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CRITICAL REVIEW

Improving life cycle assessment for carbon capture and circular product systems

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Abstract

Purpose This research aims to critically assess the suitability of current ISO life cycle assessment standards and practices for the challenges of decarbonisation through the use of carbon capture and the circular economy. Currently, the handling of wastes, including carbon dioxide, in life cycle assessment varies from sector to sector. We propose several methodological innovations to improve transparency and comparability of life cycle assessments to aid in the decarbonisation transition.
Methods Three approaches have been used to analyse the shortcomings of life cycle assessment for carbon capture and circular practices: Recent standards and practices have been assessed to determine their suitability for decarbonisation; Life cycle assessment and industry experts were consulted through a workshop held at the University of Bath in September of 2022; Case studies of industrial decarbonisation projects funded by IDRIC have been conducted to apply solutions to the shortcomings identified through the former methods. The issues identified have been categorised into three key areas: (i) guidelines and standards; (i) temporal and regional issues and (iii) data quality analysis.
Results and discussion The methods of handling carbon capture, waste valorisation and circular practices were found to vary significantly from sector to sector. Temporal aspects are frequently aggregated in a specific point of time, leading to low resolution by neglecting emissions over the duration of the process that creates them. Regionalisation was found to be hampered by regional characterisation factors being representative of larger regions but unsuitable at county or state scale. Uncertainty and sensitivity analyses, which are key to assessing the validity of the impacts of new and emerging technologies, were found to be neglected or only partially conducted.
Conclusions and recommendations The ISO life cycle assessment standards require updating to provide consistency in methodologies to make them suitable for use with carbon capture and circular systems and to avoid ambiguity. We recommend that the life cycle assessment community focuses on developing more consistent standards and practices between sectors to address carbon capture and circularity; improving the implementation of temporal aspects of impacts; increasing the number of studies including uncertainty and sensitivity analyses and moving towards global uncertainty in favour of local sensitivity.

Keywords LCA state of art · Framework · CCUS · Emerging technology · Circular economy · Temporal · Spatial · Regional · Data quality analysis · Transparency

Abbreviations

ALCA	Attributional LCA
CCUS	Carbon capture and utilisation/storage
CF	Characterisation factor
CFF	Circular Footprint Formula
CLCA	Consequential LCA
DLCA	Dynamic LCA
EoL	End of life of a product/service
GHG	Greenhouse gas emissions
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LHV	Low heat value

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MC	Monte Carlo simulation
OAT	One-at-a-time SA
PEFCR	Product Environmental Footprint Category Rules
PLCA	Prospective LCA
RLCA	Regional/geographical LCA
SA	Sensitivity analysis
TEA	Techno-economic analysis
TH	Time horizon
TRL	Technology readiness level
UA	Uncertainty analysis

1 Introduction

Life cycle assessment (LCA) is a tool used to understand the potential environmental impact of products and services by tracking different carbon sources and CO_2 emissions. Its use is widespread within industry, academia, policy and government (Bergerson et al. 2019; McManus and Taylor 2015). New technologies and strategies are rapidly being developed to meet global carbon reduction targets, such as the UK's goal of net zero by 2050 (CCC 2020). Assessing the environmental and life cycle impacts is essential to ensure that they are viable carbon reduction strategies. However, a methodological change for LCA is required to effectively model carbon over several life cycles, address the impact of moving from a linear into a circular economy and precisely account temporal and spatial aspects associated with carbon capture, utilisation and storage (CCUS) technologies.

In this paper, we have identified three key areas that need to be addressed to improve LCA for application to CCUS and circular practices: (i) inconsistent guidelines and standards; (ii) lack of temporal and regional considerations and (iii) inconsistency when conducting data quality analysis. This paper is structured so that each of these key areas is discussed as a standalone part, with a shared conclusions and future perspectives section, as shown in Fig. 1. These areas were identified through consultation with LCA experts from industry and academia at a workshop held at the University of Bath, Bath, UK, in September 2022, by assessing the recently published standards and guidelines, and by conducting case studies of emerging industrial decarbonisation technologies. Here, we discussed how these aspects are currently being handled in practice and in the current guidelines and offered recommendations to improve these aspects and allow consistent allocation of carbon. Several areas for further work were identified as critical for carbon modelling, including inconsistent use of terminology, lack of clarity in the descriptions of methodological choices or assumptions, time frame resolution, regional representativeness, technology readiness level and data quality. Tools and recommendations for the best practice are also provided.

2 PART I: Guidelines for carbon capture and storage, and circularity

Carbon modelling is critical to decarbonisation, but also to the success of several industries and businesses as they develop to meet carbon targets, and therefore in recent years several guidelines have emerged. Indeed, guidelines and case-study frameworks can be helpful to model the potential environmental impact of different products from specific manufacturing processes. However, the diversity of estimates, approaches and scopes of different guidelines could limit the precision of LCA outcomes, misdirecting investments or causing serious issues for comparing the environmental performance of technologies/products with previous studies. Six guidelines were reviewed in the next sections and their application for moving forward a circular economy were critically discussed.

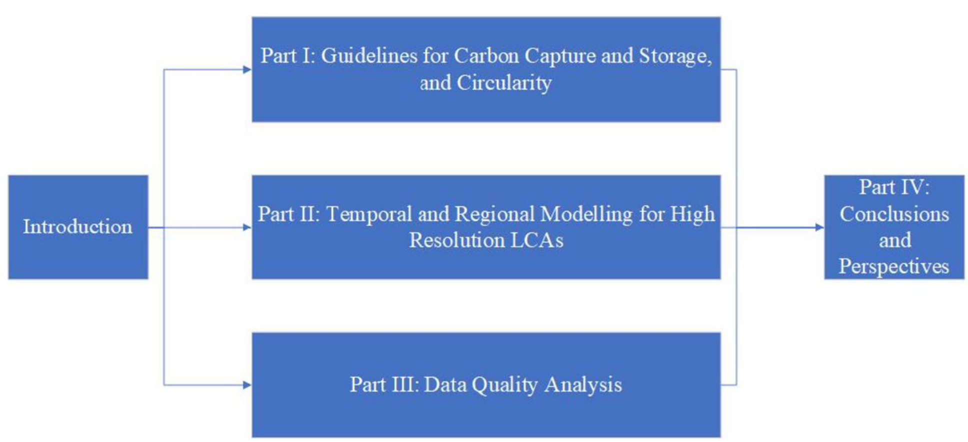


Fig. 1 Structure of this paper. Each of Parts I–III are able to be read independently of each other with shared conclusions and perspectives covered in Part IV

2.1 Life cycle assessment frameworks

Along the years many guidelines and frameworks were reported by specialists. The following sections shows a non-exhaustive presentation of the most recent/established guidelines. Table 1 summarises the key modelling aspects of some common and recent guidelines that have been used for industrial and academic assessments.

2.1.1 International Organization for Standardisation, ISO

ISO 14040 (2006) and ISO 14044 (2006) are commonly used and followed within LCA. ISO standards are generic working methodologies for best practices which allows flexibility of use over different applications. However, on the interpretation stage, there is a lack of guidance for the utilisation of uncertainty (UA) and sensitivity analyses (SA) (Igos et al. 2018). Both UA and SA are critical as products manufacturing is moving forward a circular economy since novel technologies requires the prospection of their environmental impacts. On one hand, assess the uncertainty of the environmental performance could support accuracy on comparisons of emerging technologies with the well-established production systems. On the other hand, the SA could identify the core of uncertainties or select the environmental bottlenecks to be optimised for enabling environmental gains over fossil-based products, for instance. Certainly, evaluation of uncertainties becomes more significant for low than high technology readiness level (TRL) since the data availability and quality are usually poor on the early stage of a process development. Regarding on environmental performance evaluation, a simplest LCA approach truncated on a linear modelling without uncertainty and temporal aspects of the technology deployment becomes obsolete due to low representativeness of impacts prospection of circular production systems. LCA modelling systems have developed rapidly since the ISO standards conception to address key issues of using LCA as a tool towards global net-zero targets, allowing the development of other guidelines and policies alongside in an effort to account for this rapid change and cover some of the modelling aspects associated with circularity and carbon capture and utilisation (CCUS).

2.1.2 Techno-economic assessment and LCA guidelines for CO_2 utilisation

Reported by the global CO_2 initiative (Langhorst et al. 2022) , this guideline aims to solve the lack of standardisation for CO_2 utilisation and provide methodologies for overcoming common challenges in LCA modelling for CCU. Aligned with ISO standards and attributional LCA approach, it could be applied for both the academic and industry sectors. The guideline is actively being updated on a biennial basis, the third and most recent iteration, which builds on the previous versions released in 2018 (v1.0) and 2020 (v1.1) is described here. The book offers recommendations to lessen the ambiguity of TEA and LCA for CCUS techniques. The lack of cohesiveness, openness and comparability of CCU investigations

Table 1 Summary of LCA modelling and guidelines. [1] Generic, applicable to many processes/products. [2] 'Shall, should, and may' guidelines are used. [3] The socio-economic aspects are mentioned and described, but the regionalisation modelling of the LCA characterisation impacts is just mentioned. [4] Dynamic characterisation factors are fully described for the TEA combined with LCA guidelines. [5] The circularity is regarding new strategies for mitigating environmental impacts. [6] Sector-specific guidelines.

Source		ISO 14040 & 14044	Techno-Economic Assessment & Life Cycle Assessment Guidelines for CCU	Life Cycle Assessment of Circular Systems	Responsible Steel International Standard	Whole life carbon assessment for the built environment	PEFCR
Primary Considerations	ALCA		Mention & describe	Mention only			
	CLCA		Mention only	Mention only			
	Economic Allocation	Mention only	Mention & describe	Mention & describe			Mention only
	Mass Allocation	Mention only	Mention only	Mention only	Mention & describe	Mention & describe	Mention only
	Energy Allocation	Mention only	Mention only				Mention only
	Sub-division of System	Mention only	Mention & describe	Mention & describe		Mention & describe	Mention only
	System Expansion	Mention only	Mention & describe	Mention & describe			Mention only
	Circular LCA			Mention & describe	Mention only	Mention only	Mention & describe
	CCUS		Mention & describe	Mention & describe	Mention only	Mention & describe	
Temporal	Dynamic Inventory			Mention only			
	Dynamic Characterisation Factors			Mention only			
	Delayed Emissions		Mention & describe	Mention & describe			Mention only
Regionalisation	Regionalised LCA	Mention only	Mention only				Mention & describe
Data Quality Analysis	Uncertainty Analysis	Mention only	Mention & describe				Mention only
	Sensitivity Analysis	Mention only	Mention & describe	Mention only			Mention only
Comments		[1]	[1,2,3,4,5]	[6]	[6]	[6]	[1]
References		(ISO 14040, 2006; ISO 14044, 2006)	(Langhorst, 2022)	(ICCA, 2022a, 2022b)	(ResponsibleSteel, 2022)	(RICS, 2017)	(EC, 2017)

Legend:
Mention & describe
Mention only
Do not mention

were addressed by the authors. The focus of this guideline is the technical-environmental analysis of novel technologies to support the transition of the linear to the circular economy. In this sense, the techno-economic analysis was fully described, and all aspects of the combined LCA-TEA were discussed. Combined with the TEA, a condensed, peer-reviewed paper with CCU guidelines has also been released (Zimmermann et al. 2020), where additional socio-economic issues and considerations were briefly discussed.

2.1.3 Life cycle assessment of circular systems by the International Council of Chemical Associations (ICCA)

The International Council of Chemical Associations (ICCA) have built on a case-study of plastics by Voulvoulis et al. (2020) to provide a critical overview of LCA methodologies (ICCA 2022a) and a guide accompanied by case studies (ICCA 2022b). The overview aims to increase the accessibility of LCA for circular systems by highlighting the major components of LCA studies and frequent problems addressed by analysts. The industrial case-studies offer examples and advice on establishing the primary LCA estimates, which covers the following topics: system boundaries, functional units and appropriate inventories for circular systems. Issues related to the development of the circular economy and its impact on the LCA modelling (e.g. shared burdens/gains of recycling) were fully described and discussed. Although the examples are briefly communicated, the ICCA framework offers a strong foundation for LCA analysts who are new to modelling circular systems.

2.1.4 Product Environmental Footprint Category Rules (PEFCR)

Market-based PEFCR methodology is currently being developed for use in public communication reports and does not consider projections of future scenarios (EC 2017; Zampori and Pant 2019). This guidance is focused on well-established technologies and products, as it requires a lot of information about the supply chain, details about the production, use and waste management phases. All waste streams generated during the manufacturing, distribution, use and end-of-life phases are modelled with the Circular Footprint Formula (CFF), as well as all recycled or recyclable materials entering or leaving the system (i.e. recycled materials used in the manufacturing phase and recyclable materials generated at the end of the product's life). The CFF consists of three parts which are: material formula, energy formula and disposal formula. All results are summed to calculate the total amount of emissions and resources that are part of the system's inventory due to all stages. The PEFCR method widely describes decision making guidance based on different literature documents, which includes ISO (14,040; 14,044; 14,067; 14,046; 14,020; 14,021, 14,025;14,050;14,071;14,024) and ILCD (International Reference Life Cycle Data System). The PEFCR method does not focus on carbon sequestration, but some aspects of LCA modelling may be helpful and are discussed in the following sections.

2.1.5 Responsible Steel International Standard, (Responsible Steel 2022)

The Responsible Steel is a non-profit organisation that operates a global multi-stakeholder programme to certify and standardise the steel industry with the objective of achieving sustainability. The programme evaluates steel producers based on 13 principles one of which is climate change and greenhouse gas emissions. Although it is not an LCA guideline, it provides recommendations for monitoring scope 1, 2 and 3 GHG emissions in line with the Paris Agreement's global goals. It has been included in this article as it serves as a point of reference for some of the industry experts invited to the aforementioned LCA workshop. Similar criteria exist for the other 12 principles, including responsible sourcing of input materials, noise, emissions, effluents and waste, water stewardship and biodiversity. The initiative is relevant amongst major steel manufacturers and consumers such as ArcelorMittal, POSCO, Tata Steel and Mercedes-Benz, which are all full members of the standard. Full membership is open to direct steel producers, consumers and entities with environmental interests in sustainable steel, whilst associate membership is open to government organisations, trade associations and standard bodies. However, the guideline is sector-specific for steel industry and users, which renders the application of the recommendations and guidance not suitable for other industrial processes.

2.1.6 Whole life carbon assessment for the built environment, RICS (2017)

The Royal Institution of Chartered Surveyors (RICS) developed a methodology known as a Professional Statement (PS) for the evaluation of whole life carbon for buildings. The PS is based on worldwide environmental impact assessment and sustainability standards, including ISO 14040 (2006) and ISO 14044 (2006) as well as European requirements. The system boundaries taken into account by the PS include every stage of a building project, including the extraction and transportation of raw materials, the building phase, operation and maintenance, and the end of life of the product (EoL) to calculate the global warming potential (GWP). GWP was the only indicator considered within this methodology, and it was evaluated exclusively for the building sector—which eventually limits the LCA scope, especially if the system boundaries are broad. The PS provides an extensive description of what should be relevant and included on the LCIA at each stage of the assessment and carbon sequestration accounting methods for various construction materials, which may be useful to LCA analysts looking at reuse and recycling of products.

2.2 Technology deployment of CCUS, circularity and LCA modelling

LCA can be used to identify critical points during the design of novel manufacturing processes by comparing them with commercial products/processes (Langhorst et al. 2022). Multiple scenarios can be considered through the system operating from small to large operational scale (Cucurachi et al. 2018). At the early stage of the technology development, designers can create long-term strategies to reduce emissions and compare different scenarios to evaluate the environmental performance of different products, operational conditions and processing strategies. However, the comparison of LCIA of CCUS processes can produce misleading results due to the lack of representative data to build the mass and energy inventories, resulting in high uncertainty and misleading decisions (Moni et al. 2020).

The reproducibility of an LCA or even the re-use of technology information is limited by the lack of mass and energy datasets or enough details of the process' mechanisms, kinetics or estimates. Alongside, lack of transparency in the LCI, whether deliberately (e.g. to protect commercially sensitive information) or not, makes replication of the study challenging and in turn limits the future applications of the LCA in question such as using it as an upstream process in another LCA. This leads to an overall reduction in the quality of the study (Bisinella et al. 2021). Quality examples of this are Blume et al. (2022) where the authors provide the material flows required to build an industrial-scale battery in a concise flow chart and Sharma et al. (2021) who provide the inventory in tables to identify material and energy flows for different foreground processes of a pharmaceutical manufacturing process. The comparison of the environmental performance is especially important for emerging technologies to produce commodities since they should provide high beneficial impacts to be considered as an alternative to the current production process. Although the comparison of the assessments and/or comparative assertions are the focus during the scope definition phase for all CCUS frameworks (EC 2017; ICCA 2022b; Langhorst et al. 2022), a variety of LCA modelling options are available, also hampering the comparability of LCIA of different studies.

The considerations of specific LCA guidelines vary at different levels, which includes fundamentals adjustments. Assumptions and estimates during the LCA modelling start at goal and scope definition, in which not only reference flows and functional unit are defined but also system boundaries, cut-offs, spatial–temporal considerations, co-products and waste management strategies might be established. The complexity of the model and the number of assumptions required can increase substantially as the model becomes circular, accounting for the reuse and recycling integrated with carbon capture and waste management under temporal, regional and supply–demand constraints. Indeed, the application and/or comparison of different LCA is not a straightforward task and could be challenging due to conflicting outcomes that depend on primary assumptions and interpretations. 'Traditional' LCAs are modelled with a linear approach, in which some cut offs are applied in the system boundary to determine the environmental outcomes of a specific manufacturing process or product. Qualitatively, the linearity of products manufacturing is used to simplify the complex 'carbon web' of the circular economy, which was represented by the diagram from Fig. 2.

Other key-decisions could diverge significantly, such as the allocation of burdens and benefits due to the implementation of circular strategies.

2.2.1 Allocation and circularity issues

Potential environmental impacts can be affected by the choice of allocation methods (Lauri et al. 2020). The decision hierarchy for multifunctional processes generally follows the next steps: (1) subdivision, (2) system expansion, (3) allocation based on physical relationship and (4) allocation based on other relationship (ISO 14044 2006; Langhorst et al. 2022; Zampori and Pant 2019). Subdivision and system expansion can be used to prevent allocating (ISO 14044 2006); however, the CO_2 production in CCU processes makes this unfeasible (Langhorst et al. 2022; Zampori and Pant 2019). This method can also be used to ease complications when data is limited (Langhorst et al. 2022). Theoretically, the system expansion process should be extended to model the whole technosphere. However, only major flows and processes are included due to the application of the cut-off criteria (Langhorst et al. 2022; Zampori and Pant 2019). Physical causality, economics or other non-causal physical association can be merged with system augmentation to demonstrate multifunctionality subdivision.

Normally, the allocation of a multiproduct system is based on physical (e.g. mass and energy content) and economic properties, having each of them different applications. For example, allocation using mass criteria enables an easy comparison between different systems, due to its access to readily available data. It can be used broadly with most processes aside from modelling power plants, where the energy allocation is suggested. However, when it comes to CCUS, energy allocation is not strongly recommended for processes with different low heat values LHV (e.g. O_2, CO_2) or by-products with high content of water (as the digestate from

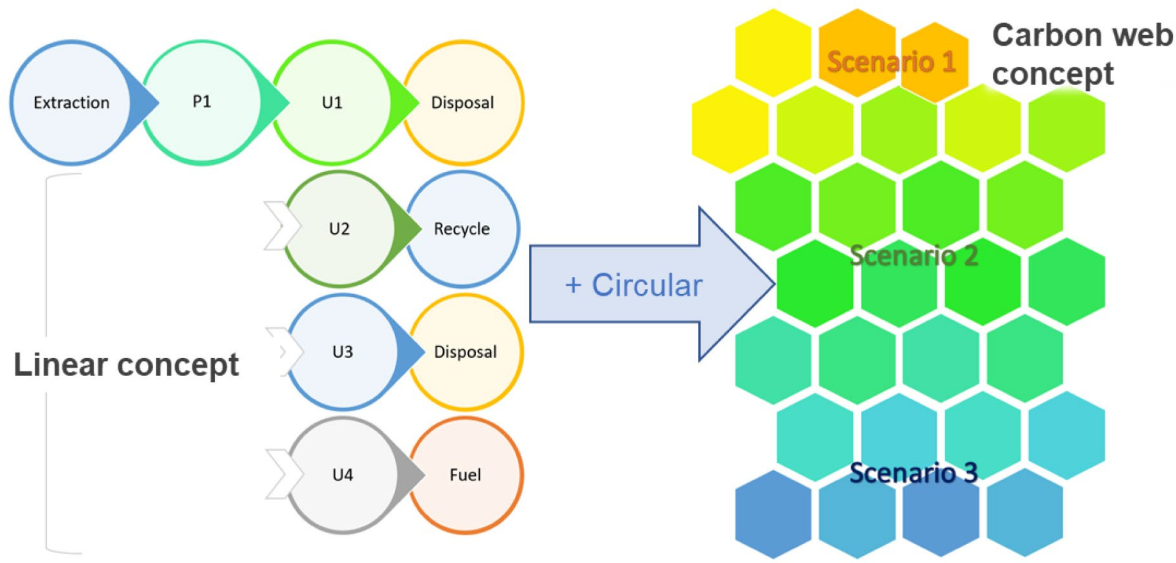


FIG. 2: Conceptual difference between linear and circular LCAs, where the links among inputs/outputs were qualitatively designed.

Fig. 2 Conceptual difference between linear and circular LCAs, where the links among inputs/outputs were qualitatively designed

biodigestion processes) where the LHV is zero (Langhorst et al. 2022). In these cases, an economic approach should be taken for allocating multifunctional systems.

The economic allocation gives more realistic impacts to low valuer by-products (Lauri et al. 2020), facilitates the comparison of both technologies and products, providing a fast analysis of different scenarios. The practical aspect of this approach could be valuable for policy makers, but it should be used carefully due to the dynamic nature of the process economics. In fact, the fluctuation of prices and inflation rates might impose a period of validity for the environmental study with this approach, which results are very sensible to the timeframe and product's market. Additionally, the carbon source can be modelled as a waste or as a by-product (Freitas et al. 2021). At the former LCA scope, Jensen et al. (2016) considers the effects of CO_2 from waste treatments being released directly to the atmosphere whereas the latter modelling could be explained by considering CO_2 as a feedstock at the cement production for enabling its capture and storage on the final product, as proposed by McDonald et al. (2022). Economic allocation could also be influenced if recycled streams in LCA are modelled as wastes (by neglecting previous environmental burdens) or as by-products from background processes (by including environmental burdens of the previous processing). The recovery of wastes into products by CCUS technologies could under valorise eco-friendly products since lower impact burdens could lead to lower prices than ones that uses raw materials. From an industrial stakeholders' perspective, the green premium value of eco-friendly production pathways could be lost. The market value from CCUS manufacturing products might be misjudged since the 'main' product has a much higher price compared to other coproducts from 'wastes'(Ardente and Cellura 2012).

The comparison of the environmental performance of different CCUS technology systems could be also facilitated by a standardised allocation of the functional unit for multiproduct and system boundary. In this context, the PEFCR guideline limits the LCA scope in three categories: (a) single application/function; (b) single function with different applications or (c) technologies/materials. The system boundary is also limited to cradle-to-gate (only for intermediate products manufacturing) or cradle-to-grave. Alternatively, the pre-stated scopes can be used as constraints for the functional unit. Langhorst et al. (2022) guideline has two main scopes: (a) CCU product or (b) energy storage. Then only mass, energy content, energy/technical services or satisfaction of energy demand are options for the function unit. The suggested system boundaries for this guideline consider chemical composition and benchmark of the products. Cradle-to-gate system boundary is appropriate for CCU products with similar chemical structure and composition. Otherwise, a cradle-to-crave approach should be employed. Likewise, other guides are malleable and allow definition of distinct function units, allocation approaches and system boundaries according to various potential scopes (ICCA 2022b). The allocation decision could be more complex for systems with more than one product, which requires an especial attention.

Allocating the environmental credits and burdens to producers and users in a complex multifunctional process involving re-used or wasted products, can be challenging. Consider, for example, a primary industry (e.g. steel, aluminium or polymers manufacturing), the products might be produced by using either virgin or recycled materials (EoL). By modelling life cycle assessments (LCA), we can understand better how to account for these credits and burdens, allowing us to compare traditional fossil-based production with greener alternatives or simply accounting for different waste management solutions at the EoL such as recycling, incineration and landfilling.

LCA allows us to view the system from a window which is movable thus taking into consideration different methods of waste management with or without its transformation back into usable products. The circularity aspect of the system expansion approach regards on sharing the benefits/burdens between the primary and secondary product (ICCA 2022b). For academic purposes, the issues of double counting the benefits of the eco-friendly alternatives could be avoided easily and the comparison of results is practical if all assumptions are stated at the same study. However, the waste generation and its management could be deployed by different stakeholders—here the system boundaries are shared, and the environmental aspects must be split to benefit all parts. Issues as the double accounting of the benefits of recycling for different industries can arise. In this context, a hybrid allocation can be effective as an alternative to other strategies.

Circular Footprint Formula (CFF) is a hybrid allocation formula that combines material, energy and disposal elements to measure the emissions and resources connected with a process including recycling, disposal and energy recovery (EC 2017; Zampori and Pant 2019). The system boundaries are flexible for applying the CFF, which could be cradle-to-grave or cradle-to-gate (limited to intermediate products); nevertheless, the differences of the modelling shall be accounted. Intermediate chemicals, for instance, can be transformed in a large variety of products with distinct applications, which hampers the EoL modelling during the LCA study and changes the CFF (EC 2017; Zampori and Pant 2019). To facilitate its commercial application, some flexibility can be considered based on negotiations amongst policy institutions and industrial clusters. The lack of temporary and permanent carbon storage and/or delayed emissions aspects (EC 2017; Zampori and Pant 2019) can be an issue of the application of this strategy for comparing CCUS technologies. Figure 3 summarises the main aspects of the LCA modelling for a linear approach.

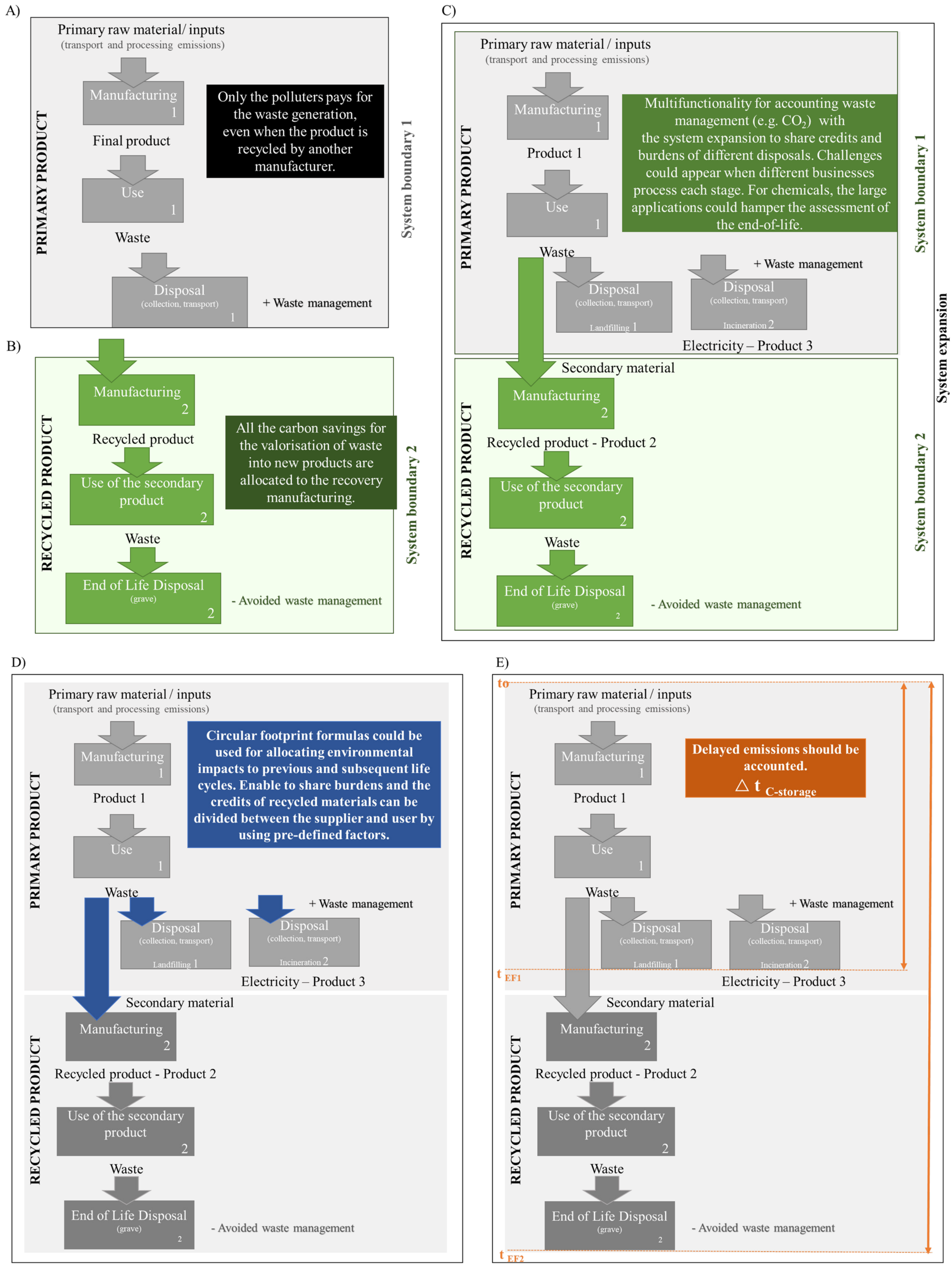
2.2.2 Time and space limitations

Temporal aspects in guidelines are more concerned with the technology development (EC 2017; Langhorst et al. 2022; Zampori and Pant 2019), rather than the dynamic aspect of the inventory or emissions. The credits for the CCUS application are not considered, which means that all emissions and removals are not discounted over time as default (EC 2017; ISO 14067 2018; Langhorst et al. 2022; Zampori and Pant 2019), especially for fuels due to low significant effect is expected—short life cycle (Langhorst et al. 2022).The timeframe of the emissions during all life cycle of the product, as well as the delayed emissions resulted from different technologies or disposals during the EoL, for instance, are recommended as additional information. It may be reported when the chemical structure of the products leads to different emission time profile over the conventional product for cradle-to-grave analysis (EC 2017; Langhorst et al. 2022; Zampori and Pant 2019). Although these temporal considerations are usually not mandatory on the carbon footprint modelling default (EC 2017; ISO 14067 2018; Langhorst et al. 2022; Zampori and Pant 2019), they are key factors for comparing the environmental performance of CCUS technologies.

Alongside temporal aspects, spatial characteristics can have a major impact on the outcome of an LCA and must be highlighted. Moving resources across different regions can lead to different impacts depending on the origin and destination. For example, the method of transportation, population density of regions, resources available, etc., can all change the final impact assessment for each geography. Furthermore, different regions may use different impact CFs, the resolution of which can be on a continental, country or county scale. Considering two identical processes with the same resource flows in Europe and South America would yield different impacts as these regions have their own CFs (Yang 2016).

2.2.3 Opportunities for circular life cycle assessments

To enhance the circularity and resolution of LCA studies, attributional (ALCA) or consequential (CLCA) are combined with economic analysis (Faber et al. 2022), dynamic inventories/emissions and market supply/demand (Aldaco et al. 2019; Ryu et al. 2022). On the industrial scope, the retrospective approach fits well-established technologies. Here the data availability is large, and the analysis usually considers commercial products or technologies. In contrast, the prospective approach uses limited data from research and development stages to assess potential impacts of new products or technologies, especially for CCUS. Indeed, the market of some products from CCU relies on the future and


A)
Primary raw material/ inputs
(transport and processing emissions)
Manufacturing 1
Final product
Use 1
Waste
Disposal (collection, transport) 1
+ Waste management
PRIMARY PRODUCT
Only the polluters pays for the waste generation, even when the product is recycled by another manufacturer.
System boundary 1
B)
Manufacturing 2
Recycled product
Use of the secondary product 2
Waste
End of Life Disposal (grave) 2
- Avoided waste management
RECYCLED PRODUCT
All the carbon savings for the valorisation of waste into new products are allocated to the recovery manufacturing.
System boundary 2
C)
Primary raw material / inputs
(transport and processing emissions)
Manufacturing 1
Product 1
Use 1
Waste
Disposal (collection, transport) Landfilling 1
Disposal (collection, transport) Incineration 2
+ Waste management
Electricity – Product 3
PRIMARY PRODUCT
Multifunctionality for accounting waste management (e.g. CO2) with the system expansion to share credits and burdens of different disposals. Challenges could appear when different businesses process each stage. For chemicals, the large applications could hamper the assessment of the end-of-life.
System boundary 1
Secondary material
Manufacturing 2
Recycled product - Product 2
Use of the secondary product 2
Waste
End of Life Disposal (grave) 2
- Avoided waste management
RECYCLED PRODUCT
System boundary 2
System expansion
D)
Primary raw material / inputs
(transport and processing emissions)
Manufacturing 1
Product 1
Use 1
Waste
Disposal (collection, transport) Landfilling 1
Disposal (collection, transport) Incineration 2
+ Waste management
Electricity – Product 3
PRIMARY PRODUCT
Circular footprint formulas could be used for allocating environmental impacts to previous and subsequent life cycles. Enable to share burdens and the credits of recycled materials can be divided between the supplier and user by using pre-defined factors.
Secondary material
Manufacturing 2
Recycled product - Product 2
Use of the secondary product 2
Waste
End of Life Disposal (grave) 2
- Avoided waste management
RECYCLED PRODUCT
E)
to
Primary raw material / inputs
(transport and processing emissions)
Manufacturing 1
Product 1
Use 1
Waste
Disposal (collection, transport) Landfilling 1
Disposal (collection, transport) Incineration 2
+ Waste management
Electricity – Product 3
t EF1
PRIMARY PRODUCT
Delayed emissions should be accounted.
△ t C-storage
Secondary material
Manufacturing 2
Recycled product - Product 2
Use of the secondary product 2
Waste
End of Life Disposal (grave) 2
- Avoided waste management
t EF2
RECYCLED PRODUCT

◂**Fig. 3** Summary of the LCA modelling (EC 2017; ICCA 2022b; Langhorst et al. 2022). **A** Polluters are responsible for the waste generation, even if that waste is recycled by another manufacturer. **B** All the carbon savings associated with the valorisation of the waste into new products are allocated to manufacture that is responsible for recycling it. **C** The system expansion approach is used to account potential environmental credits and burdens of different disposals strategies, where sharing credits and burdens are possible. **D** Temporal aspects include the delayed emissions for CCUS, and environmental benefits or drains could be shared amongst stakeholders with the CFF. **E** Emissions of stored carbon are delayed in recycled product systems leading to higher end of life disposal emissions

their deployment or comparison with well-established markets could be biassed and uncertain. In this context, foresight studies for exploring future LCA scenarios have been used to evaluate potential environmental impacts of emerged technologies by exploring future situations in policy decisions, business strategy and resource management (McDonald et al. 2022; Pinto et al. 2022).

Consequential, dynamic and prospective market demand are some of the methodologies available on the literature for future-oriented LCA modelling (van der Giesen et al. 2020). The future scenarios methodologies to assess the LCIA is complex and difficult to generalise due to a variety of possibilities, archetypes (input, output, hybrid), estimates (e.g. time-frame) and absence of systematic interpretation (Bisinella et al. 2021). According to Bisinella et al. (2021), the divergence on the definitions of these approaches in different guidelines (e.g. ISO, ILCD) and the non-existence of standards resulted in multiple approaches for future-oriented LCA modelling (Bisinella et al. 2021). Besides, the uncertainty of the inventory could be representative on the outputs of the prospective LCA.

The main sources of uncertainty on the inventory phase are data quality, TRL and market maturity (Bergerson et al. 2019). Although the complete material and energy balances are required to estimate the life cycle of CCUS products, a novel process depends on low-quality data from experimental proof of concept, or validation on pilot-scale or even lab-scale (Cucurachi et al. 2018; Piccinno et al. 2016). To avoid future misleading results and support the industrial-like scenarios of chemical processes with low uncertainties, the stoichiometric balances, thermodynamics and other physico-chemical relationships (e.g. mass-, energy-, exergy- and entropy balances) shall be considered on the inventory development (Langhorst et al. 2022). An absolute best-case scenario shall be used to assess the environmental impacts by assuming efficiency of 100% (Langhorst et al. 2022), always following the physico-chemical limitations of the system. Piccinno et al. reported qualitative and quantitative estimates for LCA practitioners when only data from laboratory experiments are available—estimates for energy use, batch reactions, purification and isolation steps were reported for different scales (Piccinno et al. 2016). Additional, performance indexes for technical, economic, environmental, health and safety hazards were reported by Sugiyama and collaborators (2008). Indicators help to model how much unwanted substances are produced in the reaction or how much energy is lost based just on the reaction information, for example (Sugiyama et al. 2008).

The maths behind the LCA plays an import role on uncertainty assessments. Both consequential (CLCA) and attributional (ALCA) approaches could be used to evaluate the environmental impacts (Schaubroeck et al. 2021) of different operational conditions or technologies through the aggregation of the emissions in a fixed time-frame (Brondi et al. 2021; McDonald et al. 2022; Pinto et al. 2022). Regarding the mathematical models, ALCA and CLCA concept should not be mixed (Schaubroeck et al. 2021) because adopting one or another strategy to the LCA modelling will change the resolution and scope of the study, which plays an important role for assessing industrial emissions or forecasting the performance of novel CCUS technologies. Some guidelines are based specifically on attributional fundamentals (Langhorst et al. 2022), whilst others just state some interpretation differences between them (ICCA 2022b). The consequential approach should be explored to enhance the circularity representativeness on LCA modelling. Figure 4 summarises the conceptual characteristics of the LCA according to resolution, circularity level, TRL and uncertainty of processes.

In fact, to ensure early design improvements in a circular economy, the LCA study shall be supported by representative information of LCIA modelling, system inventory (both foreground and background), technological landscape (e.g. TRL, spatial representativeness), clear definitions of temporal aspects and standardised conceptualisation /interpretation.

2.3 Summary

Frameworks for the best practice of LCA for both industrial processes and emerged technologies were reviewed and the key-aspects of its application on the context of a circular economy were highlighted. Temporal and regional aspects were identified as key modelling considerations that are not clearly covered on former guidelines, then their practical modelling was critically reviewed in PART II. Moreover, LCIA uncertainties and the system sensitivity under process can be decisive drivers for technologies screening on an industrial decarbonisation scope. Both uncertainty and sensitivity are strongly associated to the quality of data that is used for LCA modelling, as discussed in PART III.

3 PART II: Temporal and regional modelling for high-resolution LCAs

3.1 Time in circular systems

Temporal aspects reflect the complexity of the circular economy; if correctly accounted, they could provide important

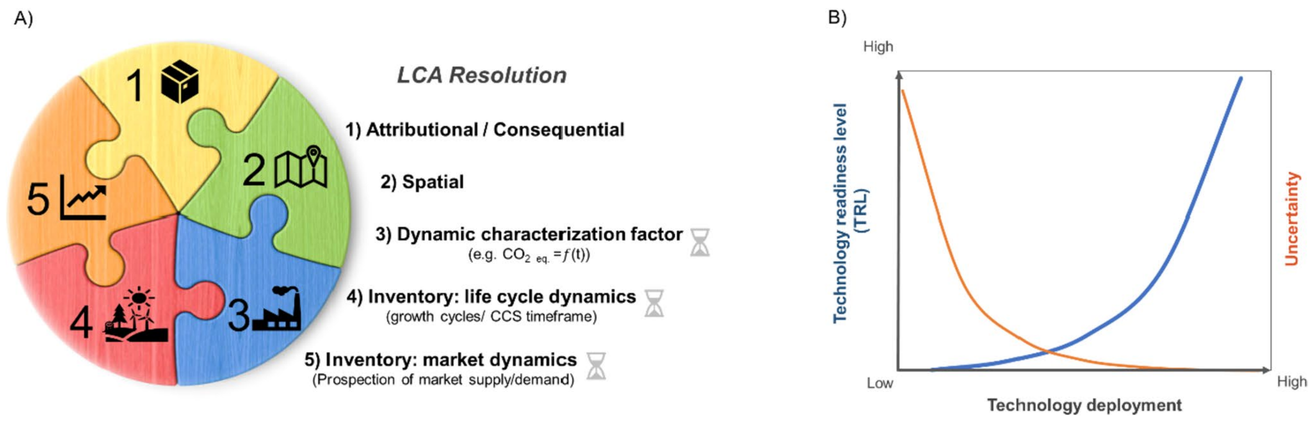


Fig. 4 Summary of LCA concept, TRL and uncertainty. LCA characteristics according to its resolution (**A**). Relationship amongst the l uncertainty of modelling, and TRL (**B**)

information related to delayed emissions, and recycled products over time, helping to build management and mitigation strategies to avoid depletion of natural resources. The gradual accountability of captured emissions over the product lifetime are required to explain CCUS systems and its modelling can be complex (Beloin-Saint-Pierre et al. 2020; Lueddeckens et al. 2020). Then, simplifications are settled by the guidelines (such as those in Table 1) to facilitate both LCA modelling and LCIA interpretation. For comparison purposes, a straightforward and simple LCIA evaluation is possible by aggregating emissions over time or neglecting some system dynamics. However, the loss of time resolution could lead to misleading conclusions, which could hamper the development of a circular economy based on CCUS. In this context, policy makers and stake holders might identify the emissions profile along the years (with high temporal resolution) to meet policies targets and/or carefully address the future generations impacts.

Circular systems consider the valorisation of alternative carbon sources to avoid emissions in the production of materials and products that would be otherwise produced from non-renewable resources, preventing with this the release of greenhouse gases ($CO_{2\,eq.}$) into the atmosphere (ICCA 2022b). The accountability of these factors is dynamic and then, strongly related to temporal assumptions on LCA. According to the most frequent guidelines (EC 2017; Langhorst et al. 2022; Zampori and Pant 2019), the amount and duration of carbon storage should be reported as additional information at LCIA. Following the LCA principals from ISO 14067 (2018), to calculate the climate change impact, the discounting of emissions over time and temporary/permanent carbon storage and/or delayed emissions shall not be included. Another approach is to consider the avoided emissions as additional to or independent of climate change indicators (Langhorst et al. 2022) and to assume that it does not contribute to climate change during a specific period. The lack of temporal resolution refers to the assumption that all input and output emissions are released at the present time (EC 2017; ICCA 2022a; Langhorst et al. 2022) by averaging the characterisation factors scores over 20, 100 or 500 years—as suggested by the IPCC guidelines. On bioenergy systems, for instance, the delayed emission of the CO_2 into the atmosphere is often relatively short due to their life cycle which is often between 3 and 30 years depending on crop type. Then, the advantage of the renewable sources for energy production relies on the carbon-savings compared to the fossil fuels options. Under the Langhorst et al. (2022) guidelines, the comparison of fuels and energy storage systems shall include each temporary storage on their cradle-to-grave LCIA; no significant effect is expected. It is important to highlight that the modelling of biofuels production provides a straightforward analysis of the whole life cycle of the final product since its final use/disposal at the EoL is not as complex as for other chemicals as in general, the carbon is released at point of use. In the latter case, different applications/uses are available to transform chemicals into new products that regards on different EoL modelling for each potential application.

The temporary or permanent carbon storage could vary according to different waste management strategies. Waste-products could be valorised by recycling or refurbishing at their EoL. Materials such as steel, aluminium or polymers can be produced from virgin, recycled or recovered mixed materials, causing or not changes on the chemical property of the final product. For a cradle-to-grave approach, the temporary storage is required for comparing final products with different composition (chemicals, material and others). Emission time profiles may be recommended as additional data by other guidelines (ICCA 2022b; Langhorst et al. 2022), but no standard practice is provided. Langhorst et al. (2022) discussed the delayed benefits of CCU and CCS. The CCU affects the emission time profile just if the conventional counterparts are replaced by CO_2-based products. For CCS

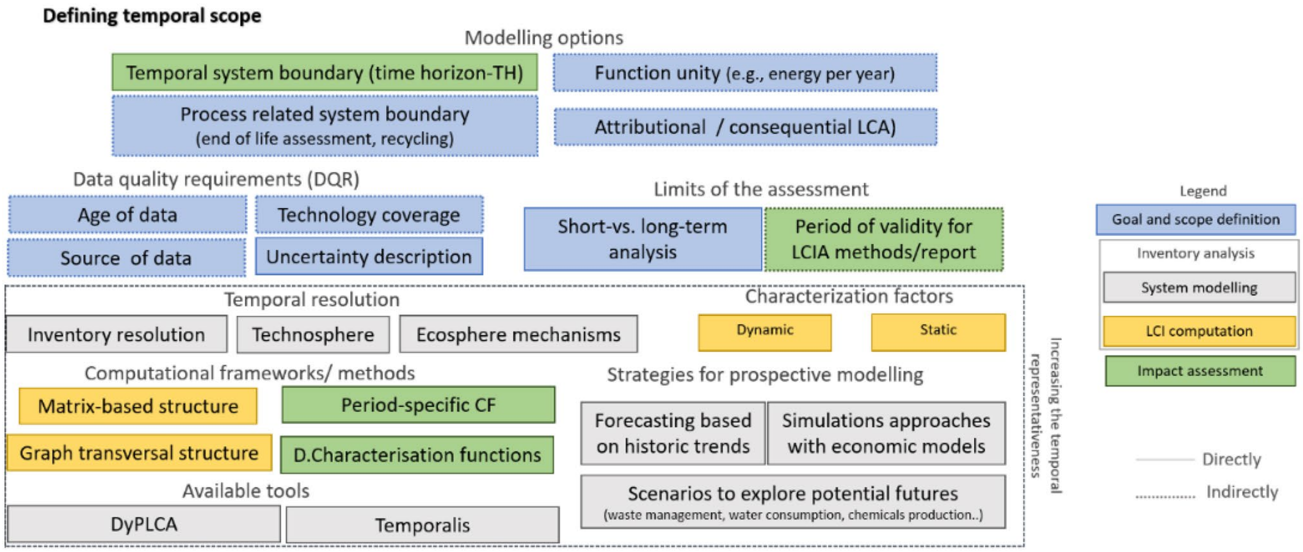


Fig. 5 Temporal considerations in relation to their purposes on the phases of the LCA methodology. Adapted from (Beloin-Saint-Pierre et al. 2020; Lueddeckens et al. 2020)

technologies, the EoL emission never occurs, which mathematically means permanent storage with zero emission.

In fact, intrinsic differences of the systems might include temporal decision on the LCA in diverse levels by establishing short- or long-term analysis, dynamic function units, different time horizons for the emissions, as well as covering the period of data validity or technological obsolescence. The indirect factors largely relate to the source, deployment and current coverage of the technology, as well as the age and source of data. Figure 5 shows a quick-reference for the key-temporal aspects and tools for LCA application. Considering the complexity of dynamic modelling and the lack of standards to its practice, an overall of the temporal modelling in LCA and the available tools were briefly reviewed in the following sections.

3.2 Time dimension

The transition towards a circular economy can only take place over a specific time frame, thus high temporal resolution on LCA modelling is essential. The lack of a precise temporal definition partly derives from the lack of consensus on how to define temporal estimates and dynamic methods (Beloin-Saint-Pierre et al. 2020). The definition of time on a LCA starts on the goal and scope phase. The first decision regards to Time Horizon (TH) of a consistent system boundary. The TH could be associated to the length of the life cycle of the product or service, to the inventory modelling, and, finally, to the TH of the characterisation factor, as shown in Fig. 6.

The temporal estimates and considerations are often related to LCA drawbacks because they are usually lost during the inventory calculation (if the static approach is used) or during the impact assessment where the potential damages/gains can be aggregated in a specific time (Levasseur et al. 2010). In a static approach, for instance, we can assume that all emissions are taking place at the time where the evaluation of the potential environmental drawbacks and benefits is made by aggregating emissions at one point (Langhorst et al. 2022; Levasseur et al. 2010). Time can be included on

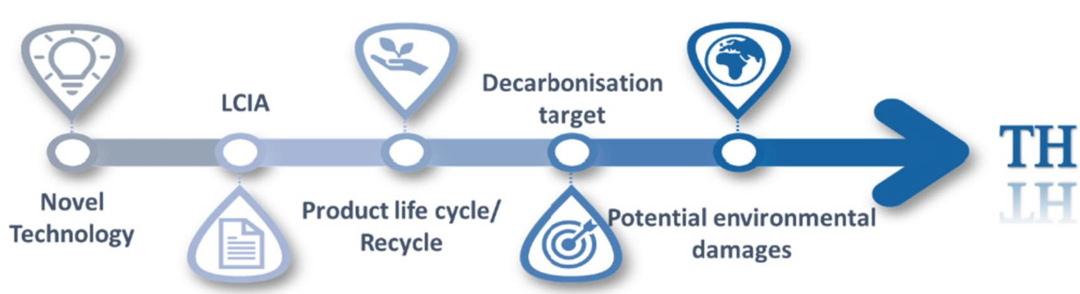


Fig. 6 Variations of the THs during LCA

LCA directly by dynamic calculations where input and outputs flows change over time and gradual impact of emissions are estimated by dynamic characterisation factors (CF). Figure 7 summarises the conceptual representation of the LCIA outcomes for both static and dynamic approaches.

Adapted from Pigné et al. (2019) and Langhorst et al. (2022).Indirect temporal aspects could be related to technology development and deployment, age of data sources and lifetime of the project. The time could also appear indirectly and limit the systems analysis by their boundaries. In this case, the end-of- life of one product can be settled outside the boundaries by using a cradle-to-gate approach, which consider just part of the emissions of the life cycle of a product. A cradle-to-gate approach is usually used to compare difference environmental performance due to changes in the production processes (e.g. efficiency or technologies) of the same products (Fernández-González et al. 2022; Pinto et al. 2022). Other cut-off approach is related to the waste processing, where just the first grave (recycled content) is accounted on the LCA modelling (ISO 14044 2006). Clearly, the real benefits over time of additional recycling are lost, leading to underestimation of environmental gains.

The inclusion of technosphere and biosphere exchanges with a CLCA, dynamic CFs or inventory increases the time representativeness of the LCA. These estimates/models could be combined or not, which means that the study can consider the temporal aspects of the inventory with or without dynamic CFs. To reduce the model complexity of the inventory resolution, Beloin-Saint-Pierre et al. (Beloin-Saint-Pierre et al. 2014) suggests that it is not necessary that the whole inventory to be dynamic, especially if there are very small emissions. On the scope of the CFs, the TH is important due to the temporal delay of several years between releases and the effective start of the potential environmental damage. The greenhouse gas emissions, for instance, show different behaviour depending on the TH considered and the IPCC provides estimates of 25, 100 and 500 years for the global warming potential (GWP). On the perspective of the LCA practice, 25 years would obviously be too short, underestimating the potential impacts of CO_2 emissions when compared to CH_4 on the GWP, which are 72 times higher than the former in a 20-year TH (Guest et al. 2012; Levasseur et al. 2012). The afore mentioned difference is reduced by 25 times in a 100-year TH, which is the most usual timeframe for GWP (Langhorst et al. 2022). Moreover, the GWP-500 can be too long leading to high complexity and uncertainty scenarios, as well, ignore the urgency of environmental problems, as an excuse for no action. Clearly, the scope has a key role for settling this timeframe in all situations and the GWP-500 are still demanded for inferring how the current technologies/strategies will impact the future generations survival,

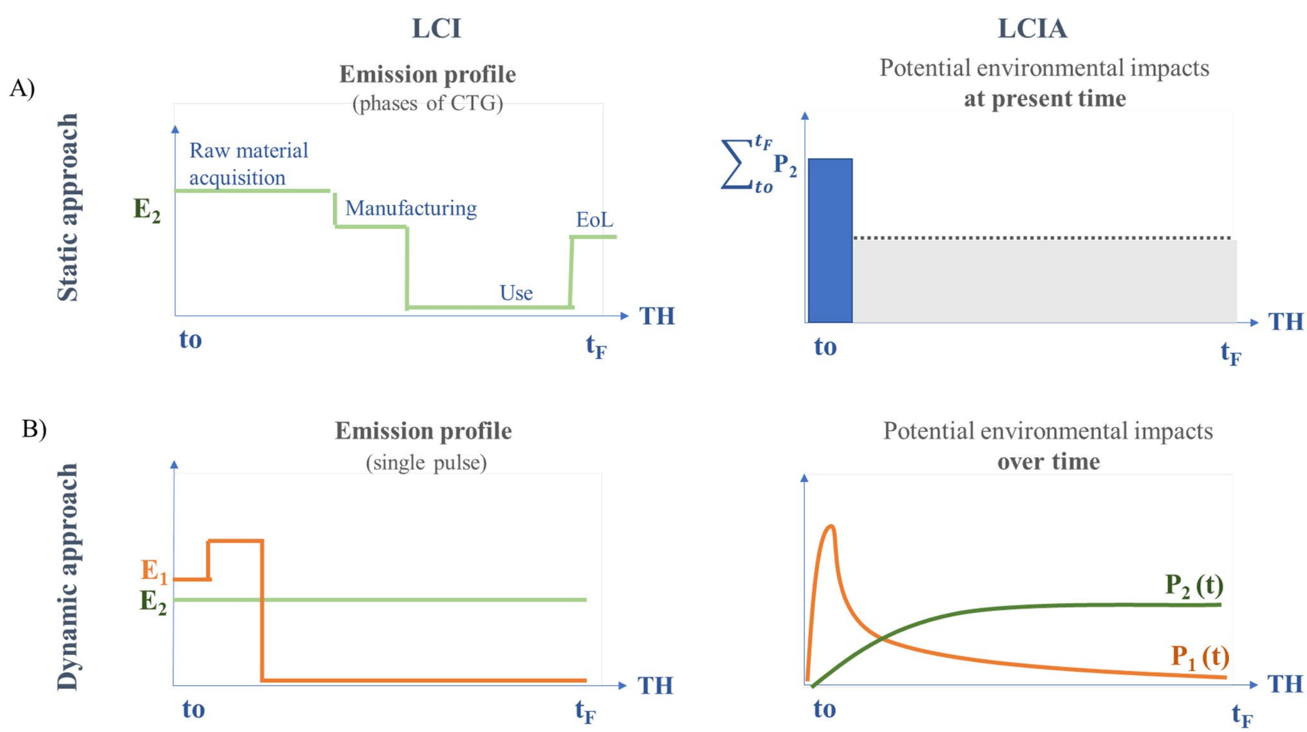


Fig. 7 Conceptual representation of inventory and LCIA for static (**A**) and dynamic (**B**) approaches

for instance. On a dynamic approach, the correct TH should be chosen carefully to avoid misleading results due to resolution loses (Levasseur et al. 2010).

The temporal aspects could be used to improve the time resolution by accounting the cycle in which the CO_2 is captured during the growth of crops and released after years to produce bioenergy or on the EoL of different products (Guest et al. 2012). For energy crops, the carbon storage in the technosphere benefits are far less pronounced for low rotation periods and high TH (Guest et al. 2012). Almeida et al. (2015) concluded that the increase of the DLCA model complexity did not add value for the analysis of GWP emissions during the energy production from perennial energy crops–short-lived product. The authors also suggested that the period of temporary carbon sequestration in the biomass is short and immediate metrics (e.g. IPCC GWP) should be used (Almeida et al. 2015). It is worth to mention that, traditionally, the impact over time is neglected and the use of biomass as a renewable source is discounted (biogenic contribution) by the difference between the carbon that is captured and the carbon that is released during the harvesting or at the EoL of the product (SETAC 2011).

Briefly, DLCA allows for an increase in temporal resolution in several aspects that include (but are not limited to) the definition of the functional unit (e.g. one year of energy consumption), the temporal distribution of elementary flows over time (foreground and/or background processes—supply chain (Aldaco et al. 2019) and marked demand (Ryu et al. 2022)), datasets (Sacchi et al. 2022), technology deployment (Faber et al. 2022) and dynamic CFs (Beloin-Saint-Pierre et al. 2020; Lueddeckens et al. 2020). To achieve the goals of industrial decarbonisation, a specific TH might be set by government policy. In this sense, increasing the temporal resolution at LCA will enable a clear understanding of the carbon capture efficiency of different CCU and CCS technologies.

3.3 Regionalisation approaches

A Generalised structure for regional LCA has been provided by Yang and Heijungs (2016). Their method allows an analyst to determine the regionalised impacts (h_r) based on the production of input materials from other regions, which is defined by the next equation:

$$h_r = \mathbf{C}_r \mathbf{B}_r \mathbf{A}_r^{-1} f_r \tag{1}$$

For hr, each element of the equation is defined by the next expressions

$$\mathbf{C}_r = \begin{bmatrix} \mathbf{C}^1 & 0 & \cdots & 0 \\ 0 & \mathbf{C}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{C}^{\mathrm{j}} \end{bmatrix} \tag{2}$$

Environmental matrix:

$$\mathbf{B}_r = \begin{bmatrix} \mathbf{B}^{11} & \mathbf{B}^{12} & \cdots & \mathbf{B}^{1\mathrm{j}} \\ \mathbf{B}^{21} & \mathbf{B}^{22} & \cdots & \mathbf{B}^{2\mathrm{j}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{B}^{\mathrm{j}1} & \mathbf{B}^{\mathrm{j}2} & \cdots & \mathbf{B}^{\mathrm{jj}} \end{bmatrix} \tag{4}$$

Technology matrix:

$$\mathbf{A}_r = \begin{bmatrix} \mathbf{A}^{11} & \mathbf{A}^{12} & \cdots & \mathbf{A}^{1\mathrm{j}} \\ \mathbf{A}^{21} & \mathbf{A}^{22} & \cdots & \mathbf{A}^{2\mathrm{j}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}^{\mathrm{j}1} & \mathbf{A}^{\mathrm{j}2} & \cdots & \mathbf{A}^{\mathrm{jj}} \end{bmatrix} \tag{4}$$

Functional unit vector:

$$f_r = \begin{bmatrix} f^1 \\ f^2 \\ \vdots \\ f^j \end{bmatrix} \tag{5}$$

Note that each of the elements of h_r, $\mathbf{C}_{\mathrm{r}}$, $\mathbf{B}_r$, $\mathbf{A}_r$ and f_r is a vector or matrix representing j regions. Even though $\mathbf{B}_r$ might appear square in the generalised form shown above the constituent matrices, $\mathbf{B}^{11}$ to $\mathbf{B}^{ij}$ may be non-square, resulting in $\mathbf{B}_r$ being non-square. By applying this methodology to LCA, analysts are able to assess the impacts of a product or process in different regions with greater precision based on local impacts such as manufacturing trends and electricity grid mixes. LCA databases such as Ecoinvent contain regionalised datasets for the majority of their processes making this method widely implemented. However, the regions used in the datasets are often broad groupings of countries and geographies such as Europe (designated as ‘RER’ in Ecoinvent) which is not technologically, geographically or ecologically homogeneous.

Regional scales vary between LCI and LCIA which is one of the major challenges in regionalised LCAs due to each being based at different regional scales (Mutel et al. 2012). For example, LCI data may be based on political borders between countries, states and regions, whereas LCIA scales are often derived from ecological factors such as population density, water courses.

The most commonly applied regionalisation method is the regional outputs approach (ROP) described by Yang (2016) which uses the basic matrix representation of LCIA with some modifications:

$$h_r = \mathbf{B}\, diag\left(\mathbf{A}^{-1} f\right) R^T \tag{6}$$

where $\mathbf{A}$ is the technology matrix and a column represents a process and a row a product, $\mathbf{B}$ is the environmental matrix that represents the quantity of emissions or natural resources emitted/consumed by the processes in $\mathbf{A}$, f is the final demand column vector related to the functional unit,

R is the regional output percentages, T transposes R and h_r consists of row vectors where each row is the quantity of a products life cycle emissions that occur in different regions. If R was representative of three regions contributing to the production of 10 kg of product with 10 kg from region 1, 8 kg from region 2 and 2 kg from region 3 it would be of the form:

$$R = \begin{bmatrix} 50 \\ 40 \\ 10 \end{bmatrix}\% \tag{7}$$

More complex and spatially accurate models exist that use Input–Output based approaches such as the interregional input output model (IRIO) also described by Yang (2016):

$$h_r = \left[\mathbf{B}^1\mathbf{B}^2 \cdots \mathbf{B}^\mathbf{n}\right] diag\left(\begin{bmatrix} \mathbf{A}^{11} & \mathbf{A}^{12} & \cdots & \mathbf{A}^{1\mathbf{n}} \\ \mathbf{A}^{21} & \mathbf{A}^{22} & \cdots & \mathbf{A}^{2\mathbf{n}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}^{\mathbf{n}1} & \mathbf{A}^{\mathbf{n}2} & \cdots & \mathbf{A}^{\mathbf{nn}} \end{bmatrix}\begin{bmatrix} f^1 \\ f^2 \\ \vdots \\ f^n \end{bmatrix}\right) \tag{8}$$

where $\mathbf{B}^i$ denotes environmental emissions from process in region i, A^{ij} denotes commodity flows from processes in region i to processes in region j. f^i denotes final demand in region i.

A hybrid approach combining IRIO and ROP models is also available:

$$h_r = \left[\mathbf{B}^1\mathbf{B}^2 \cdots \mathbf{B}^\mathbf{n}\right] diag\left(\begin{bmatrix} \mathbf{A}^{11} & \mathbf{A}^{12} & \cdots & \mathbf{A}^{1\mathbf{n}} \\ \mathbf{A}^{21} & \mathbf{A}^{22} & \cdots & \mathbf{A}^{2\mathbf{n}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}^{\mathbf{n}1} & \mathbf{A}^{\mathbf{n}2} & \cdots & \mathbf{A}^{\mathbf{nn}} \end{bmatrix}\begin{bmatrix} f^1 \\ f^2 \\ \vdots \\ f^n \end{bmatrix}\right)\begin{bmatrix} \mathbf{R}^1 & 0 & 0 & 0 \\ 0 & \mathbf{R}^2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \mathbf{R}^\mathbf{n} \end{bmatrix}^T \tag{9}$$

where R^i(i is 1, 2, …, n) contains regional output percentages for the subregions defined within region i. The ROP and hybrid approaches provide greater granularity than the method in Eq. 1, albeit with a larger input data requirement and computing time. Therefore, the application of these methods may not be suitable when running multiple LCAs such as when conducting Monte Carlo analysis.

3.4 Tools and perspectives

Regionalisation has been implemented into most of the commercially available LCA software. It is generally handled in two ways: flow-based or geo-spatially based. Flow-based approaches use elementary flows which are extended to include regional information whereas the geo-spatial approach uses GIS data to derive LCI datasets.

One alternative for increasing the temporal resolution on the LCA is addressing dynamic conditions in both the inventory and the LCIA phases with the Temporalis software tool. It supports 3 types of CFs that could be static (which means no changes over time), dynamic (where the values change over time and the impact still occur along emissions) and extended (which provides the decays rates of each CF over time) (Cardellini et al. 2018). In all approaches of this methodology, no carbon neutrality is assumed for biogenic carbon, which means its emission is accounted immediately. The dynamic impact assessment method spreads the environmental impact over time and a best-first exploratory strategy is applied to organise them as function of their priority (Cardellini et al. 2018; Zhang and Korf 1993). Then, the technosphere exchanges that contribute the most receive the highest priority and those with low relevance are neglected, as a cut-off strategy. The time of occurrence of all environmental interventions is added to a timeline satisfying the requirement of the DLCA even when the static CF are selected. The Temporalis methodology is efficient in increasing the dynamic resolution of both inventory and dynamic characterisation of emissions. The main advantage of the Temporalis approach remains on an open source generic method and tool for DLCA implementation available in Brigthway2 with framework (Cardellini et al. 2018).

Other exploratory methods are available on the literature to account the temporal aspects on LCA (Beloin-Saint-Pierre et al. 2014; Tiruta-Barna et al. 2016), but with some software limitations on running time and memory requirements. Methodological improvements considering the impact propagation over time and additional background data were suggested by (Pigné et al. 2019). The dynamic outcome of this approach considers a clear reference to process and supply chain functioning, as well as a proper temporal database linked to the background LCI (Pigné et al. 2019). Another tool software is available online for testing purposes (DyPLCA), but the access to the temporal database is protected by property rights (Pigné et al. 2019).

Temporally differentiated life cycle inventories and time-dependent, or at least TH-dependent, characterisation improve the accuracy of the LCA. DLCA are attractive for companies because the calculation results are more accurate and often lower than the static ones. However, the practical use of the former methods and tools presents barriers for their implementation in different contexts of the framework application since they are not yet available as user-friendly platforms.

Related to different perspectives, although the temporal representativeness of the supply chain have been modelled by the

DyPLCA tool (Pigné et al. 2019), the fluctuation on the market demand have not been considered during the modelling. Moreover, the existing market and surrounding product systems are not considered on the LCI of static models because they operate under steady-state conditions where the average demand and supply is generally covered in any scale (Marvuglia et al. 2013). From an industrial decarbonisation perspective, different scenarios with this scope could support the decision making process for complex systems (Marvuglia et al. 2013). The literature suggests the application of prospective modelling, where the CLCA is usually used on their calculations to project potential environmental impacts to the future and cover the interconnectivity between product system -environment. The fundamental differences on modelling can be used to classify the prospective approach in three different categories: economic models, historic trends and future scenarios (Beloin-Saint-Pierre et al. 2020). Albers et al. (2019) applied this approach to evaluate consequences of policy-driven transport strategies with time-sensitive supply–demand and dynamic CF ($C_{biogenic}$). Aldaco et al. (2019) used the prospective approach to compare the environmental outcomes of formic acid production from carbon capture and storage CCS (geological) by evaluating the potential evolution of the energy's supply system under different climate change scenarios (Aldaco et al. 2019); nevertheless, the interference of the final product on the market was not accounted by this approach. At the best of our knowledge, any tool for the application of the prospective modelling mentioned here before is available. Furthermore, the literature presents applications that are not limited to CCS and CCU (Beloin-Saint-Pierre et al. 2020), which are beyond the scope of this paper.

3.5 Summary

The inherent variations of the systems could consider time within their scope by setting short- or long-term analysis, dynamic function units and TH, and also by covering the period of validity of the data or technology obsolescence; nevertheless, the inclusion of temporal aspects in LCIA could have direct or indirect affectations to it. The indirect aspects are related mainly to the age and source of the data that is used, the technology deployment and the up-to-date coverage. Related to direct affectations, decisions regarding to LCA methods (e.g. consequential), dynamic or static inventories and CFs affect the analysis of the environmental outputs and can be assessed by different programming tools.

The complexity of the modelling, the availability of dynamic data, and the tools utilised during the study hampers the temporal calculation on LCA. Only the DyPLCA and Temporalis frameworks are available as tools. Furthermore, a limited selection of environmental categories has dynamic CFs. The process network modelling is complex due to the interaction of extensive timespans of the foreground (analysed process) and background (all supply-chain) data (Pigné et al. 2019). The temporal uncertainty and model complexity must be reduced by choosing the best compromise between accuracy and computational practicality (Pigné et al. 2019). Although the DLCA outcome provides high-quality information, its interpretation could not be as straight forward as the static approach. In this sense, the LCIA's scope, the technological state of the art, and the accessibility of the data should all be carefully considered when evaluating the inclusion of temporal aspects.

Regionalisation requires regional inventories and CFs which can be difficult to obtain at the same regional resolution. Given this, the onus of improving regionalisation relies on data collectors to improve the resolution of regional data and regional CFs, although this may be a monumental task involving the geopolitics of regions as regional CFs are often provided by state bodies. This can lead to different impacts when considering the regional impact of a process operating near and trade over international and intranational borders.

When circularity and regionalisation are considered in tandem, the processes remain the same. However, the regional vector or matrix (depending on the approach) needs to be adjusted to include a greater number of product transports between sub-regions leading to a more demanding analysis that also require temporal analysis as 'wastes' are generated and consumed cyclically.

4 PART III: Data quality analysis

4.1 Significance

In this section, we aim to address the shortcomings of the ISO guidelines with regards to data quality analysis and provide LCA analysts with methodologies to conduct UA and SA to improve the quality of their LCAs. All input data to an LCA model has some degree of uncertainty. Whether that uncertainty arises during experimental data collection, extrapolating data through time and across geographical boundaries, unverified data or from many other sources, it must be accounted for in the LCA output to accurately contextualise the importance of the results. Sensitivity analysis (SA) is then applied to the uncertainty analysis (UA) to model how the system responds to the uncertain values in the system. Properly applied, uncertainty and sensitivity analyses provide information on the predicted distribution of outputs and how a system reacts to perturbations in the inputs from a base case (Cucurachi et al. 2021).

Considering the environmental impacts of emerging technologies, it is essential to evaluate both the uncertainty associated with the technology and the sensitivity of the system to perturbations in the inputs. However, uncertainty is rarely included in published LCA studies. A meta-analysis of papers published in leading LCA journals conducted by Bamber et al. (2019) found that only 19% of ALCA and 15% of CLCA studies included some form of UA. Lo Piano and Benini (2022) found similar results as well, identifying that many authors confuse UA with SA or conduct only UA or SA, but rarely both. Most major LCA software have built in UA, SA, Monte Carlo simulations (MC) for UA, and one-at-a-time (OAT) SA (Igos et al. 2018). Bamber et al. (2019) attribute the absence of UA to several factors: a lack of understanding of the importance of UA; the time required to conduct a thorough UA; and insufficient uncertainty data available to the analyst. Additionally, the amount of information presented in the ISO 14040 and 14,044 guidelines on data quality analysis is scarce, leaving the analyst to conduct UA and SA without any specific guidance as to which methods are appropriate; therefore, many analysts choose not to conduct UA or SA.

4.2 Uncertainty analysis

4.2.1 Sources of uncertainty

In a recent review of UA in LCA studies, Lo Piano and Benini (2022) found that LCA analysts do not include all sources of uncertainty. Typically, when UA is conducted, only the uncertainty of the input parameters and/or CFs are considered. Commonly disregarded sources of uncertainty include model uncertainty and uncertainty in the context of the study; for example, two identical processes, one based in the UK and one based in mainland Europe, will have different associated geographical uncertainties when using a dataset produced from a Swiss case study. A typical LCA is traditionally done with low spatial resolution using regional, country-wide, continental or world-wide CFs during the LCI or LCIA phase depending on the availability of spatial data. Regional impacts are dependent on the impact category being applied. For example, Yang (2016) states that for the case of CO_2 the emissions, X, from producing a product, Z, in region Y would be identical when Y is varied. However, if human health were a major concern, the impact of an emission would vary with factors such as population density. For example, if benzene were emitted in Central London, it would result in a more severe human health impact compared with the same emission in Cheddar, a significantly less-dense village 180 km to the west of London.

To properly represent the uncertainty of a process, all sources must be quantified. A common approach in LCA to account for this is the use of pedigree matrices, which were introduced by Functowitz and Ravetz (1990). For example, many the datasets found in popular LCA databases, such as Ecoinvent (Wernet et al. 2016) and GaBi (Kupfer et al. 2021), are accompanied by a pedigree matrix which considers six sources of uncertainty: the reliability of the data; the completeness of the data; temporal correlation; geographical correlation; technology correlation; and a basic uncertainty based on the type of process of the dataset. A value from 1 to 5 is assigned to the first five uncertainty sources, with one being completely representative of the process and 5 being loosely representative. For example, a geographical correlation of 1 indicates that the data is from the area studied, whilst 5 indicates that the data is either from a distinctly different area, such as another continent, or is unknown. The scores are then combined to calculate the geometric standard deviation with a 95% prediction interval which can be used for the UA (Ciroth et al. 2012). The benefit of using a pedigree matrix for uncertainty representation is that it can be easily produced for a given input and, to some extent, it accounts for unknown data by assigning a pedigree of 5, leading to a high uncertainty distribution.

Applying spatial data from one region to another reduces the quality of the data and increases the geographical component of the pedigree matrix and in turn adds uncertainty. The same logic can be applied to other sources of uncertainty such as temporal relevance, technology used and reliability of data.

4.2.2 Uncertainty methodologies

When considering methodologies for UA, LCA analysts should also consider the software they are using to conduct the LCA. Igos et al. (2018) compared the functionalities of LCA software suites and found that the methods, characterisation and probability distributions differ. MC simulation propagation of the uncertainty is the most implemented method for LCA; the method iteratively calculates the LCIA scores with pseudo-randomly generated parameters based on the input distributions. MC also provides reliable outputs to users and allows the utilisation of different parameters, making it one of the best methods for uncertainty propagation. However, there are two major issues with MC in current LCA software suites. First, it is time-consuming as it requires to conduct a determine amount of iterative LCIA calculations to be statistically significant, and second, mass balance preservation is rarely, if ever, done in MC. The lack of mass balance preservation leads to a non-representative distribution outcome of the actual response of the system to perturbations.

We strongly suggest the continued use of MC for UA, in agreement with the methodology described in Langhorst et al. (2022), but encourage the LCA software developers to implement mass balance preservation and speed ups to complete a statistically significant number of iterations—typically 10,000 according to Langhorst et al. (2022) and possibly up to 1,000,000 as shown by Wei et al. (2016)—in a reasonable time frame. One such speed up is implemented in Brightway2 (Mutel 2017) where the first guess for the LCI calculation in subsequent MC iterations is the previous iterations results allowing the Brightway2 software to calculate more than 100 iterations per second. Other methodologies that give similar level of information but with faster computation times include quantitative stochastic uncertainty (Taylor series), fuzzy logic (Agarski et al. 2016) and regression analysis. However, to our knowledge, these methods have not been implemented in LCA tools yet.

4.3 Sensitivity analysis

SA is the process of determining how the uncertainty in the inputs affects the output uncertainty of a process, model or system. SA is generally conducted by recalculating outputs with small changes to two or more inputs and quantifying the impact that each varied input causes, in contrast to UA, which does not identify the assumptions responsible for uncertainty in the output (Saltelli et al. 2019). Similarly, ISO 14044 (2006) suggests to LCA analysts to conduct SA as part of their analysis but do not give a definitive method to do so.

4.3.1 Local sensitivity analysis

In a study conducted by Ferretti et al. (2016), it was found that local SA is more widely applied than global SA, as for every 100 SA studies that were reviewed, only 4 were global, with one-at-a-time (OAT) sensitivity analysis the most commonly used method, as such OAT and local SA have become near synonymous. OAT sensitivity varies one factor at a time whilst keeping the other factors at the base scenario value. The output, y (where $y = f(x)$ and x is a vector containing all inputs), local SA is more commonly applied than global SA. Along with an input, x_i, can be used to calculate the sensitivity index, S_i:

$$S_i = \frac{\partial y}{\partial x_i} \tag{10}$$

This method can be quick to calculate the sensitivity of many parameters compared to other methods, hence its popularity. However, OAT does not give any insight into how each variable of a model changes with another. Because of this the results of OAT SA quickly become very limited as the number of varied parameters increases. This concept is represented graphically in Fig. 8.

A more in-depth description of the faults of local SA methods is given by Saltelli et al. (2019). The use of OAT can however be beneficial if the input consists of one (or few) parameters of interest due to the relative simplicity and low computational times compared with global SA methods (Cucurachi et al. 2016).

4.3.2 Global sensitivity analysis

Global SA methods vary all parameters of a system proportionally to each other. This allows for the interactions of the parameters to be determined as the system changes over time. When characterising global SA, a simple Monte Carlo method can be applied with pseudo-randomly distributed factors for model inputs, CFs and so on. More complex models make more efficient use of the model input space by implementing Latin hypercube or quasi-random sampling methods, which distribute points more evenly across the space (Saltelli et al. 2008).

Global SA is appropriate in studies with large numbers of model inputs; nevertheless, its implementation in LCA is limited (Igos et al. 2018). Several studies have attempted to tackle this, some examples being Cucurachi et al. (2021), Lacirignola et al. (2017) and Cucurachi et al. (2016). However, like in the UA section above, these methods do not attempt to preserve the mass balance of the system during the variation of parameters. The co-variance of parameters is often assumed to be negligible and uncertainties to be independent of each other; thus, the correlation amongst variables in LCA studies is rarely investigated (Bisinella et al. 2016). Groen and Heijungs (2017) state that ignoring the effects of correlation of parameters is unknown, but that the risk of doing so can be quantified.

Groen et al. (2016) identify five suitable methods for global SA for matrix-based LCA: squared standard regression coefficients; squared Spearman correlation coefficient; key issue analysis; Sobol' indices; and random balance design index. Each of these methods has their benefits and drawbacks related to the size of the system, number of parameters and magnitude of input uncertainties; therefore, special considerations should be made by LCA analysts as to which method of global SA to apply. Whilst all methods considered by Groen et al. (2016) were equally suitable for small input uncertainties, the Sobol' indices and squared Spearman correlation coefficient were determined to be the best approach for large input uncertainties.

4.3.3 Outcomes

The outputs from the selected SA method are typically the variance that each parameter contributes to the system. By analysing the variance, the LCA analyst can identify the 'hotspots' of the system that are contributing the most to the environmental impact. Analysts should then consider future scenarios that could lead to reduction in the variance to improve the system in the long-term. Doing so can provide other LCA analysts, system designers and policy makers with means to implement new or developing technologies and temporally dynamic systems into the bigger picture.

4.4 Summary

The development of new LCA studies including both an UA and a SA is crucial to determine the environmental impacts of new and emerging technologies. Doing so will provide LCA analysts and policy makers with more information to understand the system as it develops or changes through time, as well as for the systems designers to visualise the contributors to environmental impact and the mitigation strategies. The framework developed here for UA and SA is presented in Fig. 9. Following these four steps ensures that the data quality analysis is complete and consistent with the state of the art described in reviews of uncertainty and sensitivity in LCA such as Lo Piano and Benini (2022), Bamber et al. (2019) and Igos et al. (2018). We also encourage LCA analysts to perform uncertainty considering more sources of uncertainty to better represent their systems, and to allow readers and decision makers to better understand the applicability of LCA studies.

Global SA methods should be considered by LCA analysts as the first choice for SA due to the quality of the analysis being higher than that of local methods. Local SA should be reserved for very simple processes with few inputs. Therefore, implementation of more robust SA methods should be a consideration of LCA software developers, such as Sobol' indices and squared Spearman correlation coefficient which were determined to be the most appropriate for LCA by Groen et al. (2016). Journal editors, and reviewers should consider the appropriateness of the sensitivity methods applied in LCA studies before approving manuscripts for publication.

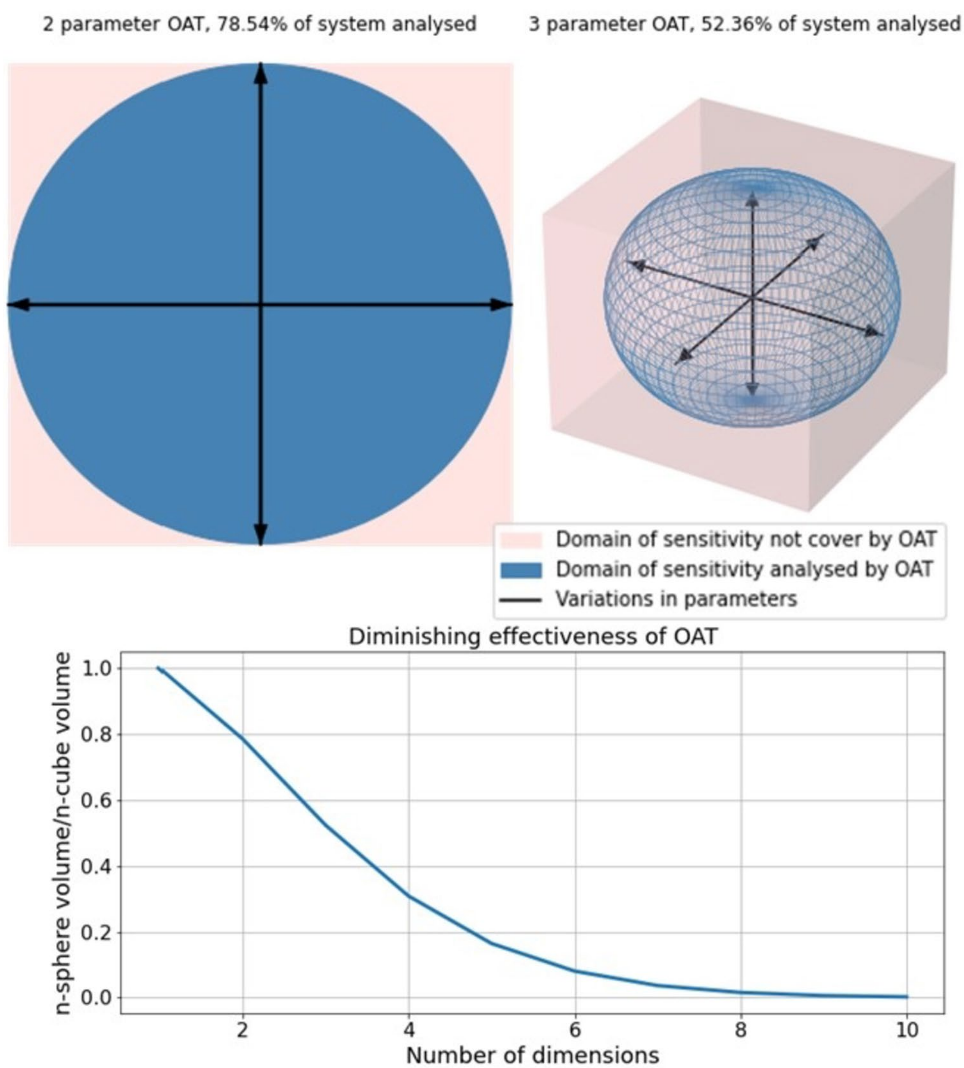


Fig. 8 *Top left*: The domain of sensitivity analysed using OAT with a two-parameter model. *Top right*: The domain of sensitivity analysed using a three-parameter model, note that the inside of the sphere should be filled as that whole volume is covered in the OAT SA but is left empty to show the extent of parameters x, y and z within. *Bottom*: Space filling ratio of hyperspheres within hypercubes of the same number of dimensions used to illustrate the shortcomings of OAT SA. As the number of varied parameters increases, the relative volume of the sensitivity space analysed decreases (illustrated by the pink area/volume in the top images). Adapted from Saltelli et al. (2019)

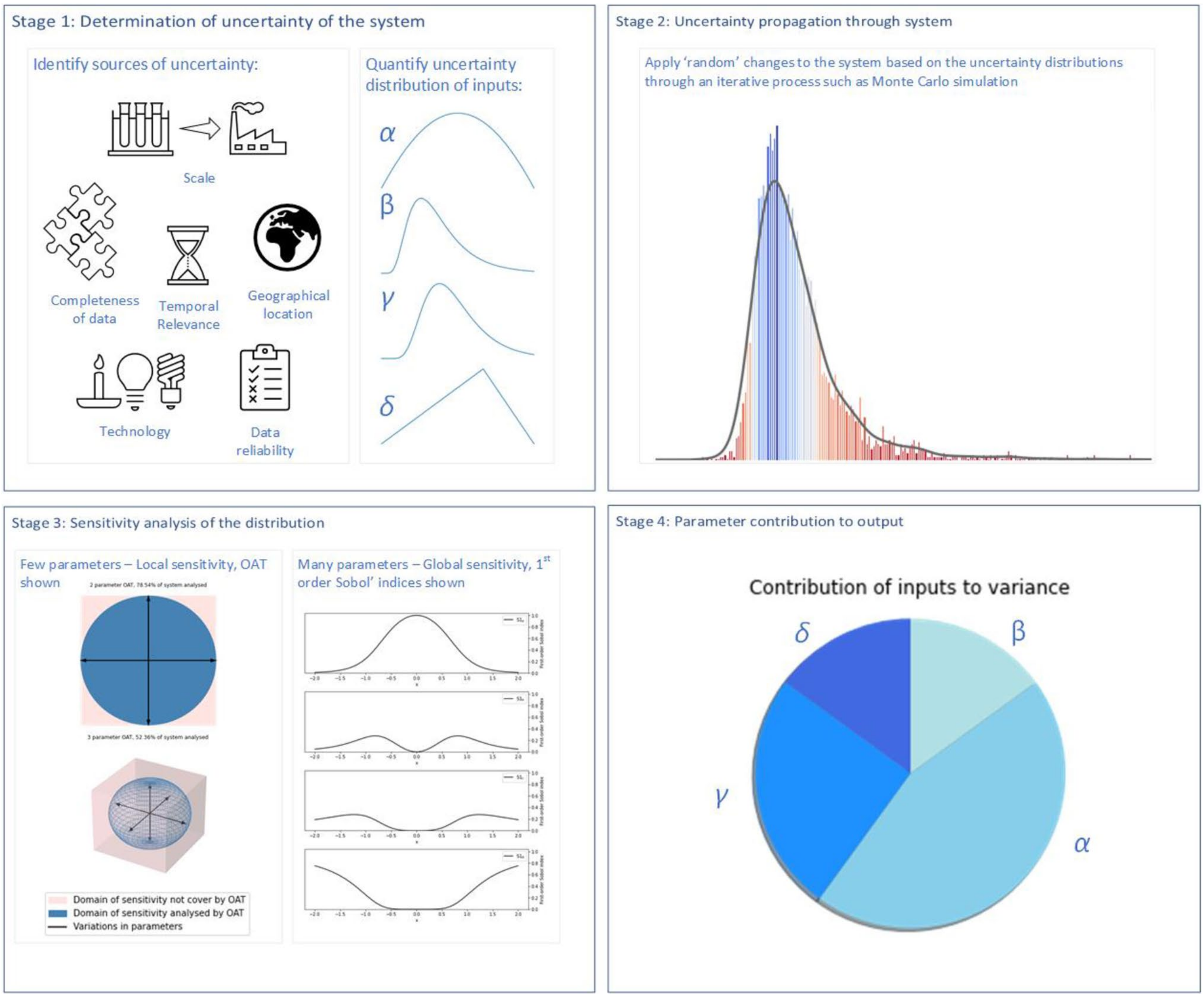


Fig. 9 The stages involved for conducting data quality analysis for LCA. Note that in this proposed framework all stages are mandatory

5 Part IV: Conclusions and perspectives

The ideal LCA modelling should be able to consider the transition to circular systems, whilst quantifying environmental, social, economic and other benefits at the largest scale with enough temporal and regional resolution, supporting with this policy makers and stakeholders.

A combination of different LCA modelling methods could help to consider both the fine resolution and broad scope required to explain the circularity distribution, and the outcomes of an LCA. Nevertheless, this potential combination could lead to a large number of interpretations, which consequently could hamper a wider application of the LCA due to the lack of transferability and comparability.

In that regard, this work provides recommendations for evaluating the LCA of CCUS by combining well known LCA guidelines with practical assumptions and applications reported on the literature. As shown before, the lack of comparability of the LCA reports must be mitigated. To support industrial decarbonisation, practitioners must apply their expertise to provide a unified method to clarify the circularity representation and to improve the representativeness of the LCA outcomes It is also considered that more transparency in LCA studies will enhance their reproducibility for other analysts, improving procedures and expanding on the body of knowledge, whilst reducing the need for reproducing LCIs and allowing LCAs of downstream and circular processes to be more agile.

Considering a circular economy, the consequential approach of LCA seems to be more appropriate than the attributional one since multifunctional background processes are linked together in a *carbon web*. For CCUS studies, prospective approaches could help to assess the potential impacts of novel products or technologies. Industrial wise, the retrospective approach can be used for well-established technologies where policy makers could manage interconnections amongst various sectors considering their shared inputs and outputs inventories. Then, the LCA could be modelled to share both benefits and burdens with suppliers and manufacturers to be implemented withing strategies like the circular footprint formula to enable a flexible system.

Better regional granularity in regionalised LCAs will aid in the incorporation of circularity and waste valorisation. Applying regionalisation could support optimising supply chains and tracking impacts over geographical boundaries. This will result in improving the quality of studies whilst making other dynamic aspects easier to model in LCA.

Temporal aspects are essential for high-resolution studies, providing a complete forecast of the emissions. Time in LCA could appear directly with dynamic inventories or CFs, for instance. The complexity of interpretation and modelling, the low availability of dynamic data, and the lack of tools hamper the application of DLCA. Time also appears indirectly for indicating aspects as period of validity of the data or deployment of technology, which indicates the excellence level of the data and its uncertainty.

Uncertainties in LCIA relies on data quality, technology readiness level and market maturity. The awareness of the importance of data quality analysis within the LCA community is essential to address the lack of information in ISO 14040 and 44. Uncertainty analysis should incorporate the mass balance preservation in processes to guarantee that 'randomised' parameters are still physically feasible possibilities, ensuring high accuracy in LCIA calculations. LCA analysts should incorporate uncertainty and sensitivity analysis when submitting their work for publication and likewise editors and reviewers should seek these analyses when considering an LCA for review. For sensitivity analysis, global methods should be chosen over local approaches since they provide a better level of sensitivity domain coverage. Local sensitivity should be confined to studies where no more than 3 parameters are of interest due to the exponential decrease in resolution of these methods as the number of parameters increases.

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Declarations

Competing interests The authors declare no competing interests.

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