# A Digital Twin-based Life Cycle Assessment framework

Theoretical and Practical contribution

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**Abstract**

The Life Cycle Assessment (LCA) is a generally accepted methodology to quantify the environmental impacts of products or systems. Nonetheless, various sources of uncertainty and complexity create barriers to its widespread adoption. Meanwhile, new technologies within the Industry 4.0 are offering innovative capabilities to overcome some of these challenges. Therefore, this work has three main objectives: (i) to review and identify research gaps in recent developments in the LCA methodology; (ii) to develop a Digital Twin (DT) based adapted LCA methodology; and (iii) to implement the methodology into a user-friendly, quick, robust and reliable DT-based LCA software. The methodology developed encompasses a theoretical proposal to adapt the traditional LCA, followed by a practical implementation and a proof-of-concept application, in a quest to develop a feasible DT-based LCA model. The practical implementation of this methodology led to a software named Towards an Online LCA for Bio-based processes (TOLCAB), providing a real-time LCA. This software targets the bio-based processing sector, but it is easily customisable for any sector. To demonstrate its capabilities, as a proof-of-concept, TOLCAB was applied in two case studies: the production of biodiesel from rapeseed and the production of the β-Galactosidase enzyme. Although in its early stages of development, TOLCAB proved to be a valuable tool for quickly providing static and dynamic results using powerful visualisation tools. Nonetheless, this approach is a first step to bridging the gap between theoretical LCA capabilities and practical applications for industries under the digitalisation paradigm.

**Keywords**: LCA, Digital Twins, Software, Industry 4.0, Digitalization, Bio-based processes.

## 1. Introduction

Decision-makers around the world frequently run against uncertainties when evaluating possible sustainable courses of action. This is particularly valid when it comes to environmental strategies (Stock and Seliger, 2016). Therefore, it is essential to have objective tools for quantifying environmental performances (Finnveden et al., 2009). The Life Cycle Assessment (LCA) is one of them and the most suitable for performing eco-assessments (Hauschild et al., 2018). It is a robust and standardised methodology that enables a holistic environmental assessment of products, processes or activities across their entire life cycle, from raw materials to the End-of-Life (EoL) (ISO:14040, 1997). This evaluation is done by undertaking a sequence of steps that essentially map all inputs and outputs of the defined system to attribute them to their respective environmental impacts (ISO:14040, 2006). After analysing the results, common goals include improving the system's overall environmental impact, comparing multiple scenarios, or communicating the findings to stakeholders, among others (Hauschild et al., 2018). Meanwhile, environmental regulations have been increasing over the years, and the trend is expected to continue (Sala et al., 2021). However, LCA is still largely associated with several sources of complexity and uncertainty. Acquiring data to assess systems properly is a significant operational barrier, as it is very time demanding and requires expertise and stakeholder coordination (Beltran et al., 2018; Teh et al., 2020). Other substantial obstacles occur, such as technological ones (e.g., complex software and unintegrated data management systems) (Pieragostini et al., 2012), disregarding temporal considerations (Beloin-Saint-Pierre et al., 2020), lacking standardisation in impact assessment methods (Hauschild et al., 2013), or difficulties in incorporating results into decision-making (Pryshlakivsky and Searcy, 2021), among others. Meanwhile, the fourth industrial revolution, commonly labelled as Industry 4.0, is taking place. New technological advancements, such as Artificial Intelligence (AI) or the Internet of Things (IoT), are creating novel and more efficient systems, especially when collecting and managing large datasets. Innovative capabilities that were previously unthinkable are now modifying both short-term performance and long-term sustainability (Ghobakhloo, 2018). In this context, the LCA has a unique potential to become automated (Culaba et al., 2022). The opportunity to merge LCA with the Digital Twin (DT) strategy is identified in the literature as promising (Barni et al., 2018). Applying this technology to LCA could potentially create a real-time bi-directional DT-based

LCA (Udugama et al., 2021). This can enable the collection of time-dependent inventory data to provide dynamic results. The ultimate goal would be to create a closed loop of environmental improvements (Thiede, 2021).

This article is organised as follows. Section 2 provides a literature review on the standard LCA methodology and the associated limitations while also outlining significant research developments suggested in recent years. Section 3 describes the methodology to adapt the LCA towards a DT-based model. The TOLCAB software is presented in Section 4. A proof-of-concept is depicted in Section 5, where TOLCAB is applied to two relevant case studies. To conclude, Section 6 summarises the final remarks and provides recommendations for future work.

## 2. Literature Review

LCA is a scientific, holistic, systematic, and multidisciplinary procedure which gained relevance during the 1990s and is now used across all industry sectors (Mannan and Al-Ghamdi, 2022). Among others, it has numerous applications in product development, strategic decisions, policy making, and marketing (ISO:14044, 2006).

### 2.1. Standard LCA methodology

According to the ISO standards (ISO:14040, 2006; ISO:14044, 2006), LCA is an environmental assessment methodology based on four main stages: (1) Goal and scope definition; (2) Life Cycle Inventory; (3) Life Cycle Impact Assessment; and (4) Interpretation. Even though they are designed to be performed sequentially, LCA allows for learning and consequent improvements across all stages, making it an iterative approach (Hauschild et al., 2018).

*1. Goal and Scope Definition.* The goal identifies the study's purpose, application, audience, and way of communication. Defining the scope consists in establishing several modelling options. Namely, setting the system boundaries, functional unit, data quality requirements, allocation regulations, assumptions, limitations, and impact assessment methods and categories (ISO:14044, 2006). The system boundaries define the unit processes to be included in the system and their respective level of detail (ISO:14040, 2006; ISO:14044, 2006). They represent the study limits: physical entities, time horizon and geographical locations (Hauschild et al., 2018).

*2. Life Cycle Inventory (LCI). This step aims* to systematically collect all the inputs and outputs of each unit process considered within the system boundaries (Hauschild et al., 2018). All inventory should follow the data quality requirements previously defined, which include ensuring that data is precise, complete, representative, consistent, and reproducible while thoroughly providing the data sources and respective assumptions in the information (ISO:14044, 2006). Collected data can be classified as primary or secondary data, depending on whether it was directly or indirectly captured from the supply chain (Mannan and Al-Ghamdi, 2022). Data can be obtained from four different main channels: (i) manual data entry; (ii) sensor-based equipment; (iii) web search (i.e., internet databases); and (iv) virtual models and ready data (i.e., engineering models loaded into the software) (Spreafico and Russo, 2021). LCI is generally considered the most critical and time-consuming phase (Ferrari et al., 2021), as data collection for the inventory phase accounts for around 70% to 80% of the total time when performing an LCA (Teh et al., 2020).

*3. Life Cycle Impact Assessment (LCIA).* This step translates the inventory flows obtained from the previous LCI phase into apprehensible environmental impacts (e.g., global warming, ozone depletion, acidification, etc.) (Hauschild et al., 2018). This stage consists of three mandatory tasks: (i) selection of impact categories, category indicators and characterisation models; (ii) classification to assign the LCI results to the selected impact categories; and (iii) characterisation to calculate the category results (ISO:14044, 2006). There are additional optional steps: (a) normalisation; (b) grouping; (c) weighting; and (d) data quality analysis (ISO:14044, 2006). The impact assessment methods must be selected since they will guide the following stage. When choosing the impact assessment methods, several options are available (e.g., ReCiPe, CML 2001, PEF, etc.). The recommended method by the European Commission is the Product Environmental Footprint (PEF) method (European Union, 2021). During classification and characterisation, the contribution of each flow is assigned and quantified to the respective environmental impact categories by multiplying the life cycle inventory value with the appropriate characterisation factors (Zampori and Pant, 2019). Normalisation usually follows to enable comparison between the impact categories (Hauschild et al., 2018). It consists in dividing the characterisation results by selected reference values (ISO:14044, 2006), which are called normalisation factors. To conclude, weighting can assign relative importance to each impact category in order to support the impact profile interpretation (ISO:14044, 2006). The weighting results are obtained by converting the normalised results using selected weighting factors (ISO:14044, 2006). This can include aggregating impact scores into several or one single indicator, commonly labelled Single Score (SS), to simplify the communication of results (Hauschild et al., 2018).

*4. Interpretation.* This final step systematically reviews and refines the results obtained in the LCA, aiming to present final conclusions, limitations and recommendations (ISO:14044, 2006). Usually, the system's environmental impact hotspots are identified at this stage. According to the United Nations (2017), environmental hotspots can be a "life cycle stage, process or elementary flow which account for a significant proportion of the impact of the functional unit". Furthermore, uncertainty and sensitivity analysis are frequently performed to evaluate the robustness of results, as well as to pinpoint areas that might require additional research to reinforce the conclusions (Hauschild et al., 2018). The uncertainty analysis allows to manage and quantify uncertainty sources, improving the precision and robustness of the study. Sensitivity analysis can determine how different values of a single variable – usually an environmental hotspot - can affect the results (United Nations, 2017). To achieve this, scenario comparisons may be useful (ISO:14044, 2006). Additionally, methodological choices, assumptions and their associated uncertainties (Hauschild et al., 2018) are considered and analysed according to the goal and scope of the study (ISO:14044, 2006). To perform a successful study, it is fundamental to perform iterative processes to refine results and accomplish the defined goal (Hauschild et al., 2018). To conclude the LCA study, the limitations, conclusions and final recommendations must also be reported (ISO:14044, 2006).

*Limitations.* Although the LCA provides valuable guidance in environmental assessment, the literature acknowledges the need for ongoing improvements (Pieragostini et al., 2012). Significant limitations hindering the LCA application are outlined in Table 1. These sources of complexity and uncertainty create barriers for LCA practitioners (Ghita et al., 2021). Ultimately, this limited applicability reduces the potential of the use of this methodology.

*Table 1 - Key limitations hindering the LCA application (Ghita et al., 2021).*

| |
|---|
| Disregard of temporal and spatial considerations |
| Uncertainty in the functional unit and system boundaries |
| Hard to obtain quality data |
| Time-consuming |
| Lack of uniformization in LCIA methods |
| Technological barriers (complex software, databases, and inexistant integrated and interoperable data management system) |
| Cost (demands experts and stakeholder coordination) |
| Problematic use in policy-regulatory context |
| Difficult application in complex industries |
| Hard to translate into strategic decision-making |

### 2.2. Methodological LCA developments

This section introduces the recent methodological developments to conventional LCA techniques presented over the years that aim to expand LCA's capabilities.

*Dynamic LCA (D-LCA). The* lack of temporal considerations in most LCA studies is concerning, as it has been demonstrated that such factors can significantly impact the outcomes, particularly in long-life cycle products or services (e.g., construction or energy industries) (Beloin-Saint-Pierre et al., 2020). Moreover, when the usage phase contributes considerably to the life cycle environmental impacts, assuming static and average-oriented usage mixes for some products (e.g., ICT products) can potentially bias the conclusions of LCA evaluations (Hagen et al., 2020; Mashhadi and Behdad, 2018). D-LCAs have been created to consider and define dynamic systems and their temporal differentiation of flows (Levasseur et al., 2010). Sohn et al. (2020) identified three forms of LCA dynamism: dynamic process inventory, dynamic systems, and dynamic characterisation. Temporal considerations are largely arising due to the capabilities of real-time data collection technologies (Ferrari et al., 2021).

*Ubiquitous LCA (U-LCA).* This new concept for assessing environmental and social impacts in the current context of industry 4.0 was proposed by Mashhadi and Behdad (2018). The authors suggest a methodology framework to improve assessments of emerging systems while aiding decision-making processes. U-LCA fundamentally reformulates the traditional definition of the functional unit. By employing IoT capabilities of real-time interconnectivity and tracking, the authors argue that future physical boundaries can be extended to encompass entire life cycle input and output flows dynamically. Perhaps the central innovation in the U-LCA proposition lies in embracing smart manufacturing capabilities to overcome traditional LCA restrictions in assessing smart infrastructure burdens. The U-LCA methodology includes smart capabilities to track product data during its entire life cycle, including the usage and End-of-Life (EoL) phases, which are typically left unassessed. These real-time computation methods ensure that the temporal and spatial considerations are addressed, contributing to a more accurate LCIA. U-LCA provides an accurate real-time assessment capable of tracking emerging systems to ultimately originate more sustainable decisions. However, U-LCA is still a conceptual framework needing further research and implementation efforts.

### 2.3. Technologies enabling LCA in the Industry 4.0

This section outlines Industry's 4.0 technologies that can be applied to enhance LCA procedures. Ultimately, these novelties provide relevant insights when developing the methodology for this project's work. Due to the unique implications offered by each Industry 4.0 technology and their *superadditive synergy* (i.e., they can provide singular sustainability implications when in a hyper-connected manufacturing ecosystem), these approaches frequently combine multiple technologies in the same environment (Ching et al., 2022).

*Smart sensor-based technologies:* Data collection and management strategies are particularly important under the Industry 4.0 paradigm. The introduction of IoT in the manufacturing field enables developments in information systems, which in turn facilitate the real-time use of potentially massive amounts of data collected from various sources (Ingrao et al., 2021). This data collection represents the bridge between the physical and the virtual world and, thus, requires investments in a capable Information Technology (IT) infrastructure - e.g., sensors, Programmable Logic Controllers (PLC), computers, and data visualisation tools (Thiede, 2018). In turn, the expansion of real-time data collecting can create a need for *on-the-fly* decision support and management systems (Culaba et al., 2022). Smart sensors are pieces of equipment that collect product data autonomously and automatically integrate it with IoT technologies, ultimately requiring no human intervention (Spreafico and Russo, 2021). A wide variety of smart sensors can be adopted at various stages throughout a product's lifecycle to monitor resource consumption, waste generation, and performance of unit operations or for safety and quality control verifications (Watson et al., 2021). Sensors are selected based on their monitoring objectives and their general characteristics. Additionally, integrating readily available data from production software systems (e.g., Enterprise Resource Planning (ERP), Manufacturing Execution System (MES), etc.) with the LCA can be an interesting and data-rich path (de Soete et al., 2014). Using actual data flows collected from sensor-based equipment might reduce the complexity, restrictions, and inconsistencies in data when performing the LCI (Ferrari et al., 2021). Furthermore, the importance of adopting more accurate data collection methods to achieve more reliable LCA results is widely discussed in the literature. For example, Watson et al. (2021) state that intelligent sensors play a more significant role in the future of food and beverages by increasing resource efficiency and lowering the sector's carbon impact. Another example is Ingrao et al. (2021), which focuses on energy consumption; it shows a significant difference between data derived using relatively advanced mathematical models and data acquired on-site using direct measurement using sensors.

*Digital Twin (DT).* DT is a digital model containing physical elements in a real space, virtual elements in a virtual space, and the bi-directional information exchange connecting them both (Grieves and Vickers, 2016; Kritzinger et al., 2018). It essentially consists of a detailed and real-time (or near real-time) representation of a physical system based on simulation (Kamble et al., 2018; Zambrano et al., 2022). A DT optimally contains all the attainable information of the depicted system (Grieves and Vickers, 2016; Kritzinger et al., 2018), allowing for "self-diagnosis, self-optimisation and self-configuration without the need for human input or intervention" (Zambrano et al., 2022). DTs of smart products enable producers to virtually evaluate and test the product's performance while assessing the respective production system (Ghobakhloo, 2018). Therefore, they have the potential to improve performance characteristics (Kamble et al., 2022) and create optimal physical solutions for both resources and operations (Yu et al., 2022). However, DT applications in environmental assessments, namely the LCA, are still in the very early stages of research. Barni et al. (2018) introduced a breakthrough LCA framework using the DT technology as a "data-rich representation of the company's products and processes". According to the authors, DT can help the LCA become more accurate and automated. Importantly, when used in conjunction with a network of sensors, DT can describe real-time processes and produce simulated data to aid LCA forecasts. DT capabilities can reduce traditional data collection burdens in the supply chain, transforming the LCA into a real-time (online) self-assessment tool. In 2021, Ghita et al. proposed a generic solution combining DT and the D-LCA methodology. Their framework introduced spatial and temporal data variability while addressing relevant, sustainable challenges, such as traceability, efficiency, and profit-sharing. Nevertheless, these ground-breaking research efforts still considerably lack practical implementation as they are conceptual contributions. Moreover, the systematic review by Kamble et al. (2022) on the DT technology for sustainable purposes shows that existing literature still needs to consider the life cycle perspective in depth.

### 2.4. Framing the Problem

At their core, LCA approaches reproduce physical systems by creating virtual models capable of performing environmental impact calculations. However, in conventional LCA procedures, the connection between the physical and virtual systems is only established by exchanging manual data flows without any automated interchange of data.

The problem is framed using Figure 1. The purpose of this visualisation is to illustrate how an ideal DT-based LCA could operate. The physical system (in red) represents events in the supply chain: its stages are represented (i.e., downstream, midstream and upstream), as well as the data collection methods that can monitor the flows occurring within them. The virtual system (in blue) contains the LCA methodology and all the necessary virtual procedures to achieve the environmental assessment objectives. These procedures include the LCA stages (see section 2.1), decision-making, and an eventual database connecting both stages. The arrows in the figure represent the data exchange between the entities. All these interactions should ideally happen in real-time. Therefore, not only should online data collection from the processes in the physical system be transcribed into the virtual system, but the decision-making conclusions arising from the virtual system should also be translated into the physical system in real-time. This demonstrates the ongoing challenge in this research field since having all the information exchange happening automatically and in real-time is not yet accomplishable. Some of the current obstacles identified in the literature are the following: (i) implementing a DT-based LCA throughout the entire supply chain; (ii) operational limitations (e.g., integrating the various architectural layers and services in a single environment); (iii) accounting for the different LCA's objectives; (iv) establishing a real-time and bi-directional connection between the physical and the virtual world capable of live environmental improvements in the system; and (v) a small number of practical applications.

Examples of practical applications are given by: (a) Barni et al. (2018), which created an automated sustainability labelling system for the woodworking sector; (b) Riedelsheimer et al. (2020), that developed a concept for the clothing industry considering the middle and EoL stages; and (c) Kaewunruen et al. (2020), which evaluated of a subway station to improve communication and asset management.

The following research question was formulated: *is it possible to overcome the mentioned research gaps while developing a feasible framework to implement a DT-based LCA*?

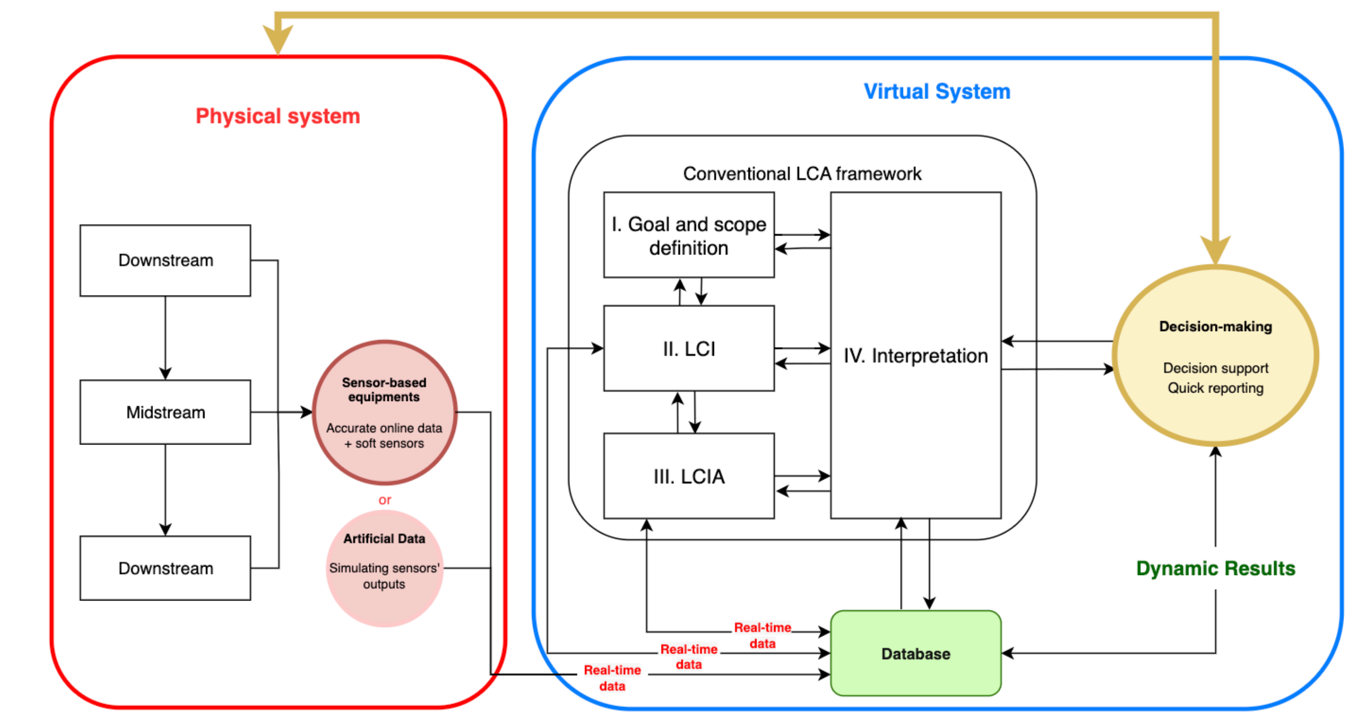


*Figure 1 - Online bi-directional connection between the physical (on the left, in red) and the virtual (on the right, in blue) systems.*

## 3. Methodology to adapt the LCA towards a DT-based model

The developed methodology comprises three phases, as schematically represented in Figure 2. They are described in detail in the following subsections.

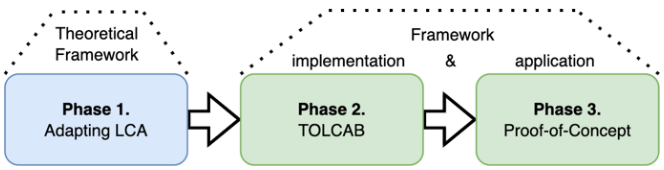


*Figure 2 - Methodology phases to adapt the LCA towards a DT-based model.*

### Phase 1 - Adapting LCA: Theoretical framework

The standard LCA methodology was reviewed in detail in section 2. Therefore, only the proposed extensions to the existing LCA standards are described in detail in the following steps.

*Step 1. Goal and Scope Definition:* The objectives, audience, functional unit, and reference flow of the LCA study should be stated (ISO:14044, 2006). As for the system boundaries, the monitoring capabilities of the Industry's 4.0 technologies enable expanding the traditional boundaries to ideally encompass the entire supply chain (Mashhadi and Behdad, 2018). Furthermore, this step includes the definition of the types and sources of data, and corresponding data-quality requirements, as detailed in ISO:14044 (2006).

*Step 2. LCI.* Due to the digitisation of the LCI, rather than relying solely on historical data, the LCA analysis can now be carried out in real-time (Ferrari et al., 2021). Therefore, the final LCI results can be portrayed as static and dynamic inventory data. This combination allows the study to consider temporal variability without compromising the ease of interpretation. LCI starts with data collection (ISO:14044, 2006). It is proposed that this process is inverted: the practitioner should define the data sources rather than the data itself. The data sources will then provide the necessary information automatically; they can include: (a) sensor-based equipment and (b) artificially generated data or existing external databases. Artificially generated data refer to probabilistic distributions that can simulate the behaviour of actual sensor-based equipment (Westermann and Evins, 2019). The chosen data collection methods can provide the LCA with real-time data flows. Static inventory data averages time-dependent flows, whereas dynamic inventory data provides flows varying with time. When selecting the data collection methods, the practitioner should balance the data-quality requirements as well as consider the inherent characteristics of the data collection equipment. Likewise, the user is encouraged to use: (i) sensor-fusion alternatives, which combine sensors to reduce uncertainty in cases where it may compromise the results' reliability; and (ii) soft sensors, which are based on models that are capable of estimating challenging process variables that cannot be measured directly in real-time (Thiede, 2021). The selected data sources provide real-time flows, creating dynamic inventory data. For instance, the consumption of a specific resource can be monitored using a sensor providing data varying with time. Depending on the sensor's inherent characteristics, such as the speed or the accuracy of data acquisition, this sensor can provide time-dependent with different degrees of uncertainty. This enables quantifying the inventory for this resource in real-time. The total inventory data includes information for each unit process contained within the system boundary (ISO:14044, 2006). This is expected to achieve the objectives defined in ISO:14044

(2006): "reach uniform and consistent understanding of the product systems to be modelled". However, calculated and estimated data must be included to encompass the background processes (Muñoz et al., 2018). Moreover, the remaining LCI procedures mentioned in ISO:14044 (2006) should be performed: validation of data, relating data to unit process and functional unit, refining the system boundary, and allocation should be considered.

*Step 3. LCIA.* Static and dynamic LCI results from Step 2 are automatically incorporated in order to begin Step 3. The PEF method should be selected since it is recommended by the European Union (2021). The consequential approach is followed because it estimates the environmental implications from the system's life cycle considering a global perspective (Ekvall, 2019), and, importantly, it is compatible with the decision-support perspective followed in this work. The following tasks include classification, characterisation, normalisation and weighting, as described in section 2.1. The main challenge here is for the practitioner to combine static and dynamic LCIA results; hence, the user is encouraged to match both static and dynamic LCIA capabilities, depending on the defined objectives. Dynamic results portray a significant amount of information and can be harder to interpret. However, whereas static results only provide average values, this time-dependent information enables the user to characterise and keep track of the system's variability. This knowledge can be used to support decision-making. For instance, by identifying maximum impact values, the user can act to reduce their likelihood instead of acting based on average values that may be misleading. Considering time-dependent results can, therefore, result in more effective and sustainable actions. Nevertheless, complete static LCIA results should also be provided. They can be very helpful for users to easily grasp the environmental impacts of the system and straightforwardly identify hotspots.

*Step 4. Interpretation.* This step is performed using automatic and explicit procedures. They are here as follows:

(i) Identify the environmental hotspots automatically by performing a Pareto analysis of the impact categories, processes units and flows in the system.

(ii) Provide iteration suggestions to improve the reliability of the results:
   a. Propose different data collection methods to reduce uncertainty when monitoring critical inputs or outputs of the system.
   b. Propose alternative options for the processes selected to reduce their environmental impacts - retrofit design (Carvalho et al., 2013).

(iii) Perform an uncertainty analysis by building a simplified uncertainty matrix, which can provide knowledge to better understand the implications of results. The user should take the automatically generated insights from the matrix and act primarily on the highest contributors to the overall environmental impact and uncertainty.

(iv) Perform a sensitivity analysis to better understand the implications of potential critical parameters. This is a valuable tool for evaluating possible courses of action.

(v) Provide a short reporting segment to facilitate the communication of results. This should be comprised of the main decisions defined in the goal and scope stage, as well as the main results from the LCA, which include the environmental hotspots and suggestions for improving the result's reliability. This report considers the user's objectives and establishes a transition between the comprehensive results and the decision-making process. Although dynamic LCI and LCIA results can provide valuable information, they are not automatically incorporated into quick reporting. Due to the significant amount of data, it is challenging to convey them clearly and thoroughly. Therefore, in this step, the practitioner is encouraged to revisit the dynamic results obtained and, in particular, to analyse the temporal variability associated with specific environmental hotspots.

**Phase 2 – TOLCAB**

In this phase, a software named TOLCAB (Towards Online LCA for Bio-based processes) is created based upon the theoretical framework developed in Phase 1 (see Figure 2). The general software architecture is schematically represented in Figure 3.

*Interface and Database:* TOLCAB incorporates the interface and database in a single environment. It was built in Excel to create a stand-alone, easy-to-use software application that facilitates user navigation and supports decisions at every level. The database includes (i) bio-based processes data, meaning all the inputs and outputs occurring in each process considered in the life cycle; (ii) the inventory data from the selected data sources; and (iii) the necessary PEF method information (i.e., characterisation, normalisation and weighting factors).

*Surrogate model:* The technical challenges inherently posed by a DT-based LCA methodology (e.g., time, resources and computational effort) require this thesis to implement a surrogate model strategy. According to Davis et al. (2017), this approach is employed when a simpler relationship with acceptable accuracy between highly complex input and output data is required. Therefore, the software will include simplifications: (i) the sensor-based equipment is substituted by artificially generated data; (ii) supply chain processes and the available technological options are simplified; and (iii) integration mechanisms across the entire supply chain are assumed to be established.

**Phase 3 – Proof-of-concept**

As shown in Figure 2, this proof-of-concept intends to demonstrate the application of TOLCAB (implemented in Phase 2). Accordingly, this software is validated using two case studies from the bio-based processing sector: biodiesel production and β-Galactosidase enzyme production.

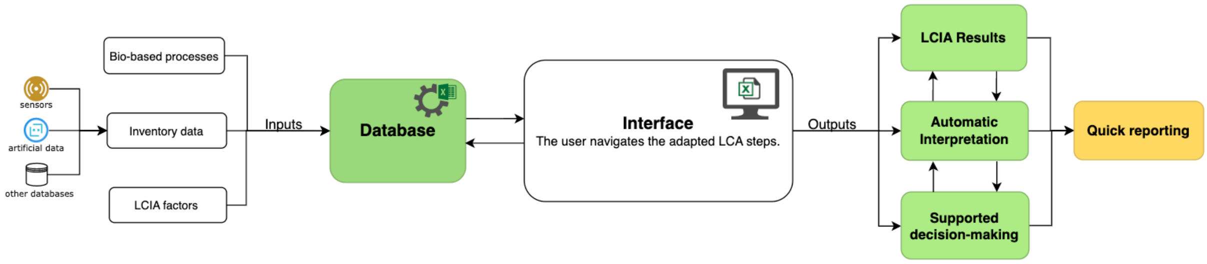


*Figure 3 - General software architecture of TOLCAB.*

For each case study, (i) the original research is contextualised; (ii) data sources used in the original study are detailed and compared with the ones employed in TOLCAB; (iii) the initial user actions are performed; and finally, (iv) the published results are visualised and compared to the results obtained with TOLCAB. A discussion follows to benchmark the results obtained, recognising the benefits and drawbacks associated with the software while addressing the associated limitations.

## 4. TOLCAB: Practical Software Implementation

The bio-based sector has been selected because it is the dominant industry in Denmark, which is used in this thesis for demonstration purposes. This section introduces the key capabilities of this software, contemplating the user's point of view: section 4.1 describes the initial user actions; section 4.2 illustrates user actions associated with the assessment and interpretation; and lastly, section 4.3 outlines potential directions for future development.

### 4.1. User inputs A: initial actions

To apply TOLCAB in a bio-based processing company, the initial actions must be followed. They are responsible for modelling the physical system to be analysed. The goal is to prepare data in order to be automatically retrieved from the system so that a real-time LCA can be performed.

### 4.2. User inputs B: assessment and interpretation actions

Assuming that the initial actions have been followed, the physical system is now completely defined. This allows for the results to be automatically generated. Therefore, the user should now be able to navigate and interpret them. Noteworthy is that the main target is for the user to gain reliable, fast and robust insights about the system's environmental impacts.

***Life Cycle Inventory.*** The user can retrieve information from the inventory data and inspect particular flows if necessary. For the dynamic flows (time-dependent), the user can also visualise their variation with time. Additionally, the total LCI results can be obtained: however, they simplify the results, which means the dynamic flows are converted in averages, thus, becoming static flows. Nonetheless, this averaging provides valuable information for future simplified calculations during the LCIA and interpretation stages.

***Life Cycle Impact Assessment.*** The calculations are carried out automatically. The LCIA static and dynamic results are ready to be visualised. As previously mentioned, the main challenge is for the user to combine different static and dynamic results into understandable data. Hence, the user is encouraged to match both static and dynamic LCIA capabilities, depending on the defined goals. Dynamic LCIA characterisation results of a particular flow can be visualised. These are described using boxplots which are used to represent graphically the numerical values of a dataset graphically. For each impact category, they present the dynamic inventory dataset of the chosen flow, illustrating the variability of the flow's impacts with time. This time-dependent information enables the user to characterise and keep track of the flow's variability. This knowledge can be used to support decision-making. Moreover, complete static LCIA results are provided. Characterisation results can be comprehensively visualised in tables, relative contributions, and customisable graphics. These features can be observed in the different tabs developed in the software. The normalisation and weighting results are also estimated automatically. The weighting results can be observed for each impact category or as a Single Score (SS).

***Interpretation.*** Several interpretation steps are automatically performed. Nonetheless, the user can perform additional analyses using the capabilities provided in the software. The automatic features are: (i) the *hotspot ranking* tool; (ii) the *environmental hotspots finder;* and the (iii) *suggestion box.* The conceptual design of features (ii) and (iii) has been designed, but due to time constraints, they are not yet totally integrated into the software flow. These tools support decision-making by (a) quickly portraying critical LCA results and (b) encouraging users to perform iterative actions to improve the results' reliability.

Dynamic results still need to be automatically incorporated into this segment. The users are encouraged to revisit the dynamic results obtained. In particular, to analyse the temporal variability associated with the specific environmental hotspots found in this step. Thanks to this time-dependent information, the user can identify and track the flow's variability. This can provide valuable insights to achieve the goals defined for the study.

***Quick Reporting.*** This final display and reporting feature presents five essential elements: (i) Starting Points – display relevant decisions made during the goal and scope definition stage. These include the Functional Unit, the Reference Flow, and System Boundaries; (ii) Life Cycle options – show the options selected within the system boundaries; (iii) Summary of Results - summarises the LCA results. They include, for example, $CO_2$ footprint, but the user can also select other categories of interest. The critical hotspots are also highlighted and displayed; (iv) Quick suggestions – summarises the potential recommendations to improve the results' reliability (e.g., propose process and supply chain design alternatives, options on other possible solvents and chemicals, retrofit designs, etc.); and (v) Additional functions - although inactivated at this point, it aims to provide three quick capabilities: update data, export quick results and create a new system.

### 4.3. Future software development

This section presents possible directions for future software development. Of note is that a key future goal is for this software to be used by different industry sectors. Thus, the aim is that the inbuilt database is to be expanded to cover such processes and supply chains. Other future paths are described here as follows:

*Improvements to the software architecture:* develop a python-based Graphical User Interface (GUI) to act as a front-end. The main goal is to provide seamless user navigation while comprehensively supporting decisions.

*Combining static and dynamic results:* as of now, dynamic results can only be visualised for a single flow at a time. Other alternatives to visualise and analyse dynamic results are being investigated and studied in order to be included in the next version of the software.

*Automating goal and scope definition:* develop the software so that the goal and scope definition step can automatically affect the following steps. For instance, making the quick reporting customisable to the user's defined goal.

*Employing actionable control data systems:* linking a control system as a new layer towards a bi-directional connection with the physical system.

*Expanding interpretation capabilities:* portray dynamic results to provide valuable information for users and enhance the uncertainty and sensitivity features.

*Improving quick reporting and decision-making:* bringing together temporal considerations and simple visualisation. Testing alternative ways to incorporate dynamic results in the Quick reporting tab is under development.

## 5. Proof-of-concept: Application

To demonstrate its capabilities and usefulness, TOLCAB was applied to two case studies: (A) González-García et al. (2013) and (B) Feijoo et al. (2017). Due to simplicity and space constraints, only case study A will be presented here.

*Approach and assumptions.* The original study is not precisely reproduced as it was performed using available published data in order to test the feasibility of TOLCAB. Therefore, the assumptions associated are: (i) Denmark as the geographic location, (ii) the PEF method to perform the LCIA calculations, and (iii) selection of different LCI data sources. Moreover, the original study embraced a cradle-to-gate perspective, whereas this proof-of-concept employs a cradle-to-grave perspective. Accounting for a larger scope of the supply chain when evaluating environmental impacts was a goal outlined in the methodology. Additionally, data collection methods were created to simulate actual direct measurements when, in fact, this data was gathered entirely from the articles. Thus, due to the lack of available dynamic data from the case studies, only static results were obtained. For the sake of simplicity, sensors retrieve the exact values stated in the case study.

### 5.1. Case study A: biodiesel production

The LCA study performed by González-García et al. (2013) evaluated the environmental impacts of biodiesel production derived from the transesterification of crude rapeseed oil from a cradle-to-gate perspective in a Spanish company. Moreover, in the original study, subsystems SS1 (Rapeseed oil production) and SS2 (Biodiesel production) were both evaluated, which was not possible to reproduce using TOLCAB since the information on flows was only available for the SS2. Therefore, only the SS2 was modelled using TOLCAB. This process includes seven subprocesses. They were all modelled in TOLCAB, and an additional one had to be added in this validation since some data from the case study was not assigned to any specific process. The study used different LCI data sources and CML 2001 as the LCIA method. Note that this was merely an approximate estimate used to facilitate relative comparison.

*Results*. Relative contributions per process to each impact category tend towards similar conclusions obtained in the original study. SS2.2 and SS2.3 were the highest contributing processes for all impact categories for both methods. Also, all categories had the same highest contributing process except for the GWP and LC categories, where SS2.2 dominated in TOLCAB and SS2.3 dominated in the original study. However, inconsistencies with the original study were found when exploring TOLCAB's possibilities in more detail. For instance, the original research mentioned ammonia and nitrate as remarkable contributors to eutrophication. However, that was not the case when using TOLCAB: Oxygen (SS2.4) was the most significant contributor, followed by Methanol and Electricity. Additional actions were performed in TOLCAB in a quest to present its possibilities, even though the original study did not pursuit them. For instance, the normalised and weighted results showed that the cancer human health effect impact category largely dominates the environmental impact. Moreover, the interpretation section of TOLCAB identified the environmental hotspots and tested sensitivity and uncertainty analyses. However, these results did not provide much value in this case study, as they were not comparable and lacked quality data to be reliable.

### 5.2. Discussion

The selected case studies posed several barriers to demonstrating the potential of TOLCAB. Data was collected from indirect sources and only static data was available. Building a real-time evaluation was, therefore, unfeasible. The proof-of-concept applications demonstrated the software usefulness and capabilities when performing an LCA. Applying TOLCAB introduces several benefits, such as: (i) it reduces time consumed due to the industry knowledge database, the automatic calculations, and the considerable decision-support features; (ii) its user-friendliness software which would facilitate the use in industrial settings; (iii) it offers powerful graphics to visualise the impact assessment results; (iv) it enables the evaluation of dynamic monitoring of results; and (v) it provides automatic support during the interpretation stage, which leads to quick and minimal resource usage that can ultimately aid decision-making.

Nonetheless, drawbacks were also identified. They are the following: (a) to perform the user actions in the tool, basic learning is needed, which can nevertheless turn away some users; (b) several envisioned functionalities are not operational at this point due to this project's time constraints; and (c) rough approximations may have compromised the reliability of the validation.

The software is still in its early stages and has a considerable margin for improvement. To achieve the possibilities envisioned in the theoretical proposal, the future development suggestions should be implemented (see section 4.3). Nevertheless, TOLCAB showed that it can be a valuable stand-alone software. Due to its industry-specificity and user-friendliness, it can substantially benefit the industry sector of bio-based processes. Noteworthy is that, although TOLCAB has been developed for the bio-based processing sector, the software is easily customizable to any sector. As companies crave quick and easy-to-use alternatives in environmental assessment, this tool can contribute to broader adoption of LCA practices.

## 6. Conclusions & Future work

A theoretical framework towards an online DT-based LCA in Industry 4.0 has been proposed in this work. By suggesting specific procedures to be added to the four stages of the conventional LCA methodology, this framework can guide practitioners in incorporating the DT technology when applying the LCA. These theoretical possibilities were implemented on a practical level by developing the software TOLCAB (Towards an Online LCA in Bio-based processes). The software architecture was defined considering the surrogate model approach. TOLCAB aims to close the gap between theoretical LCA capabilities and practical applications for industries going through the digitalisation paradigm. Hence, the user actions to visualise and interpret the results considered aiding not only real-time results interpretation and decision-making, but also user experience. Emphasis was put on supporting the interpretation stage so that sustainable decision-making could be more efficiently executed. Although TOLCAB was a successful implementation of the proposed theoretical framework, it is still in its early stages, and thus some software features are still inactive. Furthermore, several procedures still require further development; hence, forthcoming advancements were discussed in a quest to bridge the gap between the theoretical framework and its full practical implementation. Nevertheless, the software was validated using two case studies in the literature, which allowed to explore the possibilities offered using actual implementation scenarios. However, several assumptions needed to be made; thus, the comparison of results was difficult and, therefore, needs continuous and extensive future evaluation. Nonetheless, it was possible to clearly conclude that TOLCAB provides a user-friendly environment to enable automatic calculations, quick operations, enhanced visualisation and interpretation support. Final users are expected to take less time on the platform than when going through the traditional LCA procedures, and also, they do not need to be LCA experts. Further development of this user-friendly LCA software focusing on efficiency, visualisation and decision support is anticipated to promote wider adoption of environmental assessments. Additionally, for TOLCAB to become the tool of choice, further testing in a plethora of real-world applications is necessary. These efforts will enable the extension of the database of bio-based processes, the computational capabilities of the software, and its robustness and reliability. These will result in LCA applications covering most systems in the bio-based processing industry while improving the reliability of the results. TOLCAB's ultimate goal is to propose environmental improvements in a closed-loop manner with minimal need for human intervention.

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