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Use of process simulation to obtain life cycle inventory data for LCA: A systematic review

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ABSTRACT

Life Cycle Inventory (LCI) analysis is an essential and time-consuming phase of life cycle assessment (LCA). While primary data is among the most reliable and desirable data source types, it is often challenging to collect for industry-specific processes due to confidentiality concerns, in particular with respect to unique proprietary processes. In such cases, computer-based process simulation software can be used to fill gaps in inventory data based on mass and energy balances. While building process simulation models, engagement with industry is essential for verification of process models and validation of simulated data. Although process simulation-based life cycle inventory modelling is not a new research area, there has been no systematic review on this topic with respect to common methodological choices. To fill this gap, this systematic review aims to identify common practices in simulating LCI data using process simulation. Studies that used process simulation for LCI modelling were reviewed to identify the reasons for using process simulation, approaches for simulating LCI, software employed, validation processes, and processes to calculate and report uncertainty. Based on the review findings, a methodological framework was proposed to explain how process simulation-based LCI can be integrated with conventional LCA, specifically for industrial processes.

1Introduction

Life Cycle Assessment (LCA) is a widely used tool to evaluate the environmental impacts associated with a product system throughout its life cycle and to estimate the mitigation potential of specific technology or management interventions. This can facilitate improving a system/product by introducing the best possible new technologies or management alternatives in order to mitigate adverse resource/environmental impacts (Bjørn et al., 2018a; Muralikrishna and Manickam, 2017). According to the ISO 14040 and ISO 14044 standards, an LCA starts with a well-defined, organized, and deliberate definition of the goal, followed by a detailed description of the scope of the study, which will eventually shape the inventory analysis, impact assessment, and interpretation phases of the LCA (ISO, 2006a, b). Life Cycle Inventory (LCI) analysis is the second phase of an LCA study. It involves compiling data to characterize relevant inputs and outputs of the studied system within the defined system boundary according to the goal and scope of the study. Building a representative LCI can take a great deal of time and is often an iterative process. The studied product system is divided into unit processes, and all of the elementary flows (resources and emissions), product flows (material and energy), and waste flows from each unit process are identified. LCI generally culminates in the quantification of the relevant elementary flows that cross the system boundary. This quantified list of elementary flows is the input to the following Life Cycle Impact Assessment (LCIA) phase of the LCA study (Bjørn et al., 2018b; ISO, 2006a).

An inventory analysis can also be a useful decision-support resource for organizations or industries along with the outputs from other LCA phases. LCI creates a baseline for complete resource requirements and emission scenarios for a product system, which can trigger the development of a new process or product with lower resource requirements or emissions. The LCI analysis also allows organizations to compare alternative processes or products to make their systems more economically viable, efficient, and less detrimental to the environment (Bjørn et al., 2018a; ISO, 2006a). The key steps or the characteristic elements of the LCI analysis phase for a process-based model are developing a system flow diagram including all the processes involved in the study, planning for data collection, and collecting, calculating, and validating the data.

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After finalizing the system boundary with all of the relevant unit processes, data collection is the crucial next stage in developing the LCI. Before collecting data, priorities should be set about the specificity of data to balance the relevance of the data and the level of effort that acquiring it requires, as sometimes the collection of high-quality data is very time-consuming. This may not be warranted for data that have very low relevance to the intended study (Bjørn et al., 2018b; ISO, 2006a).

LCI data can be obtained through direct measurements or from supplier surveys, published data, industry databases, or other sources (Bjørn et al., 2018a; ISO, 2006a). The key task is ensuring the quality and reliability of the collected data, which can be very challenging, especially when studying highly industry-specific product systems. Development of consistent LCI in such contexts involves non-trivial effort, expertise, time, and resources in order to assemble accurate and reliable data (Kaushal and Chakrabarti, 2023; Li et al., 2018; Morales-Mendoza and Azzaro-Pantel, 2017). Other challenges associated with industry-specific LCI development are identifying and gaining access to the specific persons/organizations within a given industry, selecting a representative sample from the industry, managing confidentiality concerns, incomplete information, dynamism of industries, etc. These challenges can often lead to using secondary data from literature and/or industry reports or other data sources, which requires validation, as poor and inconsistent data can result in unrealistic findings and conclusions (Elomaa et al., 2020a; Li et al., 2018). One of the main problems with using secondary data is dealing with missing/incomplete data (Zargar et al., 2022).

There are two approaches to generating LCI data, depending on the goal and scope of the study – the top-down approach and the bottom-up approach (Li et al., 2018; Smith et al., 2017). The top-down approach (i.e., data mining) uses high-level and aggregate data from broader sources (i.e., national statistics, industry reports), and it distributes the data for specific processes within a defined system boundary based on relevant factors like production volume, economic value, or energy use (Cashman et al., 2016; Sengupta et al., 2015). The bottom-up approach mainly relies on collecting detailed and specific data for individual processes in order to create a comprehensive, representative, and accurate process-level inventory (Smith et al., 2017). Although it is sometimes possible to get realistic and accurate aggregated data from industry partners through the top-down approach, this approach can be challenged by large data gaps in terms of material and energy inputs, lack of transparency in the background information about the process technologies of concern, variations in reporting, or difficulties in the allocation of materials, energy, and emissions to a single process in a multi-process facility, etc. (Cashman et al., 2016). On the other hand, the bottom-up approach is mainly based on compiling relevant material and energy input data to complete the LCI with respect to the defined system boundary for the studied product system/process, which ensures a process-specific focus and a clear understanding of the process technology (Smith et al., 2017). However, this approach often requires systems process engineering knowledge and may involve numerous assumptions in order to achieve process-level modelling (Meyer et al., 2019; Parvatker and Eckelman, 2019; Zargar et al., 2022).

Process simulation is a flexible tool for creating specific and precise LCI (Aromaa et al., 2023). It is a bottom-up approach to generating LCI by replicating the real-world process or system in a computer-based model in order to allow virtual experimentation and various scenario analyses. It offers a cost-effective and efficient way to design and analyze complex systems, optimize operations, and make informed decisions without the need for physical trials (Cozma et al., 2013). Compared to traditional data collection methods, process simulation offers an alternative but also rigorous and detailed approach, leveraging fundamental principles of physics. It ensures adherence to the laws of mass and energy conservation, as well as the second law of thermodynamics, thereby accounting for thermodynamic losses throughout the process chains under consideration (Ali et al., 2024; Bartie et al., 2020). It is particularly useful when real, industry-specific data are scarce/missing (Christensen et al., 2020; Meys et al., 2020; Tsoy et al., 2020). It calculates the emissions based on physicochemical considerations to make the inventory robust and credible (Iosif et al., 2010). Sometimes, only laboratory-scale, measured data may be available for new and emerging technologies/processes and the environmental impacts associated with industrial-scale processes are unknown (Righi et al., 2018). Process simulation is a very useful tool to generate LCI for any novel/emerging process at a low technology readiness level (TRL) or in the early stages of process development, and/or those processes for which commercial-scale operations do not yet exist (Elomaa et al., 2020a; Mio and Fermeglia, 2022; Morales-Mendoza and Azzaro-Pantel, 2017; Zargar et al., 2022). Where industrial confidentiality concerns hamper the collection of commercial-scale data, process simulation similarly provides a reasonable alternative (Righi et al., 2018).

Although there have been numerous studies using process simulation to generate LCI and/or bridge the gap in LCI for industry-specific studies, there are very few review papers that summarize common methodological practices. Zargar et al. (2022) reviewed 18 papers from the chemical industry to identify the common methods of inventory modelling in LCA studies. They identified twelve methods within three approaches for LCI modelling – data-driven (i.e., data mining, machine learning), mechanistic (i.e., process simulation), and future inventory modelling, and summarized the main features of these methods. Liu et al. (2019) reviewed 27 articles on simulation-based LCA from the manufacturing sector to give a generic overview of those studies including their goal and scope, level of modelling detail, how they verify and validate their models, information regarding data collection and life cycle inventory, impact assessment, and means of communication. Kleinekorte et al. (2020) reviewed and discussed different methods of integrating LCA into chemical process design, products, and supply chains, including their advantages and challenges. There are also a couple of review articles that focused on the automation of LCA (Köck et al., 2023), and developing dynamic LCI for industry 4.0 applications (Cornago et al., 2022). However, there remains a gap with respect to common methodological choices and best practices for integrating computer-based process simulation to generate LCI. To fill this gap, this paper aims to systematically review industry-related LCA studies that used process simulation to generate/complete LCI data sets. The specific review questions are.

i. What are the applications/reasons/extent of using process simulation for generating LCI and/or filling the gaps in LCI?
ii. How did researchers variously generate complete LCIs using process simulation (i.e., mass balance, energy balance)?
iii. What are the prevalent software tools and modelling approaches used in these studies?
iv. What are the common practices for the validation of the process flow diagram and simulated data? How should the modelled data be evaluated and applied compared to conventional data from LCA databases?
v. How was uncertainty associated with the simulated data calculated and reported?

Based on the findings of the review questions, the common methodological practices in developing LCI through process simulation are presented in a methodological flow chart. The remainder of this paper comprises a Methods section for the systematic review using the PRISMA technique, a summary of findings for the review questions (Results section), a discussion of the integration of process simulation-based LCI into conventional LCA (Discussion section), and a Conclusions section that integrates the key findings with recognition of the limitations of the study and recommendations for future studies.

2Methods

The Preferred Reporting Items for Systematic Reviews and Meta-

Analyses (PRISMA) systematic review method (Moher et al., 2009; Page et al., 2021) was followed to identify and review the primary research articles that used process simulation to generate LCI in industry-related LCA studies. The PRISMA method comprises a 27-item checklist that is widely used for systematic reviews in different research fields including the agri-food industry (Ferdous et al., 2023), livestock farming (Heidari et al., 2021), medicine (Bei et al., 2022), and the building sector (Safikhani et al., 2022), etc. Search strategy, screening criteria, and extraction and synthesis of data are the three stages of the PRISMA method. They are discussed in detail in the following sections and the process of selecting relevant literature is illustrated in Fig. 1.

Search strategy

For identifying relevant literature, the Web of Science and Scopus search engines were used, and different search terms combined with logical operators 'AND' and 'OR' were employed. The combination of search terms was ("life cycle inventory" AND "simulat*") to identify reports of studies that developed LCI using process simulation software. Title, abstract, and keywords are only included to find the search terms. The wildcard operator '*' was used to capture all of the related words like process simulation, simulated, simulation-based, etc.

Screening criteria

An initial search on the Web of Science and Scopus gave 227 and 297 hits, respectively. Among the 227 papers in Web of Science, 192 were primary research articles published between 2001 and 2023. 218 primary research articles published between 2001 and 2023 were identified using Scopus. After removing 157 duplicates, a total of 253 articles were selected for title and abstract screening. Abstracts of these 253 articles were screened to identify the articles conducting LCA of industry-related processes/technologies which used process simulation software to develop the LCI. 50 papers remained after the abstract screening for full-text review in order to extract the information required to answer the review questions. 203 papers were excluded because they did not represent any industry-related processes (i.e., building/construction, municipal solid waste management) and/or used the 'simulation' word either as synonymous with LCA or for Monte Carlo Simulation in the context of uncertainty analysis. These shortlisted papers were published between 2003 and 2023. Among these 50 papers, 3 were data reports (Cañon et al., 2022a; Keller et al., 2022b; Sadeek et al., 2020a). The associated research articles were also retrieved and reviewed (Cañon et al., 2022b; Keller et al., 2022a; Sadeek et al., 2020b).

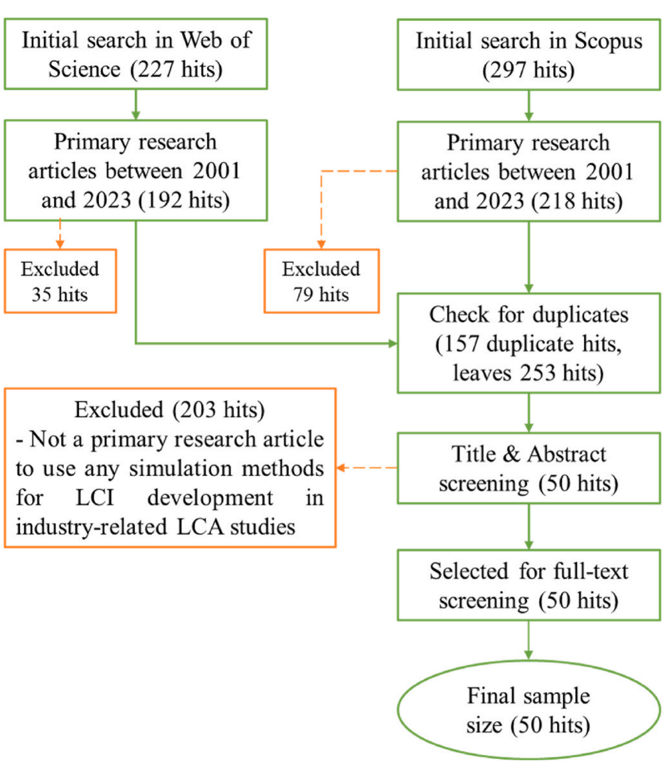

Fig. 1. Selection of relevant literature using the PRISMA systematic review method.

Extraction and synthesis of data

An Excel-based synthesis table was used to collate the extracted information from the 50 short-listed articles (Table 1). Information regarding the studied product systems, software used to simulate LCI data, data sources for process simulation and LCI, applications/reasons for using process simulation, different technical aspects of process simulation (i.e., type of process, mass/energy balance), validation methods, evaluation of simulated data and ways to integrate simulated data with LCA, and methods for uncertainty analysis/reporting for simulated data - were extracted from the reviewed articles. In the Results section, the findings for each review question are summarized and a generic methodological flow chart for integrating process simulation in LCA studies to generate LCI is illustrated and discussed in the Discussion section.

3Results

3.1Applications of process simulation to develop LCI

In total, 50 research articles were reviewed to identify current methodological choices and practices for integrating process simulation in generating LCI. Among these reviewed papers, 7 studies conducted techno-economic analysis (TEA) along with LCA (Bonatsos et al., 2020; Ioannidou et al., 2022; Larnaudie et al., 2020; Li et al., 2019a, 2019b; Riazi et al., 2019; Yang et al., 2018). The reviewed articles cover a wide range of industrial processes including biochemical production, hydrogen production, biofuel/biogas production, energy generation, manufacturing, and production of different substances from biomass and/or biowaste, etc. (Table 1). To answer the 1st review question, the reasons for and extent of using process simulation in these studies were determined. Moreover, the data sources used for process modelling were identified.

3.1.1Reasons for applying process simulation

Most of the reviewed articles (66%) mentioned the reasons/motivation to use process simulation to generate LCI (Table 1). The main reasons for using process simulation-based LCI reported in these studies were the lack of alternative sources of reliable/consistent data, lack of commercial/industrial-scale data, projection of pilot scale data, consideration of new/emerging technologies, and limitations with respect to the availability of relevant LCI data in existing LCA databases for some of the studied systems. With respect to the latter, traditional LCI databases only include LCIs for a subset of chemicals, whereas there are around 85,500 chemicals, of which 9626 are in active use in commerce according to the EPA's TSCA Chemical Substance Inventory (Li et al., 2018).

The generation of life cycle inventories for new/emerging, novel, and complex processes/products is generally a very challenging task due to the lack of reliable data in existing databases for unique processes and/or new products (Mio and Fermeglia, 2022). It is a very common practice to use LCI databases (i.e., Ecoinvent, GaBi (LCA for Experts)) for the background systems while using reliable primary data for foreground systems is desirable. The reviewed articles mainly used process simulation to generate LCI for foreground systems and included other databases for background systems to complete the inventory. So, if reliable and representative data for specific processes is not available or the studied product system is new/emerging, part or all of the foreground system LCI can be built through process simulation.

3.1.2Data sources for process simulation

Information about data sources used to build the process simulation models and to complete the LCI was also extracted from the reviewed articles. Ecoinvent and GaBi (LCA for Experts) are the most commonly used databases, mainly for background system LCIs in LCA studies. All of the articles also mentioned literature as one of their data sources (Table 1). Literature includes industry reports, patents, published LCA studies, published process models, industrial reference textbooks, etc. Some studies used primary data collected from lab and pilot-scale setups, experimental data, or data collected through personal communications with industry/technical experts to simulate and validate LCI data for industrial-scale processes (Table 1). Some studies also mentioned using simulation software databases (Baaqel et al., 2023; Daful et al., 2016; Hajjaji et al., 2016a; Hajjaji, 2014; Khalil, 2021; Mio et al., 2021). A few studies used the GREET (Greenhouse gases, Regulated Emissions, and Energy use in Technologies) model to develop the process models (Kuan et al., 2007; Riazi et al., 2020; Yang et al., 2018). Other databases specific to studied product systems and/or within particular geographical scopes were also employed in some studies, including commercial databases such as Fisher Solve and RISI (Repository of Industrial Security Incidents) (Echeverria et al., 2022), the Swiss Agricultural Life Cycle Assessment (SALCA) (Cañon et al., 2022a, 2022b), the European Database for Corrugated Board Life Cycle Studies (Helmdach et al., 2017), the USLCI database (Li et al., 2018), and the 2012 China input-output table (Li et al., 2019a, 2019b), etc. Another relatively common practice is to fill in missing information based on known chemistry and/or assumptions for specific unit processes (Beylot et al., 2021; Bonatsos et al., 2020; Elomaa et al., 2020b; Keller et al., 2020; Riazi et al., 2020). However, in such instances, sensitivity analysis to check the influence of the assumptions is also recommended (Table 1).

3.2Technical aspects of process simulation

3.2.1Types of processes simulated

Process models can be either steady state or transient. Steady-state models assume a constant system over time (Dekkers, 2017), whereas, in transient-state models, flow conditions and other properties of the processes can change with time (Feldhoff et al., 2015). The state/type of model simulated is not explicitly mentioned in most of the reviewed articles. Only 8 studies mentioned simulating steady-state processes (Table 1). Besides, the process types of these models/unit processes can be continuous, batch, or semi-batch. Continuous process refers to the production method where the input materials are continuously fed into the system, the output products are continuously produced, and it operates non-stop over an extended period (typically in industries where large volumes of uniform products are required). In contrast, the batch process involves a sequence of steps in a specific order to control the whole process and produce a specific amount of each product. In this type of production method, the process is carried out in discrete increments, where a specific amount of input materials is processed to produce a batch of the finished product. The types of models (i.e., steady state, transient) and processes (i.e., continuous, batch) mainly depend on the studied product system and the industrial setup. For instance, Riazi et al. (2020) considered continuous processes for a large-scale setup but considered batch operation for a laboratory experimental setup. Considering continuous operation for some unit processes and batch operation for others was also reported by Larnaudie et al. (2020). Most of the reviewed articles mentioned the process type for their studied systems or at least some of the unit processes. 16 studies considered continuous processes and 8 studies considered batch operations (Table 1).

3.2.2End goal of process simulation

Mass and energy balances are fundamental end goals for analyzing processes and are vital parts of any process simulation study as one or both are used in most cases. These balances mainly depend on the type of the process (i.e., steady-state or transient, batch, continuous or semi-batch), but they follow a general equation (discussed below; Fraga, 2015). Such balances help verify the integrity of the process model and ensure that the simulation represents the system accurately in terms of material and energy flows.

Mass balance (material balance) involves keeping track of the material flows throughout a process/system and ensuring that the total mass of inputs is equal to the total mass of outputs. It is based on the Law of Conservation of Mass, which states that mass cannot be created or destroyed in a closed system. Generally, this involves accounting for the quantities of materials entering the system, the internal transformations/reactions, and the quantities exiting the system. The general equation for the mass balance is (input + generation - output - consumption = accumulation), where generation and consumption mean the materials produced and consumed within the system, respectively, and accumulation is the amount of material that builds up within the system. In a steady-state continuous process, accumulation will be always zero. So, the equation for the mass balance for a steady-state process is basically (input + generation = output + consumption) (Fraga, 2015).

Energy balance (energy conservation) is based on the First Law of Thermodynamics, which states that energy cannot be created or destroyed, only converted from one form to another. It considers three types of energy for non-nuclear processes – kinetic, potential (i.e., gravitational), and internal energy (Fraga, 2015). It involves tracking the flow (input and output) and internal transformation of energy within a system and ensuring that the energy entering a system equals the energy leaving the system, accounting for any changes within the system. It considers energy in different forms – heat, work, or electric energy. The equation for energy balance is (Change in internal energy + Change in kinetic energy + Change in potential energy = Heat added – Work done by the system), which can be slightly modified based on a closed or open system (Fraga, 2015).

Implementation of mass and energy balances in LCI development ensures completeness by verifying that all inputs and outputs have been accounted for. They also check the consistency and accuracy of the assembled data and help identify any data gaps or errors. Using mass and energy balances in LCI development guarantees comprehensive and robust analysis, leading to more accurate and reliable life cycle assessments. Most of the reviewed literature used both kinds of balances (Table 1). Very few studies only employed mass balance (Beylot et al., 2021; Kulay et al., 2003; Mata et al., 2023). Li et al. (2019b) employed only energy balance, while a few studies did not specify the kind of balance they employed. In addition, a couple of studies completed the simulation by balancing stoichiometric or kinetic reactions (Li et al., 2019a; Parvatker and Eckelman, 2020), or were based on assumptions (Keller et al., 2020).

3.3Prevalent software for process simulation

There are numerous software options for performing process simulation to generate LCI data using a bottom-up approach (Parvatker and Eckelman, 2020), such as Aspen Plus, Aspen HYSYS, SuperPro Designer, ProSimPlus, CHEMCAD (Pereira et al., 2015), UniSim (Foo, 2023), PRO/II (Frutiger et al., 2018), gPROMS (Näf, 1994), and EMSO (Elias et al., 2021), etc. These global simulators have become standard tools for calculating mass and energy balances, flow rates, temperature, pressure, compositions, and physicochemical properties of different streams in unit processes (Morales-Mendoza et al., 2018). The most commonly used software found in the reviewed articles is Aspen Plus. 27 out of 50

Table 1
Key attributes of process simulation-based LCI modelling in the literature considered.

Citations	Research topics	Reasons of applying process simulation	Type of process simulated	Simulation software	Data sources for process simulation	End goal	Validation of modelled process data	Uncertainty characterization of modelled process data
Aromaa et al. (2023)	Tantalum and niobium recycling from hard metal scrap	To generate LCI due to lack of data in the literature	Batch operation in some unit processes	HSC Sim 10	Literature and typical metallurgical operation	Mass and energy balances	–	Sensitivity analysis with uncertain simulation parameters
Baaqel et al. (2023)	Dialkylimidazolium ionic liquid production	Lack of data for emerging technology	–	Aspen-HYSYS interfaced with Matlab	Literature and Aspen-HYSYS database	Mass and energy balances	–	Global sensitivity analysis for uncertainty quantification
Beylot et al. (2021)	Mining	Projection of on-site pilot tests	Continuous pilot operation	USIM-PAC®	On-site pilot test, generic data, and assumptions	Mass balance	–	Stated that there is uncertainty in both foreground and background systems and did scenario analyses
Bonatsos et al. (2020)	Biochemical production of microbial oil	Completing material and energy flows and the subsequent equipment sizing and costing	Batch operation in some unit processes	–	Literature and historical data	Material and energy balances	–	–
Cañon et al. (2022a, 2022b)	Ethyl levulinate production from Colombian rice straw	–	–	Aspen Plus v12	Literature, different emissions from IPCC methodology, and SQCB methodology	Mass and energy balances	–	Uncertainty analysis using Monte Carlo simulation and also did sensitivity analysis with different distillation columns and paddy rice yields
Cozma et al. (2013)	High-pressure water scrubbing biogas upgrading technology	Lack of reliable data	Continuous unit processes	Aspen Plus	Literature	Mass and energy balances	Compared with data from the literature	–
Daful et al. (2016)	Lignocellulosic lactic acid production	–	Continuous unit processes	Aspen Plus v8.6	Aspen Plus simulation data	Mass and energy balances	–	Uncertainty analysis using Monte Carlo simulation
De Roeck et al. (2022)	Comparing biological and catalytic biogas methanation	–	Continuous stirred tank reactor	Aspen Plus v11	Personal communication	Mass and heat balances	–	Mentioned having uncertainty in the model parameters
Echeverria et al. (2022)	End applications of dissolving pulp	To generate LCI for different scenarios	Steady-state	WinGEMS	Literature, commercial databases Fisher Solve and RISI for wood pulp mills	Mass and energy balances	Compared with data from the Fisher Solve database	–
Elomaa et al. (2020a)	Refractory gold concentrate by cupric chloride leaching	–	Steady-state	HSC-Sim	Literature	Mass and energy balances	–	Sensitivity analysis with different electricity consumptions
Elomaa et al. (2020b)	Hydrometallurgical refractory gold concentrate processing	Lack of industrial level information	Steady-state and batch operation	HSC-Sim	Known and/or published chemistry and literature	Mass and energy balances	–	Did sensitivity analysis with different electricity and water consumptions
Francois et al. (2013)	Wood gasification combined heat and power plant	Lack of reliable data	Steady-state	Aspen Plus	Literature	Mass and energy balances	Validated against measurements from a pilot plant and literature data	–
Hajjaji et al. (2016a)	Hydrogen production via	–	–	Aspen Plus v10.2	Aspen Plus database and literature	Mass and energy balances	–	–

(continued on next page)

Table 1 (*continued*)

Citations	Research topics	Reasons of applying process simulation	Type of process simulated	Simulation software	Data sources for process simulation	End goal	Validation of modelled process data	Uncertainty characterization of modelled process data
	reforming of poultry fat							
Hajjaji (2014)	Hydrogen production from steam reforming of poultry tallow	–	–	Aspen Plus v10.2	Aspen Plus database and literature	Mass and energy balances	–	–
Hajjaji et al. (2016b)	Hydrogen from biogas reforming	–	Steady-state	Aspen Plus	Literature	–	–	–
Helmdach et al. (2017)	Conversion of terpenes derived from biowaste feedstocks into reactive intermediates	Projection of commercial processes based on experimental and literature data	Steady-state and continuous stirred tank reactor	Aspen Plus	Experimental data from a plant and literature	–	Validated process models against experimental data	Mentioned having uncertainty in some model parameters
Higgins and Kendall (2012)	Using an algal turf scrubber to treat dairy wastewater	Projection of lab- and pilot-scale data	Continuous unit processes	A spreadsheet-based model	Lab and pilot-scale data and literature	Mass and energy balances	–	Mentioned having uncertainty in some model parameters and did sensitivity analysis with assumed parameters
Ioannidou et al. (2022)	Production of bio-based succinic acid and value-added co-products	Completing material and energy flows and the sizing of unit operations	Continuous operation	UniSim (Honeywell)	Experimental results from another study and literature	Material and energy balances	–	–
Iosif et al. (2010)	Steelmaking route	New technology and lack of data for large industrial scale	Continuous unit processes	Aspen Plus	Industrial data and literature	Mass and energy balances	Validated the model against an existing integrated plant and compared model results with industrial data	–
Jayasekara et al. (2022)	Polylactic acid pellets production from corn and sugarcane molasses	To scale-up	Batch operation	Aspen Plus v9	Literature	Material and energy balances	Validated by comparing with the actual plant data, reported in the published literature	Identified uncertain parameters and did sensitivity analysis by varying those parameters
Karka et al. (2017)	Biomass-to-product process chains	To generate LCI for different production pathways	–	Flowsheet based model	Industry data, patent, and literature	Mass and energy balances	Validated using pilot plant data, literature, and the knowledge acquired from industrial partners	
Keller et al. (2020)	Olefin production	Lack of consistent inventory data for all investigated pathways	Continuous unit processes	Aspen Plus v10	GEMIS database 4.95, literature, IEC pilot plant, and concept data for carbon conversion	Balanced the gaps by assumptions	–	Sensitivity analysis based on changes in the composition of power production
Keller et al. (2022a, 2022b)	Lower olefins, BTX aromatics, methanol, ammonia and hydrogen production	Lack of inventory data due to limited large scale technology application	Continuous unit processes	Aspen Plus v11	Literature	Mass, energy, and element balances	Validated with available experimental and industrial process data	Mentioned having uncertainty in some model parameters
Khalil (2021)	Glycerol-to-hydrogen conversion	Lack of inventory data in LCA databases	–	Aspen HYSYS v11	Aspen HYSYS simulation	Mass and energy balances	–	Sensitivity analysis based on varying process electricity sources and thermal energy sources
Koch et al. (2020)	Lignin nanoparticle production from what straw	Lack of data for emerging technology	–	Aspen Plus v8.6	Experimental information	Mass and energy balances	–	Mentioned having uncertainty and did sensitivity analysis with

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Table 1 (*continued*)

Citations	Research topics	Reasons of applying process simulation	Type of process simulated	Simulation software	Data sources for process simulation	End goal	Validation of modelled process data	Uncertainty characterization of modelled process data
								varying parameters
Kuan et al. (2007)	*Tongkat Ali (Eurycoma longifolia)* extract production	–	Batch operation	SuperPro Designer v6	Manufacturing database, GREET, and literature	Mass and energy balances	–	–
Kulay et al. (2003)	i-pentane purification process from the REPSOL-YPF refinery	Design of new processes and the optimization of existing installations	–	Hysys.Plant	Literature and plant data	Mass balance	Model was validated with plant data	–
Lal and You (2022)	Hydrogen production	–	Varying operating conditions	Aspen Plus	Literature	–	–	Future work should consider uncertainty.
Larnaudie et al. (2020)	Renewable diesel production	–	A mix of batch and continuous operations	Aspen Plus	Past models, literature, and experimental data	Material and energy balances	–	Scenario analysis based on overall yield of the process
Li et al. (2018)	Acetic acid production process from coal/biomass	Lack of inventory for some chemical process models	–	Aspen HYSYS and CHEMCAD	Literature	Mass and energy balances	–	–
Li et al. (2019a)	Shale gas sweetening process	–	–	Aspen Plus	2012 China input-output table and literature	Equilibrium in kinetic reactions	Compared with data reported in the literature	Sensitivity analysis with varying process parameters
Li et al. (2019b)	Shale gas dehydration process	–	–	Aspen Plus v8.6	2012 China input-output table and literature	Energy balance	–	Mentioned having uncertainty and did sensitivity analysis with different shale gas compositions and dehydrating specifications
Liao et al. (2020)	Activated carbon production from different biomass feedstock	Lack of data for emerging technology	–	Aspen Plus v10	Literature and different models	Mass and energy balances	Validated with independent experimental data	–
Mata et al. (2023)	Particleboard based on cardoon and starch/chitosan	Projection of pilot scale data	–	Aspen Plus v9	Experimental data of pilot scale and literature	Mass balance	–	–
Mio et al. (2021)	Nanostructured polymer systems in the maritime industry	Novel/early stage product design	Continuous unit processes	Multiple software	Literature and Granta CES Selector software materials database	Mass and energy balances	–	Future work should consider uncertainty.
Mirgaux et al. (2021)	Carbon capture and utilization options in an integrated plant	–	Continuous unit processes	Aspen Plus	Industrial data and literature	Mass and energy balances	Validated against industrial and literature data	–
Morales-Mendoza and Azzaro-Pantel (2017)	Energy generation	Lack of inventory data in LCA databases	–	ProSim	Literature	Mass and energy balances	Compared with literature data and the Ecoinvent database	–
Morales-Mendoza et al. (2018)	Eco-design of chemical processes - benzene and biodiesel production	–	–	COCO, ProSimPlus, and Aspen HYSYS	Previous experimental studies	Material and energy balances	Compare the model with the literature data	–
Mu et al. (2010)	Lignocellulosic ethanol production	Projection of plant level data obtained from literature	–	Aspen Plus	Literature and previously developed model	Material and energy balances	–	–
Mynko et al. (2022)	Light olefins production	Less studied technology	–	COILSIM1D and Petro-SIM®	Literature	Mass and energy balances	COILSIM1D model data was validated with an industrial furnace	–

(*continued on next page*)

Table 1 (*continued*)

Citations	Research topics	Reasons of applying process simulation	Type of process simulated	Simulation software	Data sources for process simulation	End goal	Validation of modelled process data	Uncertainty characterization of modelled process data
Parvatker and Eckelman (2020)	151 different chemical processes	Lack of inventory for some chemical process models	Batch operation	Aspen Plus	Industrial reference texts and literature	Balanced stoichiometric reactions	Compared the process simulation results with different data sources including Ecoinvent	–
Pereira et al. (2015)	Butanol production in sugarcane biorefineries	–	Continuous unit processes	Computer process simulation obtained from the literature	Literature	Mass and energy balances	–	–
Rangel et al. (2022)	Synthetic crude oil production	Technology with low TRL	–	Aspen Plus	Literature	–	–	Uncertainty analysis using Monte Carlo Simulation and scenario analysis based on varying model parameters
Riazi et al. (2019)	Isostearic acid production for pharmaceutical and personal care products	Few life cycle inventory data are available for the studied process	–	SuperPro Designer	Patent literature	Mass and energy balances	–	–
Riazi et al. (2020)	Renewable diesel from oils and animal fat waste	–	Continuous operation on a large scale but batch processing for laboratory experiments	Aspen Plus	Ab Initio methods are used for estimating missing data, literature, GREET, and assumptions	Mass and energy balances	–	–
Rinne et al. (2021)	Prospective battery-grade cobalt sulfate production from Co–Au ores	Lack of data for prospective/ emerging technology	Steady-state	HSC Sim	Literature and the state-of-the-art practices	Mass and energy balances	–	Uncertainty in process parameters was addressed by sensitivity analysis
Sadeek et al. (2020a, 2020b)	Ammonia process	Lack of reliable data	–	Aspen Plus v10	Calculated, local data and plant data	Mass and energy balances	Validated against plant operating data and measured COV	–
Santoyo-Castelazo et al. (2023)	Bioethanol production from sugarcane bagasse	Lack of reliable data	Steady-state	Aspen Plus v11	Literature	Mass and energy balances	Validated against literature data	–
Smith et al. (2017)	Chemical manufacturing process	Lack of reliable data	Continuous stirred tank reactor	CHEMCAD	Commercially available inventories and literature	Material and energy balances	–	–
Yang et al. (2018)	Manufacturing ethylene from wet shale gas and biomass	–	–	Aspen HYSYS	Literature and GREET model	Mass and energy balances	–	Sensitivity analysis with varying input process parameters

reviewed papers (54%) used different versions of this software. Aspen Plus is a flow sheet-based commercial process simulator software that can be used to model, design, and optimize (typically) steady-state processes (Francois et al., 2013). It was developed by Aspen Technology Inc. and was mainly based on simulation data from the US Department of Energy (DoE) demonstration SMR facility in Las Vegas (Hajjaji et al., 2016b). In addition, 6 studies used Aspen HYSYS (Table 1), 2 used SuperPro Designer (Kuan et al., 2007; Riazi et al., 2019), 2 used CHEMCAD (Li et al., 2018; Smith et al., 2017), and 2 used ProSim software (Morales-Mendoza and Azzaro-Pantel, 2017; Morales-Mendoza et al., 2018). Some of the reviewed articles used other software like WinGEMS (Echeverria et al., 2022), HSC-Sim (Aromaa et al., 2023; Elomaa et al., 2020a, 2020b; Rinne et al., 2021), USIM-PAC (Beylot et al., 2021), and COILSIM1D and Petro-SIM (Mynko et al., 2022).

The use of a specific process simulation software can be dependent on the type of process that needs to be simulated. Considering most of the widely used software is capable of simulating different types of processes, choosing a specific software often simply depends on its accessibility, especially for commercial software. Some software has been developed for specific product systems, such as WinGEMS, which was developed for the pulp and paper industry (Echeverria et al., 2022; Măluțan and Măluț;an, 2013). Moreover, while Aspen HYSYS is very useful for almost all types of industries, Aspen Plus is the leading software for chemical industries (Costa, 2023).

Öi (2012) compared the simulation results from Aspen Plus and HYSYS for the CO_2 capture process and found that the divergence between the two results was small. It has also been reported that the results obtained from different software often do not vary that much. For instance, Tangsriwong et al. (2020) used Aspen Plus and the open-source software DWSIM to model the petroleum production process and found the difference in the simulation results was less than 5%. Simulation results for the re-refining process of lubricant oil from Aspen Plus and CHEMCAD were also compared, and the difference was insignificant (Usman, 2016). This means that LCA practitioners can generally use any type of process simulator that suits their studied product system/process for filling gaps in LCI. However, LCA practitioners should have some knowledge of chemical processes and details of the studied product system as may be required for using the process simulation to generate LCI (Parvatker and Eckelman, 2020; Zargar et al., 2022).

3.4Validation of process simulation

Validation of process simulation covers validation of both the process model (i.e., verification of the model) and simulation results. It is a common practice to develop a process flow diagram based on information found in the literature (Rinne et al., 2021). If the process model/process flow diagram is developed based on literature, industrial reports, and/or pilot scale setups, it is crucial to check the process model for relevance to an industrial-scale setup, as the process flow diagram should be representative of the actual industrial scale system. For this, an extensive literature review combined with industry consultation should be undertaken. However, limited details are provided in the reviewed literature about developing the process simulation models and related validation processes.

This is particularly concerning given that comparing the simulation results with real-world data or experimental measurements to assess the accuracy and reliability of the model is vital for this type of study. This helps to ensure that the simulation model provides an appropriate representation of the real-world system. Validating simulation results should be based on specific, meaningful and representative parameters for the studied system such as energy consumption, the yield of the main product, the efficiency of the process, and emissions levels, etc. Different statistical analyses can be performed along with graphical comparisons, such as coefficient of variation (Sadeek et al., 2020a, 2020b). Discrepancies between the simulated and real-world data may arise due to inappropriate assumptions, input data, model parameters, etc.

Despite being a critical part of process simulation-based studies (Liu et al., 2019), validation information was reported in less than half of the papers reviewed (36%) (Table 1). Liu et al. (2019) also reported that over 80% of the papers they reviewed did not explicitly mention any information regarding the verification and validation of the process simulation models employed. Among those who did, Iosif et al. (2010) explicitly mentioned that they validated the process model with data from an established plant. Others just compared their results with data obtained from the literature (38.9%), industry (27.8%), experimental data (16.7%), pilot plants (16.7%), and databases like Ecoinvent or Fisher Solve (16.7%) (Table 1). For validating simulation data, any specific parameters (i.e., energy use, yield) can be compared with industrial or experimental data. If validation with industrial data is absolutely not possible, publicly available industrial reports, patents, and other reliable literature sources are the alternate ways to support the validation step in order to ensure the robustness of the simulated data.

3.5Evaluation of simulated data and integration with LCA

Simulated data is mostly used when reliable and representative data is otherwise lacking. The quality of LCI is crucial for carrying out a robust LCA (Khatri and Pandit, 2022), and process simulation is effective in support of arriving at accurate LCIs (Santoyo-Castelazo et al., 2023; Helmdach et al., 2017). However, it is crucial to evaluate the simulated data before integrating them into LCIs.

Though LCA practitioners need some background knowledge about the process simulation, the added complexity can be balanced against the improved LCI and the reduced modelling time (Smith et al., 2017). However, the simulated data should be evaluated to check its reliability, completeness, consistency, and representativeness (Cañon et al., 2022b), in which case, data quality assessment using the Pedigree matrix can be a vital step. The evaluation of simulated data is not mentioned in most of the reviewed articles. However, some studies suggested using some sort of primary/site-specific data and/or specific requirements of existing processes to refine the modelling quality and associated results (Beylot et al., 2021; Elomaa et al., 2020b). Another way is to perform sensitivity analysis by varying LCI data for assumed or less reliable data (Elomaa et al., 2020a, 2020b) in order to understand how changes in input parameters affect the results and to identify potential sources of error.

To integrate the simulated data with conventional LCA databases (mostly for background processes), compatibility between modelled data and conventional data in terms of functional units, system boundaries, and data formats should be confirmed. Scenario analysis to compare the impacts of different assumptions and data sources on the LCI results can be useful as well. Continuous revision and refinement of the modelling process and iteration of the process models based on feedback and new data should be carried out. Evaluating and applying modelling data in LCI development requires rigorous assessment and careful integration with conventional data. By ensuring data quality, validating against empirical measurements, and transparently documenting the process, practitioners can enhance the reliability and accuracy of their LCI studies. Integrating both modelling and conventional data allows for a more comprehensive and nuanced understanding of environmental impacts, supporting informed decision-making.

3.6Uncertainty in process simulation

LCI modelling via process simulation can lead to significant data uncertainty (Keller et al., 2022a). Reporting uncertainty in process simulation-based LCI modelling is hence recommended, along with sensitivity/scenario analysis. As the input data are generally collected from different secondary sources, uncertainty can be associated with both the model parameters and the input data. Findings from the reviewed articles, however, indicate that reporting uncertainty in input data and model parameters is not widely practiced. Only 18 (36%) papers mentioned having considered uncertainty in some of the model parameters and did sensitivity/scenario analysis based on those parameters (Table 1). Three studies mentioned having some sort of uncertainty in model parameters but did not report any associated analysis (De Roeck et al., 2022; Helmdach et al., 2017; Keller et al., 2022a, 2022b). Lal and You (2022) and Mio et al. (2021) recommended that future studies should consider uncertainty in modelling parameters and input data. Uncertainty and sensitivity analyses are highly recommended components of an LCA study and are required for studies supporting comparative assertions (ISO, 2006a), which was one of the reasons for doing sensitivity analysis that was reported in these studies.

4Discussion

Based on the findings for the review questions, the following discussion section illustrates a general methodological framework for integrating simulation-based LCI in LCA studies, explaining how to transform simulated data into LCI and the iterative process between process simulation and LCA. It also includes a discussion on the application of simulation-based data in LCA and the relative merits of using simulation-based data for LCA (see Fig. 2).

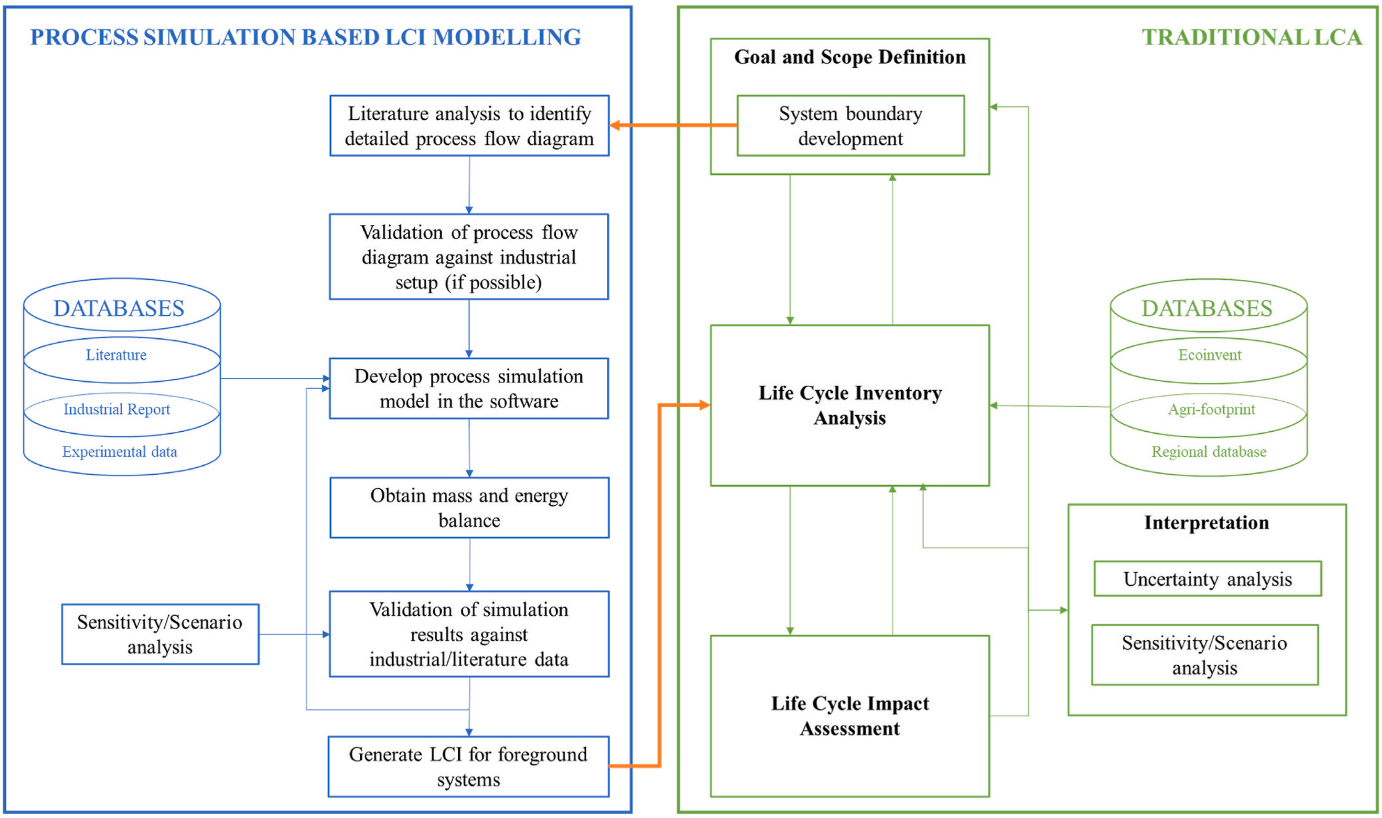

Fig. 2. Generic methodological flow chart for process simulation-based LCI modelling to facilitate LCA of industry-related processes.

4.1Methodological framework for the integration of simulation-based LCI in LCA

Based on the review findings, a general methodological flow chart for using process simulation to generate LCI was developed (Fig. 2) and is described step-by-step in this section. This is contrasted with the conventional approach of generating LCI datasets. In both cases, existing databases are used. According to ISO guidelines, goal and scope definition is the first phase of any LCA study. In the goal definition, it should be clearly defined why process simulation is integrated into the LCA. Reasons may include the lack of reliable data, improving accuracy, enhancing process optimization, etc. After establishing the system boundary, the processes that will be modelled and others that will rely on conventional data should be specified. It is common practice to consider a 'cradle to gate' system boundary in LCA studies where process simulation is used (Ferdous et al., 2023). However, process simulation is mainly used to generate LCI for foreground systems – in other words, for key 'gate-to-gate' subsystems within the system boundary (review findings; Ferdous et al., 2023). Once the boundary is established, the next task is to develop the process flow diagram. Relevant industry experts may be consulted, along with literature sources. The granularity of the process flow diagram will depend on available information and should be consistent with the defined goal and scope. Once a sufficiently detailed process flow diagram is developed, it should be validated by technical experts. It should also be noted that the necessary information might be difficult to gather due to confidentiality concerns among industrial producers (Righi et al., 2018).

The next step is to develop the process model using process simulation software (i.e., Aspen Plus, Aspen HYSYS, ProSimPlus) for the studied process. The operating condition (continuous vs. batch) can be determined based on the studied product system and especially based on the collected data for every unit process. In this step, a wide range of data sources may be consulted in order to collect the most representative and reliable data possible. Once the model is developed, mass and energy balances should be calculated in order to check completeness and consistency and generate the LCI for the specific processes of interest. The next step, validation of simulated data, is a highly recommended step, despite being seemingly uncommon in most of the literature. Validation can be done against primary data collected from industry or by using historical or experimental data. Researchers may variously consider emissions, energy use, yield, or efficiency levels when comparing the simulated data with known and reliable data. Validation can be done using graphical representation, statistical goodness-of-fit analysis, or using other statistical measures (i.e., coefficient of variation) (Sadeek et al., 2020a, 2020b). If there is a large discrepancy between the simulated and real-world data, the model parameters and assumptions (if any) should be revisited and revised accordingly. Best practices with respect to quantification and reporting of uncertainty are unclear. Some studies mentioned having uncertainty in some of the model parameters, which was typically considered using sensitivity/scenario analysis. Sensitivity analysis will identify the extent to which the uncertain parameters are affecting the results. If the uncertain parameters are found to be significant through sensitivity analysis, researchers should try to include the most reliable data possible. Both parameter and model uncertainties should be considered.

After validating and evaluating the simulated data, key output parameters should be identified from the simulation results that are relevant for the LCA (i.e., mass and energy balances, emissions, energy and resources consumptions) and compatibility between modelled data and conventional LCA data for other processes should be checked in terms of units, formats, and scope. Simulated data should be normalized to the functional unit defined in the LCA study. Finally, through these steps, a complete LCI for foreground systems will be generated that can be combined with the background models of conventional LCA databases, which can then be used in LCA software to carry out the LCIA. This integrated data can also be used to perform scenario analysis for exploring different technological, geographical, and temporal conditions. Iteratively, the insights gained from the LCA modelling can be used to refine the process models, including changing process conditions, selecting different materials, optimizing energy usage, etc.

Process simulation-based LCI modelling is an iterative process, starting with a base process model to assemble data for initial LCA modelling. Based on the LCA results, hotspots for improvement can be identified and the process models can be modified in terms of energy consumption reduction, substitution of raw materials, etc. Simulation software will produce the inventory based on the modified scenarios and another round of LCA can be performed to see the changes in results. This iterative loop can be performed until all modelling objectives are satisfied.

4.2Application of simulation-based data in LCA

Simulation-based data can significantly enhance LCA by providing detailed, process-specific information that complements conventional data from LCA databases (Pell et al., 2019). For any emerging/novel technology and/or any process with low TRL, simulation-based data can be highly useful in support of carrying out an LCA. It can provide high-resolution data for specific processes, capturing the details of operations that are often averaged in conventional databases along with filling the data gaps that may be present in conventional databases. LCI modelling based on process simulation can also be useful for scenario analysis based on different process configurations and operational conditions and for finding the optimization potential of existing processes (Morales-Mendoza et al., 2018). Additionally, simulation-based data can enable conducting dynamic LCA to consider how environmental impacts will change over time with evolving technologies (Bahramian et al., 2024). Finally, combining simulation-based data with conventional LCI data creates a hybrid approach that can strengthen the analysis (Wang et al., 2014).

4.3Relative merits of using simulated data for LCA

Integrating process simulation-based data into LCA can enhance the precision, relevance, and utility of the LCA. As it mostly provides precise and detailed data on material and energy flows, emissions, and efficiencies, it may be able to represent the studied system more accurately than would be possible using generic secondary data. The modelling can also be updated with different processing conditions as required, which allows practitioners to compare scenarios based on changes in raw materials, energy sources, or process configurations, and to find optimized processing pathways. Improved data quality through process simulation also enhances the transparency and credibility of LCA reporting. Especially for emerging and novel technologies, process simulation can help to identify potential issues in the early design phase and enable practitioners to modify the process accordingly to make it more optimized and sustainable.

Despite having several advantages, one of the main challenges of using process simulation to generate LCI is the complexity of developing process models. Sometimes, the processes are very complex, and it can be computationally intensive to model them. LCA practitioners often need specialized knowledge and expertise in process modelling and in working with specific simulation software. Substantial time and resources are required to train people for this.

Another challenge is dealing with inaccurate and incomplete data, which can lead to misleading results. Additionally, process simulation software - especially commercial, high-end software - can be very expensive to license, maintain, and update. Simulation often relies on different assumptions and simplifications, which is one of the main sources of uncertainty in LCA results. To deal with these uncertainties, sensitivity/scenario analysis should be performed to validate the robustness of the LCA results.

5Conclusions

LCI analysis is an integral and essential part of an LCA study but assembling reliable and representative data is often challenging. Industry confidentiality concerns with respect to unique proprietary processes may hinder the collection of primary data. Primary data may also be scarce for new/emerging technologies or processes at low TRL. To resolve data gap issues, process simulation-based LCI analysis is increasingly popular in LCA studies. Computer-based process simulation software enables the creation of a virtual model representing real-world processes. In this context, mass, energy, stoichiometric and kinetic balances can be used to model and generate a complete LCI for specific processes within the system boundary. Verification of the process models to check their accuracy is an essential part of such studies, along with consideration of uncertainty. Lack of engagement with industry while generating the process flow diagram and lack of primary data can lead to relying on secondary data sources (i.e., literature, industry report).

Though LCI modelling through process simulation has been used for many years, a systematic review to identify common methodological choices for this type of study was lacking. The current study hence conducted a systematic review of industry-sector-related LCA studies to identify common methodological choices made by practitioners for generating LCI through process simulation. The most common reason to use process simulation to generate LCI is the lack of reliable data. The reviewed articles developed the process models and gathered the available data from secondary sources, mostly from literature. The process models can be developed using any process simulation software as most of simulation software can handle different types of processes. Mass and energy balances can be used to fill gaps (if any) in the dataset to complete the foreground system inventory and check for completeness. The process model should be verified by industry experts, and simulated results should be validated with industry and/or literature data. If it is not possible to validate the simulated data with industrial data, industrial reports and patents can be a good source of information to support validation. Another important aspect is reporting the uncertainty associated with LCA modelling and/or process simulation, which can also be done through sensitivity/scenario analysis. Most of the reviewed articles did sensitivity analysis with respect to uncertain parameters. Overall, process simulation-based LCI analysis can greatly enhance the quality and credibility of LCA studies. However, in order to use process simulation for LCI development in LCA, practitioners should have sufficient knowledge about the studied product system and the technical specifications of the specific processes to be simulated.

This study illustrated the methodological framework for integrating process simulation with LCA and discussed how the simulated data can be converted into LCI data, which can be used in combination with LCI data from conventional LCA databases. This methodological framework should be tested using practical scenarios/case studies in the future in order to further identify potential pitfalls, refine best practices, and provide additional strategic advice on managing the complexities associated with different types of process simulation software and LCA tools.

CRediT authorship contribution statement

Jannatul Ferdous: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation, Conceptualization. **Farid Bensebaa:** Writing – review & editing, Supervision. **Kasun Hewage:** Writing – review & editing. **Pankaj Bhowmik:** Writing – review & editing. **Nathan Pelletier:** Writing – review & editing, Supervision, Project administration, Funding acquisition.

Declaration of competing interest

There is 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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