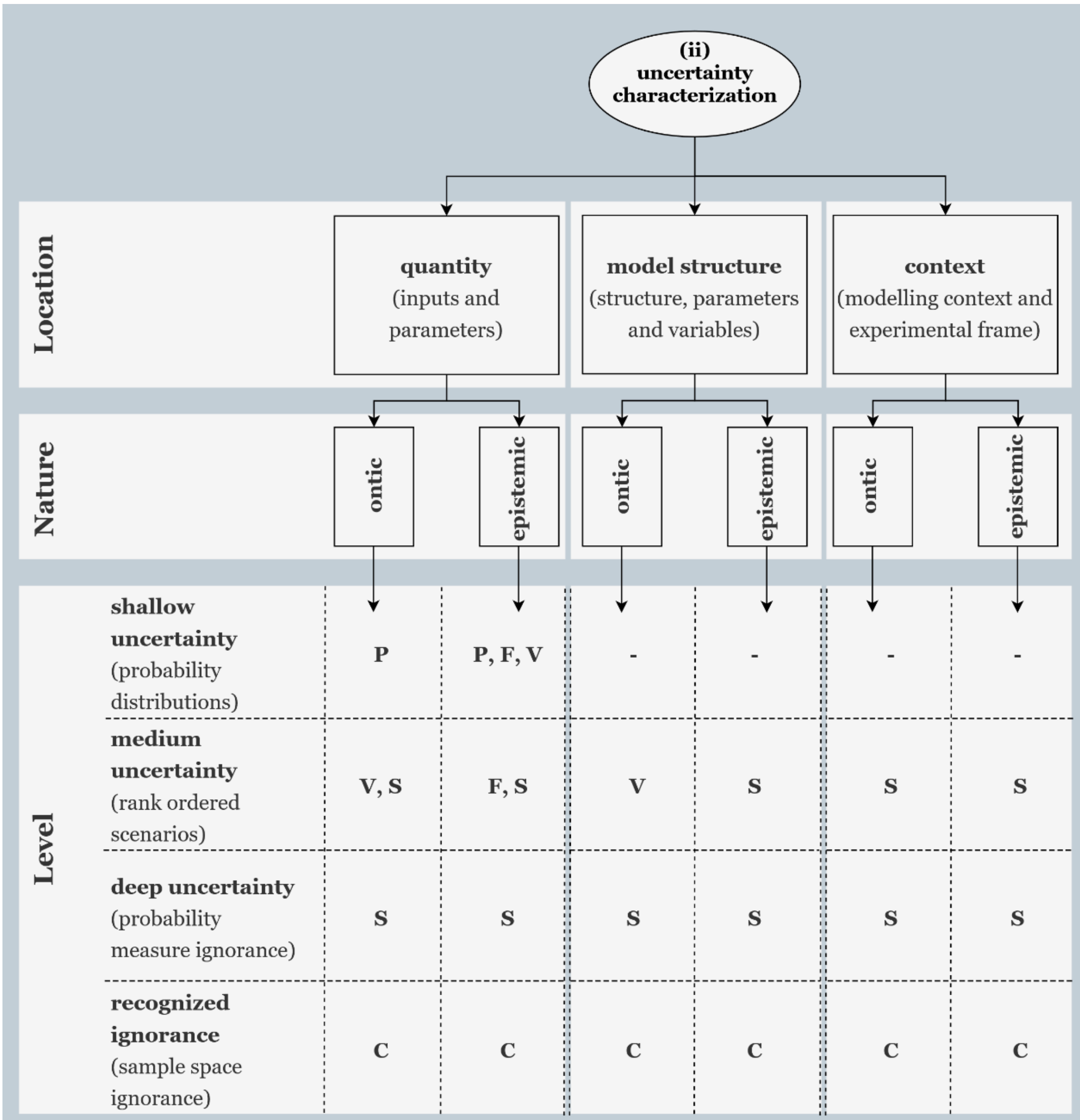
The analyst assessing a bio-based system should start with (i) localizing the sources of uncertainty in the various LCA phases (also indicated by examples in

Figure 12). Igos et al. (2018) provide a list of examples of uncertainty sources according to the most relevant LCA phase, and divide such sources into nature and location subcategories. Blanco et al. (2020) also list different uncertainty types according to the LCA phases that are most relevant to them, with a focus on emerging technologies that also applies to BbPs. We refer the reader to these works for additional details: Anderson et al (2015), Wardekker et al. (2013) and Rosenbaum et al. (2018)

6.4.2 Step (ii): Characterization

After finding the location of uncertainty in the various LCA phases (step i), the analyst moves onto characterizing the uncertainty. According to Igos et al. (2018), uncertainty can be expressed by (P) *probability distribution* (requires data and can include correlations), (V) *variance* (more easily estimated), (F) *fuzzy sets* (translate expert opinions into uncertainty ranges) and (S) *multiple scenarios* (depends on expert judgment).

Figure 13. Decision tree for uncertainty expression. Uncertainty dimensions are chosen according to Walker et al. (2003) and level subcategories adapted after Kwakkel et al. (2010). Location subcategories are according to Igos et al. (2018). For the uncertainty nature ambiguity (Warmink et al., 2010) is seen as subset of epistemic uncertainty (Baustert, 2021). The following abbreviations are used to guide the analyst to an appropriate uncertainty expression: (P) probability distribution, (V) variance, (F) fuzzy sets, (S) multiple scenarios and (C) uncertainty communication only



To combine the expression of uncertainty with the three dimensions of uncertainty (see

Figure 13), an additional expression is introduced: (C) *uncertainty communication only*, which requires the analyst to communicate the uncertainty at the various identified locations, without a quantitative characterization. If the uncertainty is in the model structure or context, they are characterized by defining alternative scenarios. This opens the possibility to compare LCA results for different combinations/assumptions (e.g. different suppliers, spatial resolutions or allocation methods).

Uncertainties inherent in the model structure should not be modelled probabilistically, but quantity uncertainties can be modelled in several ways (Morgan et al., 1992). For example, if they are epistemic in nature (second decision tree branch in

Figure 13), they can be modelled using fuzzy set theory (Igos et al., 2018). The further division into ontic and epistemic nature is also relevant, especially for bio-based products. Bio-based products are subject to environmental conditions that lead to great variability (Milà i Canals et al., 2011). A comparative life cycle assessment of biofuels with fossil fuels shows that ontic uncertainties are more prevalent for biofuels and epistemic uncertainties for fossil fuels (Michiels and Geeraerd, 2020). The degree of uncertainty can indicate whether the uncertainty can be controlled and quantified, i.e., whether it can be described either quantitatively (numerically) or qualitatively (here indicated with (C) uncertainty communication only; Baustert, 2021).

6.4.3 Step (iii): Importance ranking

Step (iii) sets the focus on the main sources of uncertainty with the intention of limiting the investment of time and modelling resources on the less important sources, while still keeping the analysis qualitative in nature. Given the size of LCA models, a qualitative approach is advised at this stage to identify those input factors to the LCA model that can fade into the background of the analysis. A suitable qualitative method is proposed by Baustert (2021), which adapted the key-issue matrix of Hauschild et al. (2018) to rank the location of the sources of uncertainty according to their degree of importance. As a result, step (iii) helps prioritize the various uncertainty locations, allowing the analyst to refine and continue the quantitative investigations on uncertainty using a limited set of inputs, and a limited set of locations.

6.4.4 Step (iv): Treatment

The following step (iv) treatment is conditioned by the previous steps. At this stage, the analyst should work on the quantitative investigation of uncertainty, using quantitative techniques of UA and SA. The treatment phase may also be limited by the available LCA tools and software and by the expertise of the analyst. Here, we further focus on a specific interpretation of UA, which focuses on the propagation of uncertainty from inputs to outputs.

We define treatment in the context of the stepwise approach as the phase in which the analyst attempts the following (Heijungs et al., n.d.; in prep.):

- UA, or the collection of uncertainty data (e.g., probability distributions) of the input variables, as well as the propagation of these into uncertain model results,
- SA, or the study of the response of a model output when one or more input variables are changed, and the subsequent study of how the input uncertainties contribute to the output uncertainty.

As earlier mentioned, both are complementary, e.g. SA can assess the contribution to variance after uncertainty propagation; we summarize the most common methods for UA and SA in Table 13 (after Igos et al., 2018).

Table 13. Methods for uncertainty propagation and sensitivity analysis (Igos et al., 2018). Uncertainty should be expressed by (P) probability distribution, (V) variance, (F) fuzzy sets, (S) multiple scenarios or (none) no expression/characterization needed.

Method groups	Available methods	Characterization (expressed by)	What is needed?	Result/ output
Uncertainty propagation	Monte Carlo sampling (MCS)	P	Distribution type (e.g. log-normal, triangular) and central values (e.g. mean, dispersion, standard deviation	Probability distribution of environmental impact (e.g. comparison of dispersion between two studies)
	Advanced sampling	P	Distribution type and central values; additional software (e.g. Oracle Crystal Ball, MATLAB, SimLab)	Probability distribution
	Analytical resolution	V	Variances of the uncertain inputs and first order Taylor approximation (only available in CMLCA)	result variance as a function of the variances of the inputs and their covariance (standard deviation)
	Fuzzy logic	F	Core value, the upper and lower bound of the possibility function and the possibility function type of each input variable	Environmental impact core value with possibility function and upper and lower bound
	Hybrid approach	P and F	See sampling methods and fuzzy logic	See sampling methods and fuzzy logic (increase in reliability and information)
Sensitivity analysis	One-at-a-time (OAT)	None, P, V or F	Variation ranges (arbitrary variation, standard variation)	Model robustness towards input parameters
	Marginal analysis	None	Partial matrix-based derivatives (only available in CMLCA)	Partial derivatives represented by sensitivity coefficients
	Key issue analysis (KIA)	V	Variances of the uncertain inputs; first-order approximation of the Taylor series	The decomposition of the uncertainty of an output result in terms of contributions by the uncertainties of the input data
	Method of Elementary Effects (MoEE)	P, V or F	Series of trajectories in the space of the inputs	Output sensitivity to variations of inputs; identification of non-influential inputs
	Correlation analysis	None	Based on the sampled results from uncertainty propagation (e.g., Monte Carlo sampling)	Sensitivity index; ability to detect correlation for non-linear models
	(e)FAST/ Sobol	P	Distribution type and central values; additional software (Simlab or R)	Ignores correlations with inputs (significance and interaction effects)
	Moment independent Global Sensitivity Analysis	P	Distribution type and central values (Brightspace 2.0 and Activity Browser)	Considers correlations with inputs (importance and interaction effects)
Both	Scenario analysis	S	Multiple conceptual models and expert judgment	Usually, output ranges from best (optimistic) to worst (pessimistic) case

Monte Carlo sampling (MCS; Brömssen and Röös, 2020) is the most commonly applied uncertainty propagation method in LCA (Groen et al., 2014; Hauschild et al., 2018; Igos et al., 2018). Based on the law of large numbers, Monte Carlo algorithms obtain numerical results by repeated random sampling (pseudo-randomness) to solve intractable or very large mathematical problems. For comparative LCA studies, the resulting probability distribution form the basis of paired comparison and hypothesis tests (Mendoza-Beltran et al., 2018). MCS is implemented in almost all LCA tools (Hauschild et al., 2018), but needs a high number of simulation runs. The identification of which uncertainty data the analyst decides to propagate typically differs by LCA phase. At the LCI phase, a distinction can be made between background system and foreground system. The most commonly used database for background LCI data, ecoinvent (Wernet et al., 2016), provides background uncertainty information by the application of the so-called Pedigree approach (Ciroth et al., 2013). In short, the Pedigree approach is typically used in LCA to turn qualitative information on the quality of inventory data (e.g. temporal resolution, geographic scope) into quantitative probability distributions (e.g. lognormal distributions) that are fed into a MC simulation (Ciroth et al., 2013; Muller et al., 2014). For the LCI foreground system, the analyst can define specific uncertainty information on the basis of collected information, sample estimation, or expert judgement. Also the uncertainty information in the foreground can be propagated using MCS. Heijungs (2021) investigated how many simulations need to be run for comparative probabilistic LCA and suggest restricting the MCSs to a number of simulation not greater than the sample size used for the input factors. Even though MCS is the most commonly applied uncertainty propagation method, several issues have been pointed out, such as the underestimation of the input uncertainties (Heijungs, 2020; Kuczenski, 2019) or the ignorance uncertainties for inputs that are correlated (Groen et al., 2017). Heijungs (2021) also concludes that when the parameters are not derived by sample estimation but through a procedure (e.g. the Pedigree approach), MCS should not be used. At the LCIA phase, characterization models do not typically come with uncertainty data, and LCA software do not always allow for the inclusion and propagation of uncertainty data at the LCIA stage. Qin et al. (2020) propose here the application of a Pedigree approach derived from expert judgement.

Advanced sampling methods, such as Latin hypercube approach or quasi-Monte Carlo (stratified and quasi-random sampling, respectively), promise faster convergence compared to MCS, but are usually not implemented in common LCA software (Igos et al., 2018). The *analytical resolution* of the LCA matrix is a first order approximation of the Taylor series expansion. On the one hand, a higher simulation speed and lower data requirements can be obtained, but on the other hand it is predominately applicable only for simple models with small uncertainties (Groen et al., 2014; Heijungs and Lenzen, 2014).

An alternative approach is that of *fuzzy logic*. Instead of general logical problems, which can only be true or false (1 or 0), fuzzy logic (many-valued logic) can be seen as a gradual logic between one very possible and zero most unlikely. A possibility function of each input variable is needed, which is usually of triangular or trapezoid shape (Groen et al., 2014). As opposed to probability density functions, the core value of height is equal to one and not the total area under the probability function. Depending on the data quality and quantity either a probability distribution or a trapezoidal fuzzy set is used for LCI inputs to the LCA model (Igos et al., 2018). When probability sampling methods are combined with fuzzy logic in a *hybrid approach*, the reliability and information provided can be increased.

Scenario analysis (see also section 5) can be used as an alternative to both UA and SA. The approach is useful for model structure and context uncertainty, but its reliability depends on expert judgment. If model validation is not possible multiple conceptual models can be defined to explore different formulations and assumptions (Igos et al., 2018). Usually, each scenario is run individually but can also be modelled by combining competing pathways in a single product system and activate or deactivate *triggers* or relevant uncertain inputs in each Monte Carlo run (Blanco et al., 2020). We refer the reader to section 6.

Once UA has been applied, SA should complement the analysis. A variety of approaches are used in the context of LCA (see also sub-section 6.3). *One-at-a-time* (OAT) is a LSA approach where one input variable is varied while keeping the others in their baseline (nominal) state. This is repeated for each parameter one at a time. The standard deviation of the input parameter can be used as the upper and lower boundaries (Heijungs and Kleijn, 2001). *Marginal analysis* or partial matrix-based derivatives (Heijungs, 1994; Sakai and Yokoyama, 2002) is also a LSA. Here, the partial derivatives of the output model depending on the individual input factors represent the sensitivity coefficients. However, the uncertainties of the parameters are not taken into account. Thus, the result can react strongly to a parameter, even if the parameter is very accurate. *Key issue analysis* (KIA) is based on the first-order approximation of the Taylor series expansion and can correct this bias consider the variance of inputs (Heijungs, 2010).

The *method of elementary effects* (MoEE) is based on OAT variations and used as an intermediate tool to prepare a global sensitivity analysis (Mutel et al., 2013). The sensitivity of model outputs is examined by systematically varying all parameters in series, thus the full range of model outcomes can be investigated. Therefore, a series of trajectories in the input space is constructed by randomly moving the inputs one-at-the-time.

With MoEE as a transition between LSA and GSA, the *correlation analysis* is a simple global sensitivity approach using the sampled results of uncertainty propagation of which the regression coefficient is calculated (Mutel et al., 2013). This method has the ability to detect correlation for non-linear models. To clarify whether the correlations are due to random variables or to interactions caused by the model, the sensitivity index (non-additivity of operations) must be calculated. Direct influences on the output variance of each input (indicated by the first-order sensitivity index) and direct/indirect contributions (total-order sensitivity index) can be calculated with the (extended) Fourier Amplitude Sensitivity Test (eFAST) or the Sobol method. For (e)FAST, a sinusoidal function is used, while the Sobol method adapts quasi-Monte Carlo sampling (Igos et al., 2018). In LCA, examples of the use of the variance-based approach of Sobol' include the work of Geisler et al. (2005), Mutel et al. (2013), Bisinella et al. (2016) and Lacirignola et al. (2017).

Cucurachi et al. (2016; Stefano Cucurachi et al., 2021) propose the application of moment-independent GSA techniques to individual components of LCA models, such as impact assessment models used for LCIA, and full-scale LCA models. Moment-independent techniques of GSA have useful properties for the application in LCA models and, in particular, can be run using the same MC sample used for UA and are suitable to assess correlated inputs. We further refer the reader to the work of Groen et al. (2017), Igos et al. (2018), and Michiels and Geeraerd (2020) for a review of GSA methods applied to LCA.

Unfortunately, the state of the art of UA and SA methods does not always go hand in hand with their availability in LCA software. Igos at al. (2018) list the availability of different methods in the most commonly used LCA software. Table 13 also indicates when additional software is needed. Nowadays, MCS is implemented in almost every LCA software available. Additional opportunities to combine UA, GSA and scenario analysis are available in open-source LCA applications, such as the Activity Browser (Steubing et al., 2020). This software offers the possibility to run MCS selecting individual components of the LCA model, including the uncertainty of techno-sphere, biosphere, characterization factors and parameters. Subsequently a GSA can be performed as well with this tool (Cucurachi et al., 2021). We refer the reader to Box 4, for additional details.

Box 4. Moment-independent UA and GSA for step (iii)

Moment-independent UA and GSA for step (iii)

The Activity Browser open-source LCA software (Steubing et al., 2020) allows for the treatment of uncertainty jointly using MCS and moment-independent GSA. The approach is presented in Cucurachi et al. (2021) and allows analysts to directly apply the proposed implementation in LCA studies. The method allows to flexibly select which uncertainty data to include in the analysis, and to flexibly exclude or include uncertainty data, depending on the uncertainty data at hand (see also github.com/bsteubing/lca-global-sensitivity-analysis).

An analyst that would want to skip the background LCI in both MCS and GSA can opt to "switch-off" the background system and ignore it when running the simulations. Similarly, should uncertainty data be available for the characterization models used, the analyst could include that information. Next, the analyst is capable of identifying the most important sources of uncertainty feeding the results of the MCS to the GSA routine used in the Activity Browser.

The general steps of implementation are the following:

- Monte Carlo simulation;
- Filtering of input data to GSA;
- Formulation of the input data for GSA;
- Moment-independent GSA and display of results.

6.4.5 Step (v): Communication

In the final step (v), a variety of techniques can be used to communicate the uncertainty of LCA results, depending on the target audience of the analysis at hand. The analyst should make sure that uncertainties in the LCA model and related results are communicated in a manner that is literally and cognitively accessible to the non-expert audience (Gavankar, Anderson, et al., 2015). Rosenbaum et al. (2018) identify the following set of questions as a basis to define a meaningful strategy to communicate uncertainty:

- Who is the target audience and how familiar is this audience with LCA and its aspects of uncertainty?
- Which information is relevant to communicate?
- How should uncertainty results be represented (see also Wardekker et al., 2013)?

In order to answer the above set of questions, the analyst should use information collected during the earlier steps of the proposed stepwise approach. We refer the reader to Rosenbaum et al. (2018) and Gavankar et al. (2015) for details on the communication of uncertainty, and on communication of uncertainty in LCA studies on emerging technologies.

6.5 Limitations and other considerations on the proposed approach

The reviewed methods can support the analyst to identify key sources of uncertainty. Still, the qualitative or quantitative treatment of uncertainty needs to be complemented with additional investments when treating, for instance, epistemic uncertainty. This can only be reduced by acquiring more knowledge, either by doing more research (measurements, literature, higher model complexity, etc.) or by consulting more experts if possible (Hauschild et al., 2018; Huijbregts, 1998; Igos et al., 2018; Walker et al., 2003).

The proposed framework has been developed to guide the LCA analyst. The ranking step (iii) is not mandatory, but can help to focus on the identification of the most severe uncertainties. Listing all sources of uncertainty is very important for the last step: (v) uncertainty communication. As steps (i) to (iv) are meant to reveal the most appropriate method to deal with uncertainties, they cannot always be executed quantitatively (method not available in the LCA software, license for another program not available, etc.). Nevertheless, all uncertainties must at least be reported qualitatively (ISO-14040, 2006; ISO-14044, 2006). To make the LCA results as reliable and credible as possible, all identified sources of uncertainty need to be stated. There is no harmonized approach to communicating uncertainties, but there are several publications that provide guidance (Gavankar, Anderson, et al., 2015) or propose and present measures, especially for comparative LCA studies (Heijungs, 2021; Mendoza-Beltran et al., 2018). Nevertheless, it is advisable to state in each assessment phase potential uncertainties, which goes hand in hand with the first step of the framework, the (i) uncertainty location and identification by LCA phases. This can also be done in form of a table summarizing all uncertainties. Qualitative assessment can be described in the text and quantitative assessments should be included in graphs (e.g. probability distributions, error bars) or added to the data tables (Igos et al., 2018). In general, it is desirable to use a common language for the subjective definition of probabilities and to facilitate access to uncertainty information (Gavankar, Anderson, et al., 2015). In summary, the sources of uncertainty in LCAs should be presented as transparently as possible, their impact on the results identified and critically discussed.

6.6 The uncertainty procedure in practice: comparison of microwave extraction and conventional acid extraction

To further illustrate the framework, the steps presented will be explored using the pectin production example from section 2. This bio-based production process valorises orange peel waste using microwave assisted extraction (MAE) as the emerging technology and conventional acid extraction (CE) as the incumbent. The functional unit and focus of the research question were structured around the product of the system and defined as 1 kg of pectin (at factory gate). Similar to previous publications (Blanco et al., 2020; Gavankar, Anderson, et al., 2015; Igos et al., 2018), the identified uncertainties are listed according to their LCA phases (see Figure 14). It should be mentioned that this is not a full LCA report and not all potential uncertainties have been captured.

An example of temporal and geographical uncertainty would be the geographical representativeness (Sicily). The region of Sicily in Italy was chosen because of the large orange production in the area (Beccali et al., 2009). To make technologies with different technology maturity levels (TRL) more comparable, the MAE technology with a TRL of 4-5 was projected to the year 2050, assuming that it will have matured to TRL 9 by then. Due to future climatic changes (from temperate to more arid; Beck et al., 2018), it is not certain whether orange production in Sicily will still be as large or not. This is a contextual uncertainty of epistemic nature. No representative statistical data are available, but rankable scenarios can be developed (e.g. worst-best case scenarios; see also section 5 on scenarios) that define this as a medium level of uncertainty. Using the decision tree in

Figure 13, the uncertainty of geographic representativeness can be expressed by using different scenarios that also represent the method for the uncertainty treatment. The geographical and temporal aspects of the target and scope phases are also crucial to produce inventory data (LCI) that adequately represent the impacts associated with water, energy and land use in this example. For this reason, variation in orange juice production is also expected. As shown in Figure 14, this uncertainty is quantifiable and of ontic nature and would also belong to the medium uncertainties. It can be expressed either by a variance or multiple scenarios, leading to several options for uncertainty treatment: scenario analysis, OAT, KIA and or MoEE.

Figure 14. Application of uncertainty and sensitivity analysis framework to the case study about pectin production from citrus peels (Garcia-Garcia et al., 2019). The same abbreviations are used for the uncertainty expression: (P) probability distribution, (V) variance, (F) fuzzy sets and (S) multiple scenarios. Methods abbreviations are: one-at-a-time (OAT), key issue analysis (KIA), method of elementary effects (MoEE), Monte Carlo sampling (MCS) and the (extended) Fourier Amplitude Sensitivity (eFAST). Further abbreviations used: foreground (FG) and background (BG).

(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

When considering impacts, it should always be questioned or discussed whether the impact categories chosen are representative of the LCA study. Thus, LCIA uncertainty is usually quantifiable, epistemic in nature and falls under shallow uncertainty. It can be expressed either by a probability distribution, variance or fuzzy sets and be treated with various methods (see figure 14). The analyst could opt here, if uncertainty data are available, for MCS and GSA as implemented by the Activity Browser.

The Activity Browser was chosen (open-source LCA software, compatible with python and brightway2, MCS and GSA are implemented) to investigate the pectin case study, which already reduces the available method options to what is implemented if the analyst cannot use additional software. Especially when many sources of uncertainty are identified, it can be helpful to rank them according to the source where the greatest uncertainty is expected (see figure 14). Everything related to the bio-based feedstock (orange peels) is expected to have the highest uncertainty (rank 1). For rank 1 uncertainties of shallow nature, MCS and GSA are advised. If a technology has to be scaled up, there is always a high probability that there will be a loss of performance or that the upscaling will not succeed at all (rank 2), due for instance to aspects related to the physical properties of the system. In the MAE example the scaling gets even more complicated due to the nature of the microwave. Some say this process might not be scalable in the conventional way at all.

The performance loss can be reduced over time by optimizing the process, but not all physical challenges can be overcome, like mass transfer of gases to the liquid. Anything at rank 3 can, for example, be subject to uncertainties that are usually difficult to manage. Let us consider that a new characterization factor (CF) is needed to measure biodiversity impacts, this is not feasible in an LCA study. The development of new CFs is very time-consuming and requires extensive experimental validation. Rank 4 is only assigned for the uncertainty of the representativeness of the flows considered. This should be implemented as accurately as possible. Interestingly, this could also be classified as recognized ignorance.

According to the ranking 1-2, scenarios should be developed following the scenario methodology explained in section 5. A local sensitivity analysis (OAT) for variability in orange juice production is also advisable and can be reported as error bars or added as variance in data tables. For rank 3 uncertainties, an MCS and also a GSA can be performed to identify the key processes or parameters that have a large impact on the outcome.

For the latter UA, it should be noted that Heijungs (Heijungs, 2020) discourages the use of MCS when deriving parameters by methods, such as the pedigree approach. This would be the case for background data provided by databases such as ecoinvent.

7. Conclusions and outlook

This report presents inputs for the development of a prospective LCA methodology for bio-based products. It addresses specific issues that require attention, including i) general issues arising during the goal and scope definition, as well as the inventory analysis phases; ii) the development of scenarios, iii) the accounting of biogenic carbon flows, and iv) specific considerations for uncertainty and sensitivity analyses. More work is required to integrate such guidance and harmonize it with existing literature, approaches and standards.

We highlight and provide guidance on a number of aspects to consider when conducting prospective LCA for bio-based products, some of which are also relevant for the application of prospective LCA to other emerging technologies that are not bio-based. Additional efforts are needed to further streamline and harmonize the application of prospective LCA for bio-based products.

Additionally, the report highlights the importance of designing and using scenario techniques as part of the prospective LCA exercise. All decisions and details of scenarios should be transparently reported by the LCA analyst, and further guidelines are needed to support the analyst. Part of the value and learnings of a study can come from the development of scenarios together with involved stakeholders rather than only from the final LCA results.

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List of abbreviations

AI	Active Ingredient
BbP	Bio-based Product
BG	Background
CCA	Cross-Consistency Assessment
CE	Conventional acid Extraction
CF	Carbon Footprint
CLD	Causal Loop Diagram
CNC	Cellulose Nanocrystals
EC	European Commission
eFAST	extended Fourier Amplitude Sensitivity
EIT	European Institute of Innovation and Technology
EoL	End-of-Life
ETEA	Educational Testing and Evaluation Agency
FG	Foreground
GDP	Gross Domestic Product
GHG	Greenhouse Gas
GMA	General Morphology Analysis
GSA	Global Sensitivity Analysis
GWPbio	Global Warming Potential of biogenic carbon
IAM	Integrated Assessment Models
IEA	International Energy Agency
IMAGE	Integrated Model to Assess the Global Environment
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
JRC	Joint Research Centre
KIA	Key Issue Analysis
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LiSET	Lifecycle Screening of Emerging Technologies method
LSA	Local Sensitivity Analysis
LUC	Land Use Change
MAE	Microwave Assisted Extraction
MCS	Monte Carlo sampling
MKS	Mango Kernel Starch
MoEE	Method of Elementary Effects
OAT	One-at-A-Time
PEF	Product Environmental Footprint

PESTEL	Political, Economic, Sociological, Technological, Environmental, Legal
PLA	Polylactic Acid
pLCA	Prospective Life Cycle Assessment
PP	Polypropylene
SA	Sensitivity Analysis
SNC	Starch Nanocrystals
SSP	Shared Socio-Economic Pathway
TRL	Technology Readiness Level
UA	Uncertainty Analysis

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The European Commission's science and knowledge service

Joint Research Centre

JRC Mission

As the science and knowledge service of the European Commission, the Joint Research Centre's mission is to support EU policies with independent evidence throughout the whole policy cycle.

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