Software and data for circular economy assessment

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5 LCI DATA FROM COMPUTER-AIDED TECHNOLOGIES AND ARTIFICIAL INTELLIGENCE: A SYSTEMATIC REVIEW

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ABSTRACT

Industrial and ecological data currently collected on supply chains is minimal in comparison with the enormous quantity and diversity of manufactured products. Meanwhile, Computer-Aided technologies (CAx) are used daily for the design and management of products' manufacturing, life cycle. As such they can generate a wealth of information about products' life cycle. Artificial intelligence (AI) methods and infrastructure are also steadily increasing society's ability to generate data, insights and automation. In this study, we investigated the combination of CAx and AI to generate, estimate and extract data for Life Cycle Inventory (LCI) modelling. We performed a systematic review of these fields covering 1995 through May 2021 using the PRISMA method. We analyzed 131 studies concerning the use of CAx (84 articles) and AI (47 articles). From the knowledge gathered in the review, we describe possible ways of using CAx and AI to obtain LCI data for existing products and their potential alternatives. Specifically, CAx provides benefits in the generation of data for life cycle stages that require industrial processing. AI provides benefits in the combination and extraction of data from heterogeneous sources, in the estimation of flows under scenarios, and it is especially helpful in highly repetitive tasks such as the creation of several alternatives. The combination of AI and CAx for LCI provides benefits for the optimization of simulated product systems from which LCI data can be obtained, generating a vast range of alternatives, estimating lifespan and maintenance of products and components.

5.1 INTRODUCTION

Products and industries need urgent changes to mitigate further negative ecological and socio-economic effects such as anthropogenic climate change and biodiversity loss. The implementation of circular and sustainable supply chains is instrumental to this objective. In order to successfully execute and track the progress of this implementation, we need to be able to promptly assess the environmental impacts of supply chains and their alternatives. The compilation of Life Cycle Inventories (LCIs) is a fundamental practice enabling this type of assessment (Guinée, 2001). However, compiling LCIs is typically a challenging and human resource intensive activity (Zargar et al., 2022). Additionally, most supply chain data has limited availability to scientists and the public due to companies' protection of intellectual property to maintain competitive advantage (Goldstein & Newell, 2019).

In order to align the need for assessment together with human limitations, estimation of LCI data through the use of Computer-Aided Technologies (CAx) and Artificial Intelligence[2] (AI) could be an attractive option. In fact, CAx are commonly used by product designers and engineers in the creation, planning manufacturing and reverse engineering of products. Similarly, AI methods such as expert systems, data mining and machine learning, can be useful to estimate and extract and process information about manufacturing activities. For example, AI methods have shown to simplify the identification of needed processes (e.g., machining such as lathing), their parameters (e.g., tooling, operating time, and energy consumption) and sequence (e.g., cutting before lathing), or the choice of materials for manufacturing (Leo Kumar, 2017). While the use of CAx for LCIs has been previously investigated (Zargar et al., 2022), a systematic use of these technologies and full integration within the data processing pipeline of LCA practitioners and product developers still remains out of reach.

[2] In the scope of this paper, we refer to first generation AI as in Artificial Narrow Intelligence. I.e. the application of intelligent systems to solve specific tasks (Kaplan & Haenlein, 2019).

In response to these developments and needs, we present a systematic review investigating how CAx and AI can be used to obtain data for LCIs. We focus on data generation, estimation and extraction, leaving prospects of LCI data collection automation to future studies. The added value of estimating data via CAx and AI include the possibility to obtain data of the highest quality short of collecting data from manufacturers (Parvatker & Eckelman, 2019; Zargar et al., 2022). This would offer the possibility to create LCIs independently from firms (i.e. reverse engineering LCIs), thereby reducing labor intensity of the LCI phase, and expanding supply chain coverage of LCIs in databases.

These objectives are addressed by following research question and sub-questions:

How can CAx and AI methods be used to obtain data for LCIs?

- How can CAx be used to obtain data for LCIs?
- How can AI methods be used to obtain data for LCIs?
- How can the combination of CAx and AI be used to obtain data for LCIs?

The remainder of this article is organized as follows. In section 2, we provide the background information for LCI, CAx and AI. In section 3, we report the methods for the systematic review. Section 4 presents summary results, insights from the studies and how these are coupled to LCIs. Section 5 describes how the methods are combined and limitation overcome. At last, sections 6 and 7 present discussions and conclusions respectively.

5.2 Background

In this section we summarize the fundamental aspects of the various technologies investigated in our work. Each of these fields is vast, as such the provided definitions are only instrumental to understand the results of the literature review and do not have the intention of describing each field to its depth. For in-depth definitions, we refer the reader to the referenced and specialized literature on the topics.

5.2.1 Life Cycle Inventories (LCIs)

LCIs are compiled during the inventory analysis phase of a Life Cycle Assessment (LCA). In this phase, practitioners compile the inputs and outputs of a product system along the life cycle (Guinée, 2001; ISO, 2006). The inventory analysis is usually considered the most time-intensive phase of LCA as all activities involved in the product life cycle are modeled. Activities are technical systems such as a process, transport and their respective aggregates (Carlson et al., 1998; Silva, 2021). Aggregates of activities form lifecycle stages (Fig. 1), from the extraction to the end-of-life (EOL) (recycle/waste management). For example the stage of manufacturing may be composed by activities such as materials manufacture, product fabrication and packaging (EPA, 1993; Silva, 2021).

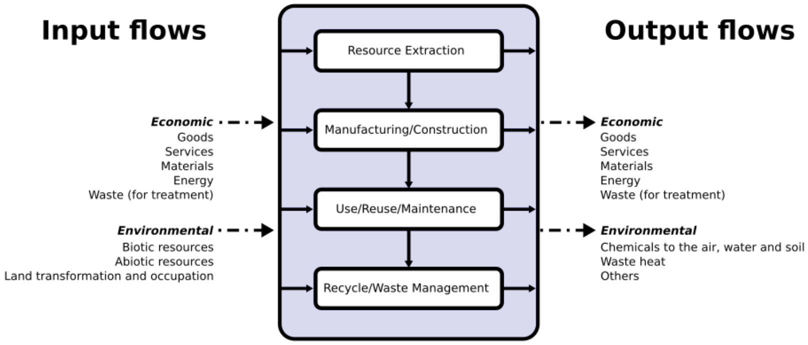

Figure 1: Lifecycle stages and flows of unit processes (adaptation from Guinée 2001; EPA 1993)

Activities, modelled as unit processes (UPs), are connected to each other by their inputs and outputs. Flows that enter and exit UPs are divided into economic and environmental flows. Economic flows are physical flows connecting UPs and concern intermediate and final products and services of positive, negative or null economic value. Environmental interventions are chemical, physical or biological anthropic interferences with the natural environment such as the extraction of resources or the emission of pollutants into nature. These quantified flows are inputs and outputs to the environment relative to the primary function(s) (i.e., functional unit) satisfied by a product system (Guinée, 2001; ISO, 2006). The wealth of information that LCIs could contain can result in heterogeneous datasets. In order to ensure a common level of information, LCA data collection is regulated by ISO (2006).

5.2.2 Computer-Aided Technologies (CAx)

CAx are a set of systems and software to support design, planning and management of products which have become indispensable to manufacturing firms and engineering education (Chryssolouris et al., 2009; Dankwort et al., 2004). They are part of a broad family of software for Product Life Management (PLM) and they compose a large ecosystem of technologies typically used in the design and planning manufacturing phase of product development. In this study, we selected a set of CAx that, to our knowledge and according to literature (Chryssolouris et al., 2009), are commonly used in engineering applications for designing products and planning their manufacturing. One additional criterion in our selection was the possibility to use CAx independently from direct interaction with firms. Such independence allows to design or reverse engineer products composition, manufacturing activities and other useful data for LCI such as economic and environmental flows. We selected the following CAx:

- ***Computer-Aided Processes Engineering (CAPE):*** The use of computer system for the design and optimization of chemical processes (Agachi, 2005);
- ***Computer-Aided Design (CAD)***: The use of computer systems for the creation, modification, analysis or optimization of a design (Elanchezhian et al., 2008);
- ***Computer-Aided Engineering (CAE):*** The use of computer software to perform simulations on physical properties of materials and goods such as structural, thermal, surface and other properties (Terzi et al., 2010). In various CAx classifications, CAE may include Computer-Aided Process Engineering and it is occasionally used to describe the totality of the computer-aided design and engineering process within a firm, however, in this study we treat these concepts separately.
- ***Computer-Aided Machining or Manufacturing (CAM):*** The use of software to plan and control manufacturing processes (Kreith & Goswami, 2004) (e.g., drills, lathes, mills or 3D printers);
- ***Computer-Aided Process Planning (CAPP):*** Tools to assist the selection, sequencing ad scheduling of manufacturing operations and their resources (ElMaraghy, 1993).

5.2.3 Artificial intelligence (AI)

AI concerns the development of *"systems that exhibit the characteristics we associate with intelligence in human behavior"* (Tecuci, 2012), such as the development of predictive models and learning complex tasks. AI is composed by 6 subfields (Russell & Norvig, 2010a): Natural Language Processing; Knowledge Representation; Automated Reasoning; Machine Learning; Computer Vision; and Robotics.

We chiefly focus on knowledge representation, automated reasoning and machine learning, and we use the following concepts to aid our study as they allow the process of obtaining and organizing knowledge useful for LCIs:

- ***Expert systems (ES)*** are knowledge-based systems that can match or exceed human experts in specific tasks, once provided with expert domain knowledge (Russell & Norvig, 2010a). These systems typically do not have learning capabilities (Negnevitsky, 2011a) and are associated with early examples of AI systems relying on Boolean logic (Russell & Norvig, 2010a). Example of expert systems may be found in decision support systems making uses of Boolean and fuzzy logic systems relying on encoded expert knowledge.
- ***Data mining (DM)*** is the process of extracting patterns from datasets, and it is an important step in the practice of knowledge discovery in databases (Fayyad et al., 1996; Han et al., 2012). While in principle data mining is not exclusive to AI, it is in practice a fundamental method in AI applications. Examples of data mining techniques are K-mean clustering, K-nearest Neighbor classification, decision trees, Bayesian Classification.
- ***Machine learning (ML)*** concerns computer systems which have the ability to learn by experience, example and analogy (Negnevitsky, 2011a). Machine learning makes great use of data mining techniques and expert systems to automatically generate rules and "*avoid the tedious and expensive processes of knowledge acquisition, validation and revision"* (Negnevitsky, 2011a). Examples of machine learning techniques are genetic algorithms, artificial neural networks and adaptive fuzzy interference systems, random forest, etc.

5.3 APPROACH TO THE LITERATURE REVIEW

This systematic review utilizes the PRISMA guidelines (Page et al., 2021) and *Web Of Knowledge Core Collection* to retrieve the relevant literature. The objective of the systematic review was to analyze how CAx and AI have been used and can be used in the compilation of LCIs. Using the definitions presented in the previous section, we created two queries: one concerning CAx and LCIs, and one for AI and LCIs. To ensure the retrieval of studies relevant to our focus but with broader labels, we included keywords for LCA and PLM in our searches.

The two searches concerned all document types in the English language from 1995 to May 2021. Any records that concerned medical research were removed before screening. We screened the articles and left out papers that incidentally contained homonyms from other fields, and those where CAx, AI and LCI were mentioned but were not employed in the methods. In the cascading phase, we analyzed the citing and cited publications in the articles that remained after screening. This step was performed to ensure the inclusion of additional literature that meets the requirements but was not in the Web of Knowledge query.

Table 1: Literature review searches

	How can CAx be used to generate data for LCI?	How can AI be used to generate data for LCI?
Keywords	Topic= ("Computer-aided" OR "PLM" OR "CAx" OR "CAD" OR "CAE" OR "CAM" OR "CAPP" OR "CAPE") AND Topic= ("LCA" OR "LIFE CYCLE ASSESSMENT" OR "LCI" OR "LIFE CYCLE INVENTORY")	Topic = ("Artificial Intelligence" OR "Machine Learning" OR "Data mining" OR "Expert system") AND Topic = ("LCA" OR "LIFE CYCLE ASSESSMENT" OR "LCI" OR "LIFE CYCLE INVENTORY")
Total Results	163	109
Removed before screening	30	15
Records after screening	58	43
Total records after cascading	84	47

We classified the studies by type of CAx and AI methods used and collected data on additional techniques that may have been employed in the study. The studies were further classified by covered sectors. In order to highlight how CAx and AI can be used for LCI data, we classified the studies further by their coverage of life cycle stages and flow types (see figure 1). Additional details on the analyzed literature can be found in the supplementary information.

5.4 Results

In this section, we present the results of the literature review. We start in 4.1 with an overview of the characteristics of the collected literature. We first analyze historical publication trends, and then provide a network analysis of technologies (CAx and AI) used in the literature. These are followed by an analysis of which sectors were covered, followed by a network analysis of which technologies are applied in which sector. In section 4.2 and 4.3 we discuss how CAx and AI respectively are used to estimate LCI data, and in section 4.4 we address their integration. The data and classifications used for the analyses can be found in the supplementary information to this study.

5.4.1 Overview of literature findings

The historical bibliographic analysis (Figure 2) shows a slow growth of interest in the use of CAx to gain information on the lifecycle of technologies from 1995. On the other hand, the use of AI for related technologies for lifecycle data is much more recent. While the first paper appeared in 2004, 45% of the papers were published only in 2020. Although the use of AI for LCI compilation is currently in its infancy, the publication of studies on these topics is growing rapidly.

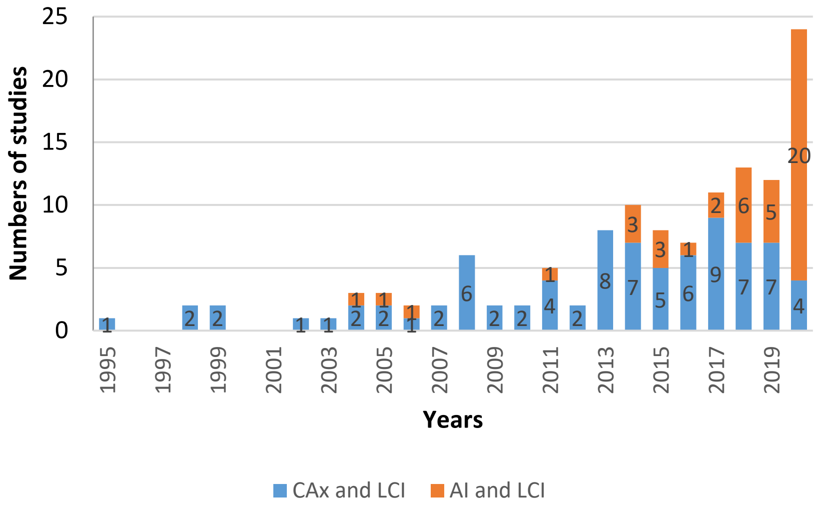

Figure 2: Published papers in the use of CAx and AI for lifecycle data in the period 1995-2020

In order to understand the attention given to each CAx and AI techniques in the context of data for LCI, we performed a network analysis (Figure 3). The circular network graph generated with the *Xnetwork* Python package show each keyword as a node, whose size is proportional to the number of articles. Each connection between nodes shows a number and is varied in thickness to indicate how frequently CAx and AI techniques were used in combination. Through this circular graph, we see that studies had a given keyword as main focus are directly connected to the main node (i.e., 131 studies (all keywords)). Combination of methods then are visible through the connections between the different keywords. For instance, one study may employ CAM as the main technology, and as a following step CAPP. The connection between these two keywords would indicate this relationship. However, the second keyword, in this case CAPP, would not have direct connection to the main node).

The network graph shows a broad use of CAD, CAPE and ML. However, they are largely disconnected with only 2 studies concerning CAPE and ML out of 45 studies concerning the two keywords. We also only found 3 articles for CAD and ML out of 80 studies for both keywords. No studies connected CAD to CAPE due to the difference in scope, as CAD focuses on the design of physical products and CAPE on the design of chemical processes. 9 studies concerned the use of ES, 6 an indirect relationship to ES through CAD. CAM, CAE, CAPP were in most cases used in combination with CAD, this is due to the fact that they rely on information provided by CAD (e.g., geometry and materials). DM, CAE, CAPP are the least employed technologies.

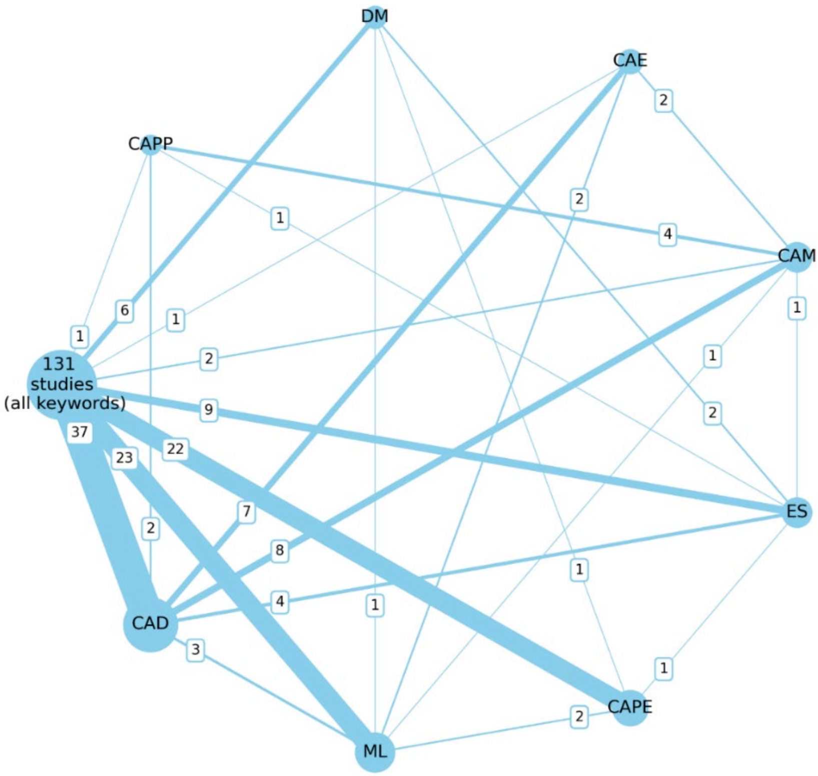

Figure 3: Technology focus in the literature and their intra-relationships. Each keyword is a node and the connections between nodes indicates combined use of the keywords. The numbers on the edges between the nodes indicate the number of studies concerning the linked CAx and AI techniques. CAD: Computer-Aided Design; CAE: Computer-Aided Engineering; CAM: Computer-Aided Machineries; CAPP: Computer-Aided Process Planning; CAPE: Computer-Aided Process Engineering; ES: Expert Systems; ML: Machine Learning; DM: Data Mining.

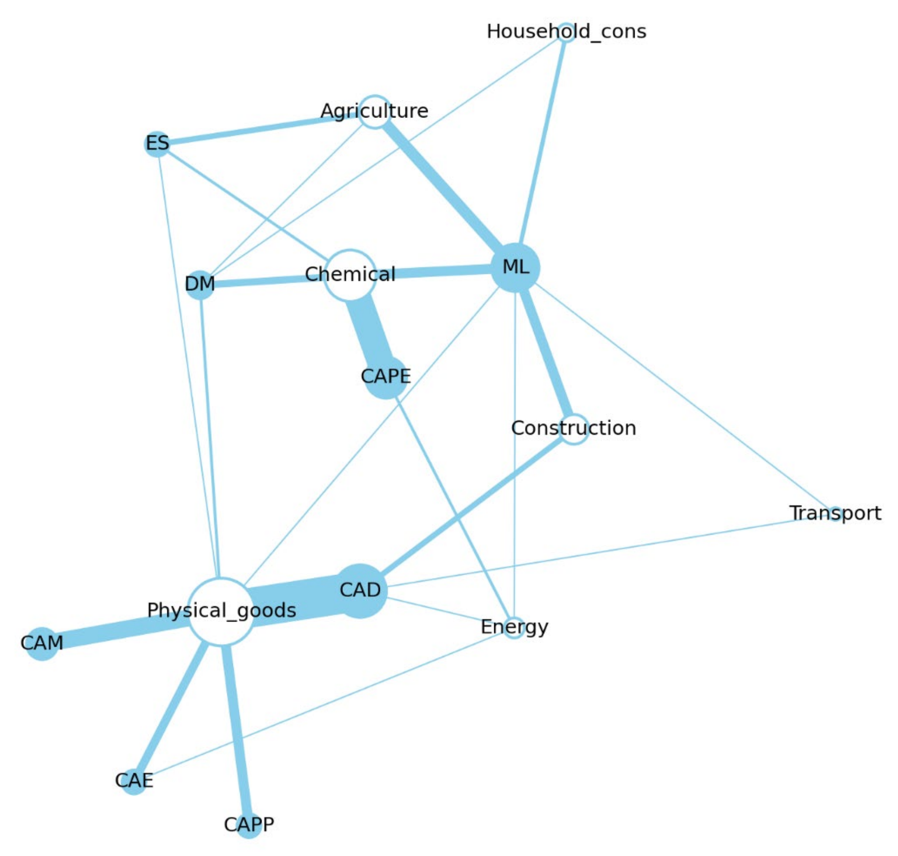

Figure 4: Sectoral focus by technology. CAD: Computer-Aided Design; CAE: Computer-Aided Engineering; CAM: Computer-Aided Machineries; CAPP: Computer-Aided Process Planning; CAPE: Computer-Aided Process Engineering; ES: Expert Systems; ML: Machine Learning; DM: Data Mining.

Figure 4 shows a network analysis of the sectors in relation to CAx and AI methods. For this analysis we used the spring layout which employs a Fruchterman-Reingold force-directed algorithm. This algorithm simulates edges as springs pulling nodes together and nodes as repelling objects. In other words, the higher the number of studies concerning the sectoral use of a CAx or AI methods the closer their nodes. From the analysis, we see that CAD, CAE, CAM and CAPP are often used in combination for LCI of physical goods (i.e., consumer and capital goods). In the construction and transportation (i.e., design, planning and assessment of transport services), the combination of ML with the use of CAD appears to be an explored avenue. However, despite the broad use of CAD for physical goods, we found little attention on how ML techniques can benefit the use of CAD for LCIs. CAPE is chiefly used in the chemical and energy sectors while ML enjoys great applications in the chemical, construction and agricultural sectors. Expert systems appear to be used mostly individually for the agricultural, and chemical sectors. Expert systems and data mining also showed some connections to CAD for physical goods. A few studies focused on general household consumption for which they employed machine learning and data mining.

Table 2: Unit process' flow types that may be estimated using the various technologies according to the literature. Each cell contains the total number of studies. Empty cells indicate no studies. A gradient from yellow (lowest number of studies) to red (highest number of studies) facilitates the identification of the least and most covered areas in data estimation for LCI.

		CAX					AI		
Stage	Flow type	CAD	CAE	CAM	CAPP	CAPE	ES	ML	DM
Resource extraction	Economic inputs	1					1	11	
	Economic outputs	1	1			1	1	11	
	Environmental inputs	1	1				3	11	
	Environmental outputs	1					3	10	
Manufacturing	Economic inputs	51	8	17	7	26	2	9	4
	Economic outputs	51	8	17	7	26	2	9	4
	Environmental inputs	27	6	10	5	26	2	9	3
	Environmental outputs	11	2	4	3	26	2	9	3
Use, Reuse,	Economic inputs	18	4	2	2			8	3
	Economic outputs	18	4	2	2			8	3
	Environmental inputs		2	1	1			5	2
	Environmental outputs							5	2
Recycling and waste	Economic inputs	11	1	1	1	2		3	2
	Economic outputs	11	1	1	1	2		3	2
	Environmental inputs				1	2		3	2
	Environmental outputs					2		3	2

Table 2 shows which flow types and life cycle stages may be generate or estimated using CAx and AI in the collected literature. The classification can be found in the supplementary information to this study. The table shows that CAx and AI have been used to estimate multiple flows and stages. The manufacturing stage has been broadly investigated both using CAx and AI. While CAx had scarce applications in the resource extraction, AI has many studies chiefly using ML with some ES applications. The distribution stage (i.e., transport and logistics from manufacturing plant to sale point) appears to not be investigated within the CAx or AI literature that we collected.

5.4.2 How CAx can be used to estimate data for LCIs

In this section we describe how CAx have been used for the estimation of each life cycle stage. The collected literature, however, revealed no CAx methods used for the estimation of LCI information for the transport stage. So this stage is discussed in the discussion section instead, together with possible ways to overcome this barrier.

Resource extraction

The analyzed literature has shown limited applications in the compilation of LCIs for the resource extraction stage. Nonetheless, in the context of agricultural products for energy or chemical production, CAPE and Computer-Aided Screening methods could be used to facilitate the identification of feedstock of agricultural origin and to be used in a specific application (Picardo et al., 2013). Once the feedstock is identified, data on the resource extraction phase could be collected or calculated. In order for this to be possible, however, the possible processes need to be modelled in CAPE software and a database needs to be provided with crops properties relevant to the modelled processes alongside information on growth conditions. However, these methods do not provide information on machineries employed for the extraction of resources.

Manufacturing

Once resources are acquired in the resource extraction stage, they are transformed into materials, parts and goods in the manufacturing stage. Most CAx applications focus on this secondary phase of the life of materials, therefore the vast majority of opportunities to estimate LCI data concerns this stage. Specifically, CAPE methods are used in the planning and design of chemical processes. CAPE achieves this by generating flowsheets containing process flow diagrams describing mass and energy balances of processes, equipment and operating conditions (Carvalho et al., 2013; Kalakul et al., 2014; Morales-Mendoza et al., 2018). This information can then be used in the simulation of plant-wide operations (Yoon et al., 2018). CAPE-generated flowsheets could be used to obtain LCI data (Romdhana et al., 2016) through the CAPE software Application Programming Interface (API) which allows to access the flowsheet of a simulated chemical production. Mass and energy balances can be used to identify all inputs and outputs, the processes and their order can be used to identify UPs, equipment tables can be used to identify equipment. Alternative processes and elementary flows, as well as uncertainties can also be identified when CAPE is linked to material property databases, knowledge based systems and optimization methods (Carvalho et al., 2013; Chen & Shonnard, 2004; Tula et al., 2017).

For goods other than chemical products, such as appliances or even buildings, the combination of CAD with CAE, CAM, CAPP and other CAx seems prominent in multiple studies (Andriankaja et al., 2017; Ben Slama et al., 2020; Tao et al., 2017, 2018; L. Zhang et al., 2019). CAD can assist in identifying economic flows linked to unit processes as the parts and materials composing the final good are known (Leibrecht, 2005). After that, CAM and CAPP can enable the retrieval of information on processes (e.g., machining), including their energy demand (Huang & Ameta, 2014b, 2014a), equipment and waste flows (Singh & Madan, 2016) as they are typically connected to manufacturing equipment databases containing specifications on operations. Specifically, CAM is used in microplanning, where processes, parameters, tooling and fluids are identified according to specific features, and CAPP is used in macroplanning, which involves the sequence of processes (Srinivasan & Sheng, 1999). The combination of multiple CAx for the design and manufacturing planning of physical goods is possible thanks to information generated by CAD software and stored within 3D CAD models, hereafter CAD models. CAD models are virtual geometric representations of goods and are stored in two types of CAD generated files (Ostad-Ahmad-Ghorabi et al., 2009):

- ***Assemblies:*** which consist of parts and subordinate assemblies (Leibrecht, 2005);

- ***Parts:*** which are made of one material and have any number of features (ibid).

Features (i.e. Feature Technology, FT) are diverse sets of information concerning for example shape, tolerances and materials (Case & Gao, 1993; Shah & Rogers, 1988). They are used to connect CAD to downstream manufacturing as they provide detailed information useful for manufacturing parts (Tao et al., 2017). The use of FT allows to automate recognition of plausible manufacturing processes and tooling and has enabled extensive investigation of the integration of CAD and other CAx such as CAE, CAM and CAPP (ibid). The reviewed studies showed that there is a long standing interest in using FT to support LCI estimation (Abad Kelly et al., 2008; Friedrich & Krasowski, 1998; Leibrecht, 2005; Otto et al., 2002). However, due to the different data structure of LCI and CAD, data transfer (i.e. interoperability) is not straightforward and prone to errors and incompleteness (Chiu & Chu, 2012; Hernandez Dalmau, 2015; Morbidoni et al., 2011). This is because LCIs focus on processes and their links to flows, while CAD models focus on the 3D representation of goods (H. Zhang et al., 2015).

This difference in ontologies across disciplines demands for common information models to allow effective transfer of data (Abad Kelly et al., 2008; Chiu & Chu, 2012; P. Yung & Wang, 2014). For this reason, Tao et al. (2017) divided FT in two main classes *Product Features* and *Operation Features*. Product features refer to the following information obtainable from CAD:

- form (e.g., name, dimensions and surface quality).
- materials[3] (e.g., name, properties, mass).
- functionality[3.]
- connectivity (e.g., connected parts, type of connection and mating relationships).

[3] n.b. not necessarily specified in CAD files

Operation features provide information through CAM and CAPP on process types, their parameters, machine and tooling specifications (e.g. resource use) and sequencing (Tao et al., 2017).

In addition to the aforementioned methods, elementary flows through unit processes can also be inventoried from CAx generated bill-of-materials (BOMs) or Building Information Models (BIM). BOMs are list of all required materials, parts and components needed to manufacture a given part or product (Cinelli et al., 2020). Building Information Modelling (BIM) offers possibilities of storing and transferring data for LCI allowing for the retrieval of buildings' parts, materials and energy performance (Mahdavi & Ries, 1998; Seo et al., 2007; P. Yung & Wang, 2014). Of particular interest, is the ability to use BIM in combination with CAD to easily generate economic inputs and outputs in construction (Seo, Tucker and Newton, 2007). However, the retrievable data from BOMs and BIMs to be used in LCI is limited (W. K. C. Yung et al., 2012). For example, while energy and auxiliary materials used in production processes may be obtained, they miss logistic information for the modelling of transportation, and in the case of BIM information on construction machineries and equipment.

Use, Reuse & Maintenance

We found no literature concerning the use of CAPE in this life cycle stage due to the fact that this lifecycle stage is typically not applicable to chemical products and substances beyond use. However, the literature showed ample opportunities to collect LCI data for physical goods and construction sectors using CAD and CAE (Chan et al., 2010; Gaha et al., 2018; Jianjun et al., 2008; Komoto & Tomiyama, 2008; Mahdavi & Ries, 1998; Umeda et al., 2012). These approaches typically involved Design-for-X (D4x) practices - where X refers to any application – and software. However, D4x applications are not common as they are typically not provided in CAx tools by default (Sy & Mascle, 2011) and often require a high level of expert knowledge to be carried out.

Some of these practices are design for disassembly, design for maintenance and design for recyclability. Maintainability and reusability (among others) can be considered life cycle features which, in addition to the product and operation features we described in the previous section, can provide information useful to compile the use, reuse and maintenance life cycle stage (Sy & Mascle, 2011). For example, knowledge on the assembly can provide information on reusability and maintenance (Rosen et al., 1996). The lifespan and score of maintainability and reuse of parts (i.e. refurbishment) can be assessed (Jianjun et al., 2008) and information on maintenance operations could be obtained through maintenance schemes generated by combining parts performance analysis in CAE. The use of CAE to assess the performance of goods though Finite Element Analysis in the use phase can provide information on the use and lifespan of a given product (Russo & Rizzi, 2014). This means that it is possible to assess uncertainty in the use stage but also in the selection of materials and processes in the manufacturing stage depending on the goods performances.

Additionally, thanks to the ability to assess performances, CAE can be of support in the identification of services related to maintenance through the generation of services oriented BOMs (Zhou et al., 2018). Service-oriented BOMs are extensive BOMs that not only contain the physical items and quantities needed to manufacture a product, but they also store service relevant information needed for maintenance, repair and overhaul throughout the product lifecycle (Zhou et al., 2018). Data concerning services can be calculated by combining users' and business/service requirement information using a Boolean approach (Xing et al., 2013). Based on these parameters, it is then possible to estimate functional, physical and economic fitness of the product (ibid). This service engineering methodologies can be replicated into CAx systems oriented toward services (i.e. Service-CAD) (Komoto & Tomiyama, 2008). Service oriented CAD tools could provide information about existing potential services that could be used for a given product (Shimomura et al., 2007) and open possibilities of Life cycle simulation approaches (Garetti et al., 2012) which could generate multiple potential alternatives. These tools could be beneficial in LCI creation and they have been shown to support Lifecycle Costing analysis (Komoto & Tomiyama, 2008; Shimomura et al., 2007). All these developments could support the creation of multiple scenarios and aiding the selection of the best alternatives using, for example, Multi-criteria Decision Support Methods (MCDSMs) in combination with CAD (Ben Slama et al., 2020).

Recycling & waste management
In section 4.2.2, we indicated that CAPE can be used to plan manufacturing activities. However, if recycling and waste management practices concern chemical processes such as in the case of processing biomass from waste sources (Romdhana et al., 2016) and reuse or conversion of CO_2 emissions (Roh et al., 2016), CAPE could be used to simulate those processes and potential alternatives. For example, various approaches such as multi-criteria decision analysis, network and graph theory and stochastic process techniques can be used to identify suitable waste and recycling treatments starting from information from the manufacturing and use stage (Fan et al., 2020).

In the life cycle of physical goods, thanks to the information on relationship among parts that is provided by assemblies and FT, it is possible to identify how a product is assembled and disassembled. Knowing this information, can be useful in understanding products' end of life and provide uncertainty values for plausible end of life treatments (Sy & Mascle, 2011). For instance, by drawing the sequence of disassembly (i.e., disassembly logic network) it is possible to map input and output flow of parts to different unit processes concerning life cycle stages after use (Jianjun et al., 2008). Graph theory in combination with CAD can also be employed to create a lifecycle model of a product in which the structure indicates connectivity and hierarchy of parts (Umeda et al., 2012). The connectivity shows relationships among parts such as how they are fixated, their signal or power transmission and motion constraints which, with the use of CAE, can support the identification of a product's fate based on its design (ibid). Once the plausible fates of a specific part or product are known, information on waste management service suppliers in a given region could be used to identify the most likely end of life treatment (Irie & Yamada, 2020). CAx could then be employed to simulate the end-of-life processes in this stage, thereby obtaining economic and environmental flows (Sy & Mascle, 2011). For example, previously developed CAx for products as complex as electronics have also helped in identify the best WEEE de-manufacturing processes according to eco-toxicity and GHG emissions levels (Chang & Lu, 2014).

At last, through the use of CAD software in construction application, BIMs and methods of construction and demolition waste assessment it is possible to identify flows concerning end of life of constructions (Mercader Moyano et al., 2019). However, this approach requires information on time of material release from construction, which is typically not readily available. However, as we have seen in previous sections, CAE could also be used to estimate the lifespan of components according to their physical performances.

5.4.3 How AI methods can be used to estimate data for LCIs

Here we describe how AI methods can be used to estimate data for LCI. The collected literature, however, revealed no AI methods used for the estimation of LCI information for the distribution stage. Therefore, distribution is presented in the discussion section instead, together with possible ways to overcome this barrier. Additionally, in this section we present only applications that did not require the combination of AI with CAx. The studies we found that describe a combination of AI methods and CAx are discussed in section 4.4 concerning the integration of AI and CAx for LCI data.

Resource extraction

The literature showed only a use of AI methods to generate LCIs for the agricultural sector. For example, in order to identify the adequate deposition of soil nutrients and other treatments in agriculture, information on specific management and operations is necessary (Renaud-Gentié et al., 2014). Additionally, farmers make choices based on a variety of factors from soil conditions to business economics, practice preferences (e.g., organic agriculture), or operations constraints that may go beyond technical aspects. This information needs to be collected from experts, literature and farming surveys and grouped according to sets of different parameters and values. Collecting and organizing this information is of course time consuming, however, if the information is already embedded within reports or scientific articles, it could be first extracted by means of text mining (e.g, Diaz-Elsayed and Zhang 2020) and organized in sets of parameters and values. These sets may be created by means of clustering techniques from data mining (e.g., K-mean clustering) to identify how frequently different choices and parameters are used in combination (Renaud-Gentié et al., 2014). This system may then also be combined with soil models and nutrients models to estimate inputs and outputs of unit processes of cropping operations

(Meza-Palacios et al., 2020). Regional data and survey (e.g., EPIC model (USDA, 2017)) can then be used to obtain regional variation of inputs and outputs (Kaab et al., 2019; Lee et al., 2020; Romeiko et al., 2020). Such applications of expert systems and data mining could present learning capabilities or be used to train an Artificial Neural Network or, in the case of fuzzy logic, to train an Adaptive Fussy Interference System (Nabavi-Pelesaraei et al., 2018). In such a case, a system would be categorized under a machine learning application. The literature has shown that such systems could be used effectively in estimating a variety of LCI data concerning future scenarios (Kaab et al., 2019; Khanali et al., 2017; Khoshnevisan et al., 2014; Khoshnevisan, Rafiee, & Mousazadeh, 2013; Khoshnevisan, Rafiee, Omid, et al., 2013; Nabavi-Pelesaraei et al., 2018). Specifically, regional climate conditions, access to water and labor may greatly influence the output of farming activities. By using these additional parameters, pre-existing LCI data and regional farming surveys (Nabavi-Pelesaraei et al., 2018), it is possible to estimate data relevant for LCIs such as energy output of biomass destined for energy generation (Kaab et al., 2019; Nabavi-Pelesaraei et al., 2018), crop yield (Khanali et al., 2017), and variety of inputs and outputs of agricultural activities (e.g., animal husbandry operations in a given region).

Manufacturing

In the context of the manufacturing stage, expert systems may be employed to transfer knowledge from one domain to the other and to identify data conversion rules (e.g., conversion of large chemical process databases to LCI data) (Meyer et al., 2021; Mittal et al., 2018a; Muñoz et al., 2018). Specifically, data that could be shared across disciplines may be labeled and organized in a different fashion than how it may be needed for the purpose of LCI modelling. In this case, the use of lineage and product ontologies have been proposed to obtain LCI data (Mittal et al., 2018a). A lineage ontology uses a family tree analogy to reconstruct all synthesis steps necessary for the production of chemicals from resource extraction to manufacturing (i.e., cradle to gate). In other words, a chemical product has own properties (e.g., the role that it plays in processes), it may be a child (i.e., the output of a reaction) and it has parent chemicals (i.e., the inputs to the reaction) defined by the reaction in which they may be involved. A process ontology is then employed to bridge this information toward LCIs to obtain elementary flows in and out of unit processes. These ontologies can help to predict products of a reaction provided that they are present in the chemical database of reference in the form of rules or algorithms (ibid). Another way to convert domain specific knowledge to LCI is through the use of machine learning applications in the field of natural language processing (Muñoz et al., 2018). Natural language processing is the field of AI that concerns the creation of systems to understand and act on text and speech in a similar way humans do. Specifically, this approach may help in the conversion of the heterogenous data that may be present in databases used by engineers and manufacturers such as facility data that may be shared with US Environmental Protection Agency through the Facility Registry Service (as shown in Mittal et al. 2018), or process recipe databases available within an enterprise (as shown in Muñoz, Capón-Garcia, and Puigjaner 2018). These databases may contain information on processes, production, materials and components and much more information that may be relevant for modelling LCIs. However, because of the diversity and large size of these databases, it is not practical to manually convert this information into LCIs. Natural language processing could be of support in this task by processing large volumes of this data, converting labels and data structures to be compatible with LCI databases (Muñoz et al., 2018).

Use, Reuse & Maintenance

The literature on this stage and the use of AI presented a vast majority of studies that focused on the combination of CAx and AI. We leave these studies for the following section concerning the integration of AI and CAx for LCI data modelling, and here we discuss the studies that did not rely on CAx software or data. The use of data mining techniques applied to regional household surveys could provide information on different regional household preferences and behaviours by creating regional household's behavioural archetypes (Froemelt et al., 2018, 2020a). While this information cannot be used directly in the compilation of LCIs, it may be useful to estimate household habits and potential variations of product's lifespan, reuse or maintenance. For instance, in studies outside of the scope of this research, households' type, composition and lifestyle have shown to have an influential factor on the tendency of adopting circular economy practices (e.g., Ottelin, Cetinay, and Behrens 2020).

Recycling and Waste management

Data mining techniques could be employed to estimate regional waste types in a given sector (e.g., food packaging) provided that access to detail data on regional consumption is available. For example, if micro data from food delivery web based services is available, likely packaging types may be associated to restaurant typologies, and by following the delivery, waste accumulation may be derived (Liu et al., 2020). If data is available on regional waste collection and treatment options, it is then possible to identify the most likely end-of-life concerning a given product system, and related energy flows. In fact, once the waste flows are known, Artificial Neural Networks could be used to estimate energy consumption due to waste transport and treatment of municipal waste management alternatives in several regions, and potential energy recovery from waste (Nabavi-Pelesaraei et al., 2017). This approach could be useful when trying to quickly estimate the data concerning the end-of-life (e.g., output flows or impacts) for one or more products in different regions. These are practices that can already be performed in current LCI modelling practices, however, the employment of machine learning methods can allow for estimating these values for a large variety of regions provided..

LCI data may also be estimated starting from laboratory data. For instance, in the case of novel waste technologies for resource recovery, it may be important to estimate potential future yield. Machine learning algorithms could then be applied to laboratory data from pyrolysis where feedstock (i.e. waste flows) can be very diverse and then estimate process outputs (Cheng, Luo, et al., 2020). Specifically, by applying the Random Forest algorithm to data collected from laboratory tests, in combination with feedstock properties (e.g., content of carbon, hydrogen, nitrogen, oxygen, and ash) and processing conditions (e.g., reaction temperature and heating rate) it is possible to estimate yields and characteristics of biochar.

At last, LCI data that may have not been added to LCI database may be concealed within the written text of previous LCA scientific publications and reports. In this case, natural language processing techniques such as text mining[4] can help in the extraction of LCI data from previous publications concerning wastewater-based resource recovery systems (e.g., functional unit, water, energy and nutrient flows) (Diaz-Elsayed & Zhang, 2020). While this technique is now being discussed within the recycling and waste management stage, it could also be employed for other life cycle stages.

5.4.4 Integration: how the combination of CAx and AI methods can be used to obtain data for LCIs

The literature presented various examples that addressed the integration of CAx and AI for the purpose of obtaining data for LCIs in the following life cycle stages: 1) manufacturing, 2) use, reuse and maintenance, and 3) Recycling and waste management. In this section we do not discuss the stages individually but we rather describe how CAx and AI can be used in combination. Specifically, we saw that the integration is typically employed for the following purposes:

- Optimization of a simulated product system from which LCI data can be obtained
- Generating a vast range of alternatives (which may or may not be optimal) from which LCI can be obtained
- Estimating values concerning component's performance over their use

System optimization concerns finding the optimal parameters or organization of processes according to one or more objectives. From an LCI perspective, it concerns the identification of the optimal alternative. For example, once livestock is raised for meat products, it is lead to slaughterhouses where the animal is killed and its meat processed. CAx simulating meat process plants (e.g., Poultry Process Plants) can be used to obtain LCI data (López-Andrés et al., 2018). A Genetic Algorithm can then be employed to select optimal process parameters according to multiple

[4] To not be confused with data mining. Text mining concerns finding and extracting data from text, data mining concerns finding patterns and relationships in datasets.

objectives. Genetic Algorithms concern metaheuristic procedures from the field of evolutionary algorithms, which are inspired by the process of natural selection and they are often used to solve optimization problems. Once optimal parameters are selected, they can be used within process simulation software, thereby generating the optimal product system alternative which can then be converted into a LCI. Similar approaches have also been used to estimate optimal solar district heating installations for urban size communities (Abokersh et al., 2020).

Besides system optimization, AI and CAx can be employed together to evaluate a vast range of design options. For example, renovation and use alternatives of buildings can be identified together with their embodied and operational energy by combining the use of Artificial Neural Networks using data from CAD models and data on properties related to building components (e.g. Roof, windows, HVAC system, location etc.) (Sharif & Hammad, 2019). Regenerative design approaches (i.e., the use of AI to generate designs) could also be employed to advance the exploration of potential design options and generate LCIs. In one study (Płoszaj-Mazurek et al., 2020), this approach was to generate 300 thousand possible building design configurations according to a multitude of parameters (e.g., type of windows, façade, height, etc.). 1500 of those configurations were then randomly selected and simulated in CAD together with their energy model to estimate embodied and operational energy. This was used as the training data for a machine learning algorithm (i.e., Gradient Boosting Regressor). The trained machine learning model was then used to estimate the carbon footprint for 100 thousand of randomly generated building designs. A similar approach is not only applicable to architectural design but also to product design and process design. Additionally, it could be employed in the estimation of flows in different stages not only for footprint analysis but also in chemical process applications, i.e., CAPE (Cheng, Porter, et al., 2020; Liao et al., 2020).

At last, the combination of AI methods with CAE for the simulation of components performance can prove useful for the estimation of flows in and out of the use, reuse and maintenance stage as well as identifying when a given product or component will reach the end of life. Specifically, in order to understand the plausible failure points (e.g., abrasion of moving parts) and maintenance requirements (e.g., when lubrification may be needed) of components and goods, engineers would typically carry out laboratory tests or perform simulations such as finite element analysis or boundary element analysis, through CAE software (Kurdi et al., 2020). In other words, CAE can therefore be used to estimate wear and tear of parts and products. However, it may be challenging to integrate within CAE the knowledge obtained during experimental data from the laboratory (e.g., physically measured failure points) and to apply large volumes of variations of system parameters. In this case, machine learning methods can be used as surrogate simulation models that take into consideration simulated and empirical data over large set of possible system properties and objectives (Ibid). This information can then be used for estimation of LCI data in the use, reuse and maintenance stage of product.

5.5 Discussions and conclusions

Our study revolved around the question of how CAx and AI techniques can be used to generate, estimate and extract data for LCIs. We reviewed 131 studies on the use of CAx (84) and AI (47) in the context of their potential to provide LCI data. The intent was to understand current developments of these applications and gain knowledge on how to improve data collection for the LCI modelling phase of LCA. We have found that there are many opportunities to obtain data through these approaches, however, there are also limitations that need to be addressed.

CAx provide most of their benefits in the generation of data for life cycle stages that require industrial processing of some kind, and in the sectors concerning physical goods, chemical products, construction, and energy. This is a logical result as CAx software and methods are developed specifically for the purpose of managing design and manufacturing activities. Therefore, CAx can offer relatively easy access to LCI data in the manufacturing stage, with some applications in estimating potential recycling and maintenance activities. In order to estimate data on use, reuse and other aspects of the product system that cannot be assessed easily through simulations (e.g., use, maintenance, reuse, etc.), the literature has shown various methods that rely on expert knowledge. Such expert knowledge, however, needs to be collected and encoded in expert systems which can then be used to estimate unit process data that does not concern industrial processes (e.g., use, reuse and maintenance, or the likelihood of a given part or product to undergo a given waste treatment option).

CAx applications in the resource extraction phase appeared to be scarce. AI methods have been shown of use in this stage, for the agricultural sector. However, the collected literature on CAx and AI did not show studies concerning the resource extraction for abiotic materials (e.g., metals and minerals). Also, the literature did not present any studies for the distribution stage. However, methods and software to simulate aspects of these stages exist, for instance planning software for logistics may be used to obtain data on warehouses and transport (e.g., ODL studio, openMAINT), and the field of operation research offers potential opportunities to employ AI methods and optimization methods to simulate aspects of distribution from which LCI data may be obtained. These represent important research gaps that should be further investigated.

We also showed that there are opportunities to extract data from previous studies and through the reuse of heterogenous data from different domains. The combination of expert systems, ontologies and natural language processing techniques such as text mining appear to be promising applications. However, more should be done to push the boundaries of their applications by performing a thorough search of all possible LCA publications beyond single sector studies, and in the combination of heterogeneous data from different domains not just in the chemical sector but also in agriculture and the estimation of LCIs for physical goods.

As previously stated, a great limitation of CAx in data generation and estimation for LCIs is the fundamental need for some level of expert knowledge input. While LCI data may be obtained through CAx software APIs, CAx always needs human intervention to at least create the first representation of the product (i.e., CAD model or CAPE flowsheets). Generative design approaches and computer vision methods (e.g., visual recognition and 3D reconstruction) may provide additional opportunities for LCI data and should be further investigated. Additionally, a broader investigation into the field of intelligent process engineering and process systems engineering could deliver additional insights into filling data gaps in LCIs.

At last, while CAx and AI methods separately and in combination show potential to facilitate the LCI modelling phase, the main work that lays ahead is in formalizing the integration of tools and methods from both disciplines, and in the search, development and curation of databases that can provide a solid base of data for these methods to fulfil their potential. In fact, we came across many studies in which very diverse data sources other than LCIs, had already been collected in other domains and curated or encoded in some fashion. While these methods show great promise, we cannot avoid that data collection and curation will still be needed. In other words, it is key that scientists working on LCI modelling shift their focus from current data collection and curation practices, to new ones such as investigation of heterogenous and unfamiliar sources, their combination and how to do more with them through the methods described in this study.

SUPPLEMENTARY INFORMATION

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ABBREVIATIONS

AI = Artificial Intelligence,
CAD = Computer-Aided Design
CAE = Computer-Aided Engineering
CAM = Computer-Aided Machining or Manufacturing
CAPE = Computer-Aided Process Engineering
CAPP = Computer-Aided Process Planning
CAx = Computer-Aided for x, where x stands for all possible applications
D4x = Design for x, where x stands for all possible applications
DM = Data Mining
ES = Expert System
FT = Feature Technology
ML = Machine Learning
LCA = Life Cycle Assessment
LCI = Life Cycle Inventory

REFERENCES

Abokersh, Mohamed Hany, Manel Vallès, Luisa F. Cabeza, and Dieter Boer. 2020. "A Framework for the Optimal Integration of Solar Assisted District Heating in Different Urban Sized Communities: A Robust Machine Learning Approach Incorporating Global Sensitivity Analysis." *Applied Energy.* https://doi.org/10.1016/j.apenergy.2020.114903.

Agachi, Paul Serban. 2005. *"COMPUTER AIDED PROCESS ENGINEERING.".*

Andriankaja, Hery, Julien Le Duigou, Christophe Danjou, and Benoît Eynard. 2017. "Sustainable Machining Approach for CAD/CAM/CNC Systems Based on a Dynamic Environmental Assessment." Proceedings of the Institution of Mechanical Engineers, Part B: *Journal of Engineering Manufacture*. https://doi.org/10.1177/0954405416629104.

Carlson, Raul, Anne Marie Tillman, Bengt Steen, and Göran Löfgren. 1998. "LCI Data Modelling and a Database Design." *International Journal of Life Cycle Assessment*. https://doi.org/10.1007/BF02978500.

Carvalho, Ana, Henrique A. Matos, and Rafiqul Gani. 2013. "SustainPro-A Tool for Systematic Process Analysis, Generation and Evaluation of Sustainable Design Alternatives." *Computers and Chemical Engineering*. https://doi.org/10.1016/j.compchemeng.2012.11.007.

Case, K., and J. Gao. 1993. "Feature Technology: An Overview." *International Journal of Computer Integrated Manufacturing,* *6*(1–2): 2–12. https://doi.org/10.1080/09511929308944549.

Chan, Clifford Chi Shing, Kai Ming Yu, and Kai Leung Yung. 2010. "Green Product Development by Using Life Cycle Assessment (LCA), Theory of Inventive of Problems Solving (TRIZ)." In Proceedings - *2010 International Conference on Manufacturing Automation*, ICMA 2010. https://doi.org/10.1109/ICMA.2010.3.

Chang, Hsiang-Tang, and Chien-Han Lu. 2014. "Simultaneous Evaluations of Material Toxicity and Ease of Disassembly during Electronics Design." *Journal of Industrial Ecology.* https://doi.org/10.1111/jiec.12052.

Chen, Hui, and David R. Shonnard. 2004. "Systematic Framework for Environmentally Conscious Chemical Process Design: Early and Detailed Design Stages." *Industrial and Engineering Chemistry Research.* https://doi.org/10.1021/ie0304356.

Cheng, Fangwei, Hongxi Luo, and Lisa M. Colosi. 2020. "Slow Pyrolysis as a Platform for Negative Emissions Technology: An Integration of Machine Learning Models, Life Cycle Assessment, and Economic Analysis." *Energy Conversion and Management.* https://doi.org/10.1016/j.enconman.2020.113258.

Cheng, Fangwei, Michael D. Porter, and Lisa M. Colosi. 2020. "Is Hydrothermal Treatment Coupled with Carbon Capture and Storage an Energy-Producing Negative Emissions Technology?" *Energy Conversion and Management*. https://doi.org/10.1016/j.enconman.2019.112252.

Chiu, Ming Chuan, and Chih Hsing Chu. 2012. "Review of Sustainable Product Design from Life Cycle Perspectives." *International Journal of Precision Engineering and Manufacturing*. https://doi.org/10.1007/s12541-012-0169-1.

Chryssolouris, G., D. Mavrikios, N. Papakostas, D. Mourtzis, G. Michalos, and K. Georgoulias. 2009. "Digital Manufacturing: History, Perspectives, and Outlook." In Proceedings of the Institution of Mechanical Engineers, Part B: *Journal of Engineering Manufacture*. https://doi.org/10.1243/09544054JEM1241.

Cinelli, Matteo, Giovanna Ferraro, Antonio Iovanella, Giulia Lucci, and Massimiliano M. Schiraldi. 2020. "A Network Perspective for the Analysis of Bill of Material." Procedia CIRP, *13th CIRP Conference on Intelligent Computation in Manufacturing Engineering,* 17-19 July 2019, Gulf of Naples, Italy, 88 (January): 19–24. https://doi.org/10.1016/j.procir.2020.05.004.

Dankwort, C. Werner, Roland Weidlich, Birgit Guenther, and Joerg E. Blaurock. 2004. "Engineers' CAx Education - It's Not Only CAD." *CAD Computer Aided Design.* https://doi.org/10.1016/j.cad.2004.02.011.

Diaz-Elsayed, Nancy, and Qiong Zhang. 2020. "Extracting the Characteristics of Life Cycle Assessments via Data Mining." *MethodsX*. https://doi.org/10.1016/j.mex.2020.101004.

Elanchezhian, C., T. Selwyn Sunder, and G. Shanmuga Sundar. 2008. *Computer-Aided Manufacturing.* Second. New Delhi: LAXMI PUBLICATIONS (P) LTD.

ElMaraghy, Hoda A. 1993. "Evolution and Future Perspectives of CAPP." CIRP Annals - *Manufacturing Technology*. https://doi.org/10.1016/S0007-8506(07)62537-2.

EPA. 1993. *"United State Environmental Protection Agency. Office of Research and Development, Life Cycle Assessment: Inventory Guidelines and Principles. EPA/600/R-92/245, US."*

Fan, Yee Van, Hon Huin Chin, Jiří Jaromír Klemeš, Petar Sabev Varbanov, and Xia Liu. 2020. "Optimisation and Process Design Tools for Cleaner Production." *Journal of Cleaner Production*. https://doi.org/10.1016/j.jclepro.2019.119181.

Fayyad, Usama, Gregory Piatetsky-Shapiro, and Padhraic Smyth. 1996. *"From Data Mining to Knowledge Discovery in Databases."* AI Magazine.

Friedrich, Jürgen, and Horst Krasowski. 1998. "Ecology-Based Product Data Model." In *SAE Technical Papers*. https://doi.org/10.4271/982227.

Froemelt, Andreas, René Buffat, and Stefanie Hellweg. 2020. “Machine Learning Based Modeling of Households: A Regionalized Bottom-up Approach to Investigate Consumption-Induced Environmental Impacts.” *Journal of Industrial Ecology*. https://doi.org/10.1111/jiec.12969.

Froemelt, Andreas, David J. Dürrenmatt, and Stefanie Hellweg. 2018. “Using Data Mining to Assess Environmental Impacts of Household Consumption Behaviors.” *Environmental Science and Technology*. https://doi.org/10.1021/acs.est.8b01452.

Gaha, Raoudha, Abdelmajid Benamara, and Bernard Yannou. 2018. “Proposition of Eco-Feature: A New CAD/PLM Data Model for an LCA Tool.” *Lecture Notes in Mechanical Engineering*, no. 207169: 763–70. https://doi.org/10.1007/978-3-319-66697-6_74.

Garetti, Marco, Paolo Rosa, and Sergio Terzi. 2012. “Life Cycle Simulation for the Design of Product-Service Systems.” *Computers in Industry.* https://doi.org/10.1016/j.compind.2012.02.007.

Goldstein, Benjamin, and Joshua P. Newell. 2019. “Why Academics Should Study the Supply Chains of Individual Corporations.” *Journal of Industrial Ecology.* https://doi.org/10.1111/jiec.12932.

Göttl, Quirin, Dominik G. Grimm, and Jakob Burger. 2021. “Automated Synthesis of Steady-State Continuous Processes Using Reinforcement Learning.” *Frontiers of Chemical Science and Engineering.* https://doi.org/10.1007/s11705-021-2055-9.

Grudziński, Jerzy Ryszard, Monika Krzywicka, and Łukasz Bolibok. 2016. “COMPUTER-AIDED ENVIRONMENTAL RISK ASSESSMENT OF POTATO CULTIVATION TECHNOLOGY USING OPENLCA SOFTWARE.” *Journal of Ecological Engineering, 17*(5): 198–202. https://doi.org/10.12911/22998993/65091.

Guinée, J. 2001. “Handbook on Life Cycle Assessment - Operational Guide to the ISO Standards.” *International Journal of Life Cycle Assessment.* https://doi.org/10.1007/BF02978784.

Han, Jiawei, Micheline Kamber, and Jian Pei. 2012. *Data Mining: Concepts and Techniques. 3rd edition*, Elsevier https://doi.org/10.1016/C2009-0-61819-5.

Hernandez Dalmau, Maria Isabel. 2015. “Eco-Design Integration into New Product Development Processes: Comparison between LCA Software and CAD-Integrated Tools.” ProQuest Dissertations and Theses, 100.

Huang, He, and Gaurav Ameta. 2014a. “A Novel Pattern for Energy Estimation Framework and Tools to Compute Energy Consumption in Product Life Cycle.” *Journal of Computing and Information Science in Engineering.* https://doi.org/10.1115/1.4025718.

———. 2014b. "Computational Energy Estimation Tools for Machining Operations during Preliminary Design." *International Journal of Sustainable Engineering.* https://doi.org/10.1080/19397038.2013.862580.

Irie, Hayate, and Tetsuo Yamada. 2020. "Decision Support Model for Economical Material Carbon Recovery and Reduction by Connecting Supplier and Disassembly Part Selections." *Journal of Advanced Mechanical Design, Systems and Manufacturing.* https://doi.org/10.1299/jamdsm.2020jamdsm0024.

ISO. 2006. "14040: Environmental Management–Life Cycle Assessment—Principles and Framework." *International Organization for Standardization.*

Jianjun, Yi, Ji Baiyang, Guan Yifeng, Dong Jinxiang, and Li Chenggang. 2008. "Research on Evaluation Methodologies of Product Life Cycle Engineering Design (LCED) and Development of Its Tools." *International Journal of Computer Integrated Manufacturing.* https://doi.org/10.1080/09511920801932486.

Kaab, Ali, Mohammad Sharifi, Hossein Mobli, Ashkan Nabavi-Pelesaraei, and Kwok wing Chau. 2019. "Combined Life Cycle Assessment and Artificial Intelligence for Prediction of Output Energy and Environmental Impacts of Sugarcane Production." *Science of the Total Environment.* https://doi.org/10.1016/j.scitotenv.2019.02.004.

Kabolizade, Mostafa, Hamid Ebadi, and Ali Mohammadzadeh. 2012. "Design and Implementation of an Algorithm for Automatic 3D Reconstruction of Building Models Using Genetic Algorithm." *International Journal of Applied Earth Observation and Geoinformation, 19*(October): 104–14. https://doi.org/10.1016/j.jag.2012.05.006.

Kalakul, Sawitree, Pomthong Malakul, Kitipat Siemanond, and Rafiqul Gani. 2014. "Integration of Life Cycle Assessment Software with Tools for Economic and Sustainability Analyses and Process Simulation for Sustainable Process Design." In *Journal of Cleaner Production.* https://doi.org/10.1016/j.jclepro.2014.01.022.

Kaplan, Andreas, and Michael Haenlein. 2019. "Siri, Siri, in My Hand: Who's the Fairest in the Land? On the Interpretations, Illustrations, and Implications of Artificial Intelligence." *Business Horizons*. Elsevier Ltd. https://doi.org/10.1016/j.bushor.2018.08.004.

Khanali, Majid, Hossein Mobli, and Homa Hosseinzadeh-Bandbafha. 2017. "Modeling of Yield and Environmental Impact Categories in Tea Processing Units Based on Artificial Neural Networks." *Environmental Science and Pollution Research.* https://doi.org/10.1007/s11356-017-0234-5.

Khoshnevisan, Benyamin, Shahin Rafiee, and Hossein Mousazadeh. 2013. "Environmental Impact Assessment of Open Field and Greenhouse Strawberry Production." *European Journal of Agronomy.* https://doi.org/10.1016/j.eja.2013.05.003.

Khoshnevisan, Benyamin, Shahin Rafiee, Mahmoud Omid, Hossein Mousazadeh, and Sean Clark. 2014. “Environmental Impact Assessment of Tomato and Cucumber Cultivation in Greenhouses Using Life Cycle Assessment and Adaptive Neuro-Fuzzy Inference System.” *Journal of Cleaner Production.* https://doi.org/10.1016/j.jclepro.2013.09.057.

Khoshnevisan, Benyamin, Shahin Rafiee, Mahmoud Omid, Hossein Mousazadeh, and Paria Sefeedpari. 2013. “Prognostication of Environmental Indices in Potato Production Using Artificial Neural Networks.” *Journal of Cleaner Production.* https://doi.org/10.1016/j.jclepro.2013.03.028.

Komoto, H., and T. Tomiyama. 2008. “Integration of a Service CAD and a Life Cycle Simulator.” CIRP Annals - *Manufacturing Technology*. https://doi.org/10.1016/j.cirp.2008.03.001.

Kreith, Frank, and D. Yogi Goswami. 2004. *The CRC Handbook of Mechanical Engineering*: Second Edition.

Kurdi, Abdulaziz, Nahla Alhazmi, Hatem Alhazmi, and Thamer Tabbakh. 2020. “Practice of Simulation and Life Cycle Assessment in Tribology-A Review.” *Materials.* https://doi.org/10.3390/MA13163489.

Lee, Eun Kyung, Wang Jian Zhang, Xuesong Zhang, Paul R. Adler, Shao Lin, Beth J. Feingold, Haider A. Khwaja, and Xiaobo X. Romeiko. 2020. “Projecting Life-Cycle Environmental Impacts of Corn Production in the U.S. Midwest under Future Climate Scenarios Using a Machine Learning Approach.” *Science of the Total Environment.* https://doi.org/10.1016/j.scitotenv.2020.136697.

Leibrecht, Sebastian. 2005. “Fundamental Principles for CAD-Based Ecological Assessments.” *International Journal of Life Cycle Assessment.* https://doi.org/10.1065/lca2005.08.217.

Leo Kumar, S. P. 2017. “State of The Art-Intense Review on Artificial Intelligence Systems Application in Process Planning and Manufacturing.” Engineering *Applications of Artificial Intelligence.* https://doi.org/10.1016/j.engappai.2017.08.005.

Liao, Mochen, Stephen Kelley, and Yuan Yao. 2020. “Generating Energy and Greenhouse Gas Inventory Data of Activated Carbon Production Using Machine Learning and Kinetic Based Process Simulation.” *ACS Sustainable Chemistry and Engineering.* https://doi.org/10.1021/acssuschemeng.9b06522.

Liu, Gengyuan, Feni Agostinho, Huabo Duan, Guanghan Song, Xueqi Wang, Biagio F. Giannetti, Remo Santagata, Marco Casazza, and Massimiliano Lega. 2020. “Environmental Impacts Characterization of Packaging Waste Generated by Urban Food Delivery Services. A Big-Data Analysis in Jing-Jin-Ji Region (China).” *Waste Management.* https://doi.org/10.1016/j.wasman.2020.07.028.

López-Andrés, Jhony Josué, Alberto Alfonso Aguilar-Lasserre, Luis Fernando Morales-Mendoza, Catherine Azzaro-Pantel, Jorge Raúl Pérez-Gallardo, and José Octavio Rico-Contreras. 2018. "Environmental Impact Assessment of Chicken Meat Production via an Integrated Methodology Based on LCA, Simulation and Genetic Algorithms." *Journal of Cleaner Production.* https://doi.org/10.1016/j.jclepro.2017.10.307.

Mahdavi, A., and R. Ries. 1998. "Towards Computational Eco-Analysis of Building Designs." *Computers and Structures*. https://doi.org/10.1016/S0045-7949(97)00146-6.

Mercader Moyano, María del Pilar, Patricia Edith Camporeale, and Elías Cózar-Cózar. 2019. "Evaluación de Impacto Ambiental Mediante La Introducción de Indicadores a *Un Modelo BIM de Vivienda Social." Revista Hábitat Sustentable, 9*(2): 78–93. https://doi.org/10.22320/07190700.2019.09.02.07.

Meyer, David E., Sarah Cashman, and Anthony Gaglione. 2021. "Improving the Reliability of Chemical Manufacturing Life Cycle Inventory Constructed Using Secondary Data." *Journal of Industrial Ecology, 25*(1): 20–35. https://doi.org/10.1111/jiec.13044.

Meza-Palacios, Ramiro, Alberto A. Aguilar-Lasserre, Luis F. Morales-Mendoza, José O. Rico-Contreras, Luis H. Sánchez-Medel, and Gregorio Fernández-Lambert. 2020. "Decision Support System for NPK Fertilization: A Solution Method for Minimizing the Impact on Human Health, Climate Change, Ecosystem Quality and Resources." *Journal of Environmental Science and Health - Part A Toxic/Hazardous Substances and Environmental Engineering.* https://doi.org/10.1080/10934529.2020.1787012.

Mittal, Vinit K., Sidney C. Bailin, Michael A. Gonzalez, David E. Meyer, William M. Barrett, and Raymond L. Smith. 2018. "Toward Automated Inventory Modeling in Life Cycle Assessment: The Utility of Semantic Data Modeling to Predict Real-World Chemical Production." *ACS Sustainable Chemistry and Engineering.* https://doi.org/10.1021/acssuschemeng.7b03379.

Morales-Mendoza, Luis Fernando, Catherine Azzaro-Pantel, Jean Pierre Belaud, and Adama Ouattara. 2018. "Coupling Life Cycle Assessment with Process Simulation for Ecodesign of Chemical Processes." *Environmental Progress and Sustainable Energy.* https://doi.org/10.1002/ep.12723.

Morbidoni, Alessandro, Claudio Favi, and Michele Germani. 2011. "CAD-Integrated LCA Tool: Comparison with Dedicated LCA Software and Guidelines for the Improvement." In Glocalized Solutions for Sustainability in Manufacturing - Proceedings of the 18th *CIRP International Conference on Life Cycle Engineering.* https://doi.org/10.1007/978-3-642-19692-8-99.

Muñoz, Edrisi, Elisabet Capón-Garcia, and Luis Puigjaner. 2018. “Supervised Life-Cycle Assessment Using Automated Process Inventory Based on Process Recipes.” *ACS Sustainable Chemistry and Engineering*. https://doi.org/10.1021/acssuschemeng.7b04154.

Nabavi-Pelesaraei, Ashkan, Reza Bayat, Homa Hosseinzadeh-Bandbafha, Hadi Afrasyabi, and Kwok wing Chau. 2017. “Modeling of Energy Consumption and Environmental Life Cycle Assessment for Incineration and Landfill Systems of Municipal Solid Waste Management - A Case Study in Tehran Metropolis of Iran.” *Journal of Cleaner Production*. https://doi.org/10.1016/j.jclepro.2017.01.172.

Nabavi-Pelesaraei, Ashkan, Shahin Rafiee, Seyed Saeid Mohtasebi, Homa Hosseinzadeh-Bandbafha, and Kwok wing Chau. 2018. “Integration of Artificial Intelligence Methods and Life Cycle Assessment to Predict Energy Output and Environmental Impacts of Paddy Production.” *Science of the Total Environment.* https://doi.org/10.1016/j.scitotenv.2018.03.088.

Negnevitsky, Michael. 2011. Artificial Intelligence: A Guide to Intelligent Systems (3rd E-Book). Addison Wesley.

Ostad-Ahmad-Ghorabi, Hesamedin, Daniel Collado-Ruiz, and Wolfgang Wimmer. 2009. “Towards Integrating LCA into CAD.” In DS 58-7: Proceedings of ICED 09, *the 17th International Conference on Engineering Design*.

Ottelin, Juudit, Hale Cetinay, and Paul Behrens. 2020. “Rebound Effects May Jeopardize the Resource Savings of Circular Consumption: Evidence from Household Material Footprints.” *Environmental Research Letters, 15*(10): 104044. https://doi.org/10.1088/1748-9326/abaa78.

Otto, H.E. E., K.G. G. Mueller, and F. Kimura. 2002. “A Framework for Structured Data Retrieval in LCA Using Feature Technology.” Proceedings - *2nd International Symposium on Environmentally Conscious Design and Inverse Manufacturing*, 250–55. https://doi.org/10.1109/.2001.992358.

Page, Matthew J., Joanne E. McKenzie, Patrick M. Bossuyt, Isabelle Boutron, Tammy C. Hoffmann, Cynthia D. Mulrow, Larissa Shamseer, et al. 2021. “The PRISMA 2020 Statement: An Updated Guideline for Reporting Systematic Reviews.” *Systematic Reviews.* https://doi.org/10.1186/s13643-021-01626-4.

Parvatker, Abhijeet G., and Matthew J. Eckelman. 2019. “Comparative Evaluation of Chemical Life Cycle Inventory Generation Methods and Implications for Life Cycle Assessment Results.” *ACS Sustainable Chemistry and Engineering.* https://doi.org/10.1021/acssuschemeng.8b03656.

Picardo, Marta C., José Luiz De Medeiros, Juliana Garcia M. Monteiro, Ricardo Moreira Chaloub, Mario Giordano, and Ofélia De Queiroz Fernandes Araújo. 2013. “A Methodology for Screening of Microalgae as a Decision Making Tool for Energy and Green Chemical Process Applications." *Clean Technologies and Environmental Policy.* https://doi.org/10.1007/s10098-012-0508-z.

Płoszaj-Mazurek, Mateusz, Elżbieta Ryńska, and Magdalena Grochulska-Salak. 2020. "Methods to Optimize Carbon Footprint of Buildings in Regenerative Architectural Design with the Use of Machine Learning, Convolutional Neural Network, and Parametric Design." *Energies*. https://doi.org/10.3390/en13205289.

Renaud-Gentié, Christel, Stéphane Burgos, and Marc Benoît. 2014. "Choosing the Most Representative Technical Management Routes within Diverse Management Practices: Application to Vineyards in the Loire Valley for Environmental and Quality Assessment." *European Journal of Agronomy.* https://doi.org/10.1016/j.eja.2014.03.002.

Rödger, Jan-Markus, Niki Bey, Leo Alting, and Michael Z. Hauschild. 2018. "Life Cycle Targets Applied in Highly Automated Car Body Manufacturing – Method and Algorithm." *Journal of Cleaner Production, 194*(September): 786–99. https://doi.org/10.1016/j.jclepro.2018.04.148.

Roh, Kosan, Rebecca Frauzem, Rafiqul Gani, and Jay H. Lee. 2016. "Process Systems Engineering Issues and Applications towards Reducing Carbon Dioxide Emissions through Conversion Technologies." *Chemical Engineering Research and Design.* https://doi.org/10.1016/j.cherd.2016.10.007.

Romdhana, Hedi, Catherine Bonazzi, and Martine Esteban-Decloux. 2016. "Computer-Aided Process Engineering for Environmental Efficiency: Industrial Drying of Biomass." *Drying Technology*. https://doi.org/10.1080/07373937.2015.1104348.

Romeiko, Xiaobo Xue, Eun Kyung Lee, Yetunde Sorunmu, and Xuesong Zhang. 2020. "Spatially and Temporally Explicit Life Cycle Environmental Impacts of Soybean Production in the U.S. Midwest." *Environmental Science & Technology.* https://doi.org/10.1021/acs.est.9b06874.

Rosen, David W., Bert Bras, Steven L. Hassenzahl, Patrick J. Newcomb, and Thomas Yu. 1996. "Towards Computer-Aided Configuration Design for the Life Cycle." *Journal of Intelligent Manufacturing, 7*(2): 145–60. https://doi.org/10.1007/BF00177070.

Russell, Stuart, and Peter Norvig. 2010. *Artificial Intelligence: A Modern Approach* Third Edition. Pearson. https://doi.org/10.1017/S0269888900007724.

Russo, Davide, and Caterina Rizzi. 2014. "Structural Optimization Strategies to Design Green Products." *Computers in Industry.* https://doi.org/10.1016/j.compind.2013.12.009.

Seo, Seongwon, Selwyn Tucker, and Peter Newton. 2007. “Automated Material Selection and Environmental Assessment in the Context of 3D Building Modelling.” *Journal of Green Building.* https://doi.org/10.3992/jgb.2.2.51.

Shah, J. J., and M. T. Rogers. 1988. “Expert Form Feature Modelling Shell.” *Computer-Aided Design*. https://doi.org/10.1016/0010-4485(88)90041-3.

Sharif, Seyed Amirhosain, and Amin Hammad. 2019. “Developing Surrogate ANN for Selecting Near-Optimal Building Energy Renovation Methods Considering Energy Consumption, LCC and LCA.” *Journal of Building Engineering.* https://doi.org/10.1016/j.jobe.2019.100790.

Shimomura, Yoshiki, Tomohiko Sakao, Tatsunori Hara, Tamio Arai, and Tetsuo Tomiyama. 2007. “Service Explorer - a Tool for Service Design.” In *Mechatronics for Safety, Security and Dependability in a New Era.* https://doi.org/10.1016/B978-008044963-0/50050-3.

Silva, Diogo Aparecido Lopes. 2021. “Life Cycle Assessment (LCA)—Definition of Goals and Scope.” In Life Cycle Engineering and Management of Products: Theory and Practice, edited by José Augusto de Oliveira, Diogo Aparecido Lopes Silva, Fabio Neves Puglieri, and Yovana María Barrera Saavedra, 45–69. *Cham: Springer International Publishing*. https://doi.org/10.1007/978-3-030-78044-9_3.

Singh, Prince Pal, and Jatinder Madan. 2016. “A Computer-Aided System for Sustainability Assessment for the Die-Casting Process Planning.” *International Journal of Advanced Manufacturing Technology.* https://doi.org/10.1007/s00170-013-5232-2.

Slama, Hadhami Ben, Raoudha Gaha, and Abdelmajid Benamara. 2020. “Proposal of New Eco-Manufacturing Feature Interaction-Based Methodology in CAD Phase.” *International Journal of Advanced Manufacturing Technology*. https://doi.org/10.1007/s00170-019-04483-7.

Srinivasan, M., and P. Sheng. 1999. “Feature Based Process Planning in Environmentally Conscious Machining - Part 2: Macroplanning.” *Robotics and Computer-Integrated Manufacturing.* https://doi.org/10.1016/S0736-5845(99)00018-6.

Sy, Mamadou, and Christian Mascle. 2011. “Product Design Analysis Based on Life Cycle Features.” *Journal of Engineering Design.* https://doi.org/10.1080/09544820903409899.

Tao, Jing, Zhaorui Chen, Suiran Yu, and Zhifeng Liu. 2017. “Integration of Life Cycle Assessment with Computer-Aided Product Development by a Feature-Based Approach.” *Journal of Cleaner Production.* https://doi.org/10.1016/j.jclepro.2016.12.005.

Tao, Jing, Lu Li, and Suiran Yu. 2018. “An Innovative Eco-Design Approach Based on Integration of LCA, CAD\CAE and Optimization Tools, and Its Implementation Perspectives.” *Journal of Cleaner Production.* https://doi.org/10.1016/j.jclepro.2018.03.213.

Tecuci, Gheorghe. 2012. “Artificial Intelligence.” *Wiley Interdisciplinary Reviews: Computational Statistics*. https://doi.org/10.1002/wics.200.

Terzi, Sergio, Abdelaziz Bouras, Debashi Dutta, Marco Garetti, and Dimitris Kiritsis. 2010. “Product Lifecycle Management - From Its History to Its New Role.” *International Journal of Product Lifecycle Management, 4*(4): 360–89. https://doi.org/10.1504/IJPLM.2010.036489.

Tula, Anjan Kumar, Deenesh K. Babi, Jack Bottlaender, Mario R. Eden, and Rafiqul Gani. 2017. “A Computer-Aided Software-Tool for Sustainable Process Synthesis-Intensification.” *Computers and Chemical Engineering.* https://doi.org/10.1016/j.compchemeng.2017.01.001.

Umeda, Yasushi, Shinichi Fukushige, Eisuke Kunii, and Yuki Matsuyama. 2012. “LC-CAD: A CAD System for Life Cycle Design.” *CIRP Annals - Manufacturing Technology*. https://doi.org/10.1016/j.cirp.2012.03.043.

USDA. 2017. *“Environmental Policy Integrated Climate (EPIC) Model | Ag Data Commons.”* 2017. https://data.nal.usda.gov/dataset/environmental-policy-integrated-climate-epic-model.

Vogel, Gabriel, Lukas Schulze Balhorn, and Artur M. Schweidtmann. 2022. “Learning from Flowsheets: A Generative Transformer Model for Autocompletion of Flowsheets.” *arXiv.* https://doi.org/10.48550/arXiv.2208.00859.

Xing, K., H. F. Wang, and W. Qian. 2013. “A Sustainability-Oriented Multi-Dimensional Value Assessment Model for Product-Service Development.” *International Journal of Production Research.* https://doi.org/10.1080/00207543.2013.810349.

Yoon, Seongkyu, Shaun Galbraith, Bumjoon Cha, and Huolong Liu. 2018. “Flowsheet Modeling of a Continuous Direct Compression Process.” In *Computer Aided Chemical Engineering.* https://doi.org/10.1016/B978-0-444-63963-9.00005-1.

Yung, Ping, and Xiangyu Wang. 2014. “A 6D CAD Model for the Automatic Assessment of Building Sustainability.” *International Journal of Advanced Robotic Systems.* https://doi.org/10.5772/58446.

Yung, Winco K.C., H. K. Chan, Danny W.C. Wong, Joey H.T. So, Albert C.K. Choi, and T. M. Yue. 2012. “Eco-Redesign of a Personal Electronic Product Subject to the Energy-Using Product Directive.” *International Journal of Production Research*. https://doi.org/10.1080/00207543.2011.571941.

Zargar, Shiva, Yuan Yao, and Qingshi Tu. 2022. “A Review of Inventory Modeling Methods for Missing Data in Life Cycle Assessment.” *Journal of Industrial Ecology*, *26*(1676-1689). https://doi.org/10.1111/jiec.13305.

Zhang, Heng, Bicheng Zhu, Yunpeng Li, Omer Yaman, and Utpal Roy. 2015. “Development and Utilization of a Process-Oriented Information Model for Sustainable Manufacturing.” *Journal of Manufacturing Systems*. https://doi.org/10.1016/j.jmsy.2015.05.003.

Zhang, Lei, Rui Jiang, Zhi feng Jin, Hai hong Huang, Xin yu Li, and Yan jiu Zhong. 2019. “CAD-Based Identification of Product Low-Carbon Design Optimization Potential: A Case Study of Low-Carbon Design for Automotive in China*.” International Journal of Advanced Manufacturing Technology.* https://doi.org/10.1007/s00170-018-2653-y.

Zhou, Chunliu, Xiaobing Liu, Fanghong Xue, Hongguang Bo, and Kai Li. 2018. “Research on Static Service BOM Transformation for Complex Products.” *Advanced Engineering Informatics.* https://doi.org/10.1016/j.aei.2018.02.008.