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A process systems engineering view of environmental impact assessment in renewable and sustainable energy production: Status and perspectives

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ABSTRACT

With the increasing concern for climate change, renewable and sustainable energy production has attracted considerable attention from the scientific community, industrial practitioners, and policy and decision-makers. There are many technological alternatives for each sub-category of complex sustainable energy systems. Life cycle assessment (LCA) can be an effective tool to compare the environmental impacts of each pathway and identify the most promising alternatives from an environmental impact perspective. This contribution first reviews the environmental assessment methods and tools developed over the years. Secondly, a comprehensive review of the contribution of the PSE community to the environmental impact analysis of renewable energy systems is performed. It is observed that while LCA is the preferred method, these studies differed widely concerning the choice of impact assessment method used, the level of details shared concerning the underlying LCA calculations, and whether or not sensitivity and uncertainty analyses were carried out, among many others. This makes the comparison of results from different studies difficult and often impossible. It is clear that the PSE community, with its emphasis on systems thinking and holistic approaches, plays a critical role in the design, integration, and operation of complex sustainable energy systems. However, the thorough calculations necessary to ensure a robust and transparent LCA analysis require a shared methodology and a detailed description of the rules. Such explicit, systematic, and transparent methods will set the bar for a minimum requirement for thorough LCA calculations, ensuring fair comparison and discussions of different technical solutions developed in the wider PSE community for sustainable renewables.

1. Introduction

Industrial activities' direct and indirect dependence on bulk and specialty chemicals, services, and energy impacts the environment. Hence, there is a shared vision of the need for a sustainable production and consumption at all scales. Among the societal challenges, solving climate change is one of the most critical challenges of the 21st century. The energy supply is the key sector responsible for greenhouse gas emissions (Azhar Khan et al., 2014). The political and public support for addressing climate change will continue to drive the energy supply in a more sustainable direction.

The breakthroughs in renewable energy technologies in the past decades have increased the momentum towards adopting these new concepts. The commonality of renewable energy sources is that they can naturally renew themselves at a pace that enables us to meet our own energy needs (Pinto et al., 2019).

Renewable energy includes hydro, biomass, geothermal, wind, solar, tidal, etc. (Qazi et al., 2019). On the other hand, sustainable energy is a broader concept that is related to sustainability. The most well-known and accepted definition of sustainability is " the development that meets the needs of the present without compromising the ability of future generations to meet their own needs" (Mahdi, 1987). Sustainable energy comes from sources that can fulfill our current energy needs without jeopardizing future generations' energy needs or the climate (Mahdi, 1987). This concept also involves collection and distribution during the energy production process, where the energy should be

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competently obtained and distributed to be sustainable.

The concepts "renewable energy" and "sustainable energy" are usually used interchangeably among practitioners and industry experts (Wigley, 2021). However, it is necessary to distinguish between renewable and sustainable energy under some circumstances. There are overlapping characteristics between both concepts, where many renewable energy sources are also sustainable. However, these two terms do not represent exactly the same. Enhancing the sustainability of fossil fuels and renewables has the potential to bring significant environmental benefits (Wigley, 2021).

In this work, the sustainable renewable energy systems term is used to emphasize renewable energy that is also deemed sustainable. The most promising and popular types of renewable energy, such as, solar, wind, and hydropower, are generally considered sustainable. There are many technologies and pathways for the utilization of renewable resources. Increasing the contribution of renewable energy to the power grid is often seen as an efficient way to reduce the environmental burdens of energy supply. However, renewable energy sources differ in their overall environmental impacts from a life cycle perspective. Although renewable energy sources are the future of the energy supply, there is still a need to investigate the environmental impacts of each renewable energy source and make the optimal portfolio decision in the energy mix considering environmental impacts.

It is important to highlight that even though these technologies are considered sustainable by their proponents, It is only by providing a rigorous assessment and benchmarking of their environmental impacts that the sustainability of technologies can be assessed. Among other challenges, the environmental burden often shifts across scales, disciplines, and processes in the value chain (Bakshi, 2019).

The design and optimization of such sustainable energy systems are complex tasks, as they are, in fact, the result of a multi-criteria and multi-objective decision-making process. It is vital to clearly and transparently consider different criteria before claiming overall sustainability, respecting the Triple Bottom Line concept (TBL). TBL is a business framework that encourages companies to prioritize people, planet, and profit, recognizing the interdependence of these three elements for long-term sustainable success.

Environmental footprint is being increasingly integrated into the decision-making process for new processes and technology development. Many methodologies have been developed and implemented over the years to quantify the environmental impact and, hence, environmental sustainability, and Life Cycle Assessment is the methodology that is by far the most frequently applied and agreed upon (Bakshi, 2019; Čuček et al., 2015).

PSE tools are the right fit to provide a systematic way to evaluate the entire value chain and devise solutions that will, among others, strive towards minimizing environmental impact and burden shifting. Several PSE methods and techniques have been developed to support decision-making and hence achieve technically feasible and sustainable engineering designs as well as optimal supply chain solutions from a potentially large number of alternatives (Yang et al., 2017). Nevertheless, the systematic and transparent integration of LCA into PSE for the design and optimization of such systems is still not optimal.

Therefore, the goal of this work is four-fold: (i) to provide a summary of current sustainable renewable energy systems; (ii) to give an overview of the environmental impact assessment methodologies developed over the years; (iii) to offer a comprehensive review of the integration of environmental impact assessment in PSE studies for the design and optimization of complex energy systems; and finally, (iv) to discuss and present our opinion and perspectives, based on solid research, on current approaches and challenges in integrating environmental impact assessment faced by the PSE community today.

The remainder of this manuscript is structured as follows. In Section 2, the principles and methodologies for environmental assessments are briefly introduced. The role of PSE in this field is highlighted, and the influential studies from the PSE community are compared and discussed in Section 3. Section 4 discusses current practices, challenges and perspectives in environmental impact assessment and PSE. Finally, conclusions and a few take-home messages are given in Section 5.

2. Principles and methodologies for environmental assessment

As mentioned above, industrial activities have led to spiking climate change, among other significant environmental impacts. The consequent environmental awareness has triggered the development of environmental assessment methodologies to proactively assess and act to reduce manufacturing's environmental burden (Jacquemin et al., 2012). Several methods, tools, and frameworks have been developed and built upon over the years to quantify environmental impact (Čuček et al., 2015; Jeswani et al., 2010). Of note is that sustainability systems thinking has started not only to be an academic exercise but has also reached industries and services (McAloone and Hauschild, 2020).

One of the first examples of environmental assessment procedures mentioned in the literature is the development of principles and guidelines, such as the 12 Green Chemistry principles (Anastas and Warner, 2000), to steer towards more environmentally friendly designs. This was quickly followed by (Anastas and Zimmerman, 2003) which proposed the 12 principles of green engineering. Both strategies are part of the first efforts to transition from reactive to preventive environmental impact control at the source. Later, Telenko et al. (2008) provided a methodology comprising 6 principles and 67 guidelines after thoroughly reviewing the published checklists, principles, and guidelines. Recently, Zimmerman et al. (2020) have updated the green chemistry principles to include resource usage and profitability, among others. Besides, these additions also highlight the great potential of driving towards zero-waste production by maximizing function and minimizing material use. In fact, the E-factor (lower E factor = less waste) is one of the most well-known and accepted green metrics used to compare different designs for producing the same product (Chang et al., 2021; Sheldon, 2017).

The Eco-indicator 99, developed first by (Ministry of Housing, Spatial Planning and the Environment, 2000), was one of the first attempts to include sustainability as a post-hoc analysis. However, as indicated in the original publication, this indicator has several drawbacks, such as the fact that there is no "clear-cut objective to define sustainable target levels" (Ministry of Housing, Spatial Planning and the Environment, 2000).

Environmental Risk Assessment (ERA) is a design tool for retrofitting/improving current processes. It assesses environmental risk due to a specific activity and/or exposure and then generates a plan to minimize harmful effects (Burgess and Brennan, 2001; Olsen et al., 2001). Moreover, Environmental Impact Assessment (EIA) targets predicting and analyzing the environmental outcomes of human activities before they even start (Morgan, 1999); it provides qualitative and quantitative information based on checklists regarding environmental and socio-economic concerns (Burgess and Brennan, 2001). Even though it enables reducing environmental impact and identifying potential benefits, it is highly project-specific.

Another method that has gained some standing for assessing energy efficiency of chemical processes and embodies a more in-depth analysis is the cumulative exergy analysis method (Bösch et al., 2007). Exergy allows quantifying the potential impact of a material or energy stream on the environment. Rosen and Dincer (1999) have shown that as the exergy efficiency of the process increases, environmental impact drops, and potentially sustainability rises. This has motivated further development of exergy-based methods, such as the cumulative exergy demand/exergy energy footprint analysis method (CExD) (Rosen and Dincer, 1999) and the water exergy footprint method (Caudill et al., 2010; Čuček et al., 2015).

Eco-efficiency is another approach that has gained some traction. It is a management strategy that implies doing more with fewer resources and focusing on creating less waste and pollution (Bengtsson, 2004).

Although a common definition has yet to be reached, a standard description is that eco-efficiency is a sustainability indicator that integrates economic and environmental performances.

The Waste Reduction Algorithm (WAR), formally introduced in 1999 by Young and Cabezas (1999) and Cabezas et al. (1999), is one of the most generally acknowledged model-based gate-to-gate methodologies that reveals the environmental performance of a production process at the early stage of design. Potential environmental impact (PEI) is applied to estimate the average environmental impact of eight impact categories (Young et al., 2000). WAR has been the quantitative basis of many other environmental assessment methods developed over the years, such as the one recently presented in the study of Heidrich et al. (2019).

There are also other model-based gate-to-gate methodologies, such as the Green Degree method (GD) and GREENSCOPE, proposed by Zhang et al. (2008) and Ruiz-Mercado et al. (2014), respectively. GD leads to estimating one aggregated indicator to quantify a system's environmental performance, either it being a product, mixture, or unit. This indicator is calculated based on 9 established impact categories and the use of simulation tools. GREENSCOPE was proposed to evaluate the sustainability of a reaction or process by assessing relevant metrics among the 140 inbuilt indicators and following a hierarchical strategy to support decision-making (Smith et al., 2015).

There has been significant interest and discussion on the benefits and drawbacks of using composite indexes (aggregated indicators) that combine several assessment methods. Benefits could be related to the potential simplification of result interpretation. However, it is rather difficult to draw detailed conclusions due to conflicting objectives in the decision-making progress (Kalbar et al., 2017; Kumar et al., 2017). They combine and/or merge different methods to decrease the complexity of interpretation, leading to a more challenging interpretation of results (Laso et al., 2022).

Although choosing greenhouse gasses as a single metric is a widespread approach (see discussion in Section 4), this leads to loss of and/or misleading information and potential burden-shifting to other resources or emission streams (Bakshi, 2019; Čuček et al., 2015; Finnveden et al., 2009). Thus, when efforts are put into transitioning to more sustainable systems it is fundamental to consider the entire life cycle of the systems under study, including all moving system parts such as processes, activities, and supply chains, in order to minimize the issue mentioned above (Čuček et al., 2015). LCA is the natural next step (Čuček et al., 2015; Pozo et al., 2012). First introduced in the late 1960s and early 1970s, LCA has become a generally accepted systematic methodology that aims at thoroughly quantifying the environmental burdens related to systems over their life cycle in terms of emissions, health impacts, and resource consumption (Čuček et al., 2015; Guillén-Gosálbez et al., 2019). Guinée et al. (2011) give a comprehensive history of the introduction of LCA and its evolution. Its structure and methodological elements are described in detail in the ISO 14,040 [37] and ISO 14,044 standards (ISO 14044, 2006).

In LCA, different approaches can be used to estimate the potential environmental impact of a product or system during its life cycle; the three common strategies are cradle-to-gate, cradle-to-grave, and cradle-to-cradle. Of note is that ISO 14,040 and ISO 14,044 are key standards, guidelines that provide support regarding the arsenal of choice of appropriate methodologies and recommend comprehensiveness and consistency.

Ideally, the application of LCA seeks to cover all activities from a "cradle-to-cradle" perspective, also known as closed-loop analysis (Čuček et al., 2015; Glavič and Lukman, 2007). The second preferred option is "cradle-to-grave", the open-loop approach (Čuček et al., 2015; Sustainable Industrial Design and Waste Management, 2007). This entails the design and development, raw material acquisition, production, distribution, use, maintenance, and end-of-life activities. It can serve numerous goals and be applied at different product life cycle stages. For example, LCA can be used to (i) evaluate the environmental impact of a sole product, (ii) compare processing alternatives for the manufacture of interchangeable products/processes, (iii) compare possible options to deliver the same function, and (iv) identify environmental hotspots in the life cycle and provide suggestions for improvement (Guillén-Gosálbez et al., 2019; Hellweg and Milà i Canals, 2014).

To summarize, the key differences between these three approaches is in the scope of the assessment: (i) cradle-to-gate, focuses solely on the manufacturing process; (ii) cradle-to-grave, considers the whole life cycle including disposal, and (iii) cradle-to-cradle, is the strategy applied to design products with a circular approach.

Noteworthy is that the wider scope of LCA such as cradle-to-cradle helps avoid the above-mentioned burden- and problem-shifting, for example, from one region to another, from one stream to another stream, and among life cycle stages (Čuček et al., 2015; Finnveden et al., 2009).

As detailed in Fig. 1, the LCA methodology is divided into four steps: goal and scope definition, life cycle inventory analysis (LCI), life cycle impact assessment (LCIA), and interpretation. The goal and scope definition depicts all the critical aspects of the LCA study; it describes the application and reasons behind the study, the target audience, the functional unit, the reference flow, and the system boundaries (*Life Cycle Assessment - Theory and Practice*, 2018). The choice of the functional unit significantly impacts the study results and conclusions as it is the basis for fruitful comparisons. The LCI is the data collection step where all inputs and outputs of the system are identified and quantified (inventory of energy and raw material inputs, products, co-products, wastes, emissions to air, discharges to water, etc.) (ISO standards). If data from measurements or literature is unavailable, generic LCI data from databases is usually used (Life Cycle Assessment - Theory and Practice, 2018). Examples of these databases are Ecoinvent (Frischknecht et al., 2003), GaBi professional (Schuller et al., 2013), and GREET (Woertz et al., 2014). Of note is that the representativeness/accuracy of the data can potentially vary among the different databases (Bueno et al., 2016; Koj et al., 2019). Once the inventory task is complete, the LCIA step is performed, where the inventory (input and output elementary flow) is categorized and assigned to different impact categories. This is immediately followed by the characterization stage, where the potential impacts are modeled by employing conversion factors to arrive at a quantified indicator for the impact category. The mentioned conversion factors depend on the LCIA method chosen; CML, ReCiPe, and TRACI are, among others, three of the most often used LCIA methods (Koj et al., 2019). Among other distinctions, the LCIA methods differ in terms of being estimated at mid- or end-point level, location/region, time horizon/temporal, and characterization model. Hence, the selection of LCIA is highly impactful and must be stated clearly in the study (Rosenbaum, 2017). Interpretation is the last stage of the LCA, where concerns and hotspots are identified, along with consistency, sensitivity analysis, conclusions, and recommendations drawn based on the LCIA results. Nevertheless, there are still some challenges and limitations to be overcome; a summary of these is as follows.

(i) While there are designated standards and guidelines to conduct LCAs (e.g., ISO 14,040 and ISO 14,044), the lack of a systematic approach can result in the unreliable application of these standards. In particular, LCA application implies making assumptions and choices at different stages, such as impact assessment models, system boundaries, and allocation methods. This **lack of standardization** leads to difficulties in comparing and interpreting LCA results across different studies due to the **subjectivity and variability** in the choices made during the LCA study.

(ii) LCA frequently depends on **simplifications and assumptions** to handle complexity and/or data gaps. These simplifications can neglect important elements and introduce uncertainties. Further, essential to note is that the choice of impact assessment methods and models affects the results, and no single impact method alone can grasp the full complexity of environmental interactions.

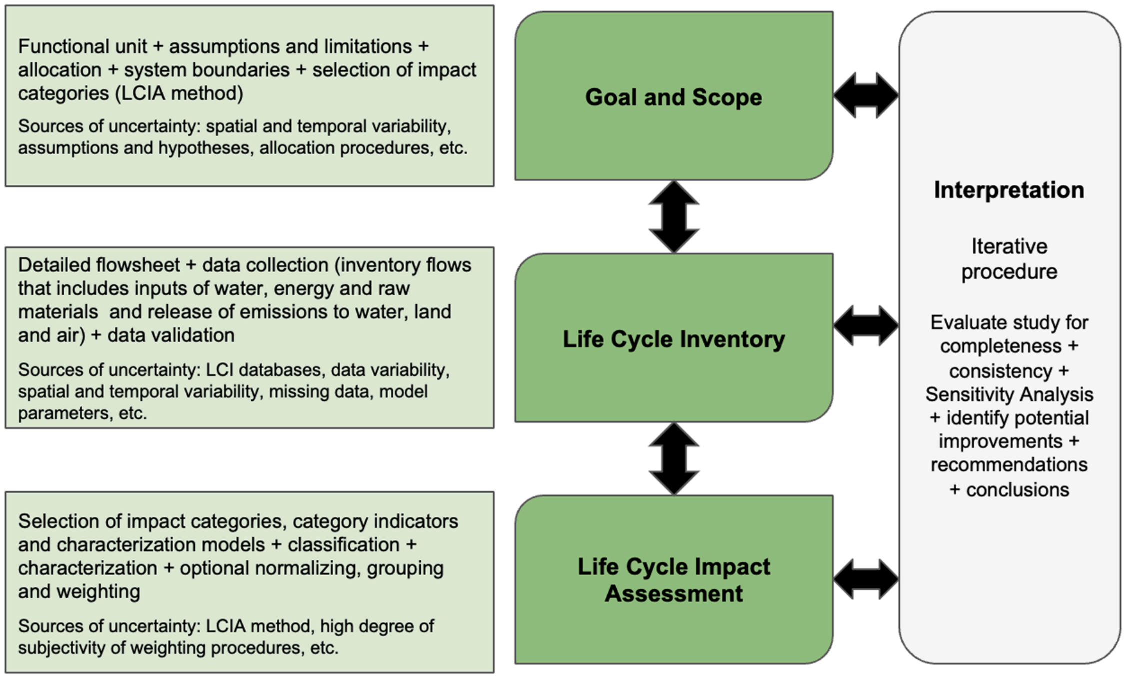

Fig. 1. The four steps of LCA. Inspired by (Čuček et al., 2015; Rebitzer et al., 2004).

(iii) Specifying the **system boundaries** determines the scope of assessment, which is another variable/limitation across LCA studies. Deciding on which life cycle stages to include and exclude and the limits of the supply chain can significantly impact the results. Different boundary alternatives can lead to inconsistent findings and make it difficult to compare and analyze different studies.

(iv) In addition to the previous point, LCA frequently employs **simplified models** to describe complex processes and systems, as it is not viable to include all the complexities of real-world processes. Regardless, the lack of a systematic approach for doing so may lead to oversimplification or dismissal of essential elements, which can then impact and influence the accuracy and reliability of the study. Securing its **quality and reliability** can be difficult even when data is available. Data may come from diverse sources with different methodologies, accuracy levels, and representativeness.

(v) LCA relies heavily on a range of input data (inventory, environmental impacts, etc.) throughout the entire life cycle of a system, product or process. Yet, **data availability** is, more often than not, limited and/or incomplete, which requires appropriate modeling/simulation to estimate the needed data (generation of so-called secondary data), particularly for emerging technologies or niche products. Collecting relevant data for all product life cycle stages can be challenging. Data may be proprietary or unavailable, notably for emerging technologies or geographical regions. These challenges lead to uncertainties, inaccuracies, and assumptions in the assessment, which consequently impacts the quality of LCA results. Data gaps and inconsistencies raise uncertainties and bias in the LCA.

(vi) Performing a comprehensive LCA is **resource-intensive**, demanding considerable resources, such as time and expert knowledge. With a systematic approach, allocating resources effectively may be more accessible, prioritizing data collection or ensuring consistency across different assessments. This can lead to incomplete or rushed analyses that capture only some of the life cycle impacts.

Of note is that the LCA community continuously works to address these challenges by enhancing data collection, increasing transparency, and advancing/improving methodologies. However, despite these limitations, LCA remains the methodology of choice for assessing the environmental impacts of products and systems and supporting informed decision-making toward sustainability. Therefore, **adopting a systematic and standardized approach to LCA is important to overcome these limitations**, which should account for reliable data, transparent methodologies, and comprehensive assessments considering the full life cycle impacts and suitable sustainability dimensions.

Another interesting recent line of research is the integration of LCA with Data Envelopment Analysis (DEA). Under this framework, LCA estimates the environmental impacts of the systems, and DEA assesses their efficiency, providing suitable benchmarks and goals for the less efficient ones. The main aim of LCA+DEA is to include both environmental and economic factors in the eco-efficiency estimation (Vásquez-Ibarra et al., 2020). Applications of said methodology can be found in Hong and Mwakalonge (2020), Martín-Gamboa et al. (2017), Rebolledo-Leiva et al. (2017), Vázquez-Rowe et al. (2010), (2011).

Finally, although the LCA methodology has not been developed within the PSE discipline, they undoubtedly have the systems approach in common (Guillén-Gosálbez et al., 2019). LCA has been increasingly integrated into the PSE studies and community by coupling LCA with process optimization under the life cycle optimization framework (LCO), first introduced by Azapagic and Clift (1999). Thence, LCA has found many applications in multiple domains. The typical approach is to benchmark a limited number of scenarios, considering their life cycle impact to identify hotspots and develop solutions/ recommendations for improvements (Guillén-Gosálbez et al., 2019; Hellweg and Milà i Canals, 2014). Examples of such efforts are given in Table 1, Section 3. The clear relationship between LCA and the PSE field, along with, among others, the challenges mentioned above, the benefits, and drawbacks, are further discussed and elaborated upon in Section 4.

3. Overview of the role of process systems engineering in renewable and sustainable energy systems

Sustainable energy system design is built on multi-criteria and multi-

Table 1
List of PSE publications reviewed limited to: (i) 2009 – 2020 (for obtaining a representative sample), (ii) performing environmental impact assessment, and (iii) complex renewable energy systems highlighted in Fig. 2. GA= Genetic Algorithm; EA= environmental assessment; NA = Not Applicable. MINFP= mixed-integer nonlinear fractional programming problem. LNG= liquefied natural gas; CED= cumulative energy demand; Fobj = objective function.

Refs.	Energy production system	Modeling approach	3 Pillars of sustainability assessment addressed?	Environmental assessment approach	Metrics used / reported	How is EA included in the study	System boundaries	LCA Life cycle impact assessment method (LCIA)	Reports decisions in all LCA 4 steps?	LCA Software used?	SA, UA, scenario analysis?
(Zamboni et al., 2009)	corn-based bioethanol	MILP, multi-objective	no	LCA	GHG	included in/as the Fobj	well-to-wheel	not mentioned	no	no	no
(Alvarado-Morales et al., 2009)	bioethanol	modeling and simulation with proii + scenarios	no	SustainPro	energy and water cost	post simulation	gate-to-gate	- (NA)	- (NA)	- (NA)	- (NA)
(Elia et al., 2011)	hybrid coal, biomass, and natural gas to liquid (CBGTL)	MILP	no	GREET model	GHG	post optimization step	well-to-wheel (gate-to-gate indirectly mentioned)	not mentioned	no	no	no
(Santibañez-Aguilar et al., 2011)	production of ethanol, hydrogen and biodiesel	LP multi-objective, e-constraint	no	eco-indicator-99	single score eco-indicator-99 and GWP	included in/as the Fobj	cradle-to-grave	Eco-indicator-99	no	no	no
(Mele et al., 2011)	production of sugar and bioethanol	MILP multi-objective, e-constraint	no	LCA	GWP and Eco-indicator 99	included in/as the Fobj	cradle-to-gate	CML and eco-indicator99	yes, in detail	no	no
(You and Wang, 2011)	biomass-to-liquids supply chains	MILP multi-objective, e-constraint	no	LCA	GHG	post optimization step	cradle-to-grave	IPCC[3]	yes, minimalist	no	economic, empirical
(Gerber et al., 2011)	combined fuel and electricity production from lignocellulosic biomass	MILP, multi-objectve	no	LCA	report several metrics estimated using the impact assessment methods	included in/as the Fobj	cradle-to-gate	eco-indicator 99 and ecoscarcity06	yes, in detail	no	no
(Modahl et al., 2012)	electricity from a fossil gas power plant with CO2 capture, transport and storage	scenarios (data comes from other sources) - not an optimization study	no	LCA	GWP, AP, EP, POCP, CED	analysis of the different scenarios + comparison of methods	cradle-to-gate	ReCiPe, EPS2000, IMPACT 2002+	yes	SimaPro	yes, process design scenarios
(Gerber and Maréchal, 2012)	cogeneration of electricity and district heating	MILP, multi-objectve	no	LCA	GWP or Eco-indicator 99	included in/as the Fobj	cradle-to-grave	IPCC[3] and Eco-indicator 99	yes	no	no
(You et al., 2012)	biofuel supply chain	MILP multi-objective, e-constraint	no	LCA	GHG	included in/as the Fobj	cradle-to-grave	IPCC	yes	no	no
(Pérez-Fortes et al., 2012)	electricity generation	MILP, multi-objective	yes	LCA	IMPACT2002+	included in/as the Fobj	cradle-to-gate	IMPACT2002+	no	no	no
(Čuček et al., 2012)	biomass to energy	MINLP, multi-objectve, multi-crireria optimization	no	LCA	GHG (Carbon Footprint[1])	included in/as the Fobj (e-constraint)	cradle-to-grave	no	no	no	no
(Kostin et al., 2012)	bioethanol/ sugars supply chain	MILP multi-objective, e-constraint	no	LCA	GWP100, EI99, DHH, DEQ, and DR.	five environmental objectives are simultaneously	not mentioned	Eco-indicator 99	no	no	no

(continued on next page)

Table 1 (*continued*)

Refs.	Energy production system	Modeling approach	3 Pillars of sustainability assessment addressed?	Environmental assessment approach	Metrics used / reported	How is EA included in the study	System boundaries	LCA Life cycle impact assessment method (LCIA)	Reports decisions in all LCA 4 steps?	LCA Software used?	SA, UA, scenario analysis?
						optimized along with the net present value					
(Bamufleh et al., 2013)	co-generation systems	combination of GA and LP, multi-objective	yes	not mentioned	GHG	included in/as the Fobj	not mentioned	no	no	no	no
(Baliban et al., 2013)	natural gas to liquids	MINLP	no	not mentioned	GHG	post calculation	not mentioned	not mentioned	no	no	no
(Yue et al., 2013)	hydrocarbon biofuels	MILP and MILFP, multi-objective, e-constraint	no	LCA	GWP or Eco-indicator 99	included in/as the Fobj	cradle-to-gate	not mentioned	yes, but as steps of their framework. So no details are given regarding the LCA itself	no	no
(Wang et al., 2013)	hydrocarbon biofuels via gasification	MINLP multi-objective, e-constraint	no	LCA	GWP or Eco-indicator 99	included in/as the Fobj	gate-to-gate	IPCC[3] and Eco-indicator 99	no	no	no
(Gebreslassie et al., 2013)	algal-based hydrocarbon biofuel production and carbon sequestration from power plant flue gas	NLP, bi-criteria, e-constraint	no	LCA	GWP	included in/as the Fobj	cradle-to-gate	IPCC[3]	yes, minimalist	no	no
(Gebreslassie et al., 2013)	hydrocarbon biorefinery via fast pyrolisis, hydrotreating and hydrocracking	MINLP, bi-criteria, e-constraint, heurisitic solution	no	LCA	GWP and Eco-indicator 99	included in/as the Fobj	gate-to-gate	IPCC[3] and Eco-indicator 99	yes	no	no
(Santibañez-Aguilar et al., 2014)	bioethanol and other bioproducts	MILP multi-objective, multi-period e-constraint	yes	eco-indicator-99	single score eco-indicator-99	included in/as the Fobj	not mentioned	eco-indicator-99	no	no	no
(Jakobsen et al., 2014)	(i) integrated gasification combined cycle, (ii) coal fired power plant, (iii) use of CO2 for oil recovery	iCCS: modular simulation of CCS chain configurations (Aspen Plus and Aspen Hysis)	no	hybrid LCA (use of Ecoinvent and IO Carnegie Mellon databases)	GHG	analysis of scenarios (not an optimization study)	not mentioned	not mentioned	no	no	yes, chain/ process design scenarios
(Hanes and Bakshi, 2015)	corn bioethanol	NLP, multi-objective	no	LCA	CO2 emissions	included in/as the Fobj	cradle-to-grave[1]	GREET model	no	no	no
(Yue et al., 2016)	bioethanol supply chain	MILP, multi-objective, multi-period e-constraint	no	hybrid LCA	GWP	included in/as the Fobj	cradle-to-grave[1]	https://ghgprotocol.org/calculation-tools	no	no	yes

(*continued on next page*)

Table 1 (*continued*)

Refs.	Energy production system	Modeling approach	3 Pillars of sustainability assessment addressed?	Environmental assessment approach	Metrics used / reported	How is EA included in the study	System boundaries	LCA Life cycle impact assessment method (LCIA)	Reports decisions in all LCA 4 steps?	LCA Software used?	SA, UA, scenario analysis?
(He and You, 2016)	shale gas processing	process design, modeling, and integration	no	LCA	energy-water-carbon nexus (HJH, water footprint, energy consumption)	post analysis	cradle-to-gate	not mentioned	no	no	no
(Ghosh and Bakshi, 2017)	corn ethanol and DDGS as by-products	NLP, multi-objective, e-constraint	no	hybrid LCA	CO2 emissions	included in/as the Fobj	cradle-to-grave[1]	not mentioned	no	no	no
(Boyaghchi and Chavoshi, 2017)	solar-geothermal driven combined cooling, heating and power (CCHP) cycle integrated with flat plat collectors	multi-objective optimization MILP and NSGA-II method	no	exergoenvironmenal analysis (combo exergy-based analysis and LCA)	total product environemental impact	included in/as the Fobj	cradle-to-grave (indirectly)	eco-indicator-99	no	no	no
(Gong and You, 2017)	algal diesel production	MINLP, multi-objective	no	LCA	11 metrics normalized into one metric	included in/as the Fobj	cradle-to-grave	IPCC	yes	no	no
(Gong and You, 2018)	shale gas processing	process simulation + multi-objective MINLP	no	LCA	GWP water footprint	included in/as the Fobj	cradle-to-gate	IPCC	no	no	SA (economics)
(Yang and You, 2018)	shale gas processing and methanol manufacturing	modeling and hysys simulation of both processes	no	LCA	ReCiPe metrics	analysis of scenarios	gate-to-gate	ReCiPe endpoint and midpoint	no	no	scenarios SA (impact of distances)
(Wheeler et al., 2018)	sugar to bioethanol	multi-attribute decision making	no	LCA[2]	11 metrics normalilzed into one objective function	included in/as the Fobj with normalizing weights	not mentioned[2]	Eco-indicator 99	no[2]	no	no
(Wu et al., 2018)	microalgae to biofuels	single objective optimization	no	LCA	GHG	included in/as the Fobj	well-to-tank	not mentioned	no	no	no
(Álvarez del Castillo-Romo et al., 2018)	lignocellulosic biomass to biofuels and bioproducts	MINLP, multi-objctive, e-cobstraint + Aspen Plus simulation	yes	eco-efficiency	Socio-eco-efficiency	included in/as the Fobj	gate-to-gate	NA	NA	NA	no
(Pérez-López et al., 2018)	oil from microalgae	not an optimization study	no	LCA	GHG, Euthrophication and CED	NA	cradle-to-gate[1]	TRACI	yes, minimalist	no	yes
(Liu and Bakshi, 2019)	corn ethanol	not an optimization study – post calculation	no	adapted LCA	net CO2 emissions	NA	cradle-to-grave	TRACI	yes	no	no
(Tian and You, 2019)	hybrid energy system for heat and coling	MINFP, multi-period	no	LCA	GWP	post optimization step	not mentioned	IPCC 2013	no	no	yes (impact of input parameter)
(Blanco et al., 2020)	power to methane	not an optimization study – post calculation	no	LCA	18 categories	NA	cradle-to-grave	ReCiPe midpoint	yes	no	no

objective decision-making procedures. During these procedures, PSE traditionally contributes to developing technically feasible engineering design, synthesis, control, and supply chain solutions. As such, the PSE discipline is well suited to integrate the LCA methodology and contribute to improving the sustainability of these processes. For example, in the future, we expect that a variety of energy production technologies will make up the large energy supply networks. In that situation, the environmental impacts of complex sustainable energy systems heavily depend on the extent of systems integration and optimization. Here, there is a natural role for PSE, with its systems approach mindset and toolset, to work jointly with LCA to contribute to sustainability by design.

Indeed, for complex sustainable energy systems design, the fundamental question to address is which technologies to adopt, which product to manufacture, and the sequence of operations needed to obtain the maximum profit and lowest environmental and social impacts. Process synthesis, integration, intensification, and optimization methods and tools from the PSE discipline can be applied to answer this question. A systematic methodology to design, analyze, and improve the process is a helpful first step in the evaluation of the environmental impacts of the energy production system. The PSE community has conducted many studies exploring this contribution to literature, which we review below.

To gather a holistic view of the studies, we performed a comprehensive literature search with the keyword PSE combined with other terms used in relation to renewable energy systems. The search results are illustrated in Fig. 2.

Environmental assessment, as highlighted in Fig. 1, primarily by applying LCA, has gradually become more important in the PSE community. As also demonstrated in Fig. 2, the research interest in renewable energy and power-to-X systems has increased tremendously, especially in the last decade. Although there are many works in the field, the goal of this work is not to present an all-encompassing literature review. Hence, a representative sample of the body of work performed in the last two decades regarding the mentioned energy systems, which includes environmental assessment in the PSE study, is collected and benchmarked in Table 1.

As mentioned in Section 2, several methods have been used in the PSE community over the years to analyze the environmental impact of energy systems. For example, eco-efficiency (Álvarez del Castillo-Romo et al., 2018) looks at a normalized quantity representing the system's environmental impact. Similarly, as observed in Table 1, Eco-indicator 99 is a quite common method, especially in older studies. This can actually represent two different aspects, where it can be used as (i) a single indicator (not LCA) (Gebreslassie et al., 2013); and (ii) as an LCA method in the Life Cycle Impact Assessment stage (Wheeler et al., 2018).

Nonetheless, it can be observed in Table 1 that LCA has gradually become the approach of choice in the PSE community. This is a welcome development, as the LCA is the most commonly accepted methodology for quantifying the environmental dimension of sustainability. However, there are some important limitations to be mentioned, as will be highlighted below.

Although most of these studies focus only on using one single impact category, the distribution is as follows: (i) 41.7% (15 out of 36 studies) mainly focus on the mid-point CO_2 eq. category of impact; (ii) 30.6% (11 out of 36 studies) use an aggregated indicator (typically end-point and the Eco-indicator 99) in the context of process and supply chain optimization, as in Santibañez-Aguilar et al. (2014) and Wheeler et al. (2018); and, (iii) 27.7% (10 out of 36 studies) use several indicators but, like in Wheeler et al. (2018), the indicators are included in the form of scenario testing. Furthermore, only 22.2% (8 out of 38 studies) performed sensitivity and uncertainty analysis. Of note is that Modahl et al. (2012) is, in fact, the only study out of 36 studies analyzed that uses professional LCA software (instead of, for example, including the calculations in the optimization problem). There is no explicit explanation in the reviewed studies as to why such specialist software is not

[1] not mentioned directly.
[2] it refers to another paper(s) for assumptions and calculations.
[3] IPCC 100-year global warming potentials.

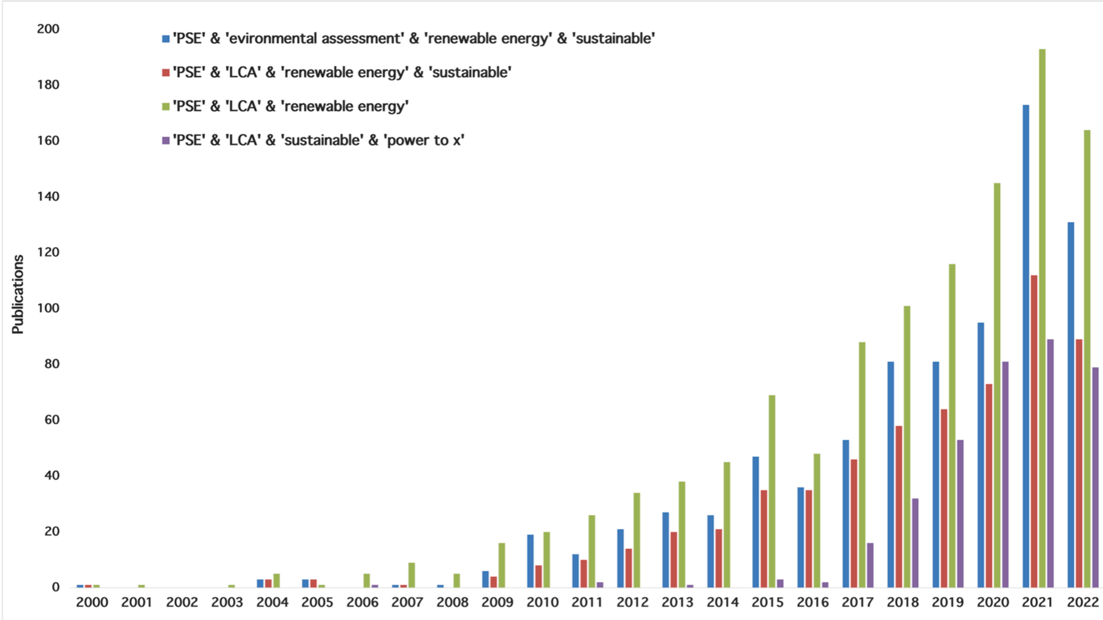

Fig. 2. Publications that fit the keyword combinations presented. Data from Web of Science, accessed on November 22, 2022.

employed. The underlying reasons could be, among others: (i) SimaPro is a license-based software, and its application requires resources as well as training, which may not be accessible to all research groups; (ii) a matter of priority and scoping of the research: it may be that there are resources yet a comprehensive environmental impact assessment and analysis of impact categories were not deemed the main focus and hence use of a specialist LCA software was not prioritized; and, (iii) it may be that integration of comprehensive LCA analysis with optimization problems (such as mathematical programming applied for supply chain analysis, process synthesis, and design, etc.) is perceived computationally too complex to solve. Irrespective of the underlying reasons, the current and future environmental impact assessment needs to perform a proper and systematic LCA analysis, ideally through an interdisciplinary collaboration with the LCA community.

Important to note is that approx. 64 % do not report all decisions made when performing the LCA study. This is critical for reproducibility and fair comparison among studies of similar or equivalent systems.

As mentioned previously, there are several impact categories calculated in the LCIA to provide a comprehensive environmental impact assessment: not only climate change but also ozone depletion, freshwater ecotoxicity, human toxicity, and water depletion, to name a few mid-point categories from the ReCiPe database. We believe that the common approach of reducing the impact categories obtained in LCIA to a few "representative" categories is very reductive, as previously mentioned, and commonly leads to less informed decisions and under-the-hood burden shifting (Bakshi, 2019; Czyrnek-Delêtre et al., 2017). The burden shifting applies not only to transfer among categories of impact but also to social and economic metrics. The next section discusses these issues, challenges, and perspectives in more detail.

A significant portion of the optimization studies, mainly based on MINLP and MILP methods, within energy systems and beyond, defend that they perform life cycle optimization by including the chosen LCA metric in the objective function through multi-objective optimization (Yue et al., 2016). However, as mentioned above, this is not representative. By using an aggregated metric, the dominance structure of the optimization problem can be altered, and thus, potentially feasible solutions could be left outside the analysis (Kostin et al., 2012). The dominance structure of an optimization problem refers to how a solution is preferred based on the problem's objectives. In Life Cycle Assessment (LCA), considering multiple environmental impact categories or objectives is crucial, but relying on aggregated metrics can oversimplify the dominance structure (Capitanescu et al., 2018). When using LCA, relying solely on aggregated metrics can oversimplify the dominance structure. These metrics combine various impact categories into a single score, which can hide the trade-offs between different environmental goals. This may result in suboptimal or even deceptive outcomes when using LCA to support decision-making (Lesage et al., 2018). Additionally, aggregated metrics assume that all impact categories are equally important, which is not always true. Different stakeholders may prioritize environmental impacts differently, and these differences can be overlooked when relying on aggregated metrics (Lesage et al., 2018). Preserving the dominance structure in LCA optimization problems can lead to a better and more precise understanding of the environmental impacts of different solutions, supporting informed and sustainable decision-making (Capitanescu et al., 2018; Rehnstrom, 2003).

All in all, this might lead to an unfair comparison and inaccurate conclusions when benchmarking these studies. This is escalated by the fact that there is a general lack of standardized and systematic descriptions of methodological assumptions as well as declared decisions in all four LCA steps (Cherubini et al., 2018; Heijungs and Dekker, 2022) .

In contrast, Gerber et al. (2011) and Gong and You (2018) are studies that more explicitly describe the methodological decisions taken when applying LCA. More details regarding the methodology used for the environmental impact assessments can be found in some review papers such as Thonemann (2020) and Koj et al. (2019).

Lastly, particularly of note is that, of all studies reviewed in Table 1, four studies (11% - 4 out of 36) perform a more holistic approach by taking into account the three aspects of sustainability (economic, social, and environmental).

4. Current practices, challenges, and future perspectives on environmental impact assessment in the PSE community

In the search for sustainable production and consumption, chemical engineering strives to identify sustainable solutions for energy systems and all applications where the triple bottom line paradigm is simultaneously respected. This commitment to pursue alternatives which are (more) sustainable requires advanced decision-support strategies and tools in order to keep the economic viability, interest, and competitiveness of the proposed solutions (Guillén-Gosálbez et al., 2019). As a subfield of chemical engineering, the PSE discipline, with its broad scope and systems thinking, developed new computer-aided methods and tools to contribute to sustainable process design problems and challenges (Bakshi, 2019; Bakshi, 2003; Grossmann and Harjunkoski, 2019; Guillén-Gosálbez et al., 2019; Klatt and Marquardt, 2009). Over the years, many sustainability metrics and indicators have been developed that cover one, two or the three dimensions of sustainability (Bakshi, 2019; Martins et al., 2007; Thonemann, 2020).

As demonstrated in Section 3, a traditional approach to integrate sustainability into PSE studies has been to minimize water and energy consumption, mainly portrayed by the greenhouse gasses and water use indicators. Even though this might presumably lower environmental impact, it potentially leads to loss of information by: (i) neglecting a range of other environmental impacts (e.g., human health, ecosystems, resources); (ii) omitting burdens beyond the production stage; and, (iii) shifting burdens to other emission flows and resources (Bakshi, 2019; Guillén-Gosálbez et al., 2019). LCA emerged as an effective method to overcome these challenges (Bakshi, 2019; Guillén-Gosálbez et al., 2019) since it shares the systems thinking with PSE and it ideally includes all phases of the process' or product's value chain (Bakshi, 2019; Guillén-Gosálbez et al., 2019). As previously mentioned, Azapagic and Clift (Azapagic and Clift, 1999) first introduced the Life Cycle Optimization framework (LCO), where optimization was coupled with LCA through multi-objective optimization (MOO) to minimize life cycle impacts and economic costs. As detailed in Section 4, this framework has been broadly applied since it was first introduced and has evolved and improved over the years. However, noteworthy is that it is seldom possible to fairly compare different studies even though they refer to the same product or process. There is an overall lack of transparency and clarity concerning the decisions taken in Step 1 of LCA, such as functional unit, time horizon, geo-location, boundaries of analysis, and a priori assumptions.

A great majority of the PSE studies published over the years (Section 3), while applying the LCO framework, only include one or a couple of environmental impact indicators as representative metrics of the whole system. This is not a one-size-fits-all solution, and it is rather important when analyzing energy systems: inferring that a particular design is a sustainable solution based on a very limited list of indicators does not provide a robust evaluation. To use these findings in a higher-level decision making (e.g., go forward with a decision to invest in a technology) could potentially be misleading.

As a future perspective for integrating environmental impact assessment into PSE, we need a clear alignment and standardization of the LCA methodology used to account for the environmental dimension of sustainability. As a minimum requirement, an LCA study must be applied with care, critical thinking, and understanding. The scope should be broadened far beyond the production boundaries (gate to gate) in order to understand the complex relationships and exchanges among subsystems and, hence, the implications of different decisions on the environment and economy. This should provide thorough insights needed to generate knowledge that must be integrated into the early stages of process and product development and decision-making to reduce impact across scales (Guillén-Gosálbez et al., 2019).

Regarding impact categories selected and used for assessment, the studies need to move beyond reporting only CO_2 and acknowledge other relevant impact categories such as mineral resource depletion, human/marine/freshwater ecotoxicity, and water depletion. The latter is becoming highly relevant for some renewable energy production systems such as wind, solar, and electrolysis technology in Power-to-X (PtX) concepts. Likewise, of note is that environmental impacts from persistent compounds (e.g., mercury) are not limited to regional scales. They can be spotted in ecosystems far from perceived human activities (Bjørn, 2015). Another point to consider in moving forward with a standardized approach is to define planetary boundaries. This has first been proposed by Rockström et al. (2009), and it is also discussed in Persson et al. (2013) and Sala and Goralczyk (2013).

The limits or thresholds of diverse Earth system processes and environmental parameters define a safe operating space for humanity are called planetary boundaries. These boundaries represent the global limits within which human activities can operate without causing irreversible or catastrophic transformations to the Earth's systems (Bjørn et al., 2020). Within this global framework, LCA can be used to evaluate the performance of the mentioned systems/products concerning the planetary boundaries, considering the impact of those categories linked to the boundaries. Of note is that although both planetary and system-specific boundaries are concerned with environmental impacts, they differ on scale level and specificity. Planetary boundaries address a global framework to evaluate the sustainability of human actions/activities on the planet. In contrast, system-specific boundaries focus on impacts within a particular life cycle assessment study. This new initiative helps provide a context for interpreting the LCA results within safe planetary limits (Ryberg, 2021). However, much work is needed in the broader sustainability assessment community and with relevant stakeholders, agreeing on principles and methods for defining safe limits for the planet in different impact categories for various sectors.

Sustainability assessment problems are encumbered by several sources of uncertainty, which are related to the LCA calculations themselves (Guillén-Gosálbez and Grossmann, 2009). LCA is accompanied by uncertainty sources regarding the inventory data and the damage factors that need to be analyzed and mended if possible (Gargalo et al., 2016; Huijbregts, 1998; Santos et al., 2022). A crucial/outstanding contributing factor to the propagation of uncertainty and difficulty in comparing different LCA studies is that different LCIA methods can be selected (Chen et al., 2021; Heijungs and Dekker, 2022; Landis and Theis, 2008; Owsianiak et al., 2014). Often, they do not lead to exactly the same value (e.g., ReCiPe, ILCD, CML, IMPACT2000+) since different mathematical models are employed to estimate the indicators (mid-point and end-point methods) (Bueno et al., 2016; Müller et al., 2020). Noteworthy is that some of these impact assessment methods are also outdated (Verones et al., 2020). A detailed review of uncertainty propagation due to using different LCIA methods is given in Chen et al. (2021) and Heijungs and Dekker (2022). Hence, for the sake of robustness, we recommended justifying the approach/methods used for the LCIA method by doing a benchmarking (does the interpretation and sustainability picture differ when using different LCIA methods?).

As an example, we will illustrate our point using an example study of environmental impact assessment of a pharmaceutical compound A (production scale analysis) (Wernet et al., 2010). This study assessed the impact assessment of pharmaceutical compound A using different methods and databases (CED, GWP, Eco-indicator99, TRACI, LCA with ReCiPe, and Impact2002+). Here, the study aimed to compare the environmental impact of pharmaceutical product A against the sustainability impact of bulk chemicals using different methods. In conclusion, the study found that the sustainability metrics are two orders of magnitude higher for producing pharmaceutical compounds versus bulk chemicals, which is consistent among different methods (Eco indicator, ES2006, LCA recipe, Impact2002+, etc.). However, as the results clearly show, one cannot directly compare the results among different methods as each method uses different expert rankings to aggregate the results (especially for end-point indicators). For instance, IMPACT2002+ and ReCiPe, as different LCIA methods, use different units and nomenclature as well as aggregation. As a result, while ReCiPe gives a score of 7 points/kg of A as the overall LCA score, Impact2002+ gives a score of 6.7E-3 points/kg A. Clearly, these two databases cannot be compared against each other, and only a relative comparison can be made to compare different products using the same method (e.g., Product A versus Product B comparison using ReCiPe is possible).

A second example is from the work of Vollmer (2022). The latter study aims to perform the environmental impact assessment of the production of xylitol from renewable feedstock (such as lignocellulosic wood chips), which is a frequently studied process (Vollmer, 2022).

When using renewable energy (such as wind energy), the global warming potential in CO_2 equivalents is relatively low, as the xylitol biorefinery just releases biogenic CO_2. However, freshwater and marine ecotoxicity impacts are rather high, as well as the human carcinogenic potential. The first two can be associated with the biorefinery's energy demand since it is presumed that the energy is used from wind power. The windmills need copper for the generators, typically obtained using toxic chemicals that can potentially damage freshwater and marine life if not disposed of carefully and correctly. Indeed, this is a clear example of the importance of properly identifying the relevant impact categories and reporting them. As the review shown in Table 1 illustrates, most studies only focused on one impact category and miss the opportunity to identify other relevant categories.

Obtaining data for the complex life cycle activities of the systems under study (from "cradle to grave") and the uncertainty it carries is a significant challenge. Software and databases have been developed over the past two decades to simplify this task; however, most of the available databases are based upon regional facility-level data that result from the combination of multiple manufacturing processes (Bakshi, 2019). Efforts should be applied to avoid the use of this secondary data and gather primary data for emerging technologies and individual processes through, for example, process models (Bakshi, 2019; Geisler et al., 2004; Jiménez-González et al., 2000; Li et al., 2018; Yao and Masanet, 2018), data reconciliation (Ilagan and Tan, 2011; Yi and Bakshi, 2007), and extended input-output models (Yang et al., 2017). Nonetheless, when using these techniques, system boundaries are still seen as incomplete, especially when new products are included (Guillén-Gosálbez et al., 2019; Majeau-Bettez et al., 2011) show that unaccounted processes may be up to 80% of the total flows. To overcome this, integrated hybrid LCA has been investigated; an example is given by Gao and You (2018). Integrated hybrid LCA combines process-based and input-output data to assess environmental impacts, avoiding truncation and double counting.

Another recent trend is the potential use of AI and ML algorithms to build surrogate models for different unit operations for optimization problems, as exemplified in Gonzalez-Garay and Guillen-Gosalbez (2018). Besides, the uncertainty in the inventory could and should also be included in optimization studies in the form of stochastic programming or robust optimization. Stochastic programming is particularly useful for decision-making under uncertainty since it can accommodate several time points, optimizing the expected objective function value over all uncertainty realizations (Birge, 1997; Guillén-Gosálbez et al., 2019). A good example is given by Gao and You (2017). Robust optimization is of simpler implementation since it does not require prior and accurate information of probability distributions of uncertain parameters. An example is given by Calvo-Serrano et al. (2019) for the design of a biomass processing network for the production of fuels, electricity, and chemicals. Nevertheless, these approaches are computationally expensive, and that requires a natural need for more efficient algorithms to solve complex large-scale problems (Guillén-Gosálbez et al., 2019). Targeting to solve this, combining machine learning and big data is gaining ground (Ning and You, 2019). For example, Gao et al. (2019) use this new strategy for the energy supply chain LCO under uncertainty.

LCA has demonstrated its usefulness towards the assessment of a better environmental performance of given alternative technologies/products over the years. As such, LCA is considered valuable to reduce the burden/impact per function of a system/product under study. On the other hand, since the population and consumption profiles continue to rise at an increasing pace, there is a growing need and call for verifying this premise. In other words, there is actually a need to develop strategies to assess whether the current technologies are indeed "sufficiently good to contribute to a sustainable lifestyle" and not just "relatively better than the alternatives" (Hauschild, 2015; Ryberg, 2021).

In summary, many new technologies are being developed, pursuing sustainable production and consumption, here illustrated in the area of renewable energies. However, to avoid unexpected and unobserved environmental impacts as seen in the past, future efforts need to focus on establishing a strong relationship between PSE and environmental assessment strategies (LCA in particular, due to the mentioned similarities). This relationship must be conveyed in the form of a systematic, standardized, and transparent framework in order for the studies to be comparable and usable for practical purposes. This will lead to significant advances in accounting for ecosystems and supporting industrial activities while minimizing environmental burden.

5. Conclusions

There are many complex renewable and sustainable energy systems. A significant research effort has been dedicated to environmental assessment, primarily based on LCA. The open literature has shortcomings in terms of transparency, reproducibility, etc. The critical role of PSE is highlighted, and influential studies from the community are reviewed. The application of PSE tools for the synthesis, design, and optimization can further enhance the benefits of renewable and sustainable energy systems.

The challenges, perspectives, and potential guidelines collected and presented in this article are based on experience and a comprehensive literature review. To successfully integrate LCA into PSE studies, the following recommendations are made to overcome the above-discussed challenges. These suggestions aim to become the best practice and require careful consideration and implementation. They are as follows.

(i) Define the objectives and boundaries of the LCA study as clearly as possible at the beginning. This entails specifying the following: functional unit, system boundaries, and pertinent life cycle phases that are to be included. Of note is that it is paramount to clearly **define the scope** in order to avoid data gaps and inconsistencies.

(ii) Define **suitable system boundaries** in agreement with the scope of the analysis, and ensure these are exhaustive; include upstream processes (e.g., raw material acquisition) and downstream processes (e.g., waste management and disposal). This is crucial in order to avoid the problem of burden shifting by considering the entire life cycle of the product/process/system.

(iii) Accurate and reliable data is crucial for an LCA study. Ensure that the **data** used for the inventory analysis (e.g., mass and energy inputs, emissions) is **high-quality, updated, and representative.** Well-known databases such as coinvent are good sources of data, and the use of secondary data (such as modeling and simulation) needs to be clearly mentioned.

(iv) Temporal and geographical variations in the data and impact assessment are essential to consider since the environmental impact of a product/process might change with time and across different locations. Thus, using **site- and time-specific dat**a and characterization factors is a way to reduce the associated uncertainty.

(v) When conducting Life Cycle Assessment (LCA) studies, it's common to encounter **data uncertainties**. To address this issue, a few strategies can be implemented, such as data estimation approaches, proxies, and expert judgment based on past experiences. Additionally, performing **sensitivity and uncertainty analyses** is beneficial as it allows for the identification of important data gaps and the **assessment of result robustness**. This analysis also evaluates the sensitivity of results to **critical input parameters**, assumptions, and hypotheses. Overall, this process helps to identify the most significant and impactful factors, such as technology and energy mix choices, ensuring the trustworthiness of the conclusions.

(vi) When a process/product/system has multiple co-products, or system expansion is required, one needs to apply allocation. It is crucial to **appropriately select the allocation methods** that best align with the study's purposes and avoid allocation methods that can lead to the misinterpretation of the results.

(vii) There must be **transparent and thorough reporting of the LCA study**, including methodology, data sources, assumptions, and limitations. This facilitates others to understand and assess the study's validity and enables a trustworthy comparison with other studies. For the sake of transparency, these need to be disclosed in scientific publications as supplementary material.

(viii) Adopting a **holistic approach** considering multiple environmental indicators is necessary. This ensures a comprehensive understanding of the environmental performance and impacts of a system, process, or product.

By enforcing these suggestions and recommendations, the reliability and quality of LCA studies in PSE are improved, along with the understanding of the environmental impacts of processes and products.

In summary, we call for a shared systematic and transparent methodology where detailed LCA calculations are performed and reported in a consistent and robust framework such that results from different studies can be fairly compared and discussed.

CRediT authorship contribution statement

Carina L. Gargalo: Conceptualization, Visualization, Data curation, Formal analysis, Writing – review & editing, Writing – original draft. **Haoshui Yu:** Data curation, Formal analysis, Writing – review & editing, Writing – original draft. **Nikolaus Vollmer:** Data curation, Formal analysis, Writing – review & editing, Writing – original draft. **Ahmad Arabkoohsar:** Data curation, Formal analysis, Writing – review & editing. **Krist V. Gernaey:** Formal analysis, Writing – review & editing. **Gürkan Sin:** Conceptualization, Visualization, Formal analysis, Writing – review & editing.

Declaration of Competing Interest

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

Data availability

No data was used for the research described in the article.

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