A Digital Twin-based Life Cycle Assessment framework

Theoretical and Practical contribution

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Declaração

Declaro que o presente documento é um trabalho original da minha autoria e que cumpre todos os requisitos do Código de Conduta e Boas Práticas da Universidade de Lisboa.

Declaration

I declare that this document is an original work of my own authorship and that it fulfils all the requirements of the Code of Conduct and Good Practices of the Universidade de Lisboa.

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To my family, for the unconditional love.
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To her, for reminding me what truly matters during our short stay on this planet.

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 Twin, Software, Industry 4.0, Digitalisation, Bio-based processes

Resumo

A Análise de Ciclo de Vida (ACV) é uma metodologia geralmente aceite para quantificar os impactos ambientais de produtos ou sistemas. No entanto, várias fontes de incerteza e complexidade colocam barreiras à sua adoção generalizada. Para superar alguns destes desafios, novas tecnologias trazidas pela Indústria 4.0 estão a oferecer possibilidades inovadoras. Este trabalho tem três objetivos principais: (i) rever e identificar lacunas na investigação nos desenvolvimentos recentes da ACV; (ii) desenvolver uma metodologia para adaptar a ACV tradicional, baseada em Digital Twin (DT); e (iii) implementar a metodologia num software de fácil utilização, rápido, robusto e fiável. A metodologia desenvolvida engloba uma proposta teórica, seguida de uma implementação prática e de uma aplicação de prova de conceito, para desenvolver um modelo viável de ACV baseado em DT. A implementação prática desta metodologia levou a um software denominado TOLCAB (*Towards an Online LCA for Bio-based processes*), capaz de fornecer uma ACV em tempo real. Este software tem como alvo o setor dos processos biológicos, mas é personalizável para outros setores. Para demonstrar as suas capacidades, o TOLCAB foi aplicado em dois casos de estudo: produção de enzimas e produção de biodiesel a partir de colza. Embora ainda numa fase inicial de desenvolvimento, o TOLCAB provou ser uma ferramenta valiosa para fornecer resultados estáticos e dinâmicos rapidamente, utilizando poderosas ferramentas de visualização. No entanto, esta abordagem é um primeiro passo para colmatar a lacuna entre as capacidades teóricas da ACV e as aplicações práticas para as indústrias sob o paradigma da digitalização.

Palavras-chave: Análise de Ciclo de Vida, Digital-Twin, Software, Indústria 4.0, Digitalização, Processos biológicos

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List of Abbreviations

- Artificial Intelligence (**AI**)
- Big Data (**BD**)
- Business Intelligence (**BI**)
- Characterisation Factor (**CF**)
- Circular Economy (**CE**)
- Cleaning-In-Place (**CIP**)
- Cyber-Physical Production Systems (**CPPS**)
- Cyber-Physical Systems (**CPS**)
- Digital Twin (**DT**)
- Distributed Ledger Technology (**DLT**)
- Dynamic Life Cycle Assessment (**D-LCA**)
- End-of-Life (**EoL**)
- Enterprise Resource Planning (**ERP**)
- European Commission - Joint Research Centre (**EC-JRC**)
- Gate Operating System (**GOS**)
- Global Positioning Systems (**GPS**)
- Graphical User Interface (**GUI**)
- Greenhouse Gas (**GHG**)
- Human Health (**HH**)
- Industrial Internet of Things (**IIoT**)
- Information and Communication Technologies (**ICT**)
- Information Technology (**IT**)
- International Organisation for Standardisation (**ISO**)
- Internet of Things (**IoT**)
- Life Cycle Assessment (**LCA**)
- Life Cycle Cost (**LCC**)
- Life Cycle Costing of Organisations (**O-LCC**)
- Life Cycle Impact Assessment (**LCIA**)
- Life Cycle Inventory (**LCI**)
- Machine Learning (**ML**)
- Manufacturing Execution System (**MES**)
- Non-Governmental Organisations (**NGOs**)
- Normalisation Factor (**NF**)
- Organisational Life Cycle Assessment (**O-LCA**)
- Product Environmental Footprint (**PEF**)
- Programmable Logic Controller (**PLC**)
- Radio-Frequency Identification (**RFID**)

- Single Score (**SS**)
- Small and Medium-sized Enterprises (**SMEs**)
- Small and Medium-sized Manufacturers (**SMMs**)
- Smart Data (**SD**)
- Smart Factories (**SF**)
- Social Life Cycle Assessment (**S-LCA**).
- Technology Readiness Level (**TRL**)
- Triple Bottom Line (**TBL**)
- Ubiquitous Life Cycle Assessments (**U-LCA**)
- United Nations Economic Commission for Europe (**UNECE**)
- Wastewater Treatment Plant (**WWTP**)
- Weighting Factor (**WF**)
- World Economic Forum (**WEF**)

1. Introduction

1.1. Contextualization

Coupled with the world's growing population, severe environmental problems are imposing significant global challenges for humanity. Governments and industries around the world are being pressured to adopt more sustainable practices associated with safeguarding the economic, social and environmental requirements of present and future generations (United Nations, 2015). These three dimensions are known as the Triple Bottom Line (TBL). However, 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, 2016a). 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, among others, improving the system's overall environmental impact, comparing multiple scenarios, or communicating the findings to stakeholders (Hauschild et al., 2018). Nonetheless, the potential applications of LCA are enormous since they can encompass every type of product, process, or activity in all organisations and quantify corresponding environmental impacts that would otherwise be extremely hard to predict (Yang et al., 2019). Meanwhile, environmental regulations have been increasing over the years, and the trend is expected to continue (Sala et al., 2021). Having that said, organisations should be able to carry out these assessments. 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. 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. These obstacles are being discussed while the fourth industrial revolution, commonly labelled as Industry 4.0, is taking place. New technological advancements, such as Artificial Intelligence (AI), the Internet of Things (IoT) or Digital Twin (DT), 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). Consequently, a single joint global endeavour should together strive for both digitalisation and sustainability, as these two are immensely interconnected (Patyal et al., 2022).

LCA has a unique potential to become automated (Culaba et al., 2022). From automatically performing data collection in real-time with reliable sensor-based equipment to utilising more powerful platforms to manage and interpret Big Data (BD). The possibilities are significant and, in many cases, yet to be explored.

1.2. Master’s Dissertation Objectives

This work aims to develop and apply an innovative framework to perform the LCA in the Industry 4.0 context by developing a software tool. To achieve that, this master’s dissertation is structured to accomplish three intermediate objectives: (1) a literature review on the LCA topic to comprehend the methodology and the associated limitations while also outlining significant developments suggested in recent years by scientific research; (2) the development of a methodology to maximise the potential of the LCA by attempting to digitalise common bottleneck procedures using the DT strategy; (3) the development and validation of a software tool that applies the framework’s principles in practice.

1.3. Master’s Dissertation Structure

This master’s dissertation is constituted of seven chapters.

Chapter 1 provides the context of the problem under study and establishes the objectives for this work. It also defines the structure of the document.

Chapter 2 provides a literature review of the LCA methodology. The standard methodology is described, along with why it is still relevant. The limitations associated with the LCA are also outlined. The LCA is then framed in the Industry 4.0’s context. Both methodological and technological proposals of recent years are introduced. This opens space for framing and characterising the problem to be addressed in this master’s dissertation. To conclude, the relevant remarks of this chapter are summarised.

Chapter 3 establishes the research methodology. Four stages are listed, along with their specific goals.

Chapter 4 presents a framework to develop the LCA as a DT model. This theoretical framework adapts the LCA, suggesting procedures to move towards a real-time and bi-directional LCA.

Chapter 5 introduces an original software named TOLCAB (Towards an Online LCA for Bio-based processes), which implements the theoretical framework focusing on the bio-based processing sector. This industry was selected due to its relevance in Denmark, which was the country where this approach was developed. The Initial actions (to configure the physical model) and the assessment and interpretation actions are presented. To conclude, future software development suggestions are mentioned.

Chapter 6 tests and validates TOLCAB by applying the tool to two published LCA studies. The first refers to biodiesel production using rapeseed oil, and the second to β-Galactosidase enzyme production. A discussion segment follows to analyse the tool’s applicability.

Chapter 7 concludes the master’s dissertation by stating final remarks and recommendations for future work.

2. Literature Review

This chapter explores the relevant scientific literature on the latest LCA developments while analysing how and why this practice remains significant. To do so, in the first subchapter (section 2.1), the LCA is introduced and contextualised in a quest to grasp its methodology and purpose. The following subchapter (section 2.2) presents an overview of the recent innovations concerning LCA approaches in the current Industry 4.0 context. Innovative methodological and technological approaches are introduced, as well as the challenges they face across various industries.

Using these findings, the problem that will be addressed in this master's dissertation is framed in the next segment (section 2.3). To close this chapter, both the significant findings and implications of this review are stated (section 2.4).

2.1. Life Cycle Assessment

The LCA methodology is the industry standard to quantify environmental impacts considering the entire life cycle of a product, process, or activity (ISO:14044, 2006). It is a holistic, systematic, and multidisciplinary procedure which gained relevance during the 1990s and is used across all industry sectors (Pieragostini et al., 2012). This section presents the LCA methodology in detail while addressing its significant limitations.

The LCA is a comprehensive, effective and robust scientific tool which measures products, processes or activities' potential environmental impacts across their entire life cycle, from raw materials to the final stages of waste disposal or recycling (ISO 14040, 2006; Mannan & Al-Ghamdi, 2021).

The LCA is used for a wide variety of purposes in government and international organisations, as well as in industry and enterprise sectors (Yang et al., 2019). The European Union recommends using the LCA methodology for environmental assessment and is an active endorser of the implementation of LCA policies (Sala et al., 2021). Manufacturing can benefit largely from this analysis, as testing various combinations of product design, manufacturing process, and material selection can help find more efficient options while significantly impacting sustainability (Escoto et al., 2022). Many review articles performed on several other different sectors, such as energy, agriculture, construction, or bio-based processes, present the LCA as a highly valuable applicable tool (Gangolells et al., 2016; Ingrao et al., 2021; Venkatraj & Dixit, 2022; Culaba et al. 2022). The sustainability pursuit in terms of energy, process, material, environmental friendliness, waste management, as well as the need for a Circular Economy (CE) that prioritizes waste elimination are widely accepted ideas (Daniyan et al., 2021). Moreover, according to research, conducting LCA can have other beneficial side effects. Organisations that assess their products or services have the potential to additionally boost their business activities' value and performance, thus creating competitive advantages at the industrial and corporate levels (Pryshlakivsky and Searcy, 2021). Therefore, by accomplishing better environmental solutions, LCA emerges as a universal proposition.

2.1.1. Standard LCA methodology

With the growing concern towards environmental issues in the last decades of the 20th century, the International Organisation for Standardisation (ISO) created numerous standards. In 1997, the first ISO 14040 series (e.g., ISO 14040 and ISO 14044) was published: a general methodological framework which has harmonised the procedures when performing an LCA. These series were then updated in the following years (i.e., ISO 14040 and ISO 14044, 2006), providing a new framework with principles to guide the LCA's implementation. According to the ISO standards, LCA is an environmental assessment methodology based on four main stages (Figure 1). 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).

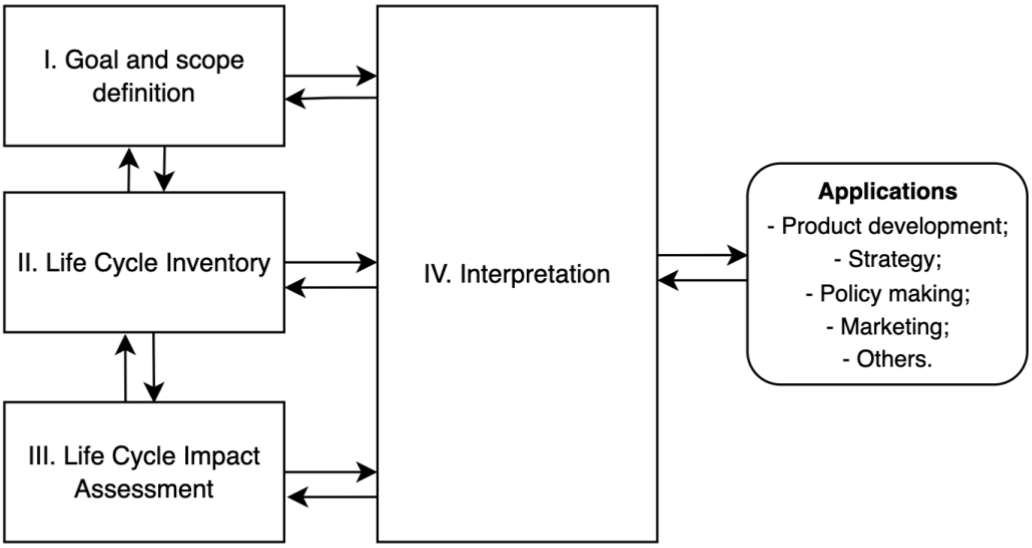


Figure 1 – Life Cycle Assessment framework, adapted from ISO 14040 (2006).

I. Goal and scope definition

The objectives and the scope of the LCA are defined in the first step of the methodology. The goals should clearly identify the study 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 corresponding 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).

A study taking a full life cycle perspective considers all activities from upstream to downstream, to the use phase and disposal in a so-called *cradle-to-grave* study. However, the study may intend to follow a partial life cycle perspective rather than a complete one, according to the objectives and intended applications previously defined. Additionally, it is not practical to include all supply chain data (inputs and outputs) in the LCA (Mannan and Al-Ghamdi, 2022), as their evaluation may lead to enormous efforts when capturing all the necessary inventory data. Also, it may complicate the comparison between systems (Hauschild et al., 2018). Therefore, the study may intend to assess activities occurring from material extraction to the end of the factory system boundary in so-called a *cradle-to-gate* research or even only the activities occurring in the factory system boundary in a *gate-to-gate* study (ISO:14040, 2006). One additional option aligned with the CE concept is to embrace a cradle-to-cradle perspective "through the application of reuse, recovery, and recycling of materials and energy" (Mannan and Al-Ghamdi, 2022). These decisions affect the definition of the functional unit. The functional unit should clarify the function of the product or process in analysis while considering the system boundaries (ISO 14044, 2006) and serves as a reference to scale the following data collection (Hauschild et al., 2018). The functional unit has to be measurable and allow for comparison between systems (Mannan and Al-Ghamdi, 2022). The reference flow can also be defined as the quantity of the product required to produce the functional unit (Hauschild et al., 2018). This definition can be especially relevant in studies considering industrial-scale productions. Moreover, the types and sources of data, the associated data-quality requirements should be determined in this stage, and the existent assumptions and limitations in that data collection (ISO:14044, 2006). A precise and transparent documentation of all the products, processes, or technological methodologies within the system boundaries, must be presented (ISO:14044, 2006). Besides, the data quality requirements should be settled since they will determine the overall quality of the LCA. They include the following criteria (defined in ISO 14044:2006): time-related coverage, geographical coverage, technology coverage, precision, completeness, representativeness, consistency, reproducibility, type of source and related uncertainty. Moreover, the allocation procedures (i.e., the partitioning of inputs and/or outputs in the processes to the product system under analysis) are determined during this stage. Finally, the scope definition should decide on the perspective to apply in the study, whether it is (i) a consequential approach when evaluating the anticipated impacts is a consequence of selecting one choice over another or (ii) an attributional approach when only evaluating the impacts associated with the assessed activity (Hauschild et al., 2018; Ekvall, 2019).

The LCA is an iterative approach: the original scope settings will typically need to be updated as additional information becomes available during data gathering in the life cycle inventory or the subsequent impact assessment and interpretation stages (EC-JRC, 2010).

II. Life Cycle Inventory

The next step of the LCA is the Life Cycle Inventory (LCI). It systematically collects all the inputs and outputs of the processes considered within the system boundaries. To start, the LCI presents the functional unit in detail so that it contains information about the product's quality, quantity, and duration. The function quantification of a product or service intends to enable comparisons between different options in the study. Afterwards, a detailed data collection is required. All inventory flows, meaning all inputs and outputs, 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). Inputs are divided between water, energy, and raw materials; and outputs are between air, land, and water (Mannan and Al-Ghamdi, 2022). The Product Environmental Footprint (PEF) method suggests classifying the flows as elementary or non-elementary (Zampori and Pant, 2019). Elementary flows are any material or energy that entered or left the system without prior or post-human transformation, making it directly linkable to characterisation factors in the LCIA phase (ISO:14040, 2006). Contrarily, non-elementary flows are the remaining flows demanding additional models be translated into elementary flows (Zampori and Pant, 2019).

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). Collected data can be classified as primary or secondary data. Primary data refers to data collected directly in the supply chain process, whereas secondary data refers mainly to robust data collected from different literature sources (Mannan and Al-Ghamdi, 2022). Data for the background system or the portions of the foreground system where more precise data cannot be retrieved are sourced from LCI databases. Several LCI databases are available (e.g., ecoinvent, ELCD, Agri-footprint, LCA food, etc.). However, ecoinvent is the most comprehensive and presumably the most widely used (Hauschild et al., 2018).

Data management comes after comprehensive data collection. As this step deals with large datasets, it demands computational support. Therefore, software (e.g., SimaPro, open LCA, GaBi, among others) analyses and aggregates the data so that it becomes possible to obtain results, according to the functional unit set previously in the goal and scope definition phase (Hauschild et al., 2018). The life cycle inventory (i.e., the list of all the quantified physical elementary flows of the system) is the outcome of the LCI stage (Hauschild et al., 2018).

LCI is generally considered in the literature as 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).

III. Life Cycle Impact Assessment

The following phase is the Life Cycle Impact Assessment (LCIA). It aims to translate the mass data obtained from the previous LCI phase into environmental impacts. This is carried out by converting the inventory flows into apprehensible environmental impacts (e.g., global warming, ozone depletion, acidification, human toxicity, resource consumption, land use, etc.) (Hauschild et al., 2018). This phase 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: (i) normalisation, (ii) grouping, (iii) weighting, and (iv) data quality analysis (ISO:14044, 2006). However, this section will only expand on normalisation and weighting.

The impact assessment impact categories and 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 European Commission recently recommended using the PEF method (European Union, 2021). Even though this method is based on previously existing ones, it leads to more accurate and comparable studies by providing detailed requirements for thoroughly considering supply chain activities (Zampori and Pant, 2019).

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). Characterisation results can be portrayed using the midpoint or the endpoint level. The midpoint is oriented towards a specific environmental problem (e.g., aquatic toxicity, photochemical oxidation, land occupation, or global warming). In contrast, endpoint level is further-down in the cause-effect of environmental damages (e.g., human health, ecosystem quality, climate change and resources) (Hauschild et al., 2018).

Normalisation usually follows to enable comparison between the impact categories (Hauschild et al., 2018). It divides 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 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), generated to simplify the communication of results (Hauschild et al., 2018). However, weighting steps are based on individual choices and are not scientifically based (ISO:14044, 2006). In particular, discussions regarding the final single value obtained appear since it absorbs various hard-to-measure factors (e.g., distance to policy or scientific targets, social evaluation, prevention or repairing costs, energy consumed or panel weighting) and, thus, portrays inherent subjectivity (Hauschild et al., 2018).

IV. Interpretation

The interpretation phase systematically reviews and refines the results obtained in the LCA, aiming to present final conclusions, limitations and recommendations (ISO:14044, 2006).

The first task usually identifies the impact hotspots in the study. According to the Hotspot Analysis report by 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." This is frequently performed using Pareto analysis, where the highest contributors to a given indicator result (e.g., impact category or process) are plotted in descending order (Carvalho, 2015). Their identification can help prioritise potential environmental actions (ISO:14044, 2006). Moreover, the methodological choices, assumptions made during the study, and their associated uncertainties are considered and analysed (Hauschild et al., 2018) according to the goal and scope of the study (ISO:14044, 2006).

Furthermore, uncertainty and sensitivity analyses 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). Uncertainty analysis allows to manage and quantify uncertainty sources, improving the precision and robustness of the study. According with Gargalo et al., (2016), uncertainty analyses include: "(1) evaluating and quantifying errors in the input data, (2) evaluating the propagation of errors in the computations, and (3) evaluating and interpreting errors in the output data*".* Sensitivity analysis can determine how different values of a single variable – usually an environmental hotspot - can affect the results (United Nations, 2017).

To achieve, scenario comparisons may be helpful (ISO:14044, 2006). Depending on the study's goal, they can allow testing different parameters to consider future decision alternatives (Hauschild et al., 2018). To conclude, the study limitations, conclusions and final recommendations must also be reported (ISO:14044, 2006). Note that the LCA may involve many feedback loops between the different phases of the LCA. Therefore, to perform a successful study, it is fundamental to perform iterative processes in order to refine results and accomplish the defined goal (Hauschild et al., 2018).

2.1.2. Limitations

The LCA is an extensively accepted methodology. However, it is widely acknowledged in the literature and requires continuous development (Pieragostini et al., 2012). This section presents key limitations hindering LCA studies. They are summarised in Table 1.

Table 1 - Key limitations hindering the application of LCA.

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

An inherent limitation of the LCA has always been neglecting temporal considerations (Levasseur et al., 2010). The absence of temporal profiles in the life cycle inventory can lead to uncertainty when performing the LCIA (Beloin-Saint-Pierre et al., 2020). LCA provides a single static snapshot of time and does not allow for quickly identifying hotspots and trade-offs (Hagen et al., 2020). Beloin-Saint-Pierre et al. (2020) stated that ignoring temporal considerations is especially severe in sectors like construction or energy since it disregards long lifespan cycles. For example, averaging the CO_2 emissions or the energy consumption values may disguise extreme and undesirable variations. Dynamic Life Cycle Assessment (D-LCA) has been created to consider and define dynamic systems and their temporal differentiation of flows (Levasseur et al., 2010). To date, however, it is tough to predict system lifespans (Gangolells et al., 2016). Thus, D-LCAs are generally not employed and require considerable refinements. The difficulty in accomplishing the novel concept of Live LCA - a real-time environmental assessment - is also part of the issue (Hagen et al., 2020). Due to technological barriers and difficulties in acquiring continuous real-time data, Live LCAs seamlessly gathering data have been scarcely developed into practice (Mashhadi and Behdad, 2018).

There are several uncertainties associated with LCA. According to Mendoza Beltran et al. (2018), among the more common are: “variability, imperfect measurements, gaps, unrepresentativeness of inventory data, methodological choices made by practitioners throughout the LCA, and mathematical relationships (also known as model uncertainty).” The nonlinearity of the environmental impacts, which means that emissions per unit do not scale linearly with the total product produced, is also a substantial source of uncertainty (Gençer et al., 2020). Additional uncertainties are associated with the definition of the functional unit and the system boundaries since it involves generalisations and simplifications in the modelling of the product system (Hauschild et al., 2018). The subjective nature of these classifications may make it difficult to draw comparisons between various evaluations (Beltran et al., 2018). This issue is especially relevant in emerging smart manufacturing contexts since innovative virtual approaches impose new difficulties in defining physical boundaries (Mashhadi and Behdad, 2018). Moreover, data collection and management introduce significant limitations. Collecting data fulfilling high-quality requirements while coping with a complex data management process is a daunting task (Hauschild et al., 2018). Determining a system boundary, which does not contain all conceivable flows and unit processes for a product or service system, creates cut-offs and data gaps (ISO 14040, 2006). Therefore, the availability of accurate input data is commonly referred to in the literature as an LCA limitation (Escoto et al., 2022). Besides, discrepancies in allocation and aggregation processes can provide inadequate data for the LCI (ISO:14044, 2006).

Furthermore, the lack of uniformisation in the methodology creates complications for decision-makers (Hauschild et al., 2018). This is particularly true in the LCIA, as using different assessment methods leads to different results (Wernet et al., 2010), to name a few: (i) different names for similar impact categories or similar names for different impact categories, (ii) contrasting characterisation, and (iii) normalisation factors (Wernet et al., 2010). Performing the LCIA using different methods simultaneously and then comparing them is a way to achieve more robust conclusions. Again, however, this is time-consuming (Hauschild et al., 2018).

Additionally, technological barriers are significant obstacles when performing an LCA. While the software provides essential tools for the eco-assessment (Spreafico and Russo, 2021), its complexity, on the other hand, demands the involvement of experts (Hauschild et al., 2018). This usually implies the assistance of consulting forms in the set-up and maintenance of the LCA, with associated fees and time expenses (Barni et al., 2018).

For example, this is a significant drawback for Small and Medium-sized Manufacturers (SMMs), which account for the vast majority of manufacturing firms worldwide, as many of them are still unsure whether and how to embrace sustainability as a driving business imperative (Escoto et al., 2022). Moreover, the review performed by Spreafico and Russo (2021) on eco-assessment software highlights a tendency toward increased software specialisation concerning the application field. Furthermore, the lack of unified and interoperable data management systems facilitating the user experience in industrial systems is a relevant limitation (Watson et al., 2021).

LCA may also be challenging and expensive to utilise, given the various stakeholders participating in interrelated activities along the supply chain (Teh et al., 2020). Due to the potential lack of trustworthiness between stakeholders, the *trust tax* concept defined by Zhang et al. (2019) highlights the necessary but costly additional contributions (e.g., extra information or resources) to maintain the systems' reliability. Moreover, stakeholders usually resist adopting new technologies (Ghobakhloo, 2018). This slows the essential development of LCA techniques or similar eco-assessment practices.

Besides, utilising the LCA in a policy-regulatory context is problematic since it does not provide a single metric to assist policymakers, and its main strength lies in comparative premises (de Benedetto and Klemeš, 2009). For instance, in the case of new Information and Communication Technologies (ICT) products, negative or positive results of total environmental impacts can depend on how the policies are designed (Hilty et al., 2006). Nonetheless, new ways of dealing with this subject are being introduced, and some sectors have presented novel approaches.

LCA application in complex sectors (e.g., energy, biochemical, construction, etc.) is also of problematic feasibility (Gençer et al., 2020; Ögmundarson et al., 2020; Venkatraj and Dixit, 2022). Their vast technological diversity and the wide variety of materials used across long product life cycles make the LCA a daunting task (Karaszewsk et al., 2021).

Even though LCA is involved in environmental issues, there are other assessments regarding the economic and social sustainability pillars: Life Cycle Cost (LCC) and Social Life Cycle Assessment (S-LCA). However, the lack of unity in these assessments makes it harder to understand possible trade-offs in decision-making (Mahmud et al., 2021), failing to connect LCAs to the strategic perspective of business (Pryshlakivsky and Searcy, 2021). In a quest for both simplicity and reliability, a growing desire to unite these pillars of sustainability in one powerful computer-aided tool has been discussed thoroughly (Pieragostini et al., 2012). Nonetheless, it is relevant to note that environmental concerns do not always imply economic or social drawbacks. In long-term speaking, CE activities can lead to economic growth by promoting responsible and sustainable industrial consumption (Culaba et al., 2022) by utilising fewer resources and valorising waste. Simultaneously, Industry 4.0 is a significant driver for this economic model transition (Sahu et al., 2022).

2.2. LCA in the Industry 4.0

Industry 4.0 has introduced novel paradigms. In this new context, the LCA has the potential to become automated (Culaba et al., 2022). Section 2.2.1 presents the ongoing Industry 4.0 and how it can provide new capabilities when pursuing more sustainable solutions. Next, recent methodological and technological LCA developments are described in sections 2.2.2 and 0.

Ultimately, this section intends to find research gaps to frame the problem addressed in this master's dissertation.

2.2.1. Industry 4.0 and sustainability

Since the first industrial revolution at the end of the seventeenth century, followed by the second and third industrial revolutions, the world has changed drastically. By introducing entirely new ways of production, these revolutions led to improvements in efficiency and productivity, giving rise to overall better conditions for populations (Commission on Environment, 1987). We are currently experiencing the fourth industrial revolution, commonly labelled as the ongoing Industry 4.0. This term was first introduced in 2011 in Germany as various breakthroughs were amalgamating manufacturing with information technology (Kamble et al., 2018). The increasing automation of smart machines has created Smart Factories (SF). Machines are interconnected with web-related services in a concept known as the Internet of Things (IoT). This has enabled large amounts of data, labelled Big Data (BD), to be collected. By analysing and facilitating evidence-based decision-making, this BD can turn into Smart Data (SD), which can generate value (Vacchi et al., 2021). The current technological breakthroughs and modifications to existing business environments are modifying both short-term performance and long-term sustainability (Ghobakhloo, 2018). Furthermore, unlike earlier industrial revolutions, Industry 4.0 has the potential to promote greater operational efficiency without increasing emissions or generating waste (An et al., 2021).

However, Industry 4.0 is still recent, and there is some ambiguity surrounding the concept. Some authors tend to define it using two components: design principles and technological trends (Ghobakhloo, 2018). Design principles are the requisites enabling digital industrial transformation. For instance, the most addressed principles relate to real-time capabilities, virtualisation, interoperability, decentralisation, and virtual/horizontal integration. Technological trends comprehend a wide range of information, digital, and smart manufacturing technologies (Ching et al., 2022). These include facilitating, mature, and accessible technologies (e.g., existing networking systems, software, computer-aided design and manufacturing tools, and sensors), which enable the integrated implementation of recent core technologies providing adaptability and automation. Recent developments include Cyber-Physical Systems (CPS), additive manufacturing, AI, and cloud computing.

From the environmental sustainability standpoint, Industry 4.0 provides enormous opportunities. Industry 4.0's technologies can tackle TBL challenges in sustainable manufacturing at the plant and value chain levels (Ching et al., 2022). New possibilities include, among others, (i) efficient coordination of product, material, and energy throughout the entire product life cycle; (ii) sustainable product design; (iii) sustainable process design and resource efficiency; (iii) increased worker efficiency thanks to Industrial Internet of Things (IIoT) infrastructure; or (iv) the implementation of green business models (Stock and Seliger, 2016). These possibilities can be explored to improve the LCA procedures and tackle some of its limitations: data collection and management difficulties, lack of uniformisation, or complexity in its various forms are just some of the multiple LCA limitations that can be tackled using new technological possibilities (e.g., integrating AI with the LCA, genetic programming to optimise processes, etc.) (Culaba et al., 2022).

Therefore, in the past few years, the pressing necessity of incorporating environmental sustainability in manufacturing has been extensively recognised by politicians, researchers, and industrial enterprises (Thiede, 2018). Governments and industries are calling for investments. Developments in increasing the reliability and maturity of these technologies can eventually lower their costs and ease their adoption (Kamble et al., 2018). Besides, the digitalisation initiatives at the organisational and value chain levels should consider both the unique implications offered by each new Industry 4.0 technology and their *superadditive synergy* (i.e., they can provide singular sustainability implications in a hyper-connected manufacturing ecosystem) (Ching et al., 2022). However, companies face several challenges when adopting Industry 4.0 approaches in production processes. There is still an absence of understanding of the mechanism by which Industry 4.0's technologies enable sustainable manufacturing (Ching et al., 2022). Also, while smart infrastructures can be used to improve current LCA practices, they can impose new considerable environmental burdens, which conventional LCA practices cannot measure (Ferrari et al., 2021). Moreover, these recent technologies can encourage sustainable manufacturing through an intricate, costly, and knowledge-based mechanism, which leaves aside manufacturers without these capabilities (e.g., a large SMM portion) (Escoto et al., 2022). Several other barriers also come into play, such as data security and privacy concerns or difficulties in integration and compatibility between systems (Sahu et al., 2022). Besides, critical organisational and managerial readaptations are necessary to face this ongoing revolution.

Moreover, a new need for standardising LCA integrations with recent technologies brought along by Industry 4.0 appears to be arising. Venkatraj and Dixit (2022), for instance, mention the lack of standardised methodologies as a key factor blocking the integration with Machine Learning (ML) techniques. These and other technological innovations and their implementation challenges will be further explored in the following sections.

2.2.2. Methodological LCA developments

This section introduces the recent methodological developments in conventional LCA techniques. The described proposals intend to expand LCA capabilities. Ultimately, these procedures may provide relevant insights when developing the methodology for this master's dissertation. For each methodological proposal, its own methodology is described, as well as the required inputs and obtained outputs. Potential applications are then addressed, along with their benefits and drawbacks. Finally, recommendations for future work are presented. Table 2 summarises the methodological developments to conventional LCA techniques described in this section.

Dynamic LCA

Putting aside temporal considerations (i.e., all features described concerning the time dimension or dynamic of systems in the LCA Framework) has been identified as a significant cause of uncertainty when performing the LCA (Hauschild et al., 2018), especially regarding LCAs performed in the industry sector (Rovelli et al., 2022). By assuming a static world, conventional LCA techniques disregard the environmental implications of constantly evolving social, economic, and material circumstances (Sohn et al., 2020). This lack of temporal considerations in most LCA studies is concerning, as it has been demonstrated that such factors can have a significant impact on its 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. The same study reviewed many D-LCA applications and found that their implementation varies widely. Namely, it identified (i) the full D-LCA - where temporally induced changes are incorporated in all phases of the assessment; (ii) the prospective D-LCA – when the assessment is made for a single point in the future; and (iii) the partially D-LCA – when dynamism is only applied in specific parts of the LCA. While dynamic elements are critical, implementing them with existing software might be challenging (Sohn et al., 2020). Operational methods for calculating time-differentiated inventory and impacts are still insufficient (Pigné et al., 2020). However, the need for such dynamic capabilities must increase for this form of software to be developed (Sohn et al., 2020).

The first operational framework for implementing an entirely temporally differentiated full LCA was conducted by Pigné et al. (2020) based on the model developed by (Tiruta-Barna et al., 2016). The study includes the temporalisation of the background and foreground systems while introducing several key ideas. Combined with appropriate impact calculation methods, a time-differentiated LCI is the first requirement for a consistent D-LCA approach. Rather than being based on an accounting perspective, the dynamic LCI model is based on supply chain modelling - meaning time dependency in demand-supply relationships is considered. When Tiruta-Barna et al. (2016) first introduced this approach it was a breakthrough. The inputs for this approach consist of (i) unit processes – including background and foreground operations - that demonstrate a pattern of behaviour throughout time; (ii) unit and material or energy interventions with their respective temporal profile; (iii) specific supply models, which determine intermediary exchanges between unit processes; and (iv) temporal parameters and functions to describe production and supply. These efforts are further processed using dynamic LCIA models, such as dynamic characterisation factors for limited time intervals. Although the results proved difficult to be translated over time, the case study presented in the same research (Pigné et al., 2020) demonstrated that addressing temporal differentiation across the whole life cycle, particularly in the background system, can drastically alter LCA results and their interpretation. By conducting a full D-LCA, including the use of dynamic LCIA models, one can leverage the full potential of temporally differentiated LCI results. Accounting for temporal considerations has a considerable impact on the outcomes of several case studies, especially long-term systems, which can benefit from models and methods that address the dynamics of energy and material flows in even greater depth (Beloin-Saint-Pierre et al., 2020). Furthermore, the D-LCA framework developed is a flexible tool. A new temporal database can be built up for any other LCA database, and a relatively small number of temporal parameters can be analysed for many processes, thus characterising generic supply chains. On the other hand, this framework presents some disadvantages. Because the algorithm is computationally intensive, calculation time reveals to be crucial. Large datasets can also pose problems with storage and induce latencies. Overall, it is a costly and time-consuming assessment due to its complexity.

To overcome these limitations, some recommendations include the development of temporal databases for products and processes, including the option to create calendar-specific timings (e.g., to include seasonal aspects); modelling supply-demand; coupling with other LCIA modules; and improving computational efficiency, user-friendliness, and compatibility with other software (e.g., OpenLCA) (Pigné et al., 2020). These elements represent interesting opportunities for future research studies.

The framework presented here only represents a fraction of the developments in this area since fully conducted D-LCAs are scarcely mentioned in the literature (Pigné et al., 2020). However, that is not the case for partial D-LCAs, which are conducted regularly and are expected to continue (Beloin-Saint-

Pierre et al., 2020). Temporal considerations are largely arising due to the capabilities of real-time data collection technologies (Ferrari et al., 2021). To obtain reliable results, it is, therefore, fundamental for LCA practitioners to understand the dynamism of the systems they assess (Levasseur et al., 2010).

Organisational LCA

Although the LCA was initially created for products, its potential can be used to evaluate organisations. Therefore, the ideas, rules, and requirements of ISO 14040 and ISO 14044 serve as the foundation for Organisational Life Cycle Assessment (O-LCA) (Hauschild et al., 2018). However, some adjustments are necessary. Thus, the O-LCA methodology is defined in the ISO/TS 14072 and thoroughly covered in the Guidance on Organisational Life Cycle Assessment publication (UNEP, 2015) as a compilation and evaluation of the inputs, outputs, and potential environmental impacts of the activities associated with the organisation as a whole or portion thereof adopting a life cycle perspective. It was developed to expand the scope of LCA from products to organisations, considering their value chains (Marx et al., 2020).

The O-LCA tends to be much more complex than the conventional LCA: assessing multiple product life cycles or coordinating the various stakeholders in the value chain can introduce a vast spectrum of resources, emissions, and waste to be analysed in a whole organisation (de Camargo et al., 2019).

The O-LCA encourages a great effort in performing a complete cradle-to-grave assessment, and only if the organisation holds no influence in specific downstream life-cycle stages (i.e., usage and EoL) can it employ a cradle-to-gate perspective (UNEP, 2015) Due to the wide range of activities and processes to be addressed, inventory data gathering is one of the most challenging tasks in O-LCA (Forin et al., 2019). Having available disaggregated data (e.g., by activity, geography, brand, or facility) is strongly advised, especially for organisations with diverse product portfolios (UNEP, 2015). By doing so, organisations can distribute environmental impacts among different chosen product categories and even derive product LCAs from the O-LCA. In general, to collect data, the O-LCA methodology encompasses three distinct ways: (i) a top-down or inventory-oriented approach – reporting the organisation as a whole and adding upstream and downstream models; (ii) a bottom-up or product-oriented approach – summing the different LCAs of products, including the supporting activities; or (iii) the possibility of combining both approaches in a hybrid or intermediate approach (UNEP, 2015). For the bottom-up approach, more disaggregated data is expected, which is helpful, as mentioned. However, the top-down approach also includes advantages, for instance, when collecting a given plant's fixed energy or water consumption. Nonetheless, findings from both perspectives should be consistent, even if not equal (UNEP, 2015). Either way, due to the collaborative nature when sharing data between upstream and downstream portions, O-LCA is expected to improve the quality and transparency of data (Cucchi et al., 2022).

The impact assessment and interpretation stages are essentially the same as in conventional product LCAs. Thus, the same standards apply (UNEP, 2015). In 2012, the European Commission recommended using the Organisational Environmental Footprint method (Pelletier et al., 2012). Therefore, a complete O-LCA model can help to identify environmental hotspots, forecast and compare scenarios testing trade-offs between categories, or track environmental performance according to pre-defined targets (Forin et al., 2019). Environmental reports can then be stated to communicate findings with stakeholders, encourage innovation, minimise risks, or prepare for future regulations (UNEP, 2015). As a result, O-LCA provides environmental information that can be well translated into actual organisational decision-making (Rimano et al., 2021). The internal operations and value chain knowledge provided by this methodology have, thus, a valuable prospective strategic potential for organisations. The O-LCA efforts can encourage the development of new data collection and management systems (UNEP, 2015).

The O-LCA can be applied to every type of organisation, regardless of its size, location, or sector; this includes less digitalised SMEs since also they can benefit from applying the O-LCA (Cucchi et al., 2022; Marx et al., 2020). On the other hand, this wide applicability range means there is no *one-size-fits-all solution*, and each organisation should build their own application (Forin et al., 2019). Manufacturing organisations, in particular, must focus not only on specific environmental consequences but simultaneously on measuring sustainability holistically by assessing the whole supply chain (Cucchi et al., 2022). Furthermore, every social sector (e.g., NGOs, governments, or universities) should seek to use organisational environmental evaluation methodologies, not just profit-driven companies (UNEP, 2015). Industrial symbiosis contexts can benefit especially from this application due to its unique collaborative environment between economic agents in the supply chain (Cucchi et al., 2022).

The following authors emphasised the capabilities of Industry 4.0's digital technologies to provide long-term sustainability, and, therefore, encouraged future efforts to connect them with the O-LCA methodology: (i) by studying 12 *road-testing* organisations Forin et al. (2019) presented some challenges for the O-LCA application, but ultimately verified its usability and effectiveness; (ii) Marx et al. (2020) showed that, while service-provider organisations may face additional methodological challenges when implementing the O-LCA, they may benefit from its use; (iii) Alejandrino et al. (2022), by combining the O-LCA Framework with an innovative Life Cycle Costing of Organisations (O-LCC), proposed and executed an eco-efficiency technique capable of assessing and prioritising CE solutions at the organisational level based on their environmental and economic performance; and (iv) Cucchi et al. (2022) developed an O-LCA integrated into a ceramic manufacturing company, successfully combing Industry 4.0 technologies with this methodology, as they allow to perform a quicker and more dynamic data collection.

Moreover, previous use of the LCA methodology is referred to as beneficial to ease the O-LCA application (Forin et al., 2019). However, the inherent hard replicability and scalability are major barriers hindering O-LCA adoption (Cucchi et al., 2022). They persist, in part, because there is yet to be a specific O-LCA software solution (Forin et al., 2019; Marx et al., 2020). Additional challenges discouraging O-LCA application include the inherent complexity involved in processes such as identifying and classifying activities, assessing data quality, interpreting results, preparing environmental reports, reducing operational costs or enhancing stakeholders' environmental tools (Forin et al., 2019). Moreover, although O-LCA is a broad assessment, social and economic sustainable pillars are left behind (Alejandrino et al., 2022).

Therefore, the literature agrees that O-LCA is still under-researched and lacks application examples. According to Forin et al. (2019), creating O-LCA-specific software and regional databases, as well as building frameworks to make data quality assessment easier, might go a long way. Integrating this complex methodology with Industry 4.0 technologies also represents significant opportunities (Cucchi et al., 2022). Future research efforts should aim to broaden the use of O-LCA, as it has proven to be a beneficial tool for providing a holistic environmental evaluation.

Ubiquitous LCA

Mashhadi and Behdad (2018) proposed a new concept for assessing environmental and social impacts in the current context of Industry 4.0. The authors suggest a methodology framework to improve assessments of emerging systems while aiding decision-making processes. Ubiquitous Life Cycle Assessment (U-LCA) fundamentally reformulates the traditional definition of the functional unit fundamentally. 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. Furthermore, they propose a proactive LCA framework capable of reaching optimum sustainable decisions across the TBL requirements. 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. Even though defining system boundaries has for long been a challenge in the LCA due to its inherent subjectivity, this obstruction has become preponderant nowadays: organisations are finding it difficult to understand the full scope of their responsibilities, as current Industry 4.0's business models work according to non-trivial boundaries. Therefore, as the environmental burdens imposed by smart infrastructures should not be discarded (Hilty et al., 2006), there is a greater need to develop techniques capable of measuring those impacts. The U-LCA methodology includes smart capabilities to track product data during its entire life cycle, including the usage and EoL phases, which are typically left unassessed. To do that, the authors propose a *Self-Monitoring, Analysis and Reporting Technology (S.M.A.R.T)* using *product identity data,* continuously monitoring individual product flows. This real-time computation method ensures that the temporal and spatial considerations are addressed, contributing to a more accurate LCIA. Smart enterprises can benefit a lot from using this contemplated methodology. U-LCA provides an accurate real-time assessment capable of tracking emerging systems to ultimately originate more sustainable decisions. On the other hand, U-LCA is still a conceptual framework, lacking further research and implementation efforts. Moreover, companies lacking a smart infrastructure may fall behind (Ferrari et al., 2021). Future research endeavours are, thus, recommended to extend U-LCA's practical utilisation while aiming to expand the use of smart capabilities in sustainable assessments. Table 2 summarises the methodological developments to conventional LCA techniques described in this section.

Table 2 - Methodological LCA developments reviewed in this work.

	Ubiquitous Life Cycle Assessments (U-LCA)	Organisational Life Cycle Assessment (O-LCA)	Dynamic Life Cycle Assessment (D-LCA)
Inputs	Smart manufacturing infrastructure (IoT sensor, BD, real-time computation, cloud computing); Considers entire life cycle and respective temporal, spatial and global impacts.	Data for the impacts of the whole or a portion organisation's activities; Disaggregated data is preferable.	Unit processes – background and foreground operations – patterns of behaviour over time; Unit and material or energy interventions with their own temporal profile; Specific supply models that define intermediary exchanges between unit processes; Temporal parameters and functions to describe production and supply.
Methodology	Real-time methodology; Product identity data (self-monitoring, analysis and reporting technology).	Bottom-up or top-down approach for inventory analysis; IoT data collection linked with the company's ERP; Possible simplifications: deriving the organisation' s impacts from the inventory analysis of a single plant.	1) a dynamic LCI model; 2) a temporal database including temporal characterisation; 3) a graph search algorithm; 4) dynamic LCIA models.
Outputs	Traceability of products; Real-time computation and assessment of impacts; Self-awareness; Temporal, spatial and global impact assessment; Accurate and exclusive impact assessment.	Identification of environmentally critical phases; External communication with stakeholders; Simple model to account for the global organisation's impact.	Impact curves over time for each individual procedure or substance or aggregated by impact category.
Advantages	Emergent systems - measurement of smart manufacturing environmental impacts; Real-time assessment; Encompasses entire life cycle and respective temporal, spatial and global impacts; Traceability - enables usage phase impacts; TBL sustainability; Comprehensive understanding of the functional unit.	Quality of data for LCI - collaboration, transparency and responsibility between shareholders; Knowledge - internal operations and value chain; Broader life cycle perspective - relevant for industrial symbiosis scenarios; Preparatory to single product category-specific LCAs - O-LCA as the initial step in identifying the organisation's environmental baseline; Suitable for less digitalised organisations; Detects unique environmental hotspots; Standardised approach - ISO/TS 14072 technical standard and the UNEP 2015 guidelines; Prospective strategic relevance.	Results - time considerations affect results and their interpretation; Flexible - Few parameters and adaptable to other studies.
Disadvantages	Singular and recent conceptual methodological proposal; Requires a smart ICT infrastructure; Uncertainties regarding long-term environmental impacts of smart capabilities.	Under-researched methodology: High complexity - organisations producing a variety of products or where supporting activities are more relevant may find it complex to assess everything; Lacking an O-LCA-specific software solution; Databases need further improvements; Still lacking application tests in various contexts and organisations; Difficult application for some sectors (e.g. building sector, service sector).	High complexity - manual data collection and insertion for foreground processes and extensive databases for background processes; Difficult interpretation of results - only presented as impact curves over time; Computationally intensive.
References	Mashhadi & Behdad, 2018.	Pelletier et al., 2012; UNEP, 2015; Forin et al., 2018; Manzardo et al., 2018; de Camargo et al., 2019; Marx et al., 2020; Rimano et al., 2021; Alejandrino et al., 2022; Cucchi et al., 2022.	Levasseur et al., 2010; Tiruta-Barna et al., 2016; Pigné et al., 2020; Sohn et al., 2020; Beloin-Saint-Pierre et al., 2020; Rovelli et al., 2021; Ferrari et al., 2021.

2.2.3. Technologies enabling LCA in the Industry 4.0

The limitations associated with the LCA (presented in section 2.1.2) are multifaceted and require actions on multiple fronts. Several authors mention various opportunities to overcome them using technologies brought by Industry 4.0 (Ching et al., 2022; Hagen et al., 2020). Therefore, this subchapter aims to analyse different Industry's 4.0 technologies that can be applied to enhance LCA procedures. They were chosen based on perceived novelty and impact in an attempt to highlight recent scientific efforts. Ultimately, these novelties may provide relevant insights when developing the methodology for this master's dissertation. The key findings from the enabling technologies for the LCA development in Industry 4.0 are compiled in Table 3.

It is worth noting that the approaches employed frequently combine multiple technologies. For instance, several studies mention using smart sensors as primary data sources while also relying on IoT to manage data or BD analytics to interpret it (Ferrari et al., 2021; Mieras et al., 2019; Zhang et al., 2019; etc.). For each technology presented, respective methodologies and the corresponding inputs and outputs are introduced. Then, potential applications are discussed as their advantages and disadvantages. In the end, general future work recommendations are addressed.

Smart sensor-based technologies

Data collection and data management strategies are of special importance under the Industry 4.0's 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, 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. Potential monitoring objectives, meaning the determination of the sensor's desired outputs, include measuring pressure, temperature, energy, consumption, spatial dimensions, and light intensity, among many others. General sensor characteristics include their inherent reliability, speed of data acquisition and analysis, cost, energy consumption, accuracy, invasiveness, security, and autonomy (Watson et al., 2021). It is relevant to mention that not all these smart sensor equipment is on the same page regarding the Technology Readiness Level (TRL). Hence, this factor should also be considered. Some typical sensor examples operating in hands with LCAs are smart electricity metres, smart water metres, Radio-Frequency Identification (RFID) readers, intelligent heat metres, intelligent gas metres, fibre optical sensors, or Global Positioning Systems (GPS) (e.g., to measure transportation routes).

Typically, each module is connected to a server via its own PLC, thus enabling the detection of incoming and outgoing goods (Hagen et al., 2020). The information collected by monitoring systems in the data acquisition layer is then transferred to the upper layers. Namely, the data transmission, platform and application layers, can differ substantially as they include various enterprise information tools.

Regarding data entry modalities, Spreafico and Russo (2021) mention a discordance between academia and industry: academia prefers manual entry, while the industry shows more interest in automatic sensors. The same study argues that in the industry case, the diffusion of sensors is increasing despite other modalities. In this context, another relevant topic is soft sensors, also labelled as hybrid or model-based sensors. They provide inferential sensing technology to estimate unmeasurable parameters (Udugama et al., 2021).

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). Ferrari et al. (2021) studied this integration by implementing an Industry 4.0 factory design for dynamic data gathering, integrating an ERP application with a customised LCA tool for the specific industrial system (a ceramic manufacturer) through Business Intelligence (BI) software. Using real data flows collected from sensor-based equipment might reduce the complexity, restrictions, and inconsistencies in data when performing the LCI.

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 contributing to increasing resource efficiency and lowering the sector's carbon impact. Another example is given in Ingrao et al. (2021), which particularly 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. The same study claims that direct measurements consider certain aspects that fail to be addressed in mathematical models (e.g., malfunctions or consumption of control circuits, displays and other electronic parts).

By enabling sensors to link to the internet with cloud computing capabilities, cost and size reductions of on-site gear are achieved (Watson et al., 2021). Moreover, by monitoring and tracking a product's life cycle and respective impacts, they are emerging as promising approaches for improving traditional physical machines' abilities (Zhang et al., 2020). By recording waste data in real-time during manufacturing and sharing it with all stakeholders in the food supply chain, Jagtap and Rahimifard (2019) reduced food waste by 60.7%. An et al. (2021) also presented a real-time IoT system exclusively designed for wind turbines, and when compared to conventional LCA systems in the sector, they managed to considerably reduce the workload attributed to data collection while improving LCA's accuracy and response time.

Additionally, intelligent network sensors and PLCs collecting data can be used for production control. Real-time sensor-based LCAs can incorporate temporal and potentially spatial dynamics of systems, while tracking production resources, ultimately resulting in competitive advantages (Karaszewski et al., 2021). Therefore, implementing a monitoring infrastructure can serve multiple purposes, both environmentally and economically.

On the other hand, even though IoT has been effectively utilised in a variety of disciplines, its use in LCA is still in its infancy (An et al., 2021). Implementing and maintaining such infrastructures, capable of collecting and managing BD generated by the monitoring system, is costly (Ingrao et al., 2021). Certain challenging industrial environments (e.g., the food and agriculture sectors) are delaying the adoption of these technologies due to the current lack of cost-effective monitoring options (Watson et al., 2021). Stakeholders in the supply chain are sometimes reluctant to share data concerning their internal processes (Ferrari et al., 2021). Moreover, LCA experts that can effectively integrate the given sensing technologies with the LCA lack guidance to ensure platform interoperability and compatibility. Thus, standardisation is crucial for the widespread adoption of IoT since it ensures scalability and compatibility throughout various industrial environments (An et al., 2021).

Future work recommendations on this topic include: (i) integrating sensor-based capabilities with other Industry 4.0 technologies (e.g., blockchain, ML, etc.); (ii) incorporating in enterprise production systems; and (iii) developing sensor fusion options, meaning, merging diverse sensors to provide less uncertain information (Watson et al., 2021).

Blockchain

Blockchain technology first appeared as a technology to support transactions in the crypto-currency field (i.e., bitcoin) (Nakamoto, 2008). However, blockchain applications are not restricted to financial services. They can include any computerised information transport, as they are essentially a database which allows vast amounts of data to be accessed and transmitted in real-time (Ghobakhloo, 2018; Karaszewski et al., 2021).

Recent blockchain applications include financial services, insurance, food, health care, supply chain management, and governments. Blockchain technology is widely considered to have the potential to disrupt many existing industries (Zhang et al., 2020). Both the United Nations Economic Commission for Europe (UNECE) and the World Economic Forum (WEF) has incited the adoption of blockchain as a strategy for transforming societies into more sustainable and resilient ones (Teh et al., 2020). Blockchain can be used to verify numerous sustainability-related aspects in the supply chain, both upstream and downstream, such as worker living conditions, pay, and environmental impacts (Teh et al., 2020).

Blockchain is a form of Distributed Ledger Technology (DLT), which refers to the technological architecture and procedures that enable information transactions between peers in a decentralised way. This technology comprises a shared database formed by a digital ledger and a distributed peer-to-peer network (Teh et al., 2020). It stands apart from other information systems thanks to four primary characteristics: decentralisation, involving the exchange of control from a centralised entity to distributed network; security, ensured through a transaction log saved across many distributed nodes; audibility, occurring when the majority of nodes approve the transaction; and smart execution, guaranteed since the processes can be executed by smart contracts (Figueiredo et al., 2022; Kouhizadeh et al., 2021).

There is already a scientific discussion about how blockchain's transparent and open character can benefit LCA applications. As available quality data is vitally crucial in an LCA analysis (Venkatraj and Dixit, 2022), blockchain applications can reduce information uncertainty, minimise data collecting time, and guarantee flawless data source traceability (Kouhizadeh and Sarkis, 2018). Moreover, blockchain technology benefits other LCA stages, as it ensures traceability and transparency of the goal and scope definition and creates analytical forms at the LCIA level (Karaszewski et al., 2021). (Carrières et al., 2021) add a blockchain-based LCA would also be advantageous for eco-conception design. Consequently, blockchain technology is a compelling tool for achieving operational excellence in LCA (Zhang et al., 2020).

Zhang et al. (2020) propose a framework to guide the implementation of a blockchain-based LCA. The authors combine blockchain with other Industry 4.0 technologies, namely IoT and BD analytics and visualisation. Data collection requires a physical infrastructure powered by IoT technologies, enabling large-scale real-time data generation. The physical inputs are automatically translated to the blockchain services layer through hardware (i.e., smart sensors, local servers and storage, and network) in the supply chain, followed by a Gate Operating System (GOS) software. Without the need for central verification, these transactions or digital events are confirmed and updated in real-time by the consensus of system members (Teh et al., 2020). Then, BD and supply chain analytics provide powerful data management capabilities in the service and application layers, thus guiding decision-makers toward more informed decisions. The authors of this framework were pioneers, mainly due to the disruptive nature of the technology.

As for the advantages when using a blockchain-based LCA, this technology supports companies in implementing more robust supply chain management practices (Teh et al., 2020), which can minimise natural resource usage by enabling data integrity through transparency and traceability (Figueiredo et al., 2022). This tractability allows for the retrieval of sub-level impact queries based on multiple parameters, such as product model or type of use (Mashhadi and Behdad, 2018). Since tracking is improved, the relationship between blockchain and CE is clear – it facilitates authentication, resale, and materials recovery. As a result, this system design extends beyond the traditional cradle-to-grave approach, embracing a cradle-to-cradle one – crucial for transitioning to a CE model (Zhang et al., 2020). Moreover, while providing a reliable, efficient, secure, and up-to-date service (Carrières et al., 2021; Zhang et al., 2019), blockchain can bring together stakeholders from the entire supply chain, from acquirers, producers, and intermediaries, to end consumers (Teh et al., 2020).

Besides, constructing a blockchain-based system is not prohibitively expensive (Zhang et al., 2020). However, costs may vary depending on the existing infrastructure across the supply chain. There is a gap between large tech companies with existent infrastructure and Small and Medium-sized Enterprises (SMEs). The full potential of blockchain cannot be realised without smart enabling technologies like IoT, BD analytics, cloud computing, and data visualisation. Thus, SMEs using blockchain must build competencies in smart enabling technologies (Zhang et al., 2020).

There are other technical barriers when implementing blockchain-based LCA. Large quantities of transactions can pose computational and data-storing issues, as rising block sizes are a challenge when dealing with enormous amounts of data in real life (a problem labelled as *bloat* in cryptocurrency) (Kouhizadeh et al., 2021). These issues can also result in higher levels of energy consumption and system latency (Figueiredo et al., 2022). Moreover, the blockchain's inherent characteristics of immutability and interoperability can pose problems, as possible information transaction errors are forever recorded, and the integration with different information systems can be complex (Carrières et al., 2021). There is also a lack of research regarding methods for verifying the legitimacy of subjective sources, as most extant research relies on data from objective sources (Karaszewski et al., 2021).

Furthermore, privacy is a big concern. Although blockchain helps significantly to minimise *trust tax* expenses (mentioned before in section 2.1.2), decentralisation can pose problems since data can be publicly accessed. Different data privacy demands may exist among supply chain players, and some players may even have a solid incentive to profit from exchanging false data with other supply chain participants (Zhang et al., 2020). Coordinating and managing stakeholders can simultaneously pose serious organisational difficulties (Karaszewski et al., 2021).

Even though blockchain technology has been promoted for years, it has yet to gain widespread acceptance (Kouhizadeh et al., 2021). Because of its origins in cryptocurrency, this technology has a poor public impression (Zhang et al., 2020). Therefore, blockchain technology is less widely addressed than other Industry 4.0 innovations (Zheng et al., 2021). There is also a general lack of understanding about blockchain applications in sustainable practices, which results in an overall absence of governmental regulation (Carrières et al., 2021). Figueiredo et al. (2022) concluded that there is a delayed adoption of process and technological advancements in the construction industry and real estate cases. And these sectors are not alone in their reluctance. A complete paradigm shift is required to persuade governments and corporations to invest more in blockchain capabilities.

Artificial Intelligence

Artificial intelligence (AI) studies machines that can perform intelligent tasks like problem-solving and learning (Akhshik et al., 2022). AI can have various applications (e.g., pattern recognition, modelling, simulations, and predictions) for a wide range of sectors. Some of these applications can be categorised as Machine Learning (ML) techniques, which are focused on steadily improving accuracy by using data and algorithms (Philipp Schume, 2020). ML approaches have become increasingly popular as large-scale data has become more accessible (Venkatraj and Dixit, 2022) since they are typically suited for scenarios with large amounts of available data (Watson et al., 2021). (Akhshik et al., 2022) even state that the creation of vast amounts of data due to the advent of IoT has left us with no other method to cope with the zettabytes of data other than ML. However, ML has yet to be significatively developed in the field of environmental assessment, fundamentally due to the absence of sufficient quality data (Akhshik et al., 2022). Nevertheless, there are opportunities to automate LCA using AI. These opportunities are especially relevant in data collection and management processes.

Regarding data collection, Watson et al., (2021) claim that ML models that turn sensor data into meaningful, actionable information are at the heart of intelligent sensors. Culaba et al. (2022) add that a relatively small number of sensors in the system can have a great capacity to forecast and analyse the system performance and environmental effect, thanks to the use of genetic programming – an AI approach to create evolving computer programmes that answer pre-defined automated programming and ML issues (Schwender, 2010).

Regarding data management, several opportunities also arise. The absence of large-scale data in some industries, such as the building sector (D'Amico et al., 2019) and others, can present low accuracies for environmental assessments. However, AI and ML techniques offer ways to cope with that. The research performed by Akhshik et al. (2022) compared and predicted carbon emissions when substituting materials in automotive parts by using ML. Through applying several AI algorithms and input matrices, they managed to predict and compare Greenhouse Gas (GHG) emission options. This study presented a unique way of dealing with a minimal quantity of data, which typically discourages researchers from performing a reliable LCA. This appears to be a promising approach for predicting the environmental impacts of material options. However, further developments and discussions are fundamental.

ML techniques can differ widely based on the desired tasks, the most common being classification or regressive, and they can also be further classified depending on their learning approach (Watson et al., 2021). Nonetheless, practitioners' methodologies follow similar patterns: determining the required output, choosing the most suited ML algorithm; setting the model hyperparameters; training; validating, and finally, testing the model.

There seems to be a generalised trend in literature to enhance the collection of large-scale quality data (D'Amico et al., 2019). AI techniques, and particularly ML algorithms, require large datasets, and researchers agree that gathering data is more difficult than training the ML models themselves (Venkatraj and Dixit, 2022). However, through prediction models, a quick and low-cost analysis can be performed even before design, while not fully compromising the reliability of results (Akhshik et al., 2022). Integrating AI with LCA also presents a viable method for translating large-scale data into apprehensible operational guidance (Culaba et al., 2022).

Even though AI approaches still require further developments, the Culaba et al. (2022) review concluded that the implications of employing AI in a smart biorefinery system have no significant adverse impact but have the power to improve existing processes. This statement is likely to be true for other industry sectors. However, research efforts in developing LCA techniques capable of measuring the impacts of new technologies in different sectors must be carried out (Mashhadi and Behdad, 2018). Recent research efforts have been inconsistent and fragmented, not focusing on generalising and transferring findings to different scenarios (Venkatraj and Dixit, 2022).

Nonetheless, the possibility of AI in managing large-scale data still needs to serve its potential. Creating large datasets will allow for more robust assessments. Currently, there is a general lack of consistency and transparency in collecting, evaluating, and structuring data, which makes it challenging to evaluate and compare the performances of different ML approaches (Venkatraj and Dixit, 2022; Watson et al., 2021). Therefore, creating standardised ML methodologies is vital to expand their use. Even though these data-driven strategies need significant initial efforts to design and test computational algorithms, once they are established, they can provide faster and more reliable evaluations (Akhshik et al., 2022; Venkatraj and Dixit, 2022). This is a critical issue to promote the use of AI for the LCA.

Besides, integrated AI methodologies need to address temporal considerations. This thesis has pointed out their relevance (section 2.1.2). Efforts in performing full D-LCAs should join AI endeavours, as current prediction models struggle to introduce dynamic situations (Venkatraj and Dixit, 2022).

Moreover, using scarce data sources to accurately predict scenarios is a recent topic, and there is still a long way ahead (Akhshik et al., 2022). Having multiple stakeholders contributing to creating anonymised and aggregated databases would contribute immensely (D'Amico et al., 2019). Also, adopting transparent, open-source platforms for LCA users to insert data could help create large-scale databases (Venkatraj and Dixit, 2022). This way, large-scale data could be translated into apprehensible operational guidance by integrating AI with LCA (Culaba et al., 2022).

It is also important to emphasise that AI technologies are constantly developing. Computational intelligence may still be simplified while maintaining its prediction and optimisation effectiveness (Culaba et al., 2022).To conclude, combining AI improvement efforts with LCA developments can widen the LCA user base, thus increasing the total number of decisions based on sustainability indicators (D'Amico et al., 2019).

Cyber-Physical Systems

Cyber-Physical Systems (CPS) are disruptive technologies promoting interconnectivity between physical assets and computational capabilities (Ghobakhloo, 2018). By integrating CPS with current operational practices, the economic potential of factories can increase, helping them to become Industry 4.0 smart factories (Lee et al., 2015). CPS are operated and monitored using computer-based algorithms which are tightly connected over the internet to their users (e.g., machines, products, materials, or humans) (Ghobakhloo, 2018). Therefore, they offer vast possibilities for managing BD (Lee et al., 2015). In particular, systems that improve factories by interconnecting production machines and process chains are called Cyber-Physical Production Systems (CPPS) (Thiede, 2018).

Nowadays, many production systems include a variety of IT-related hardware and software (e.g., sensors, PLCs, ERP, MES) to facilitate operations. However, CPPSs are unique due to their specific use with designated functionalities (Thiede, 2018). There may be various CPPSs in the same production environment, each possibly requiring extra components (Thiede, 2018).

Integrating CPPS systems with LCA was conceptually explored in the framework developed by Thiede, (2018) and further explored by Hagen et al. (2020). The framework examines and displays the environmental assessment database formed by the link between the cyber and physical worlds. These studies present innovative LCA approaches using CPPS to perform a real-time product LCA.

The inputs for this conceptual model include all the elements (i.e., materials, energy, and water) leading to the dynamic impact of the final product. Information is obtained from real-time measurements of the physical system, collecting data both from the production equipment and their respective control infrastructure (e.g., installed sensors or PLCs). Having the physical system dynamically characterised allows for creating large datasets establishing the foundation for the LCI. Afterwards, the cyber world analyses data and forecasts processes. The evaluation is performed via the LCIA, which leads to visualising the results to support stakeholders in their decision-making processes.

The technical implementation of this environmental assessment framework evolves interconnected production process modules. Each module is connected to a server using PLCs. They are responsible for detecting inbound, and outbound flows through RFID chips. Afterwards, the cyber world consists of industrial-grade middleware, connecting the shop floor with the software layer. This information is then processed by the developed code of Live LCA, programmed using python. Finally, a visualisation tool facilitates understanding and empowers decision-makers to compare different scenarios.

It is important to note that CPPS viability is primarily determined by the specific case study and its respective design and operational parameters (Thiede, 2018). Nonetheless, the application of CPPS systems enables LCA users to reflect on their actions and corresponding environmental consequences while making decisions (Hagen et al., 2020).

Due to their innovative nature, the mentioned works still possess several limitations. The existent studies lack a full life cycle perspective, a full D-LCA approach, or a practical application in complex scenarios, as significant simplifications were made during the data collection and management processes. Overall, the TBL sustainable perspective needs to be considered to its full potential.

On the other hand, there is evidence that CPPS systems can provide practical tools to adjust operational management to high-level sustainability objectives by improving productivity and resource efficiency in a wide range of industrial processes (Ballarino et al., 2017). The successful application presented by Kumar et al. (2022) for 3D printed products or the smart energy grid application performed by Ballarino et al. (2017) provides tangible examples of success.

Therefore, future research integrated into more complex production systems is recommended, as well as further technological development and testing (Ching et al., 2022). Nonetheless, CPPS have the potential to achieve intelligent, robust, and self-adaptable machines capable of handling BD and leveraging machine interconnectivity (Lee et al., 2015).

Digital Twin

Digital Twin (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 at 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 company’s products and processes.” According to the authors, DT can help the LCA become more accurate and automated. When used in conjunction with a network of sensors, DT not only can describe real-time processes but also produce simulated data to aid LCA forecasts. DT capabilities can reduce traditional burdens of data collection 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 essentially conceptual contributions. Moreover, the systematic review presented by Kamble et al. (2022) on the DT technology for sustainable purposes mentions that existing literature still needs to consider the life cycle perspective in depth.

This section introduces a general DT methodology for sustainable assessment practices based primarily on the mentioned research efforts by Barni et al. (2018) and Ghita et al. (2021). First, when developing the DT model, sustainable goals should be emphasised right from the beginning as they will define the rest of the methodology (Riedelsheimer et al., 2020). The inputs for any DT require data from the actual physical model. Therefore, a holistic DT-based LCA gathers data from the entire life cycle. This data should be collected in real-time by complementing the DT technology with IoT data collection (Kamble et al., 2022), enabling systems to become intelligent and autonomous.

The framework presented by Ghita et al. (2021) consists of five layers: the context layer; the perception and interrogation layer; the mirroring and cognitive layer; the intelligence layer; and finally, the services layer. These layers continually interact with the involved stakeholders, whether they act on the physical or the virtual system. The initial layers are in charge of comprehending the system and allocating the appropriate methods for data to be collected and transmitted to the DT model. The mirroring and cognitive layer are responsible for mimicking the actual system while providing the occurring dynamic interrelations with the environment across its entire life cycle. The last layers are then in charge of acquiring the system's knowledge, enabling an intelligent decision structure. According to Kaewunruen et al. (2020), DT technology allows for improved management and communication by combining all life cycle stages into a single complete model. The authors mention several considerations when building a DT-based LCA system: "interoperability, security and trustworthiness, ergonomics, persistence, and traceability." Other authors (Barni et al., 2018; Kamble et al., 2022) added the scalability and the heterogeneity of the assessment as the essential requirements when building such DT systems. Nevertheless, these studies successfully showed that DT-based LCA models can provide and optimise sustainable performance outcomes while tackling conventional LCA limitations.

Moreover, the capabilities of DT applications in the supply chain can be enhanced by recent Industry 4.0 innovations. IoT, blockchain, CPPS, cloud computing, AI, and ML, among others, coupled with DT models, offer interesting possibilities for smart manufacturing systems. They can use large volumes of real-time data to recommend more efficient solutions (Kamble et al., 2022).

As for the applications, DT models can be used for a variety of sustainable purposes. Their applications vary widely as they can virtually represent the entire life cycles of products, not only aiding to improve pre-production planning and design but also optimising and maintaining production lines (Zambrano et al., 2022). Kaewunruen et al. (2020) and Riedelsheimer et al. (2020) implemented innovative DT-based LCA case studies in different sectors. Riedelsheimer et al. (2020) developed a user-oriented DT sustainable framework for the clothing industry. By providing the product user with continuous information about all life cycle stages, they managed to reduce energy and detergent consumption while preventing waste. On the other hand, Kaewunruen et al. (2020) developed an unprecedented DT-based LCA for a subway station case study and managed to complement the LCA model accurately. The authors showed the enormous potential across the construction sector, as DT models can optimise the project information, leading to a variety of more sustainable decisions. Moreover, Yu et al. (2022)

reviewed DT applications in energy management and concluded that DT technology provides immense possibilities for designing energy-efficient sites and improving maintenance, among others. Kamble et al. (2022) extensively reviewed DT applications to meet sustainable goals, including various forms of design, simulation, or operations optimisation, in a wide range of industry sectors. They also identified prognostics and health management (i.e., the prediction of errors in production without provoking damages, thus aiding in re-designing products or systems) as the most promising DT application in manufacturing in the coming years.

A DT-based LCA can bring many advantages by facilitating data collection and interpretation while being able to translate results into action. Regarding production processes, it aids in structuring complex systems, thus reducing operational failures while improving accuracy and agility when implementing changes (Kamble et al., 2022). Therefore, it promotes product quality with increased transparency and eased communication between stakeholders (Riedelsheimer et al., 2020). Since these capabilities consider real-time status assessments, a DT-based LCA encourages the rapid implementation of environmentally sustainable solutions (Kamble et al., 2022). Moreover, this type of integration can further promote economic and socially sustainable courses of action (Kritzinger et al., 2018; Riedelsheimer et al., 2020). On the other hand, a DT-based LCA poses significant challenges right from the beginning when planning and designing the model (Kamble et al., 2022). A balance has to be obtained between the different framework layers and their intensive computing capacity and need for storage (Ghita et al., 2021). Integrating this tool into traditional enterprise systems while being able to capture real-time data may also pose serious operational constraints (Kamble et al., 2022). Moreover, conflicting gaps between the virtual system and the actual physical, generated by human failures or miscommunication, can also impose major uncertainties on the results (Kaewunruen et al., 2020). Furthermore, DT-based LCA models face issues regarding information security, the lack of standardisation, and the complex multidisciplinary coordination between stakeholders (Kamble et al., 2022; Yu et al., 2022). There is still a considerable lack of research when implementing the DT technology coupled with the LCA. The literature encourages the need to integrate the entire life cycle perspective in these models, considering the environmental burdens created across the whole value chain (Kamble et al., 2022). Future research is, therefore, encouraged to proceed with these efforts and develop a fully DT-based LCA. This could be achieved in a highly digitalised organisation, where automatic data exchange could quickly occur across the entire supply chain. In this case, the environmental assessment results could be automatically translated into improvements in the physical system without the need for human intervention in the decision-making process.

The key findings from the enabling technologies for the LCA development in Industry 4.0 are compiled in Table 3.

Table 3 – Enabling technologies for LCA under the Industry 4.0 umbrella.

	Blockchain	Smart sensor-based technologies
Inputs	Resource consumption data and waste emission data: instant data from all the supply chain.	Direct real-time measurements from the physical product's life cycle world: resources, unit processes and waste; Potential data sources form the entire life cycle.
Methodology	1) Hardware (Smart sensors, Local servers and storage, and network) - IoT enabled automatic and real-time data collection; 2) Gate Operating System (GOS) software; 3) Blockchain services layer - including blockchain-based LCA, and BD and supply chain analytics; 4) Applications layer - data visualisation tools to produce graphical insights; 5) Users.	1) Data acquisition layer: including sensor identification, placement, tracking, monitoring, and management; 2) 3) 4) Data transmission, Platform and Application layers - require the use of IoT and other technologies; Merging with production softwares (e.g., ERP, MES, etc.)
Outputs	Real-time LCA; Including, other applications: energy-saving management, ecosystem quality management, waste management, reuse/recycling management, product information management, and uncertainty treatment management.	Direct measurements of real-time quality-data; Connection with IoT capabilities.
Advantages	Collection and process of vast amounts of real-time data, accounting for complex supply chains; Data security; Reduces consumption of natural resources; Quality data - transparency, traceability and integrity; Transactions - virtually immutable; Minimise the need for subjective judgment of the functional unit; Quantify the material regeneration and restoration effects within a circular supply chain.	Real-time and direct measurements avoid significant uncertainties in the LCA; Relevant for safety and quality control; Potential reduction of data collection workload.
Disadvantages	Smart infrastructure required; Stakeholders coordination and management; Computational power; Storage problem: Data - transmission challenges and lack of approaches to verify subjective data authenticity; Privacy; Scalability; Requires expertise; Can reduce transaction costs; Under-researched technology in this context; Throughput and latency; Interoperability; Lack of governmental regulations; Negative public perception; Lacks investment.	Implementation and maintenance costs; Experts to integrate data with LCA; Lack of cost-effective sensing technologies; Lack of guidance and standardisation - due to the recent nature of IoT technologies; Stakeholders reluctancy to share data.
Studies	Nakamoto, 2008; Kouhizadeh & Sarkis, 2018; Ghobakhloo, 2018; Saberi et al., 2019; Zhang Y. et al., 2019; Zhang et al., 2020; Teh et al., 2020; Karaszewsk et al., 2021; Carrières et al., 2021; Figueiredo et al., 2022.	De Soete et al., 2014; Thiede, 2018; Ingrao et al., 2021; Ferrari et al., 2021; Thiede, 2021; Watson et al., 2021; An et al., 2021; Ferrari et al., 2021; Vacchi et al., 2021; Culaba et al., 2022.

	Digital Twin (DT)	Cyber-Physical Systems (CPS)	Artificial Intelligence (AI)
Inputs	Real-time data from the physical world.	Elements from the physical world: production equipment and respective control infrastructure.	Data from real-time sources or databases.
Methodology	1) Context layer; 2) Perception and interrogation layer; 3) Mirroring and cognitive layer; 4) Intelligence layer; 5) Services layer.	1) Physical Elements - e.g., RFID chips; 2) Programmable logic controllers (PLCs); 3) Middleware; 4) Software; 5) Python code for Live LCA; 6) Visualisation tool;	1) Specify the required output for the model; 2) Choose algorithm - AI genetic programming, or other ML algorithms; 3) Set model hyperparameters; 4) Model training; 5) Model validation; 6) Model testing.
Outputs	Life cycle information in one comprehensive model; Intelligent decision structure; Allows simulations.	Visualised results to compare different scenarios.	Predicted environmental impacts.
Advantages	Improves transparency and interconnectedness between product, company and user; Reduces operational failures; Reduces downtime; Enables structuring complex systems; Monitors processes with increased agility and accuracy; Provides real-time status; Enables TBL sustainable assessment.	Useful in specific approaches for industrial contexts.	Generates data - a small number of sensors, collecting limited input data can lead to good results; No significant environmental impacts; Improves efficiency in existing processes; Supports operational decision-making.
Disadvantages	Complex multidisciplinary cooperation; Lacks consistent and standardised framework; Demands computational power and storage; Gaps between physical and virtual model; Challenges designing the DT model; Operational constraints: difficult integration with traditional systems while demanding high-performance real-time data collection systems; Security concerns.	Under-researched and still a conceptual framework.	Issues of data - collection, quality, and availability; Lack of standardised methodologies; Temporal representativeness and granularity of prediction; Prediction models - still in early developments; Black-box models lacking transparency
Studies	Grieves, 2015; Grieves & Vickers, 2017; Barni et al., 2018; Kritzinger et al., 2018; Zhang & Ji, 2019; Riedelsheimer et al., 2020; Kaewunruen et al., 2020; Ghita et al., 2021; Kamble et al., 2022; Zambrano et al., 2022; Yu et al., 2022.	Lee et al., 2015; Ballarino et al., 2017; Ghobakhloo, 2018; Thiede, 2018; Hagen et al., 2020; Kumar et al., 2022.	Schwender, 2010; D'Amico et al., 2019; ; Watson et al., 2021; Venkatraj & Dixit, 2022; Culaba et al., 2022; Akhshik et al. 2022

2.3. 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 data interchange. As a result of this *modus operandi*, LCA endeavours are faced with significant challenges (Ghita et al., 2021).

Therefore, given the immense possibilities in the automatic exchange of data brought by Industry 4.0's innovations, it is this author's conviction that the model conception itself has to change. To accomplish that, merging the DT strategy with the LCA methodology is a promising path supported in the literature (Barni et al., 2018; Ghita et al., 2021; etc.).

Accordingly, the problem is framed using Figure 2. This visualisation aims to illustrate how an ideal DT-based LCA could operate. By realising that some of the illustrations are not yet realistically achievable, it is possible to describe the problem. In this schematic representation, the physical and virtual systems are characterised. 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, decision-making and an eventual database connecting both stages. The arrows in the figure represent the data exchange between the entities. All interactions within the physical and virtual systems should ideally happen in real-time. Additionally, real-time communication in both ways between the physical and virtual systems is required. Therefore, not only should online data collection from the processes in the physical system be transcribed into the virtual system, but also should the decision-making conclusions arising from the virtual system be translated into the physical system in real-time.

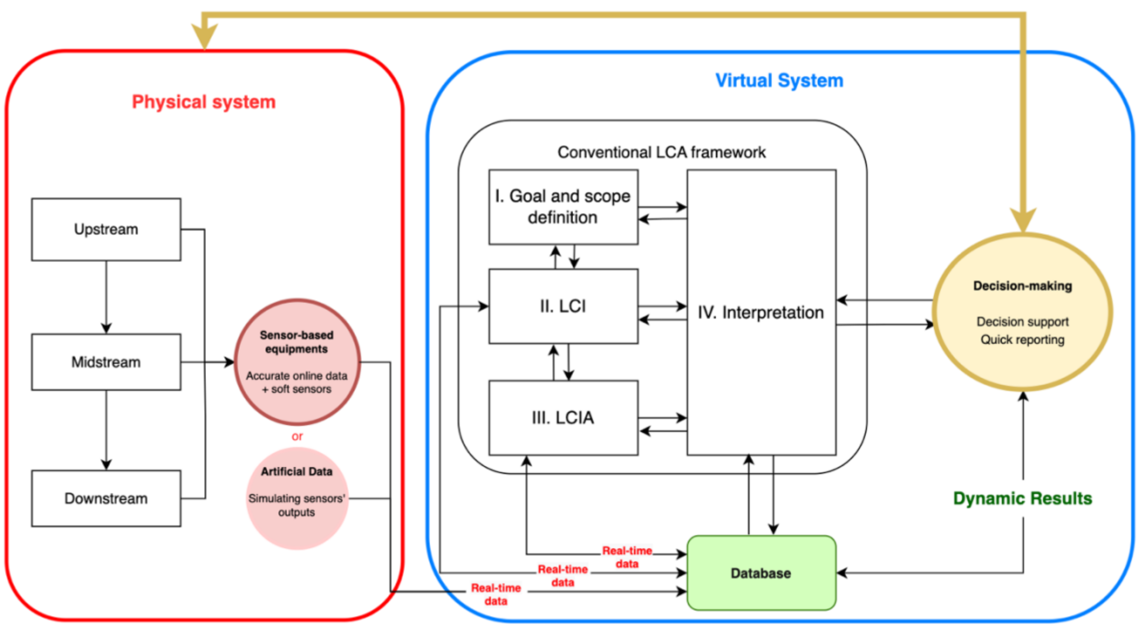


Figure 2 - Online bi-directional connection between the physical (on the left, in red) and the virtual (on the right, in blue) systems.

This demonstrates the ongoing challenge in this research field since it is still not possible to have all information exchange occur automatically and in real-time. Therefore, this idealisation faces many obstacles grounded in literature. Some of the current obstacles identified in the literature (see the Digital Twin segment in section 0) are the following:

(i) Implementing a DT-based LCA **throughout the entire supply chain** (Barni et al., 2018; Ghita et al., 2021; Riedelsheimer et al., 2020).

(ii) **Operational limitations.** Integrating different data collection methods in the same DT environment and the computing power of the various architectural layers and services is challenging. Namely, incorporating databases, direct data from the system (e.g., sensor-based equipment in real-time) and artificially generated data (Barni et al., 2018; Ghita et al., 2021).

(iii) **The heterogeneity of the assessment scope** (Barni et al., 2018), which means taking into account the different LCA's objectives.

(iv) Establishing a **real-time and bi-directional connection** between the physical and the virtual world (Udugama et al., 2021) **capable of live environmental improvements in the system** (Thiede, 2021) by supporting decision decision-making.

(v) **There is 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; Riedelsheimer et al. (2020), that developed a concept for the clothing industry considering the middle and end-of-life stages; or the Kaewunruen et al. (2020) which evaluated of a subway station to improve communication and asset management. However, appliances in a variety of sectors are still lacking.

These knowledge gaps served as the motivation for the subsequent work in this thesis. Therefore, the following research question is formulated: *Is it possible to overcome the mentioned research gaps while developing a feasible framework to implement a DT-based LCA?*

2.4. Chapter conclusions

From the LCA methodological developments subchapter, several research gaps were identified. The D-LCA introduced relevant considerations in addressing temporal issues from cradle-to-grave but lacked implementation due to the inherent complexity to collect and interpret temporal data. The O-LCA introduced a holistic assessment of environmental impacts for whole organisations and their value chain, although faced technical barriers due to the lack of organisational activities' databases and O-LCA-specific software. The U-LCA proposed integrating Industry 4.0 innovations into the LCA methodology, by suggesting the collection of real-time data and product' tracing throughout the entire life cycle, however, it is still a conceptual framework.

Afterwards, a number of Industry 4.0 technologies applied to LCA approaches were review. A general trend was noticed in integrating the LCA with manufacturing systems interconnected with real-time control tools. The DT technology showed to be powerful strategy to perform real-time simulation of industrial systems, thus, considerably improving LCA's capabilities in proactive assessments.

The research gaps found in literature provided various insights for future work directions. These insights were explored and are summarised in Appendix A. Nonetheless, they led to the problem framing: how would an ideal integration between the DT strategy and the LCA look like. This way, the motivation for the remaining research was established: moving towards an ideal DT-based LCA model by tackling the existing research gaps.

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

This chapter introduces the methodology to develop the proposed framework towards a DT-based LCA. The three phases composing the methodology are schematically represented in Figure 3. The word *towards* indicates that the comprehensive DT-based LCA is not yet achievable, as previously stated in the problem framing (section 2.3). The goal is instead to accomplish a feasible DT-based LCA moving *towards* a comprehensive DT strategy.

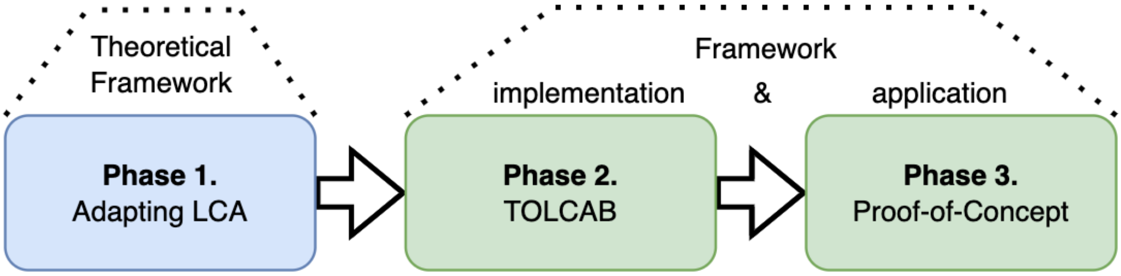


Figure 3 - Methodology phases to adapt the LCA towards a DT-based model.

Phase 1 - Adapting LCA: Theoretical framework

As shown in Figure 3, the theoretical framework is developed in Phase 1 by adapting the standard LCA methodology. The key proposals to adapt the traditional LCA are summarised in Figure 4. These include partially D-LCA and U-LCA procedures facilitated by different technological capabilities from Industry 4.0 (reviewed in sections 2.2.2 and 0).

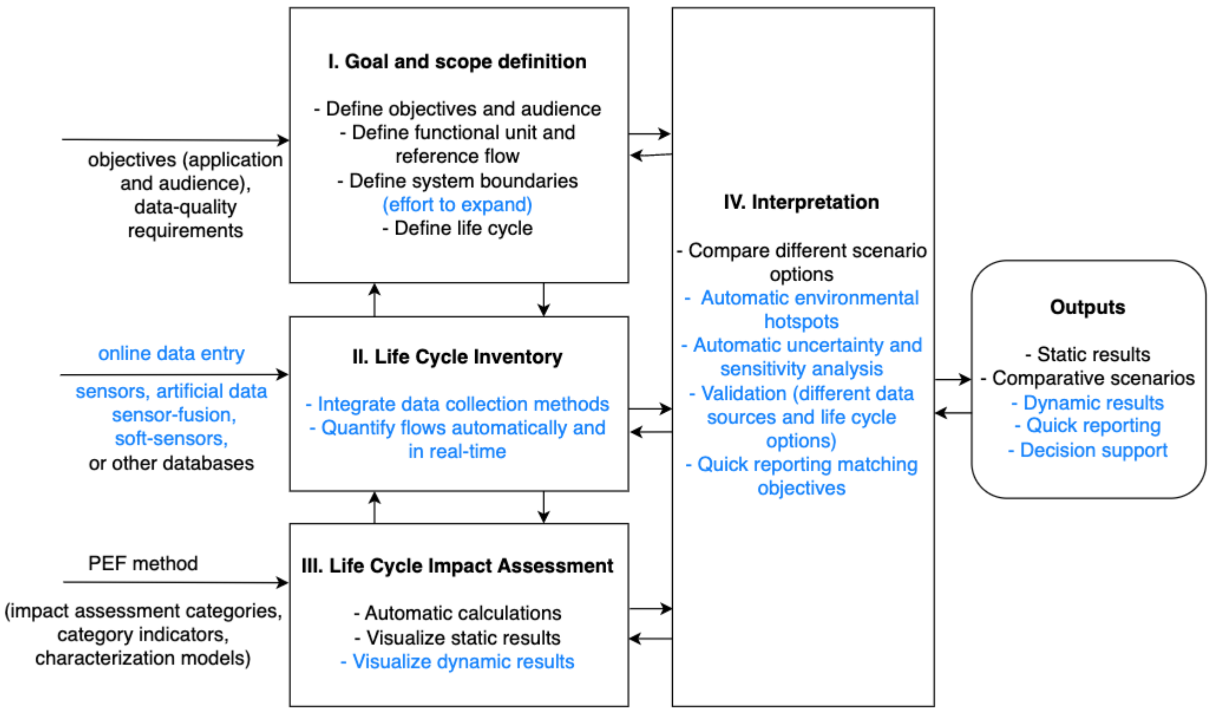


Figure 4 – Summarised illustration of Phase 1, including the four LCA steps. Essential procedures from the conventional LCA are highlighted in black, and key propositions to adapt the LCA are highlighted in blue.

The standard LCA methodology was reviewed in detail in chapter 2 (section 2.1.1). Therefore, only the proposed extensions to the existing LCA standards are described in detail in the following steps.
As established when framing the problem (section 2.3), whereas the goal would be for all data exchanges between the physical and virtual systems to be automated, that is not achievable. Therefore, figures throughout this first step (Figure 5, Figure 6 and Figure 7) will help understand the information flows occurring in the assessed system, which are divided between manual and automatic.

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 Industry 4.0's technologies enable expanding the traditional boundaries to ideally encompass the entire supply chain (Mashhadi and Behdad, 2018). Therefore, it is possible to evaluate the environmental impacts of the activities whose boundaries are traditionally unclear, such as the ones of emerging technologies (e.g., Cloud Computing, IoT, etc.).
Furthermore, this step includes the definition of the types and sources of data, and corresponding data-quality requirements, as detailed in ISO 14044:2006, here as follows: time-related coverage, geographical coverage, technology coverage, precision, completeness, representativeness, consistency, reproducibility, source type and related uncertainty.
As shown in Figure 5, from left to right, the information flow into Step 1 is manually introduced, taking into consideration the physical system to be assessed (the supply chain highlighted in grey). By determining the goal and scope of the LCA study, the practitioner defines the data sources to be used (highlighted in red). These choices will define the conditions of the database to perform the following calculations.

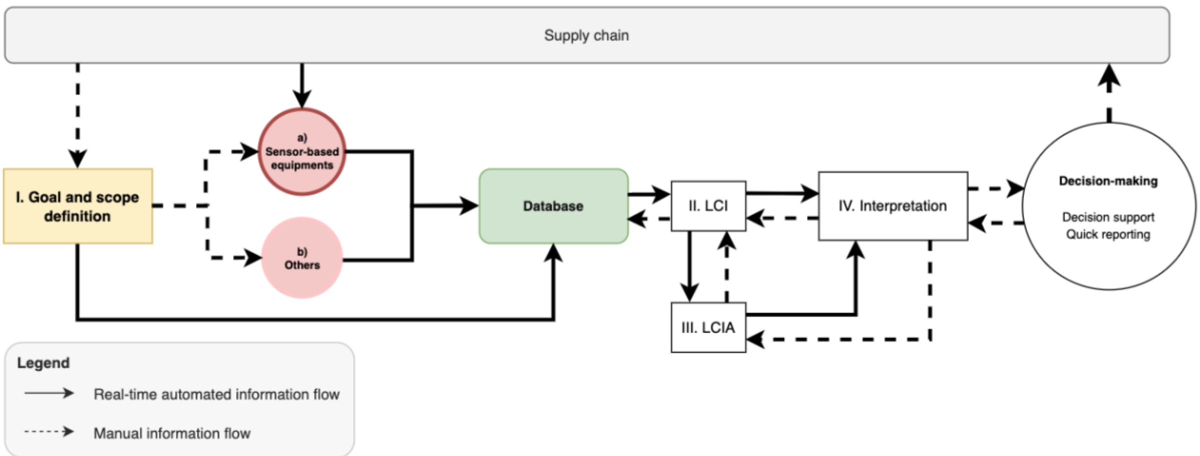


Figure 5 - Information flows in Step 1. The supply chain represents the assessed physical system and is highlighted in grey. Step 1 is highlighted in yellow. The data sources are highlighted in red. The database is highlighted in green.

Step 2. Life Cycle Inventory

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 the data collection process is somewhat 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 or (b) artificially generated data or existing external databases, as shown in Figure 5. Artificially generated data refer to probabilistic distributions that can simulate the behaviour of actual sensor-based equipment (Westermann and Evins, 2019). 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. In the case of sensors, these characteristics include their reliability, speed of data acquisition and analysis, accuracy, invasiveness, energy consumption, security, price and autonomy (more detail in section 0). Likewise, the user is encouraged to use (i) sensor-fusion alternatives, which combine sensors to reduce uncertainty in cases where it may compromise the result's reliability, and (ii) soft sensors, which are based on models capable of estimating challenging process variables that cannot be measured directly in real-time (Thiede, 2021).

The chosen data collection methods can provide the LCA with real-time data flows. 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 data for each unit process contained within the system boundary (ISO:14044, 2006). Potentially, the total inventory data for the LCI can be collected using sensor-based equipment in the supply chain within the system boundaries defined. 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.

When selecting the data collection methods, the practitioner should describe them in terms of the following parameters: type of data collection method, type of flow measurement, input or output, process, unit, time period, time unity and uncertainty. These registrations describe each method's operability. The time period and time unit refer to the frequency of data measurement and must consider the specific method's capabilities (e.g., some sensors may be programmed to collect data at a different frequency). The uncertainty level is selected from the literature and should be based on the

measurements' reliability and the data input quality. According to ISO 14044:2006, the uncertainty of the results can be expressed in terms of data ranges, probability distributions or assumptions.
As Figure 6 shows, data can travel automatically from the database into Step 2 (highlighted in yellow), creating real-time inventory data.

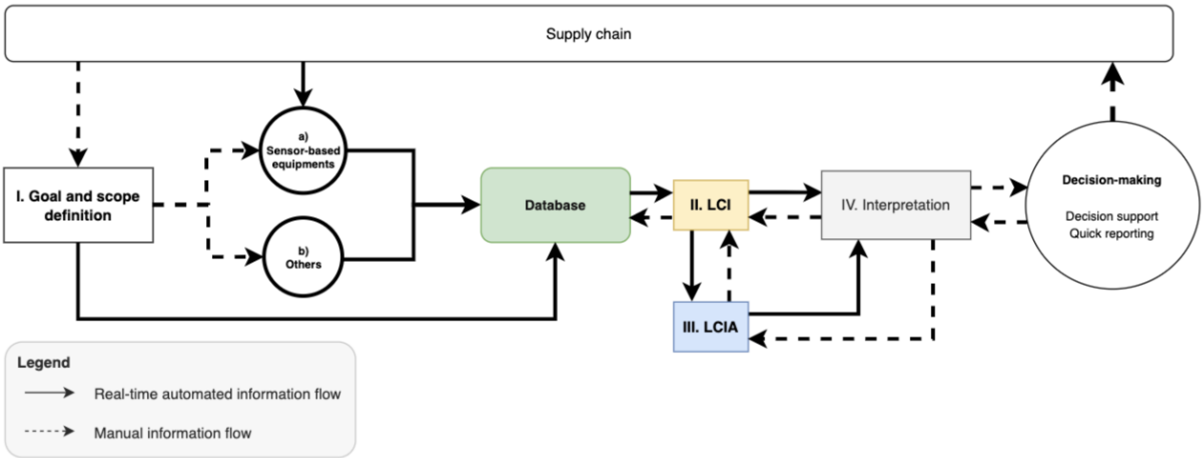


Figure 6 - Information flows in Step 2 and Step 3. The database is highlighted in green. Step 2 is highlighted in yellow. Step 3 is highlighted in blue. Step 4 is highlighted in grey.

Step 3. Life Cycle Impact Assessment

Dynamic LCI results from Step 2 are automatically incorporated in order to begin Step 3, as shown in Figure 6. The PEF method should be selected since it is recommended by the European Union (2021). The environmental impacts are described according to the impact categories in Table C 1 (see Appendix C – PEF method impact categories).
The consequential approach is followed due to the fact 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, as shown in Figure 4. The following tasks include classification, characterisation, normalisation and weighting. 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 with the appropriate characterisation factors (Zampori and Pant, 2019). Although normalisation and weighting are optional, they are recommended since they aid non-experts in understanding the results (Hauschild et al., 2018). Normalisation enables comparison between the impact categories, and it consists in dividing the characterisation results by selected normalisation factors (ISO:14044, 2006). 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, the SS, which is generated to simplify the results (Hauschild et al., 2018).
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 larger 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.

Figure 6 shows that Step 3 obtains the results from Step 2 automatically. It also provides automatic information to perform the following Step 4. Manual inputs can, however, reverse the process if some iteration is needed.

Step 4. Interpretation

This step systematically reviews and refines the results obtained in the LCA, aiming to present final conclusions, limitations and recommendations (ISO:14044, 2006). In this methodology, the interpretation is supported 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. For each critical flow, the matrix plots a point based on two parameters: uncertainty and environmental impact. The uncertainty value refers to the uncertainty inherent to the data collection methods used to monitor the critical flow. The environmental impact value corresponds to that critical flow's weighted environmental impact results. This way, 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 analysing possible courses of action by quickly determining the outcomes of certain decisions.

(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 results' 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 information, 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.

As Figure 7 shows, the inputs to perform Step 4 are automatically obtained from the previous steps. The information flows from Step 4 into Decision-making (the green circle on the right) are also manual since the practitioner should visualise and interpret the results to plan decisions. These decisions are then manually translated to the supply chain since the actions performed depend on human action.

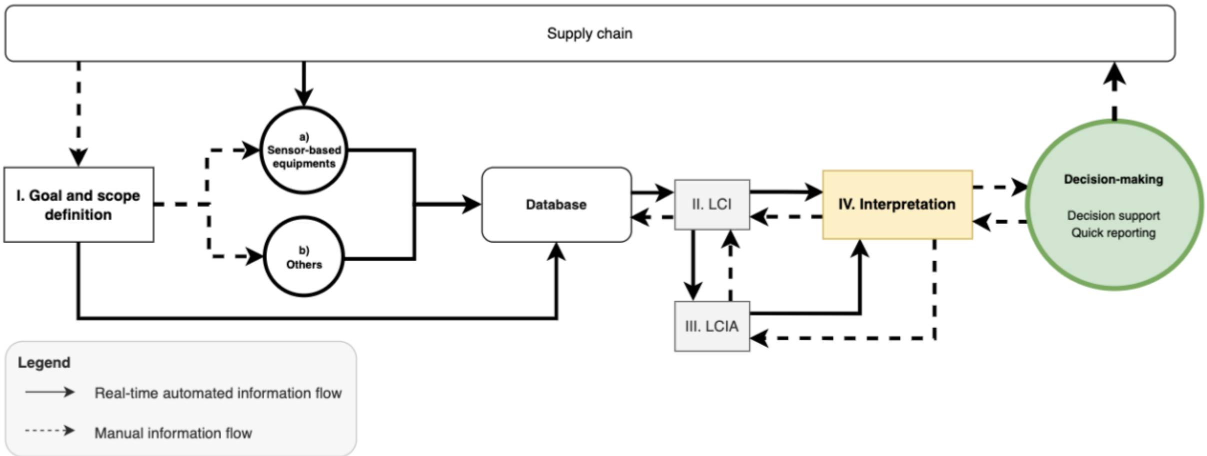


Figure 7 - Information flows in Step 4. Step 2 and Step 3 are highlighted in grey. Step 4 is highlighted in yellow. The Decision-making is highlighted in green.

Phase 2 - TOLCAB (Towards an Online DT-based LCA of Bio-based processes)

In this phase, a software named TOLCAB (Towards Online LCA for Bio-based processes) is created based upon the theoretical framework defined in Phase 1 (see Figure 4). This practical implementation is performed for the bio-based processing sector. This is a lead industry in Denmark, thus will be used in this thesis for validation. TOLCAB's software architecture is schematically represented in Figure 8. The surrogate model considered in this architecture is described.

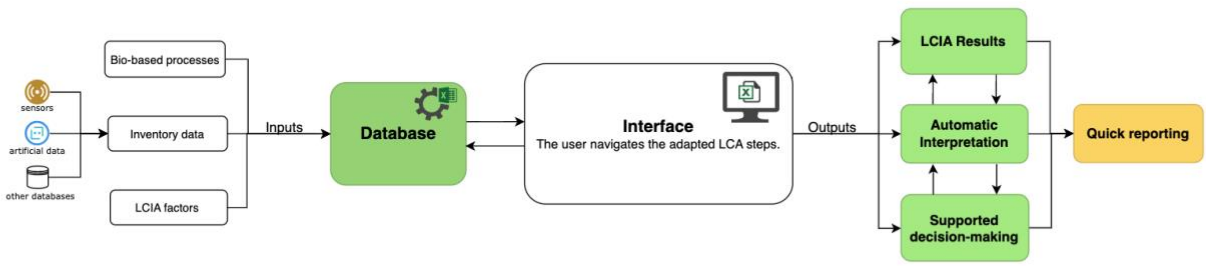


Figure 8 - General software architecture of TOLCAB.

Interface and database

TOLCAB is a software built in Excel, which integrates the database and the interface in a single environment, as shown in Figure 8. The objective is to create a stand-alone, easy-to-use software application that facilitates user navigation and supports decisions at every level. Moreover, customising the platform to individual industries is the strategy followed. This enables building a customisable database, which includes comprehensive information on the specific sector. For this to occur, the database is incorporated into TOLCAB. The database consists of (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). This way, TOLCAB can possess detailed industry knowledge and suggest relevant user inputs. Additionally, developing a user-friendly LCA software focusing on efficiency, visualisation and decision support is anticipated to promote wider adoption of environmental assessments (Buchert et al. 2019).

In this platform, both the back- and front-end segments are included: (a) the back-end segment includes the database information and the necessary computational models to perform all the calculations, and (b) the front-end provides the necessary capabilities to perform the desired user actions. Therefore, the software tabs are according to this architecture. Hence, they are divided into two main groups: the back-end and the front-end tabs. These tabs enable the user to perform the instructions described during Phase 1. However, the software developed is still in its early stages. The back- and front-end boundaries still need to be clarified, as the user has to insert data in the database manually. The future goal, however, is for the user to only interact with the front-end interface.

Surrogate Model

The technical challenges inherently posed by a DT-based LCA methodology (e.g., time, resources and computational effort, among others introduced in chapter 2) 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. In this context, a surrogate model means that the physical system is not fully characterised. 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 3, this proof-of-concept intends to demonstrate the application of theoretical framework (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. 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 ones 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: Towards an Online DT-based LCA of Bio-based processes

The software tool presented here is named TOLCAB - Towards Online LCA for Bio-based processes. The logo is shown in Figure 9. It embodies the methodology developed in Phase 1 and the practical implementation guidelines described in Phase 2, as shown in Figure 3. This software targets the sector of bio-based processes. This is a novel tool that aims to provide the industry with a quick LCA analysis inspired by the DT strategy. The bio-based sector has been selected because it is the dominant industry in Denmark, which is used in this thesis for demonstration purposes. The future goal, however, is for this tool to be customisable for multiple industry sectors, potentially covering a more comprehensive range of processes and supply chains.

Figure 9 – TOLCAB logo.

TOLCAB was built considering the software architecture presented in Figure 8. The Excel tabs are described in Table B 1 shown in Appendix B. Users should access the front-end tabs to perform the assessment. The back-end tabs are characterised by the letters BE in brackets. These tabs mainly present the information of the database, as described in the software architecture (Figure 8). Moreover, LCA experts and non-experts are recommended to perform an LCA using TOLCAB. Nevertheless, as it is advised to recognise the basic principles of the LCA methodology, LCA non-experts are advised to gather a basic understanding of this topic (read section 2.1 or other relevant literature on LCA principles). This chapter introduces the capabilities of this software in three sections while contemplating the user's point of view: section 4.1 describes the initial user actions in order to model the physical system, section 4.2 illustrates the user actions associated to the assessment and interpretation, section 4.3 outlines potential directions for future software development, and lastly, section 4.4 presents final remarks.

4.1. User inputs A: initial actions

The initial actions must be followed to apply TOLCAB in a bio-based processing company. 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. These initial actions are presented in Figure 10. Note that even though they are in order, they are iterative. Therefore, adjustments can be performed without strictly respecting the pre-established hierarchy.

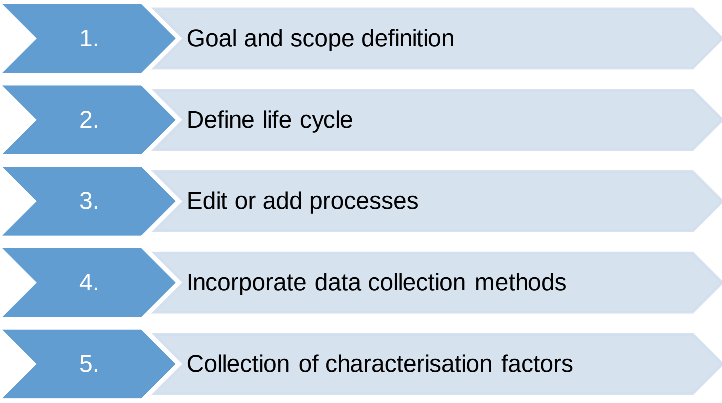


Figure 10 – User inputs A: Initial actions.

1. Goal and scope definition

This initial action is performed in the *1. Goal and scope definition* tab, as shown in Figure 11. The users should fill in the gaps, which include drop-down menus to facilitate the user's decisions. The system boundary definition now consists of the options: cradle-to-grave, cradle-to-gate, gate-to-gate, and gate-to-grave. The geographical location definition includes Denmark and Europe as the available options.

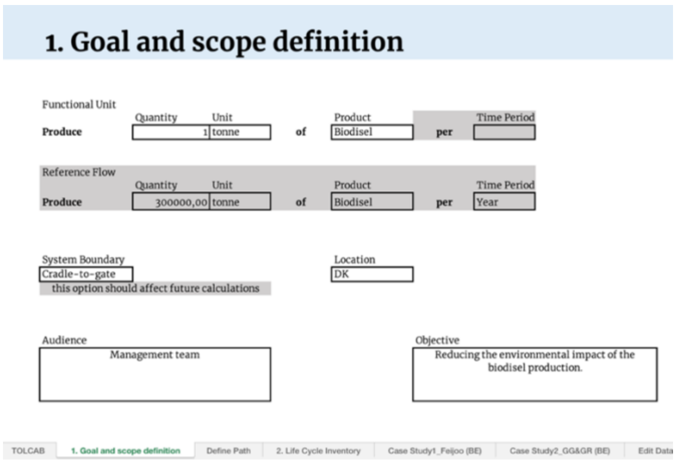


Figure 11 – 1. Goal and scope Definition. At this stage, the inactive features are highlighted in grey.

2. Define Life Cycle

This initial action is performed in the *Define Life Cycle* tab, as shown in Figure 12. The software is prepared from the get-go to accept bio-based process systems. As a result, it already comprises a range of processes for the sector. To this point, only two options for each process are provided. They can be selected by using the drop-down menus. Nonetheless, the user can edit the existing process options or add new ones. This is explained in the following action (3 - Edit or add processes).

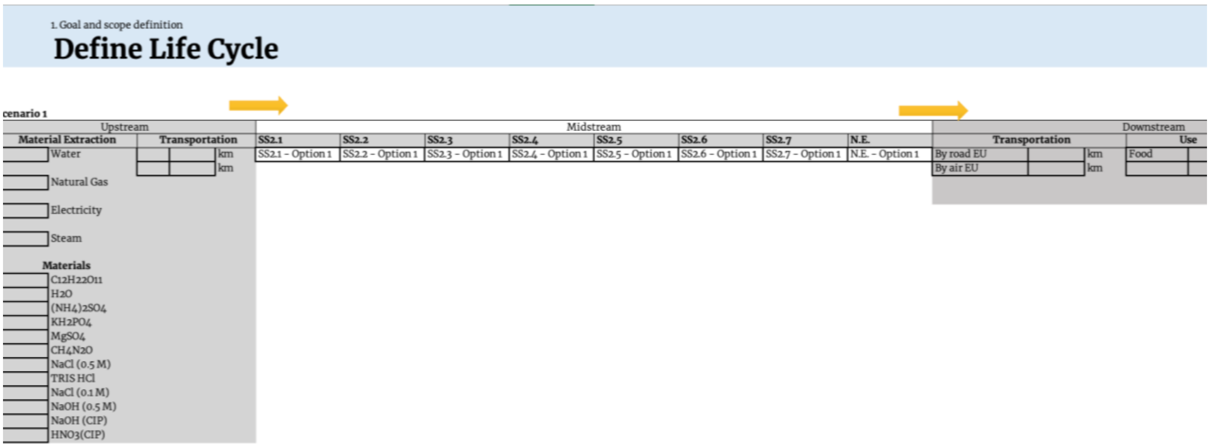


Figure 12 - The user defines the life cycle by selecting from the range of process options. At this stage, the inactive features are highlighted in grey.

3. Edit or add processes

This initial action is performed in the *Description of Processes* tab, as shown in Figure 13. This action has two main objectives. The first is to check and edit processes to ensure they match the assessed system's life cycle previously defined during initial action 2 (Define Life Cycle). Additionally, since the software still lacks several process options, the user is welcome to add new processes to the software. This addition must be followed by an update of the *LCI Summary* tab to ensure the flows match the corresponding processes.

Moreover, when editing or adding processes, the user must undergo the following procedures if new inputs or outputs are needed: add the flows in the tab *LCI Summary*, and assign them to the corresponding characterisation factors in the tab *LCIA – CFs (BE)*. The second objective is to assign a unique data collection method for each flow. By doing this, each flow measurement can be translated by the results of the chosen strategy. The user can move on to the next phase when all the processes are stated, their flows declared, and the corresponding data collection methods selected in agreement with the evaluated system.

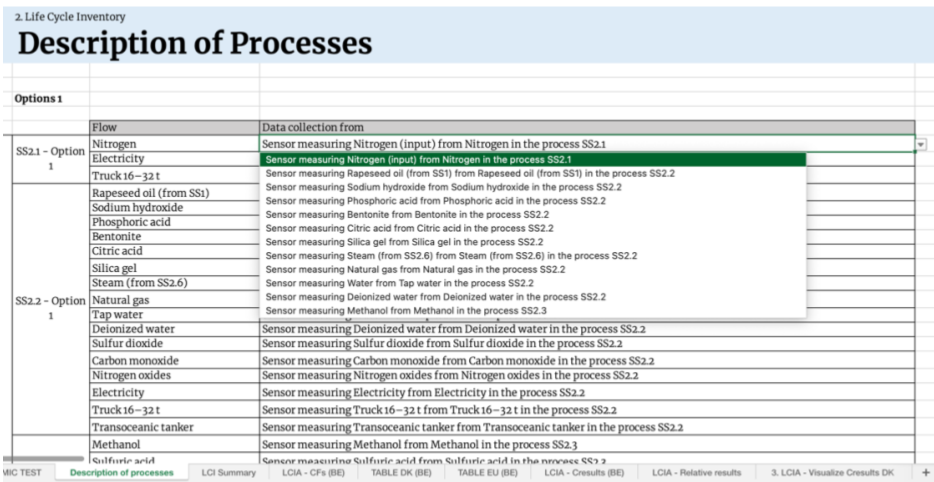


Figure 13 - The user edits or adds processes in the Description of Processes tab.

4. Incorporate data collection methods

After defining the desired data quality requirements, the user is responsible for selecting the available data sources: (i) sensor-based equipment, (ii) soft sensors, (iii) artificially generated data, and (iv) other external databases. However, as the quality of the LCA depends mainly on its data collection strategies and the data quality itself, the user is reminded to consider the guiding criteria. That said, it is recommended *a priori* that data is collected using smart sensor-based equipment, as the goal is to create a dynamic LCA in real-time. They may include both sources already present in the system and freshly installed ones for the purpose of this analysis.

As shown in Figure 14, the selected data collection methods should be described in terms of the required parameters to describe each method's operability. They are quite straightforward, as each parameter includes the available options selected from a drop-down menu. Soft sensors can also be defined and added. It is worth repeating that this software was built to combine static and dynamic data to produce the LCI results (more details in section 4.2.).

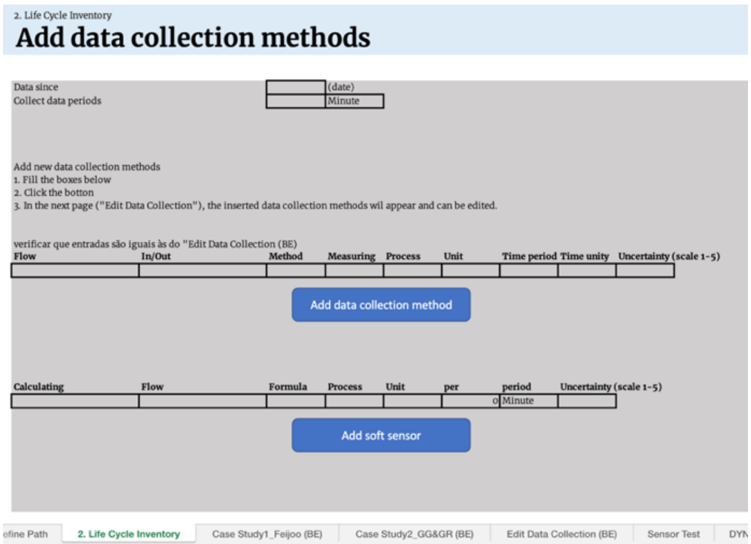


Figure 14 - Incorporate data collection methods in the 2. Life Cycle Inventory tab. At this stage, the inactive features are highlighted in grey.

5. Collection of characterisation factors

This initial action aims to prepare the LCIA calculations. The characterisation factors from the PEF method were extracted using the SimaPro 9.2 software (PRé Sustainability B.V., 2021). For this, the Ecoinvent 3 database (Wernet et al., 2016) was used to obtain most characterisation factors, with some exceptions (i.e., project EU & DK Input Output Database and Agri-Footprint 5). The complete list of the used characterisation factors can be observed in the *LCIA – CFs (BE)* tab and are detailed in Table D 1 in Appendix D. The normalisation and weighting factors were extracted from (European Commission - Joint Research Centre, 2022) and are detailed in Table E 1 and Table E 2 in Appendix E.

2. Life Cycle Inventory

Edit data collection methods (BE)

new data collection methods can be added in the '2. Life Cycle Inventory' tab

Flow	In/Out	Method	Measuring	Process	Unit	Time period	Time unity	Uncertainty (scale 1-5)	Automatic name
Nitrogen	Input from tec	Sensor	Nitrogen (input)	SS2.1	kg			1	Sensor measuring Nitrogen (input) from Nitrogen in the process SS2.1
Rapeseed oil (from SS1)	Input from tec	Sensor	Rapeseed oil (from SS1)	SS2.2	kg			2	Sensor measuring Rapeseed oil (from SS1) from Rapeseed oil (from SS1) in the process SS
Sodium hydroxide	Input from tec	Sensor	Sodium hydroxide	SS2.2	kg			3	Sensor measuring Sodium hydroxide from Sodium hydroxide in the process SS2.2
Phosphoric acid	Input from tec	Sensor	Phosphoric acid	SS2.2	kg			4	Sensor measuring Phosphoric acid from Phosphoric acid in the process SS2.2
Bentonite	Input from tec	Sensor	Bentonite	SS2.2	kg			2	Sensor measuring Bentonite from Bentonite in the process SS2.2
Citric acid	Input from tec	Sensor	Citric acid	SS2.2	kg			3	Sensor measuring Citric acid from Citric acid in the process SS2.2
Silica gel	Input from tec	Sensor	Silica gel	SS2.2	kg			2	Sensor measuring Silica gel from Silica gel in the process SS2.2
Steam (from SS2.6)	Input from tec	Sensor	Steam (from SS2.6)	SS2.2	kg			1	Sensor measuring Steam (from SS2.6) from Steam (from SS2.6) in the process SS2.2
Natural gas	Input from tec	Sensor	Natural gas	SS2.2	kg			1	Sensor measuring Natural gas from Natural gas in the process SS2.2
Tap water	Input from tec	Sensor	Water	SS2.2	kg			1	Sensor measuring Water from Tap water in the process SS2.2
Deionized water	Input from tec	Sensor	Deionized water	SS2.2	kg			1	Sensor measuring Deionized water from Deionized water in the process SS2.2
Methanol	Input from tec	Sensor	Methanol	SS2.3	kg			1	Sensor measuring Methanol from Methanol in the process SS2.3
Sulfuric acid	Input from tec	Sensor	Sulfuric acid	SS2.3	kg			1	Sensor measuring Sulfuric acid from Sulfuric acid in the process SS2.3
Chlorhydric acid	Input from tec	Sensor	Chlorhydric acid	SS2.3	kg			1	Sensor measuring Chlorhydric acid from Chlorhydric acid in the process SS2.3
Sodium hydroxide	Input from tec	Sensor	Sodium hydroxide	SS2.3	kg			1	Sensor measuring Sodium hydroxide from Sodium hydroxide in the process SS2.3
Nitrogen	Input from tec	Sensor	Nitrogen (input)	SS2.3	kg			1	Sensor measuring Nitrogen (input) from Nitrogen in the process SS2.3
Tap water	Input from tec	Sensor	Water	SS2.3	kg			1	Sensor measuring Water from Tap water in the process SS2.3
Steam (from SS2.6)	Input from tec	Sensor	Steam (from SS2.6)	SS2.3	kg			1	Sensor measuring Steam (from SS2.6) from Steam (from SS2.6) in the process SS2.3
Potassium methylate	Input from tec	Sensor	Potassium methylate	SS2.3	kg			2	Sensor measuring Potassium methylate from Potassium methylate in the process SS2.3
Citric acid	Input from tec	Sensor	Citric acid	SS2.3	kg			1	Sensor measuring Citric acid from Citric acid in the process SS2.3
Ureum	Input from tec	Sensor	Ureum	SS2.4	kg			1	Sensor measuring Ureum from Ureum in the process SS2.4
Sodium hydroxide	Input from tec	Sensor	Sodium hydroxide	SS2.4	kg			1	Sensor measuring Sodium hydroxide from Sodium hydroxide in the process SS2.4
Coagulant	Input from tec	Sensor	Coagulant	SS2.4	kg			1	Sensor measuring Coagulant from Coagulant in the process SS2.4
Acetone cyanohydrin	Input from tec	Sensor	Acetone cyanohydrin	SS2.5	kg			1	Sensor measuring Acetone cyanohydrin from Acetone cyanohydrin in the process SS2.5
Helium	Input from tec	Sensor	Helium	SS2.5	kg			1	Sensor measuring Helium from Helium in the process SS2.5
Heptane	Input from tec	Sensor	Heptane	SS2.5	kg			1	Sensor measuring Heptane from Heptane in the process SS2.5
Ultrapure water	Input from tec	Sensor	Ultrapure water	SS2.5	kg			1	Sensor measuring Ultrapure water from Ultrapure water in the process SS2.5
Packaging materials	Input from tec	Sensor	Packaging materials	SS2.5	kg			1	Sensor measuring Packaging materials from Packaging materials in the process SS2.5
Tap water	Input from tec	Sensor	Water	SS2.6	kg			1	Sensor measuring Water from Tap water in the process SS2.6
Sodium chloride	Input from tec	Sensor	Sodium chloride	SS2.6	kg			1	Sensor measuring Sodium chloride from Sodium chloride in the process SS2.6
Natural gas	Input from tec	Sensor	Natural gas	SS2.6	kg			1	Sensor measuring Natural gas from Natural gas in the process SS2.6
Sulfur dioxide	Input from tec	Sensor	Sulfur dioxide	SS2.2	kg			1	Sensor measuring Sulfur dioxide from Sulfur dioxide in the process SS2.2

Case Study1_Feijoo (BE) | Case Study2_GG&GR (BE) | Edit Data Collection (BE) | Sensor Test | DYNAMIC TEST | Description of processes | LCI Summary | LCIA - CFs (BE) | TABLE DK (BE) | +

Figure 15 - Edit data collection methods in the Edit Data Collection (BE) tab. At this stage, the inactive features are highlighted in grey.

4.2. User inputs B: Assessment and Interpretation actions

In TOLCAB, 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. Thus, although the organisation of this section follows the suggested sequence of the LCA procedures described in Phase 1 (Figure 3), users may find it more pertinent to proceed directly to the analysis.

Life Cycle Inventory

The LCI procedures have been performed to this point. Therefore, 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, as shown in Figure 16. Additionally, the user can inspect the total LCI results by visiting the *LCI Summary* tab. This tab, however, shows the dynamic flows converted in averages, thus, becoming static flows. Nonetheless, this averaging provides valuable information for future simplified calculations during the LCIA and Interpretation stages.

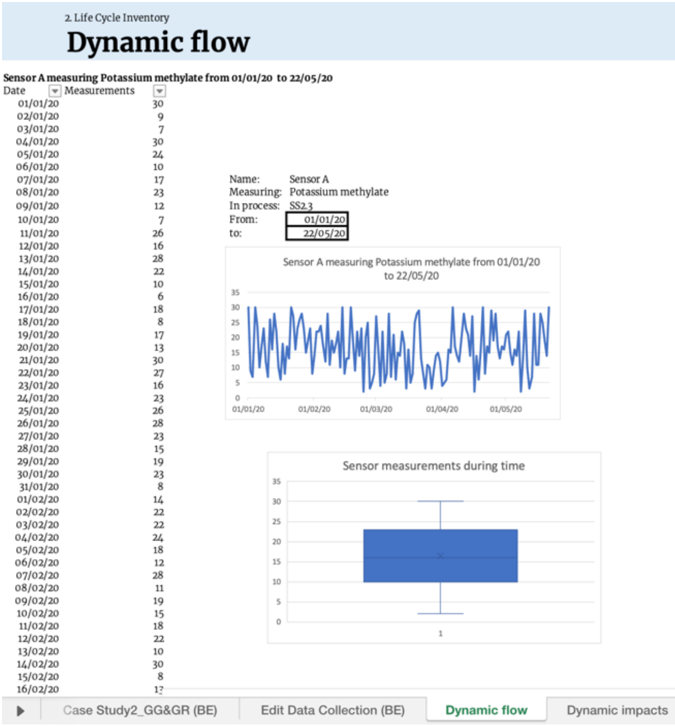


Figure 16 - Visualisation of the example of a dynamic flow.

Life Cycle Impact Assessment

The LCIA calculations are carried out automatically, assuming all the data required to run the LCIA was gathered during the initial user actions. Therefore, 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, as shown in Figure 17. These are described using boxplots which are used to represent graphically the numerical values of a dataset. For each impact category, they present the dynamic inventory dataset of the chosen flow, illustrating the variability of the flow's impacts with time. The boxplots provide information about the maximum and minimum values in the dataset, the first and third quartiles, the mean (represented with a cross) and the median (denoted with a horizontal line). 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 SS.

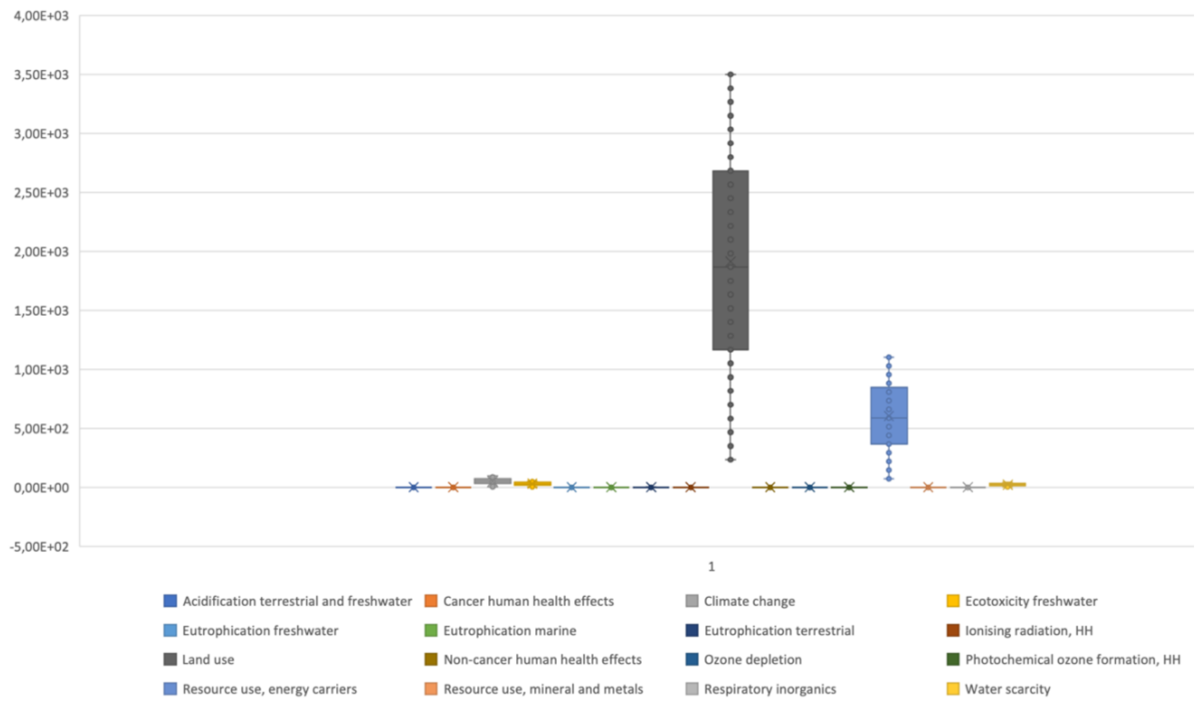


Figure 17 – Demonstration using random inventory data to produce dynamic results. The boxplots represent the flow's characterisation impacts varying with time for each impact category. The units considered for the impact categories are detailed in Table C 1 in Appendix C.

Interpretation

Several interpretation steps are automatically performed. Nonetheless, the user can perform additional analyses using the capabilities provided in the software. The automatic interpretation results can be visualised, as shown in Figure 18, Figure 19 and Figure 20. These features aim to facilitate the user's interpretation of results without providing an overwhelming amount of information. In the first tab, three tools were conceived, as shown in Figure 18: (i) the *hotspot ranking* tool sorts the impact categories, processes, and flows in descending order considering their overall contribution. This quick analysis helps the user to identify the highest contributors for each parameter, quite similarly to a Pareto analysis, although not showing the actual contribution values, as they can be observed during the previous LCIA stage; (ii) the *environmental hotspots finder* takes the information from the three highest contributing aggregated flows defined in the *hotspots ranking*, to exhibit the highest individual contributor and its respective unit process; and the (iii) *suggestion box,* which provides suggestions to perform iterations in previous user actions. These iterative actions entail data collection improvements. They are targeted on flows with both high relative impact and uncertainty. For instance, if the flow with the highest environmental impact is measured according to less reliable data sources, it can be better monitored using appropriate sensor devices. 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.

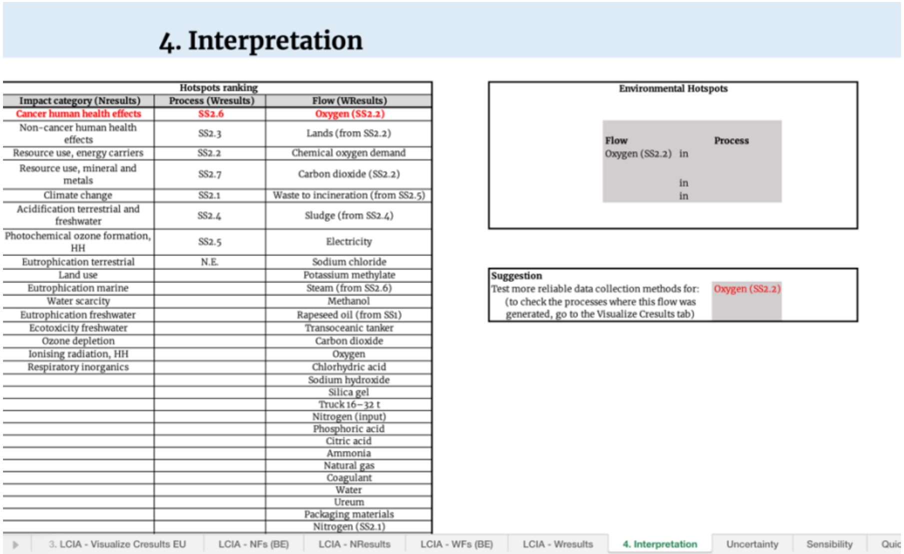


Figure 18 – 4. Interpretation tab. At this stage, the inactive features are highlighted in grey.

The uncertainty analysis is automatically performed, as shown in Figure 19. Here, an uncertainty matrix is generated. It assists users in comparing the three critical flows identified on the Hotspots ranking, as shown in Figure 18. The user should take the automatically generated insights from the matrix and act primarily on the highest contributors to the overall environmental impact (Y-axis) and uncertainty (X-axis). TOLCAB considers the flow with the higher ratio between environmental impact and uncertainty to be the uncertainty environmental hotspot.

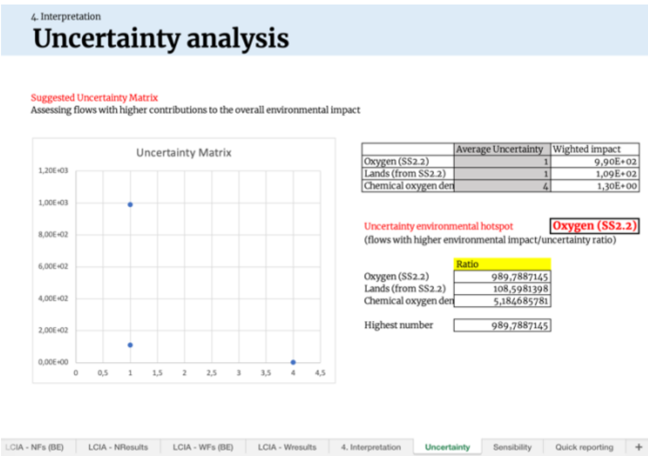


Figure 19 – Uncertainty analysis tab.

Lastly, a sensitivity analysis is suggested (Figure 20). The goal is to answer the question of what would happen to the environmental burdens of each impact category if a specific percentage reduced a given flow. This evaluation is performed automatically for the uncertainty environmental hotspot established previously. This evaluation makes it possible to determine quickly whether the possible action has the desired outcome.

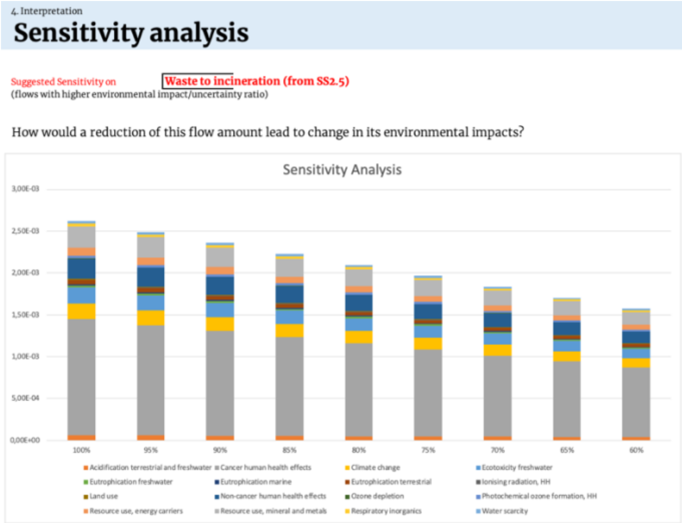


Figure 20 – Sensitivity analysis tab. The unit considered for each impact category is detailed in Table C 1 in Appendix C.

Quick Reporting

The software's final display and reporting feature is shown in Figure 21. It 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.).
v. Additional functions - although inactivated at this point, it aims to provide three quick capabilities: update data, export quick results or create a new system.

The quick report still needs to include dynamic information since no path was found to portray crucial dynamic results in a clear manner. However, users are recommended to revisit the dynamic results obtained. In particular, to analyse temporal variabilities over various time scales and for multiple processes. This can lead to fresh insights into the causes of results variability and corresponding potential solutions. Moreover, it is important to highlight that the LCA is an iterative methodology. Users are encouraged to make continuous adjustments at various stages, even if it includes changing the initial assumptions. Testing and validating different data sources for given flows can improve the results' reliability. Expanding the system boundaries to include other relevant processes that were not considered initially is another way to capture a more comprehensive understanding of the value chain's environmental impacts. Ultimately, decisions obtained through this methodology and its implementation through the TOLCAB software can improve the actual physical system, thus contributing to environmental sustainability.

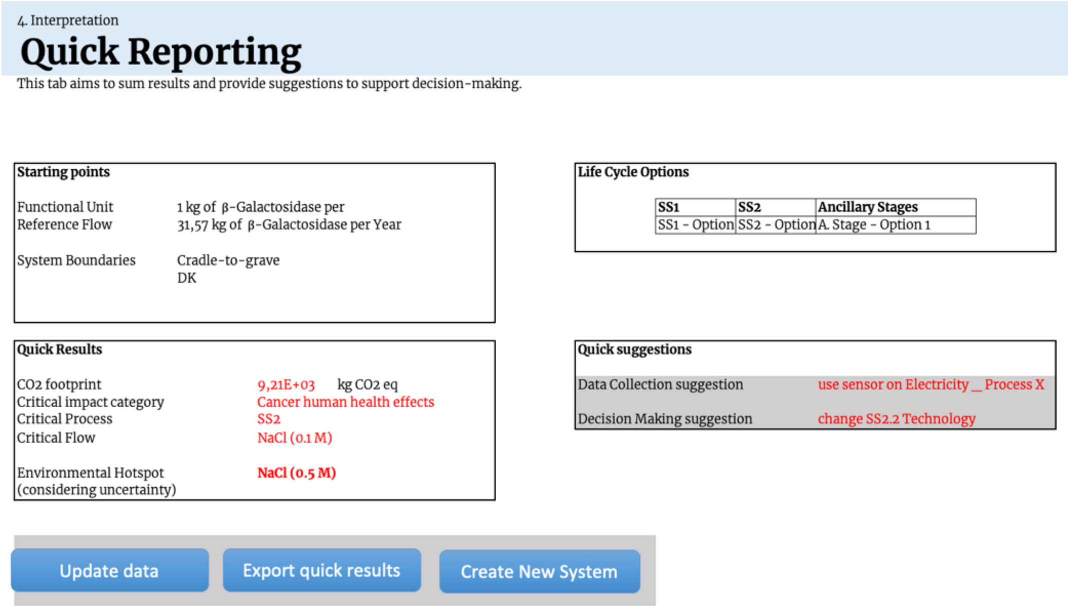


Figure 21 – The Quick reporting tab automatically presents the summarised results. At this stage, the inactive features are highlighted in grey.

4.3. Future software development

The methodology presented in Chapter 3 was influenced by both recent LCA developments and Industry 4.0's capabilities. It was, therefore, a proposition based on achievable milestones. However, the work developed in this chapter showed that theoretical and practical possibilities are often misaligned. Creating software from scratch in an individual endeavour, facing time constraints and computation lack of expertise, were significant challenges to this work. As a result, the TOLCAB tool still has a way to go to deploy its full potential. On the other hand, this section seeks to cover some potential future directions that will help the TOLCAB software to realise its total capacity to become the envisioned tool. To accomplish this, some strategies are summarised in Figure 22.

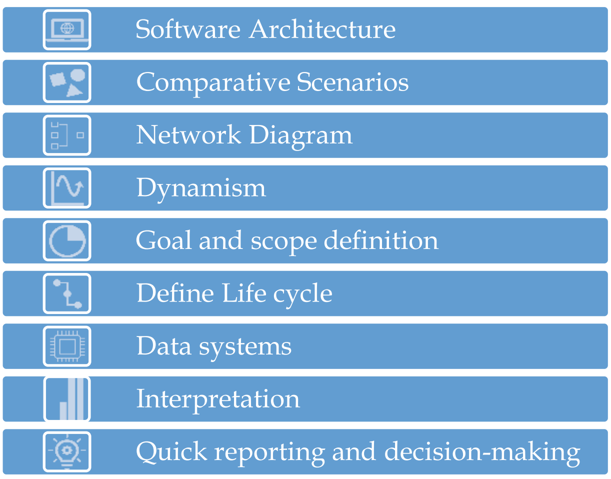


Figure 22 – TOLCAB's recommended future development directions.

Improvements to the software architecture

Currently, TOLCAB is an excel-based platform acting both as the software's back- and front-end. A future direction proposal is to develop a python-based Graphical User Interface (GUI) to act as a front-end (Figure 23). The objective is that the user would use the GUI interface for input and output without having to go through the software's back-end. The main goal is that the GUI provides seamless user navigation while comprehensively supporting decisions.

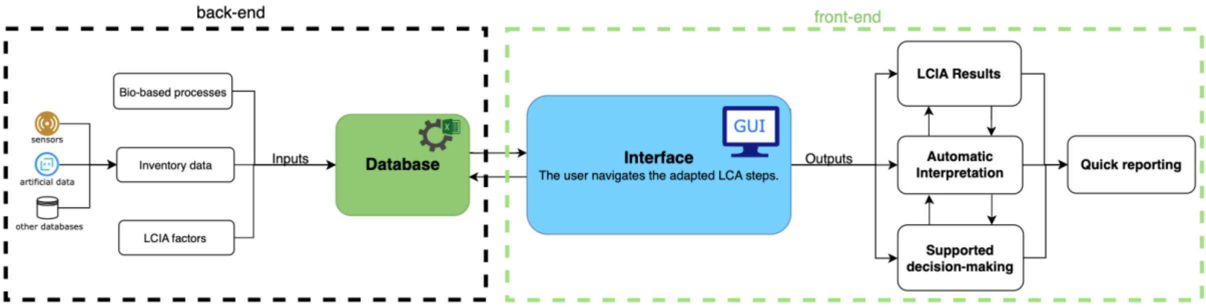


Figure 23 - Future software architecture suggestion with more precise boundaries between the back-end and front-end to facilitate user navigation.

Creating comparative scenarios

Creating multiple scenarios for environmental impact comparison is a common feature in most LCA software. Scenarios are created in the goal and scope definition stage and influence the other following stages (Pesonen et al., 2000). To allow for comparison, according to ISO:14044 (2006), they should all use *the same functional unit and equivalent methodological considerations, such as performance, system boundary, data quality, allocation procedures, decision rules on evaluating inputs, and outputs and impact assessment*. In TOLCAB, scenarios could be defined to compare, among others: (i) geographical contexts; (ii) processes selected in the life cycle; (iii) data collection methods; and (iv) LCIA methods. Creating hypothetical scenarios and comparing them with the current physical system is highly advisable as new environmentally sustainable courses of action can be found.

New visualisation tools would have to be implemented to compare the scenario's static and dynamic results. Additionally, the *Quick reporting* would include an option to present a report comparing options. This is believed to be a significant improvement towards facilitated decision-making.

Adding a network diagram

This is an extra tool to visualise the results from the LCIA stage. It is a standard and helpful tool to visualise environmental processes in the life cycle. It displays the defined processes in a clear flowchart that enables the user to identify environmental concerns in the system quickly. For each scenario, a cut-off selection can allow users to designate the amount of material or energy flows or the degree of environmental relevance connected to individual processes or product systems to be disregarded (ISO 14044, 2006). As TOLCAB aims to provide quick results in an improved user experience, this would be an exciting upgrade to the software. A new tab would be created to achieve this goal. There, users could visualise the physical system's life cycle and spot the main areas of concern. The main benefit would be to combine the life cycle perspective with a straightforward visualisation of environmental impacts.

Combining static and dynamic results

To include interpretation and quick reporting results based on dynamic results, future development needs to find a way to integrate and combine static and dynamic results throughout the platform. As of now, dynamic results can only be visualised for a single flow at a time. Additionally, the boxplot tool on its own may be restrictive. Other alternatives to visualise and analyse dynamic results are recommended to be studied and eventually included in the software. Testing TOLCAB in situations providing dynamic data (time-dependent) could facilitate the generation of ideas for new approaches.

Moreover, future software development efforts should include a full temporalisation of background and foreground LCI processes as they can considerably affect results (Pigné et al., 2020). These efforts can include dynamic LCIA models, using, for instance, dynamic characterisation factors (see section 2.2.2).

Automating goal and scope definition

The main objective here is to develop the software so that the goal and scope definition step can automatically affect the following steps. For this to happen, the inactive boxes (in grey) can be activated to perform automatic actions: the time period, the reference flow, the system boundary and the location (see in Figure 11). The time period box is the time interval related to the functional unit and reference flow. The activation of this time period box is related to the environmental impact results. Only data from a specific time interval would be assessed if this box was activated. The reference flow addition would be especially relevant for the bio-based processing sector since the impacts from the industrial production of a batch often differ from those of small-scale productions. Comparing results between the reference unit and the actual reference flow could allow measuring the non-linear scaling of environmental impacts. The system boundary still needs to affect future calculations. Activating it could mean that the users would obtain more precise results regarding the environmental impacts of the desired processes supply chain. Moreover, expanding geographical options in the database would allow for more reliable results if this software were to be used outside Denmark or Europe. Furthermore, the heterogeneity of the assessment scope can be automatically addressed. This would be possible if the audience and objectives selected during the goal and scope definition could affect how quick reporting is performed. Hence, the quick reporting could be customisable and tailored to the user's goal. For instance, if marketing purposes were to be the goal of the LCA study, the quick reporting tab could generate a sustainable label, e.g., similar to the one developed by Barni et al. (2018). This allows for the LCA study to consider the different goals defined by the users.

Improving the definition of the Life Cycle

The tab *Define Life Cycle* was conceived as a crucial action in TOLCAB. The idea was to allow a holistic visualisation of the life cycle while providing the user with different options for each process that would characterise the uniqueness of that specific life cycle included in the bio-based processing sector. This was inspired by Gençer et al. (2020), who developed a modular representation in the SESAME tool for the energy sector. In this tool, the various technology options possible for each standard process in the energy sector are included in the software using drop-down menus. This way, the user can choose the ones that better apply to the system. However, this has not yet been implemented in TOLCAB.

Nonetheless, it would also be possible for the bio-based processing sector if a continuous effort were devoted to creating a database that would include most standard bio-based processes. This way, the user would only have to choose from the several available standard bio-based process options instead of having to model them.

This tab could also include allocation possibilities, especially in processes where the pathway would diverge. To achieve this, for instance, additional alternatives could be added where the user could include the percentages of the reference unit assigned to each flow. Upstream and downstream process options would also need some development as they are crucial to achieving a more comprehensive assessment.

Developing data systems

The integration of sensor-based equipment and soft sensors has not yet been tested in TOLCAB. Future efforts will focus on the actual incorporation of these data collection methods. As mentioned, these efforts should also consider the correct collection and management of dynamic data.

Moreover, it is recommended to create a control system to introduce a new layer towards a bi-directional connection with the physical system. To achieve this, actuators can be integrated. According to Gajjar (2017), actuators take "one form of energy as input and produce some form of motion, movement or action". Figure 24 illustrates the potential of actuators in triggering actions in the DT system, by acting between the virtual and physical worlds. This could mean that the results obtained from the software could trigger actuators to change the sensor's way of operating. These actions could be performed, for instance, to reduce the uncertainty of measurements or to change the time intervals of the data collection. This subject can explore many possibilities (Udugama et al., 2021).

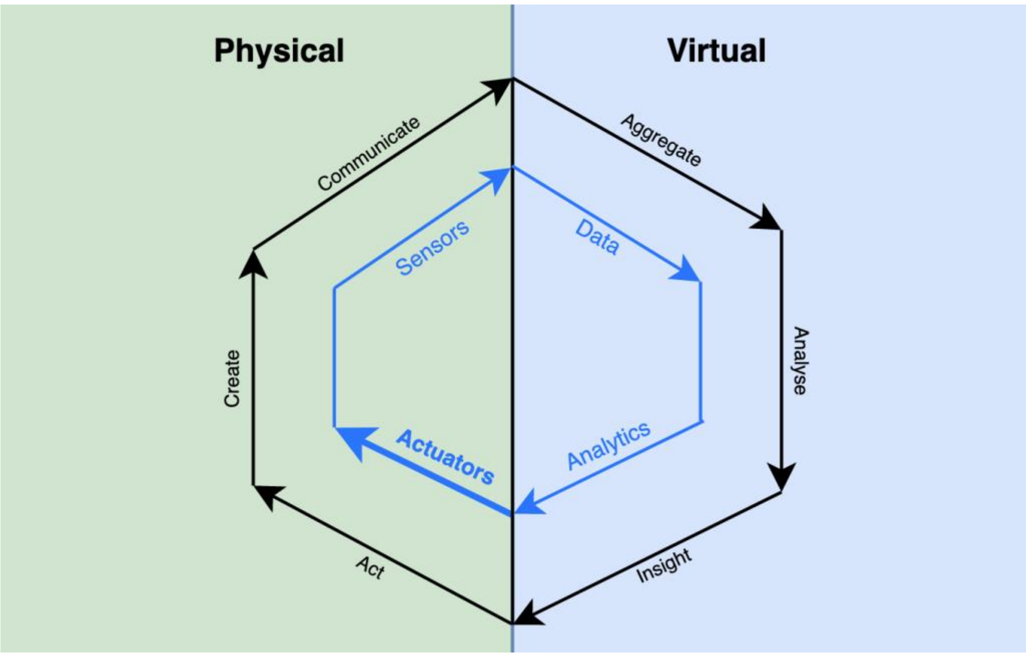


Figure 24 – Potential role of actuators in a DT strategy, adapted from Lisachuck (2018).

Expanding interpretation capabilities

The interpretation step should find ways to portray dynamic results as they can provide valuable information for users. Moreover, the *environmental hotspots finder* and the *suggestion box* still need to be activated, as shown in Figure 18. Future efforts are planned to achieve this. Additionally, uncertainty and sensitivity analyses can be enhanced to provide a more robust assessment, improving the interpretability and trustworthiness of the results (Beltran et al., 2018). For the sensitivity analysis, this can be done by expanding the number of parameters assessed. For the uncertainty analysis, an attempt to evaluate and quantify errors was developed only for the input data. Future development should expand these partial efforts to encompass the propagation of errors in model computations and output data (Gargalo et al., 2016). Adding these analyses can guide users to evaluate, among others, variability in methodological choices, spatial or temporal assumptions, or variability in characterisation factors (Beltran et al., 2018). Statistical methods coupled with powerful visualisation tools could help achieve this. Interval calculation, fuzzy logic, Gaussian formulas or Monte Carlo Simulation are some statistical methods that could be explored (Gargalo et al., 2016). Also, using the variability boxplots tool (presented in Figure 17) could help users better comprehend the sources of uncertainty. Further studies should be performed on how to achieve these possibilities.

Moreover, it is suggested that the uncertainty and the sensitivity analyses reverse order. The sensitivity analysis could be re-designed to identify the parameters influencing the environmental impacts the most. This way, the uncertainty analysis could then target those particular critical parameters.

Improving quick reporting and decision-making

Temporal considerations and simple visualisation should be brought together. Testing alternative ways to incorporate dynamic results in the *Quick reporting* tab should be a future concern. For instance, these could include mentioning the temporal environmental impact peaks for the critical flows.

Moreover, the theoretical framework presented in Phase 1 - Adapting LCA (see section 3) outlined prospects for creating an online bi-directional DT-based LCA. This may be achieved if environmental decision-making becomes automated. There are many possibilities to be explored. The main idea is to create a closed loop between the virtual LCA model and the physical system. Depending on readings from the physical plant, the automated assessment would suggest changes or even activate the changes itself (e.g., using actuators). This is part of ongoing work.

4.4. Conclusions

This chapter presented the TOLCAB software. This outcome represented the methodology implementation of Phase 2, as illustrated in Figure 3. A complete overview of the software was provided. The initial actions were introduced to configure a physical system to be analysed using the LCA. Next, the assessment and interpretation capabilities offered by this tool were outlined. To conclude, recommendations for future software development were indicated.

5. Proof-of-concept

This chapter aims to apply and validate the TOLCAB software. Section 5.1. provides application demonstrations using two case studies selected from the literature. Firstly, the approach and assumptions considered for these applications are described. Then, the case study applications are exhibited: case study A is applied in section 5.1.1, and case study B is applied in section 5.1.2. Finally, section 5.2 discusses the results, their corresponding limitations, and the benefits and drawbacks when applying this tool.

5.1. Approach and assumptions

This section reproduces two LCA case studies using the TOLCAB software. Both these studies belong to the bio-based processing sector. For each case, the approach employed in the original papers is introduced and compared with the approach used when adopting TOLCAB. Similar to chapter 4, TOLCAB's results are presented here considering the user perspective, thus following the recommended user actions in order. It is important to emphasise that this validation does not attempt to repeat the studies precisely as they were performed but rather to use their available data to test the feasibility of TOLCAB. Accordingly, the reproduction of these studies includes the inherent assumptions and capabilities associated with TOLCAB: (i) Denmark as the geographic location, (ii) the PEF method to perform the LCIA calculations, and (iii) LCI data sources presented in Appendix D. Note that regarding the inventory data, only the Denmark location option is tested. Although the software includes a location option for Europe, it is decided that it does not add anything to this demonstration other than the notion that it exists. As previously indicated, the PEF method was used because this tool was designed to contribute to future LCA implementations, and the European Commission currently advises utilising this strategy (European Union, 2021). Moreover, landfill waste and wastewater are simplified in this chapter - all flows corresponding to these two groups have been assigned to the same references for each case study. Also, although the consequential approach is followed, two references considering the allocation at the point of substitution (APOS U) are selected (see Appendix D) due to a lack of acceptable alternatives. Furthermore, the selected case studies do not provide all the necessary information in-depth. Simplifications regarding the modelling of the system's processes, the inexistence of dynamic LCI data, or the non-sharing of inventory data create limitations for this validation. Nonetheless, sufficient information is provided in both case studies regarding the input and output flows of these systems. Therefore, the following case studies A and B (see sections 5.1.1 and 5.1.2) were found to be suitable for performing this proof-of-concept.

Both original studies embraced a cradle-to-gate perspective. However, this chapter employs a cradle-to-grave perspective. This choice was made because accounting for a larger scope of the supply chain when evaluating environmental impacts was a goal outlined in the methodology, as described in Phase 1 (see section 3). Furthermore, data collection methods were created to simulate actual direct measurements from the system when, in fact, this data was gathered entirely from the articles. These data collection methods are not implemented in an actual plant and only aim to mimic what would happen in a real context application. For the sake of simplicity, sensors retrieve the exact values stated in the case study, and the artificial data generators retrieve those values doubled. The user can choose between the available data collection methods when modelling the system. Moreover, two alternative life cycle options are defined for every process in the system: Option 1 for measuring processes' flows with the sensors and Option 2 for measuring the processes' flows with the artificial data generators. This chapter will not compare the options since their results bring no additional value. They were only created to demonstrate that TOLCAB allows the selection of alternative processes with different inputs and outputs. Moreover, only static results were obtained due to the lack of available dynamic data from the case studies. Nonetheless, the test presented in Figure 17 (section 4.2) shows that if dynamic data had been available, dynamic results could have been obtained for each flow and presented in boxplots for each impact category.

5.1.1. Case study A: rapeseed-based 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. The study additionally examined its energy balance and the usage of biodiesel versus petroleum-based fuel in a standard 28-t vehicle. Figure 25 provides a visual description of the evaluated system.

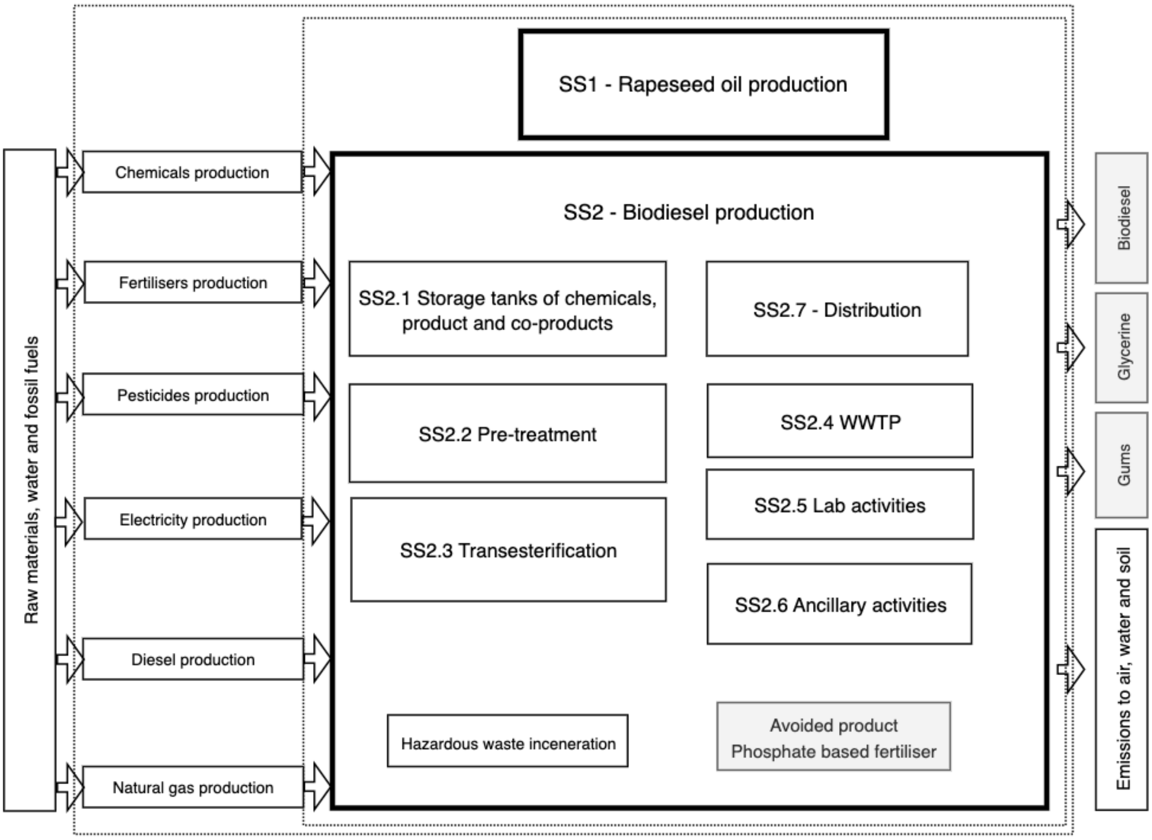


Figure 25 - System boundaries and the process chain for biodiesel production from rapeseed oil, adapted from González-García & García-Rey (2013).

Data sources

In the original study, data for the background system was acquired from databases. In contrast, the inventory data for the foreground system used average annual data that had been measured on-site in the company. The referred data from databases includes mostly references from the Ecoinvent

database, with some exceptions mentioned in the article. The exact references used, however, are not detailed in the paper. Moreover, they used the characterisation factors reported by the Centre of Environmental Science of Leiden University (CML 2001 method), which includes the following impact categories: abiotic depletion (ADP), acidification (AP), eutrophication (EP), global warming (GWP), land competition (LC), ozone layer depletion (ODP), and photochemical oxidants formation (POFP).
Therefore, the TOLCAB software validation approach significantly differs from the original study. Due to the references' lack of detail, it was challenging to find comparable characterisation factors. Also, the impact assessment method used is the PEF method, which implies distinct impact categories. Moreover, in the original study (Figure 25), 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 comprehensibly available for the SS2. Therefore, only the SS2 was modelled using TOLCAB.

Initial actions

The initial actions presented in section 4.1 are followed here to model the system of case study A using TOLCAB. They include: (i) inserting the goal and scope definition details, as shown in Figure 26; (ii) creating sensors and artificial data generators assigned to specific inputs or outputs in the *Edit Data Collection (BE)* tab; and (iii) inserting the information regarding the processes' flows into the tool, and defining two options for each process (Option 1 is detailed in Appendix F – Description of processes). Note that several output emissions were not assigned to a specific process (i.e., Phosphorous, Suspended solids, Ammonia and Chemical oxygen demand). Thus, in this work, they were assigned to a new process called N.E. (Not Expressed). The life cycle was then defined, and Option 1 was chosen for all the processes in the life cycle (see Figure 27). These processes are descripted in detail in Figure F 1 in Appendix F. The characterisation factors are presented in the *LCIA – CFs (BE)* tab (detailed in Appendix D). The only exception was the biogenic CO2, for which the characterisation factors were altered in the climate change category (-1 for uptake and +1 for release), following the original case study's approach.

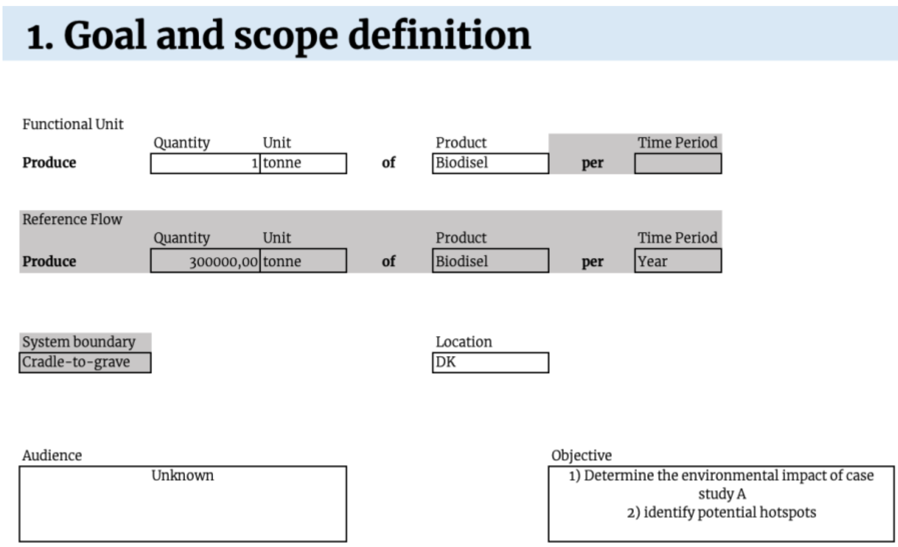


Figure 26 - 1. Goal and scope definition tab for case study A.

Midstream							
SS2.1	**SS2.2**	**SS2.3**	**SS2.4**	**SS2.5**	**SS2.6**	**SS2.7**	**N.E.**
SS2.1 - Option 1	SS2.2 - Option 1	SS2.3 - Option 1	SS2.4 - Option 1	SS2.5 - Option 1	SS2.6 - Option 1	SS2.7 - Option 1	N.E. - Option 1

Figure 27 - Define Life Cycle tab for case study A.

Results

Since the system has been configured, results can now be retrieved. The total value for each flow is calculated according to the chosen data collection methods options. All the flows in the system can be visualised using the *LCI Summary* tab. Since Option 1 was selected for all the processes, the LCI results coincide with the information provided in the case study. The static characterisation results can be visualised in various ways, depending on the user's interests. Relative contributions per process of the system can be seen in Figure 28. They tend towards similar conclusions obtained in the original study. SS2.2 and SS2.3 are the highest contributing processes for all the impact categories of both methods. The conclusions were similar for most categories except for the GWP and LC categories, where SS2.2 dominated in TOLCAB and SS2.3 dominated in the original study.

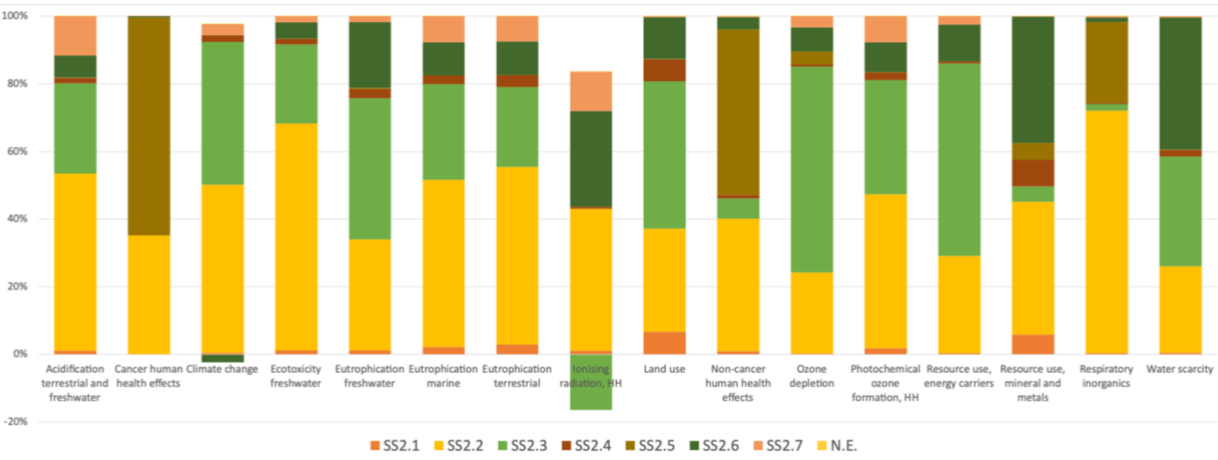


Figure 28 - Relative contributions per impact category for case study A.

Figure 29 shows other possibilities offered by the software to visualise results. Figure 30 shows an example of how a flow can be selected to observe whether it affects the impact categories, in this case, for the Waste to incineration (from SS2.5) output. However, incongruencies with the original study were found when exploring these possibilities in more detail. For instance, the original research mentions ammonia and nitrate as remarkable contributors to eutrophication. However, that was not the case for the TOLCAB proof-of-concept, where Oxygen (SS2.4) was the most significant contributor, followed by Methanol and Electricity.

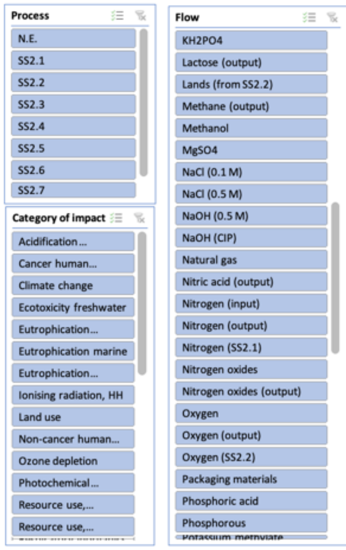


Figure 29 - Flexibility in visualising characterisation results in 3. LCIA – Visualise CResults DK for case study A.

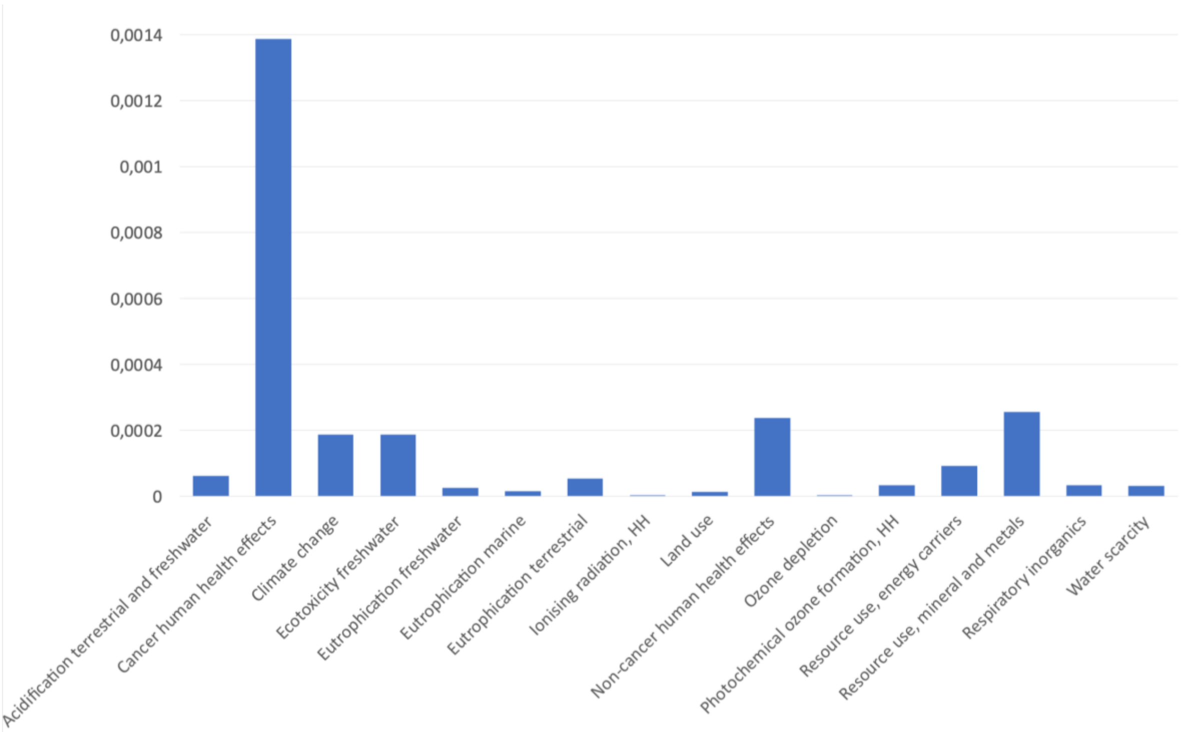


Figure 30 – Characterisation results of the Waste to incineration (from SS2.5) flow for case study A. The units considered for each impact category are detailed in Table C 1 in Appendix C.

The normalised and weighted results were not performed in the original study (González-García et al., 2013) as the authors did not consider it would provide additional robust information. Nonetheless, in a quest to present TOLCAB's possibilities, normalised results are shown in Figure 31 and weighted results in Figure 32. In both cases, the cancer human health effect impact category dominates the environmental burdens expressively.

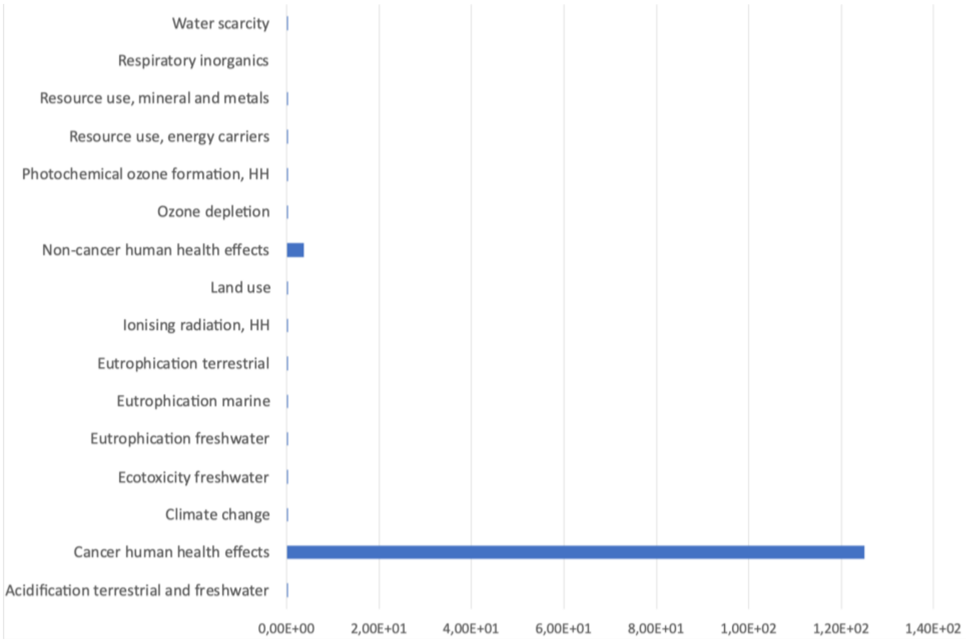


Figure 31 - Normalised results in tab LCIA - NResults for case study A. The units considered for each impact category are detailed in Table E 1 in Appendix E.

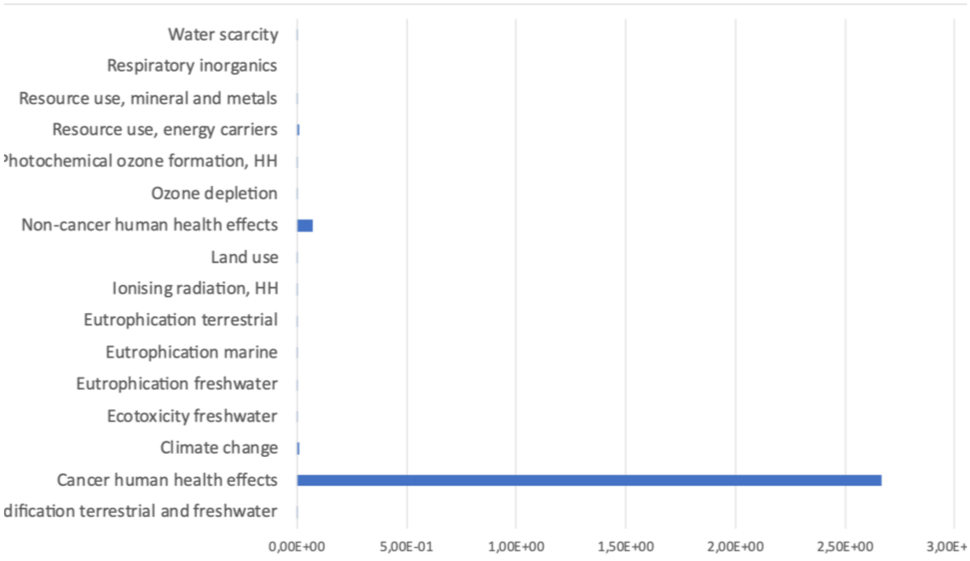


Figure 32 - Weighted results in tab LCIA - WResults for case study A. The units considered for each impact category are detailed in Table E 2 in Appendix E.

The interpretation procedures are automatically presented. The *Hotspots ranking* provides a concise summary of the findings (see Figure 33). The process with the higher environmental impact is SS2.6; the flow with the highest environmental impact is “Carbon dioxide (SS2)”, followed by “Waste to incineration (from SS2.5)” and “Oxygen (SS2.2)”. To gather more details about the contribution of each impact category, process or flow, the user is recommended to go back to previous tabs.

4. Interpretation

Hotspots ranking		
Impact category (Nresults)	**Process (Wresults)**	**Flow (WResults)**
Cancer human health effects	**SS2.5**	**Waste to incineration (from SS2.5)**
Non-cancer human health effects	SS2.2	Carbon dioxide (SS2.2)
Resource use, energy carriers	SS2.6	Oxygen (SS2.2)
Resource use, mineral and metals	SS2.3	Electricity
Climate change	SS2.7	Sodium chloride
Acidification terrestrial and freshwater	SS2.4	Steam (from SS2.6)
Land use	SS2.1	Methanol
Photochemical ozone formation, HH	N.E.	Potassium methylate
Eutrophication terrestrial		Rapeseed oil (from SS1)
Eutrophication marine		Transoceanic tanker
Water scarcity		Oxygen
Ecotoxicity freshwater		Chlorhydric acid
Eutrophication freshwater		Sodium hydroxide
Ozone depletion		Carbon dioxide
Ionising radiation, HH		Silica gel
Respiratory inorganics		Truck 16–32 t
		Phosphoric acid

Figure 33 – Hotspots ranking in the 4. Interpretation tab for case study A.

The uncertainty, sensitivity and quick reporting analyses were also automatically performed. The sensitivity analysis (see Figure 34) show how reducing the Waste to incineration (from SS2.5) flow would affect the environmental burdens per impact category.

The quick reporting results summarise findings (see Figure 35). The starting points, life cycle options, quick results and quick suggestion tools are automatically presented. This way, the major findings from case study A are summarised in a single tab which can facilitate communication and potential fulfilment of the objectives established.

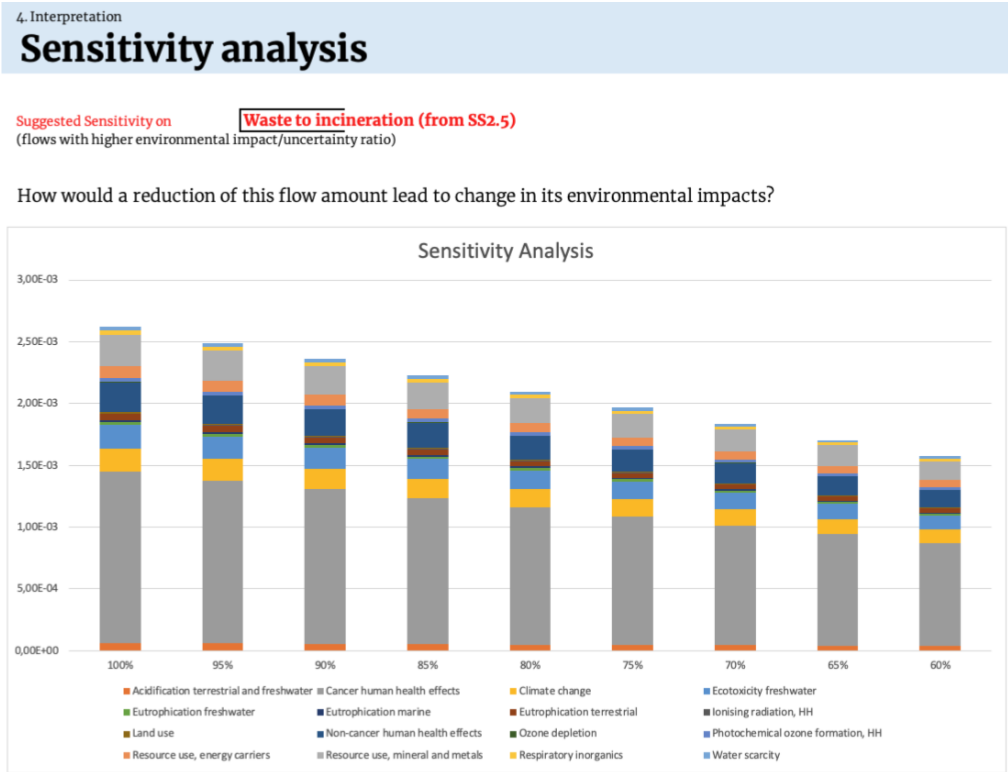


Figure 34 – Sensitivity analysis tab for case study A: how would reducing the Waste to incineration (from SS2.5) flow affect the environmental burdens per impact category? The units considered for each impact category are detailed in Table C 1 in Appendix C.

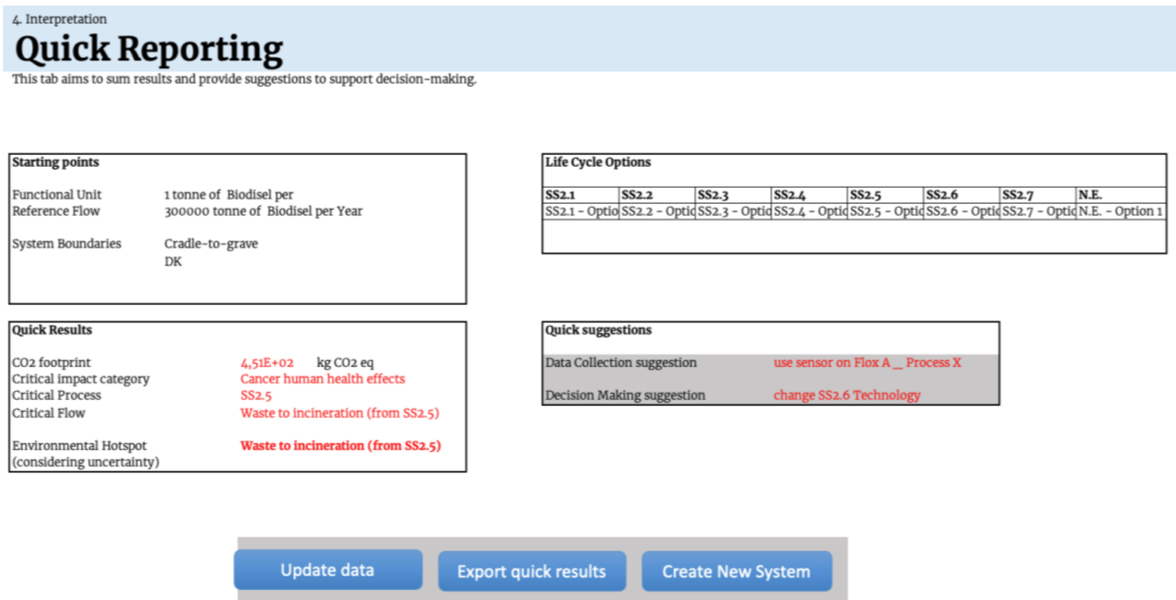


Figure 35 - Quick reporting tab for case study A.

5.1.2. Case study B: β-Galactosidase enzyme production

The LCA study performed by Feijoo et al. (2017) evaluated the β-Galactosidase enzyme production in an industrial-scale facility from a cradle-to-gate perspective. The production process alternative chosen for this evaluation was the use of recombinant *Saccharomyces cerevisiae* yeast expressing the lacA gene of *Aspergillus niger*. Figure 36 provides a visual depiction of the assessed system.

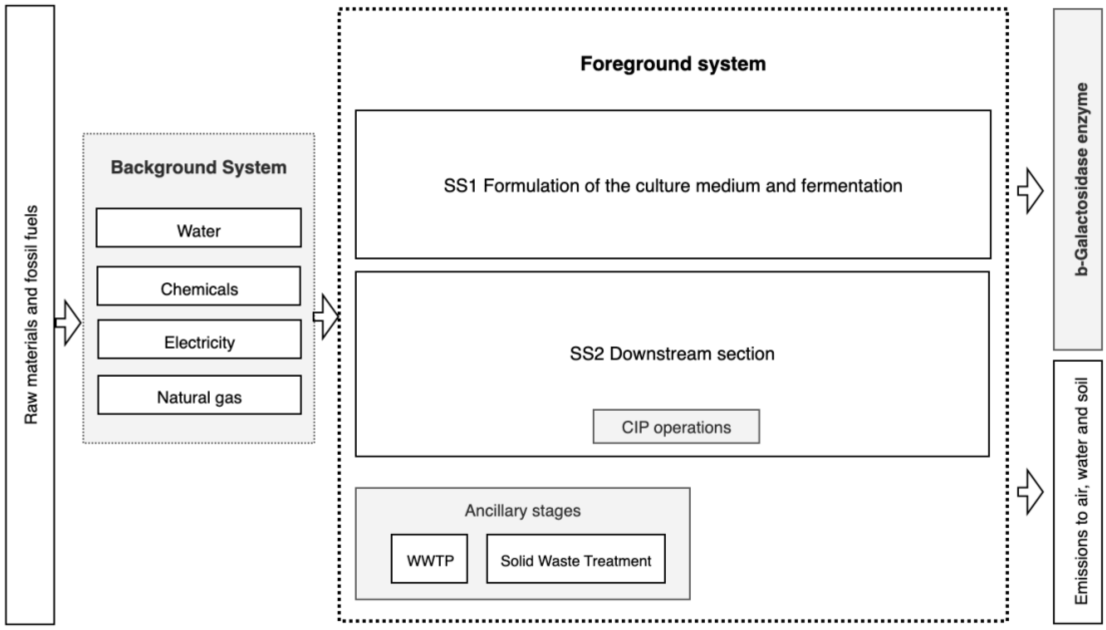


Figure 36 - System boundaries of the production of β-Galactosidase enzyme, adapted from Feijoo et al. (2017).

Data sources

The original study used the SimaPro 8.2 software to perform the LCA. The inventory data was completed using the Ecoinvent database, especially for background processes and the ancillary stages, and the inventory related to wastewater treatment activities was taken from Doka (2007). However, the specific inventory references employed are not detailed in the study. The characterisation stage was performed using the ReCiPe midpoint method – hierarchist perspective. The assessment included the following environmental impact categories: climate change (CC), ozone depletion (OD), terrestrial acidification (TA), freshwater eutrophication (FEU), marine eutrophication (MEU), human toxicity (HT), photochemical oxidant formation (POF), terrestrial ecotoxicity (TE), freshwater ecotoxicity (FE), marine ecotoxicity (ME), water depletion (WD) and fossil depletion (FD).

As a result, the TOLCAB approach has significant discrepancies from the original study. The references used for the inventory are likely to be different from those in the original analysis. Additionally, the PEF method is the impact assessment approach used, which denotes distinct impact categories.

Initial actions

The initial actions are performed. The goal and scope definition details are inserted, as shown in Figure 37. Regarding the modelled system, the subprocesses within the processes defined in this stage could not be later interpreted since they were aggregated in the main processes SS1, SS2 and Ancillary Stages. This is true for the CIP (Cleaning-in-Place) operations which are a part of the SS2, and for the

WWTP (Wastewater Treatment Plant) and Solid Waste Treatment, which are part of the Ancillary stages (see Figure 36). These processes are descripted in detail in Figure F 2 in Appendix F.

Additionally, in this approach, the air emissions are allocated to the ancillary stages, although it was unclear where they were generated. This decision was based on the fact that ancillary stages are related to the system's emissions management. This may lead to more significant impacts occurring in this stage. As for the remaining initial actions, the same approach as the one performed in the previous the González-García & García-Rey (2013) proof-of-concept is followed, and the information regarding the processes' flows was inserted into the tool (Option 1 is detailed in the Appendix F – Description of processes). Option 1 is again selected for all the processes in the system (see Figure 38).

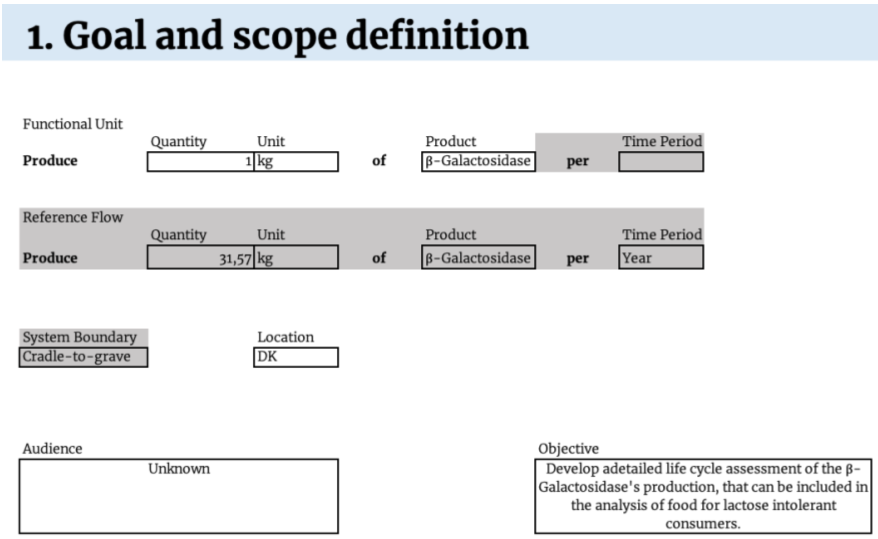


Figure 37 - 1. Goal and scope definition tab for case study B.

Midstream		
SS1	**SS2**	**Ancillary Stages**
SS1 - Option 1	SS2 - Option 1	A. Stage - Option 1

Figure 38 - Define Life Cycle tab for case study B.

Results

All the flows in the system can now be visualised, and once again, depending on the user's preferences, the static characterisation findings can be shown in various ways. Relative contributions of the processes of the system to the impact categories can be visualised in Figure 39. The tendency towards SS2 being the hotspot process with the overall highest contributions across most environmental impact categories is similar both in the original study and in this proof-of-concept approach. Most categories adopted in the original research (i.e., CC, OD, TA, HT, POF, WD and FD) showed analogous results when compared to the PEF categories used in the TOLCAB approach (i.e., correspondingly, Climate change, Ozone depletion, Acidification terrestrial and freshwater, Non-cancer human health effects and cancer human health effects, Photochemical ozone formation Human Health - HH, Water scarcity, and Resource use energy carriers). Although it was more challenging to compare the other impact categories related to eutrophication and ecotoxicity, it was found that there were some disparities. Again, it is relevant to note that comparing these impact categories is a rough approximation with several reliability drawbacks. Furthermore, the original study presented additional relative environmental contribution graphs for specific flows and processes, which are not performed in this approach.

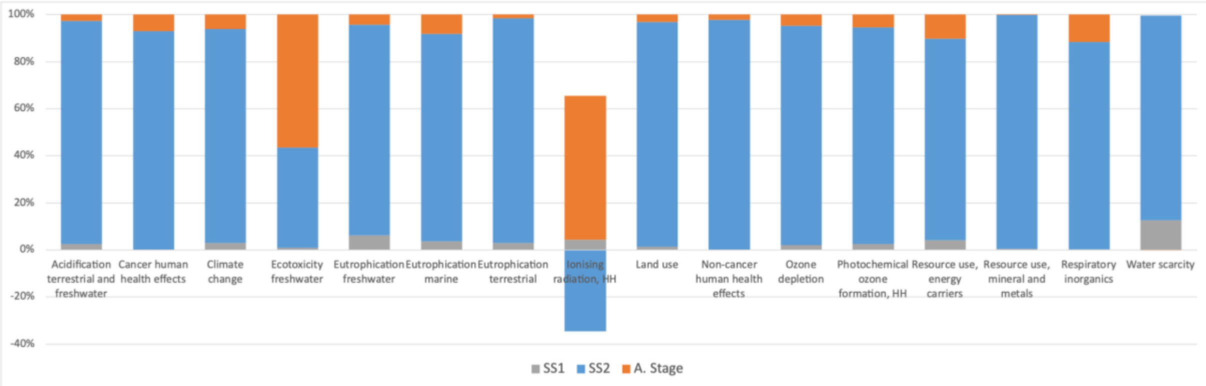
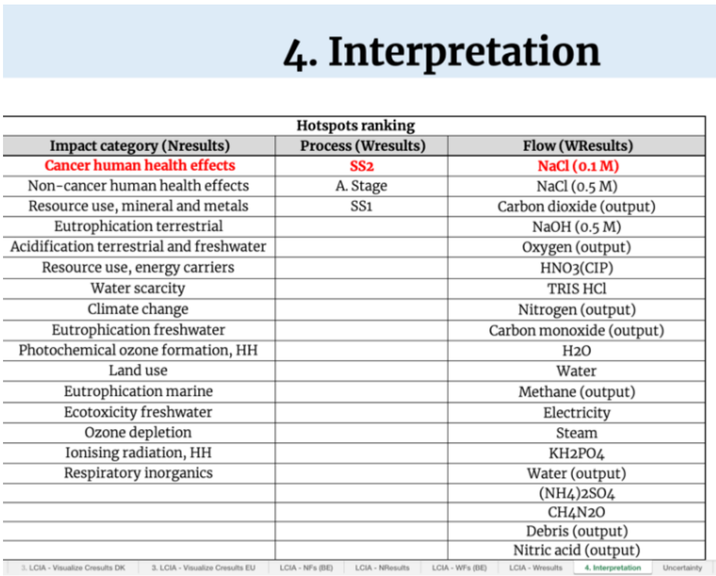


Figure 39 - Relative contributions per impact category for case study B.

The normalised and weighted results showed the same tendency observed in the previous proof-of-concept approach (see section 5.1.1). Cancer human health effects stand above all the other categories with a weighted contribution of 91%, followed by non-cancer human health effects (7%).

The interpretation results are presented in Figure 40 and show the *Hotspots ranking*. The impact category and the process hotspots were already mentioned. The highest contributing flow is NaCl (0.1M), followed by NaCl (0.5M) and Carbon dioxide (output), among the others in the list. These findings contradict the original study, where the environmental burdens associated with the β-Galactosidase enzyme production were reported to be primarily related to the consumption of the chemicals present in the CIP operations (included in the process SS2), especially NaOH and HNO3. This conclusion led the original study to evaluate and compare alternative scenarios for CIP operations. These assessments were not conducted in this proof-of-concept.



4. Interpretation

Hotspots ranking		
Impact category (Nresults)	**Process (Wresults)**	**Flow (WResults)**
Cancer human health effects	SS2	NaCl (0.1 M)
Non-cancer human health effects	A. Stage	NaCl (0.5 M)
Resource use, mineral and metals	SS1	Carbon dioxide (output)
Eutrophication terrestrial		NaOH (0.5 M)
Acidification terrestrial and freshwater		Oxygen (output)
Resource use, energy carriers		HNO3(CIP)
Water scarcity		TRIS HCl
Climate change		Nitrogen (output)
Eutrophication freshwater		Carbon monoxide (output)
Photochemical ozone formation, HH		H2O
Land use		Water
Eutrophication marine		Methane (output)
Ecotoxicity freshwater		Electricity
Ozone depletion		Steam
Ionising radiation, HH		KH2PO4
Respiratory inorganics		Water (output)
		(NH4)2SO4
		CH4N2O
		Debris (output)
		Nitric acid (output)

Figure 40 – Hotspots ranking in 4. Interpretation tab for case study B.

The remaining results consist of uncertainty (Figure 41) and sensitivity (Figure 42) analysis, as well as the quick reporting results (Figure 43). In this approach, arbitrary values were inserted in the uncertainty column of the highest contributing flows to demonstrate one additional capability of these tools. This change generates a more complex uncertainty matrix when compared to the previous one (section 5.1.1) where all the uncertainty values had been assigned to the same value. This variability leads to the NaCl (0.5M) flow being assigned the uncertainty environmental hotspot, even though it presents a lower impact value than the NaCl (0.1M) flow. This result affects both the sensitivity analysis and the quick reporting that followed. The sensitivity analysis is determined for the NaCl (0.5M) since that is the uncertainty environmental hotspot flow. In turn, the quick reporting results show a different critical flow - NaCl (0.1M) - and environment hotspot result - NaCl (0.5M).

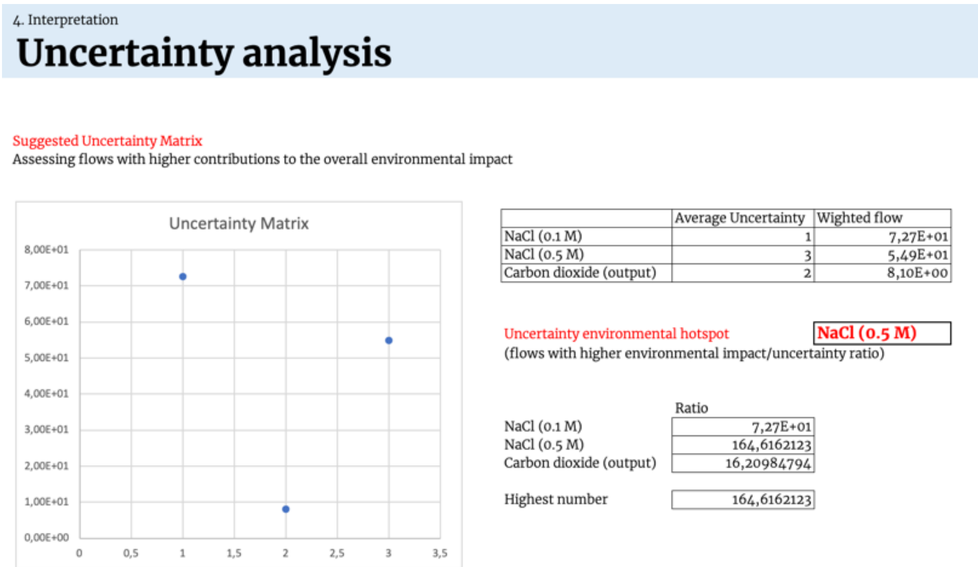


Figure 41 – Uncertainty analysis tab for case study B.

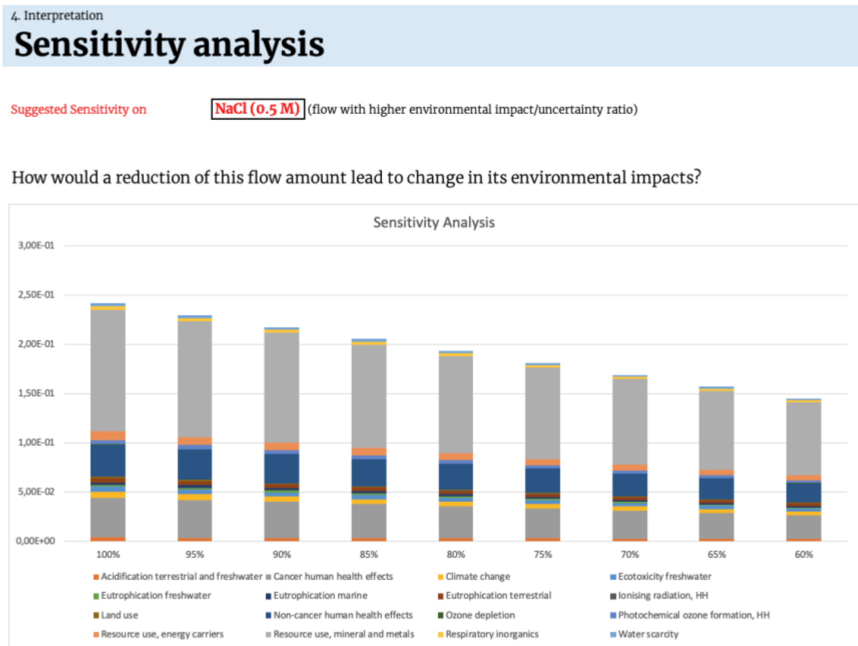


Figure 42 – Sensitivity analysis tab for case study B: how would reducing the NaCl (0.5 M) flow affect the environmental burdens per impact category? The units considered for each impact category are detailed in Table C 1 in Appendix C.

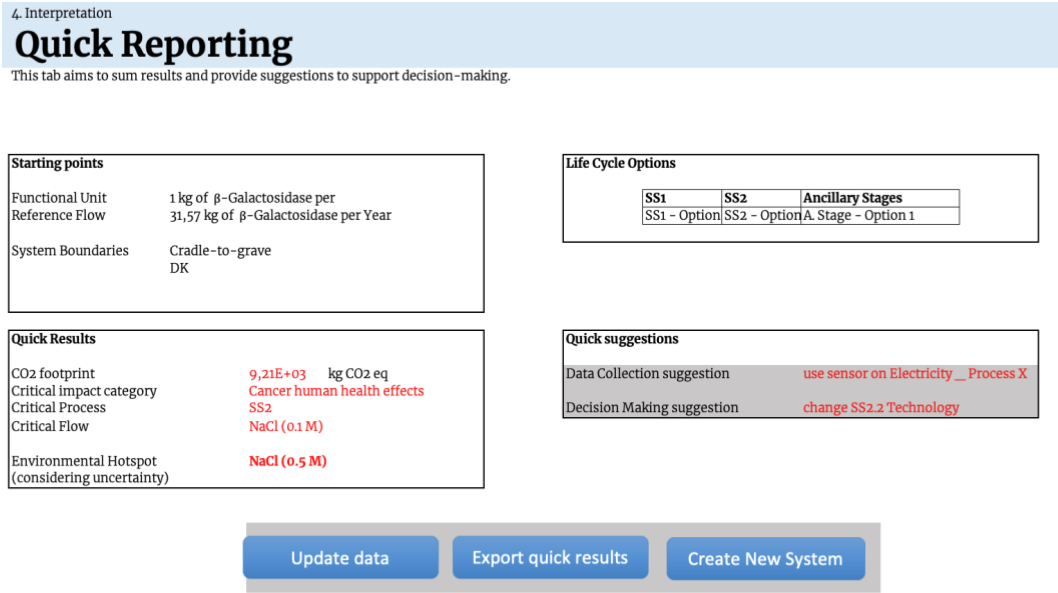


Figure 43 – Quick reporting tab for case study B.

5.2. Discussion

The proof-of-concept applications demonstrated the software usefulness and capabilities when performing an LCA for the bio-based processing sector. It has been shown that applying TOLCAB can introduce several benefits, such as: (i) reduce time consumed due to the industry knowledge database, the automatic calculations, and the considerable decision-support; (ii) user-friendly software which facilitates the use in industrial settings; (iii) offers powerful graphics to visualise the impact assessment results; (iv) enables the evaluation of dynamic monitoring of results; (v) 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, such as (a) to perform the user actions in the tool, basic learning is needed, which can nonetheless turn away some users; (b) several envisioned functionalities are not operational at this point due to time constraints; and (c) rough approximations may have compromised the reliability of the validation.

Of note is that the selected case studies posed several barriers to demonstrating the potential of TOLCAB. Given the fact that these were study recreations, data was collected from indirect sources and only static data was obtained. Building a real-time evaluation was, therefore, unfeasible. Additionally, the cradle-to-grave assessment was not entirely possible since the complete knowledge of the inputs and outputs of the supply chain was not reported in the case studies. This is especially true of the lack of information regarding the use phase. Therefore, comparing the original studies with the results obtained with TOLCAB was challenging. In summary, this was due to mainly two reasons: (i) the inventory data provided was, for the most part, unclear; (ii) they used different LCIA methods CML and ReCiPe, whereas in this work we have used the PEF method. This emphasised the consequences of choosing different impact assessment methods to the same case study, as they produce, in some instances, different outcomes (Wernet et al., 2010). Important to highlight is that, as above-mentioned, the PEF method was employed due to the fact that the goal was to contribute towards a unified and standardised LCA and LCA applications, and PEF has now been recommended of the method of choice (European Union, 2021). Moreover, intending to expand the system's boundaries, the validations performed cradle-to-grave studies instead of a cradle-to-gate ones, which were used in the original study. This led to additional differences in results.

The software is still in its early stages and has a considerable margin for improvement. The surrogate model approach should be transformed into a real implementation approach. This would enable actual real-time data collection methods to be incorporated into the platform.

Furthermore, there are other minor limitations, and they are as follows: (i) there is no integration with surrounding technologies in the industry environment, such as Cloud Computing capabilities or existing manufacturing software (e.g., MES or ERP); (ii) the bi-directional flow of information is not yet implemented which would allow to automatically bring decision-making power to the physical system; and (iii) sharing data between various stakeholders remains an issue to assess the entire supply chain.

To achieve the possibilities envisioned in the theoretical proposal, future development suggestions detailed above (see section 4.3) should be implemented. To name a few, further developing the software architecture in order to improve user navigation, include additional tools such as comparing scenarios and network diagram, or including actuators in the platform establishing a real-time bi-directional connection.

It is recommended that future practical applications choose real implementation scenarios where data collection methods can be implemented to create a live dynamic LCA. Efforts to build a comprehensive bio-based processes database encompassing the most common processes in the industry should also occur. These additions can increase the reach of this proposal.

Nevertheless, TOLCAB showed 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 processing. Noteworthy is that, although TOLCAB has been developed for the bio-based processing sector, the software is easily customisable 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 and future work

The LCA methodology is a robust and scientific approach to quantifying the environmental impacts of processes or product systems. However, several challenges are still preventing its widespread adoption. In the meantime, the ongoing Industry 4.0 introduces new technologies with ground-breaking possibilities, including automation, real-time monitoring, and decision-making capabilities.

This thesis attempted to merge these two subjects to maximise the potential of the LCA. To accomplish that, the literature review started by presenting the methodology standards and their associated limitations. Then, the latest research developments to overcome these obstacles were reviewed. They include methodological and technological proposals in the Industry 4.0 context. The methodologic proposals encompass the Dynamic, Organisational and Ubiquitous LCA. The Industry's 4.0 technologies applied to the LCA consist of smart sensor-based equipment, blockchain, artificial intelligence, cyber-physical systems, and digital twins.

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 conventional four stages of the LCA, this framework guides 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. The software's attempt to apply the ideas presented in the framework was overall successful but insufficient. Several propositions still require further development; thus, forthcoming developments were discussed in a quest to bridge the gap between the theoretical framework and its practical implementation.

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. 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. TOLCAB's ultimate goal is to propose environmental improvements in a closed-loop manner with minimal need for human intervention.

Furthermore, general future work recommendations emerge from this work. They are here as follows: (i) create guidelines to support the implementation and selection of data sources; (ii) study the integration of product identity data (Mashhadi and Behdad, 2018) as an additional data collection method; (iii) study ways to automatically integrate dynamic results in interpretation and quick reporting; (iv) investigate efforts in integrating background and foreground LCI and LCIA data considering temporal variability; (v) expand the system's boundaries by integrating all the supply chain data in the platform; (vi) investigate further automation of decision-making processes; (vii) customise the software to apply the theoretical framework in other sectors; (viii) follow a user centred design approach to reach an superior user-experience – this a proposal firstly introduced by Gould and Lewis, (1985), and recently applied by Riedelsheimer et al. (2020) using the DT technology with interesting outcomes; (ix) test an alternative framework conceptualisation where the LCA software is coupled with other existing manufacturing software (e.g., MRP, ERP, SCADA, among others); (x) consider expanding the theoretical framework to the economic and social sustainability pillars; (xi) use the planetary boundaries perspective (i.e., an environmental assessing concept attracting both the scientific and industry communities) (Ryberg et al., 2016); and (xii) conduct a systematic literature review on the recent research efforts on Industry 4.0 developments applied to the LCA.

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Appendix A – Research Gaps and Potential Ideas

The literature review (section 2) identified several research gaps. Table A 1 summarises these findings in a simplified manner. When creating this table, the goal was to generate ideas for framing the problem to be addressed in this master's dissertation. Nonetheless, it is this author's belief that this table can also help other researchers generating ideas for future work.

Table A 1 – Research gaps from the literature review on recent LCA developments, and corresponding drawbacks and ideas for future work.

Reseach Gaps	Drawbacks	Potential ideas for future work
Real-time LCA assessments	Need for smart infrastructures; Integrating LCA with smart infrastructures; Implementation and maintenance costs; Experts required.	Integrating sensor-based equipment in smart factories; Creating product identity data systems.
Apply intelligent sensor methodologies	Lack of cost-effecting sensing solutions; Required developments in sensor-based solutions; Lack of guidance and standardisation; Little research on the sensor fusion topic; Under-researched applications in certain sectors.	Study sensor fusion; Expand application of sensor-based LCA frameworks.
Tracking products through their entire life cycle	Stakeholders' reluctancy to share data; Hardware and software infrastructure required; Technology in early stages of development; Insufficient usage phase data.	Create open-source platforms for LCA users to insert data; Blockchain technology to bring stakeholders together; Creating product identity data systems for the usage phase.
Proactively predicting environmental impacts during the design phase	Uncertainties regarding product's life cycle; Lack of usage phase information.	Performing advanced simulation with digital-twin models; Using predicting AI algorithms.
Integrate Sensors-Blockchain-LCA	Need for smart infrastructures; Implementation and maintenance costs; Difficult stakeholder coordination; Blockchain solutions lack investment.	Practically implement a proof-of trial of the framework proposed by Zhang et al. 2020; Create a software solution combining sensors-ERP-blockchain-LCA; Further investigate barriers hindering blockchain-LCA application.
Applications in industrial symbiosis' contexts	Very complex coordination of stakeholders.	Blockchain technology to bring stakeholders together; O-LCA methodology for a holistic perspective.
Uncertainty when integrating LCA with emerging technologies	Lack of standardised integration methodologies; Need for smart infrastructures; Implementation and maintenance costs; Lack of trust surrounding new technologies.	Create new ISO standardised methodologies; Expand smart infrastructures; Research efforts.
Addressing spatial and temporal considerations from cradle-to-grave or cradle-to-cradle	Lack of temporal and region-specific databases; Need for manual data insertion; Computationally intensive; Difficult interpretation.	Perform real-time assessments, using sensor-based LCAs; Develop product identity data systems; Create net temporal databases; Create open-source platforms for LCA users to insert data.

O-LCA is under-researched and has limited uses in manufacturing	Lack of a O-LCA-specific databases and software solutions.	Applications in industrial symbiosis' contexts.
Uncertainties measuring emerging systems' impacts	Inexistent datasets, difficult to define smart technologies' physical boundaries.	Create open-source platforms for LCA users to insert data; Develop real-time monitoring and product identity data systems.
Predicting scenarios using scarce data sources	Under-researched topic.	Development of ML solutions to predict scenarios.
Time-consuming and evolving experts	Complex data collection during LCI; LCA software.	Implement real-time LCA assessment solutions; Develop easier software interfaces.

Appendix B – Tabs of the TOLCAB software.

Table B 1 describes the existing tabs in the TOLCAB software.

Table B 1 - TOLCAB tabs and corresponding descriptions.

Tab (in order of appearence)	Description
TOLCAB	Introduction to the software.
1. Goal and scope definition	Definition of the goal and scope.
Define Life Cycle	Definition of the life cycle being assessed.
2. Life Cycle Inventory	Mapping and integrating data sources into the platform.
Edit Data Collection (BE)	Data sources comprehensive collection.
Dynamic flow	Introducing dynamic inventory data.
Dynamic impacts	Dynamic characterisation results.
Description of processes	Processes comprehensive collection.
LCI Summary	LCI final results.
LCIA - CFs (BE)	Characterisation factors comprehensive collection.
TABLE DK (BE)	Characterised results - for Denmark location.
TABLE EU (BE)	Characterised results - for Europe location.
LCIA - Cresults (BE)	Characterised results - additional tables.
LCIA - Relative results	Characterised results - relative contributions.
3. LCIA - Visualize Cresults DK	Visualisation of characterisation results - for Denmark location.
3. LCIA - Visualize Cresults EU	Visualisation of characterisation results - for Europe location.
LCIA - NFs (BE)	Normalisation factors comprehensive collection.
LCIA - NResults	Normalised results.
LCIA - WFs (BE)	Weighting factors comprehensive collection.
LCIA - WResults	Weighted results.
4. Interpretation	Interpretation prompt results.
Uncertainty analysis	Automatic uncertainty analysis.
Sensitivity analysis	Automatic sensitivity analysis.
Quick reporting	Automatic quick reporting communication.

Appendix C – PEF method impact categories

Table C 1 describes the impact categories used in TOLCAB, and their corresponding units.

Table C 1 - PEF impact categories and corresponding units according to European Commission - Joint Research Centre (2022).

Impact categories	Unit
Acidification terrestrial and freshwater	mol H+ eq
Cancer human health effects	CTUh
Climate change	kg CO2 eq
Ecotoxicity freshwater	CTUe
Eutrophication freshwater	kg P eq
Eutrophication marine	kg N eq
Eutrophication terrestrial	mol N eq
Ionising radiation, HH	kBq U-235 eq
Land use	Pt
Non-cancer human health effects	CTUh
Ozone depletion	kg CFC11 eq
Photochemical ozone formation, HH	kg NMVOC eq
Resource use, energy carriers	MJ
Resource use, mineral and metals	kg Sb eq
Respiratory inorganics	disease inc.
Water scarcity	m3 depriv.

Appendix D – LCI data sources used in the Proof-of-Concept section

Table D 1 describes the LCI data sources extracted using the SimaPro 9.2 software (PRé Sustainability B.V., 2021). The Ecoinvent 3 database (Wernet et al., 2016) was used to obtain most data, with some exceptions (i.e., project EU & DK Input Output Database and Agri-Footprint 5).

Table D 1 - LCI data sources used in the Proof-of-Concept section.

Flow	Unit	LCI data sources
Electricity	KWh	1 kWh Electricity, medium voltage {DK}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Steam	kg	1 kg steam, in chemical industry {RER}| market for steam, in chemical industry | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Water	kg	1 kg Tap water {Europe without Switzerland}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
C12H22O11	kg	1 kg Sugar, from sugar beet {RoW}| beet sugar production | Conseq, U (of project Ecoinvent 3 - consequential - unit)
H2O	kg	1 kg water, ultrapure {RER}| market for water, ultrapure | Conseq, U (of project Ecoinvent 3 - consequential - unit)
(NH4)2SO4	kg	1 kg ammonium sulfate {RER}| market for ammonium sulfate | Conseq, U (of project Ecoinvent 3 - consequential - unit)
KH2PO4	kg	1 kg inorganic potassium fertiliser, as K2O {DK}| market for inorganic potassium fertiliser, as K2O | Conseq, U (of project Ecoinvent 3 - consequential - unit)
MgSO4	kg	1 kg Magnesium sulfate {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
CH4N2O	kg	1 kg urea {RER}| market for urea | Conseq, U (of project Ecoinvent 3 - consequential - unit)
NaCl (0.5 M)	kg	1 kg Sodium chloride, powder {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
TRIS HCl	kg	1 kg Hydrochloric acid, without water, in 30% solution state {RER}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
NaCl (0.1 M)	kg	1 kg Sodium chloride, brine solution {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
NaOH (0.5 M)	kg	1 kg Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
NaOH (CIP)	kg	1 kg Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
HNO3(CIP)	kg	1 kg nitric acid, without water, in 50% solution state {RER w/o RU}| market for nitric acid, without water, in 50% solution state | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Nitrogen (input)	kg	1 kg Nitrogen, liquid {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Rapeseed oil (from SS1)	kg	1 kg Crude rapeseed oil (pressing), at processing/DK Economic (of project Agri-footprint 5 - economic allocation)
Sodium hydroxide	kg	1 kg Sodium hydroxide, without water, in 50% solution state {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Phosphoric acid	kg	1 kg Phosphoric acid, industrial grade, without water, in 85% solution state {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Bentonite	kg	1 kg Bentonite {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)

Citric acid	kg	1 kg Citric acid {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Silica gel	kg	1 kg Activated silica {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Steam (from SS2.6)	kg	1 kg Steam, in chemical industry {RER}| production | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Natural gas	kg	1 kg Natural gas liquids {GLO}| production | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Deionized water	g	1 kg water, deionised {Europe without Switzerland}| market for water, deionised | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Methanol	kg	1 kg Methanol {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Sulfuric acid	kg	1 kg Sulfuric acid {RER}| market for sulfuric acid | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Chlorhydric acid	kg	1 kg Hydrochloric acid, without water, in 30% solution state {RER}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Potassium methylate	kg	1 kg Methanol, from biomass {RoW}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Ureum	kg	1 kg urea {RER}| market for urea | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Coagulant	kg	1 kg Polyaluminium chloride {GLO}| market for polyaluminium chloride | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Acetone cyanohydrin	kg	1 kg Acetone cyanohydrin {RER}| market for acetone cyanohydrin | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Helium	kg	1 kg Helium {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Heptane	kg	1 kg Heptane {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Ultrapure water	kg	1 kg water, ultrapure {RER}| market for water, ultrapure | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Packaging materials	kg	1 kg Packaging glass, white {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Sodium chloride	kg	1 kg Sodium chloride, powder {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Sulfur dioxide	kg	1 kg Sulfur dioxide, liquid {RER}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Carbon monoxide	kg	1 kg Carbon monoxide {RER}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Nitrogen oxides	kg	1 kg NOx retained, by selective catalytic reduction {GLO}| selective catalytic reduction of nitrogen oxides | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Carbon dioxide	kg	1 kg Carbon dioxide, liquid {RER}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Oxygen	kg	1 kg Oxygen, liquid {RER}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Phosphorous	kg	1 kg Phosphorus, white, liquid {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Truck 16–32 t	t km	1 tkm Transport, freight, lorry 16-32 metric ton, EURO6 {RER}| transport, freight, lorry 16-32 metric ton, EURO6 | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Transoceanic tanker	t km	1 tkm Transport, freight, sea, transoceanic tanker {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)

Transoceanic freight ship	t km	1 tkm Transport, freight, sea, transoceanic ship {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Nitrogen (output)	kg	1 kg Venting of nitrogen, liquid {RER}| venting of nitrogen, liquid | APOS, U (of project Ecoinvent 3 - allocation at point of substitution - unit)
Oxygen (output)	kg	1 kg Basic oxygen furnace waste (waste treatment) {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Carbon dioxide (output)	kg	1 kg venting, from carbon dioxide in chemical industry {GLO}| market for venting, from carbon dioxide in chemical industry | APOS, U (of project Ecoinvent 3 - allocation at point of substitution - unit)
Carbon monoxide (output)	kg	1 kg Carbon monoxide {RER}| production | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Methane (output)	kg	1 kg biomethane, low pressure, vehicle grade {RoW}| biomethane production, low pressure, vehicle grade | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Nitrogen oxides (output)	kg	1 kg NOx retained, by selective catalytic reduction {GLO}| selective catalytic reduction of nitrogen oxides | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Dinitrogen oxide (output)	kg	1 kg Nitrous oxide {RoW}| production | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Sulfur dioxide (output)	kg	1 kg Sulfur dioxide, liquid {RER}| production | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Amino acids (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Beta-Galactosidase (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Lactose (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Proteins (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Water (ouput)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Salts (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Sodium chloride (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
TRIS HCl (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Sodium hydroxide (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Nitric acid (output)	kg	1 m3 Wastewater, average {RoW}| treatment of, capacity 5E9l/year | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Biomass (output)	kg	1 kg 107 Waste treatment, Landfill of waste, Food, DK (of project EU & DK Input Output Database)
Debris (output)	kg	1 kg 107 Waste treatment, Landfill of waste, Food, DK (of project EU & DK Input Output Database)
Lands (from SS2.2)	kg	1 kg 107 Waste treatment, Landfill of waste, Food, DK (of project EU & DK Input Output Database)
Sludge (from SS2.4)	kg	1 kg 107 Waste treatment, Landfill of waste, Food, DK (of project EU & DK Input Output Database)
Waste to incineration (from SS2.5)	kg	1 kg Hazardous waste, for incineration {Europe without Switzerland}| treatment of hazardous waste, hazardous waste incineration | Conseq, U (of project Ecoinvent 3 - consequential - unit)

Nitrogen (SS2.1)	kg	1 kg Venting of nitrogen, liquid {RER}| venting of nitrogen, liquid | APOS, U (of project Ecoinvent 3 - allocation at point of substitution - unit)
Carbon dioxide (SS2.2)	kg	1 kg venting, from carbon dioxide in chemical industry {GLO}| market for venting, from carbon dioxide in chemical industry | APOS, U (of project Ecoinvent 3 - allocation at point of substitution - unit)
Oxygen (SS2.2)	kg	1 kg Basic oxygen furnace waste (waste treatment) {GLO}| market for | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Suspended solids	kg	1 m3 Wastewater, average {Europe without Switzerland}| market for wastewater, average | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Ammonia	kg	1 m3 Wastewater, average {Europe without Switzerland}| market for wastewater, average | Conseq, U (of project Ecoinvent 3 - consequential - unit)
Chemical oxygen demand	kg	1 m3 Wastewater, average {Europe without Switzerland}| market for wastewater, average | Conseq, U (of project Ecoinvent 3 - consequential - unit)

Appendix E – Normalisation and Weighting factors

Table E 1 describes the normalised factors used in TOLCAB, and their corresponding units. Table E 2 describes the weighted factors used, and their corresponding units.

Table E 1 - PEF normalisation factors according to the European Commission - Joint Research Centre (2022).

Impact categories	**Unit**	**Normalisation factors**
Acidification terrestrial and freshwater	mol H+ eq./person	5,56E+01
Cancer human health effects	CTUh/person	1,73E-05
Climate change	kg CO_2 eq./person	7,55E+03
Ecotoxicity freshwater	CTUe/person	5,67E+04
Eutrophication freshwater	kg P eq./person	1,61E+00
Eutrophication marine	kg N eq./person	1,95E+01
Eutrophication terrestrial	mol N eq./person	1,77E+02
Ionising radiation, HH	kBq U-235 eq./person	4,22E+03
Land use	pt/person	8,19E+05
Non-cancer human health effects	CTUh/person	1,29E-04
Ozone depletion	kg CFC-11 eq./person	5,23E-02
Photochemical ozone formation, HH	kg NMVOC eq./person	4,09E+01
Resource use, energy carriers	MJ/person	6,50E+04
Resource use, mineral and metals	kg Sb eq./person	6,36E-02
Respiratory inorganics	CTUe/person	5,67E+04
Water scarcity	m^3 water eq of deprived water/person	1,15E+04

Table E 2 - PEF weighting factors according to the European Commission - Joint Research Centre (2022).

Impact categories	**Weighting Factors [%]**
Acidification terrestrial and freshwater	6,20%
Cancer human health effects	2,13%
Climate change	21,06%
Ecotoxicity freshwater	1,92%
Eutrophication freshwater	2,80%
Eutrophication marine	2,96%
Eutrophication terrestrial	3,71%
Ionising radiation, HH	5,01%
Land use	7,94%
Non-cancer human health effects	1,84%
Ozone depletion	6,31%
Photochemical ozone formation, HH	4,78%
Resource use, energy carriers	8,32%
Resource use, mineral and metals	7,55%
Respiratory inorganics	8,96%
Water scarcity	8,51%

Appendix F – Description of processes for the Proof-of-Concept

Figure F 1 describes the unit processes in case study A, and the corresponding flows and data collection methods. Figure F 2 describes the unit processes in case study B, and the corresponding flows and data collection methods.

2. Life Cycle Inventory

Description of Processes

Options 1

		Flow	Data collection from
Inputs	SS2.1 - Option 1	Nitrogen	Sensor measuring Nitrogen (input) from Nitrogen in the process SS2.1
		Electricity	Sensor measuring Electricity from Electricity in the process SS2.1
		Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.1
	SS2.2 - Option 1	Rapeseed oil (from SS1)	Sensor measuring Rapeseed oil (from SS1) from Rapeseed oil (from SS1) in the process SS2.2
		Sodium hydroxide	Sensor measuring Sodium hydroxide from Sodium hydroxide in the process SS2.2
		Phosphoric acid	Sensor measuring Phosphoric acid from Phosphoric acid in the process SS2.2
		Bentonite	Sensor measuring Bentonite from Bentonite in the process SS2.2
		Citric acid	Sensor measuring Citric acid from Citric acid in the process SS2.2
		Silica gel	Sensor measuring Silica gel from Silica gel in the process SS2.2
		Steam (from SS2.6)	Sensor measuring Steam (from SS2.6) from Steam (from SS2.6) in the process SS2.2
		Natural gas	Sensor measuring Natural gas from Natural gas in the process SS2.2
		Tap water	Sensor measuring Water from Tap water in the process SS2.2
		Deionized water	Sensor measuring Deionized water from Deionized water in the process SS2.2
		Sulfur dioxide	Sensor measuring Sulfur dioxide from Sulfur dioxide in the process SS2.2
		Carbon monoxide	Sensor measuring Carbon monoxide from Carbon monoxide in the process SS2.2
		Nitrogen oxides	Sensor measuring Nitrogen oxides from Nitrogen oxides in the process SS2.2
		Electricity	Sensor measuring Electricity from Electricity in the process SS2.2
		Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.2
		Transoceanic tanker	Sensor measuring Transoceanic tanker from Transoceanic tanker in the process SS2.2
	SS2.3 - Option 1	Methanol	Sensor measuring Methanol from Methanol in the process SS2.3
		Sulfuric acid	Sensor measuring Sulfuric acid from Sulfuric acid in the process SS2.3
		Chlorhydric acid	Sensor measuring Chlorhydric acid from Chlorhydric acid in the process SS2.3
		Sodium hydroxide	Sensor measuring Sodium hydroxide from Sodium hydroxide in the process SS2.3
		Nitrogen	Sensor measuring Nitrogen (input) from Nitrogen in the process SS2.3
		Tap water	Sensor measuring Water from Tap water in the process SS2.3
		Steam (from SS2.6)	Sensor measuring Steam (from SS2.6) from Steam (from SS2.6) in the process SS2.3
		Potassium methylate	Sensor measuring Potassium methylate from Potassium methylate in the process SS2.3
		Citric acid	Sensor measuring Citric acid from Citric acid in the process SS2.3
	SS2.4 - Option 1	Electricity	Sensor measuring Electricity from Electricity in the process SS2.3
		Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.3
		Transoceanic tanker	Sensor measuring Transoceanic tanker from Transoceanic tanker in the process SS2.3
		Ureum	Sensor measuring Ureum from Ureum in the process SS2.4
		Sodium hydroxide	Sensor measuring Sodium hydroxide from Sodium hydroxide in the process SS2.4
	SS2.5 - Option 1	Coagulant	Sensor measuring Coagulant from Coagulant in the process SS2.4
		Electricity	Sensor measuring Electricity from Electricity in the process SS2.4
		Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.4
		Acetone cyanohydrin	Sensor measuring Acetone cyanohydrin from Acetone cyanohydrin in the process SS2.5
		Helium	Sensor measuring Helium from Helium in the process SS2.5
		Heptane	Sensor measuring Heptane from Heptane in the process SS2.5
		Ultrapure water	Sensor measuring Ultrapure water from Ultrapure water in the process SS2.5
	SS2.6 - Option 1	Packaging materials	Sensor measuring Packaging materials from Packaging materials in the process SS2.5
		Electricity	Sensor measuring Electricity from Electricity in the process SS2.5
		Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.5
		Tap water	Sensor measuring Water from Tap water in the process SS2.6
		Sodium chloride	Sensor measuring Sodium chloride from Sodium chloride in the process SS2.6
		Natural gas	Sensor measuring Natural gas from Natural gas in the process SS2.6
		Carbon dioxide	Sensor measuring Carbon dioxide from Carbon dioxide in the process SS2.6
		Oxygen	Sensor measuring Oxygen from Oxygen in the process SS2.6
		Sulfur dioxide	Sensor measuring Sulfur dioxide from Sulfur dioxide in the process SS2.6
		Nitrogen oxides	Sensor measuring Nitrogen oxides from Nitrogen oxides in the process SS2.6
		Carbon monoxide	Sensor measuring Carbon monoxide from Carbon monoxide in the process SS2.6
		Electricity	Sensor measuring Electricity from Electricity in the process SS2.6
		Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.6
	SS2.7 - Option 1	Truck 16–32 t	Sensor measuring Truck 16–32 t from Truck 16–32 t in the process SS2.7
		Transoceanic tanker	Sensor measuring Transoceanic tanker from Transoceanic tanker in the process SS2.7
		Transoceanic freight ship	Sensor measuring Transoceanic freight ship from Transoceanic freight ship in the process SS2.7
	N.E. - Option 1	Phosphorous	Sensor measuring Phosphorous from Phosphorous in the process N.E.
Outputs		Lands (from SS2.2)	Sensor measuring Lands (from SS2.2) from Lands (from SS2.2) in the process N.E.
		Sludge (from SS2.4)	Sensor measuring Sludge (from SS2.4) from Sludge (from SS2.4) in the process N.E.
		Waste to incineration (from SS2.	Sensor measuring Waste to incineration (from SS2.5) from Waste to incineration (from SS2.5) in the process N.E.
		Nitrogen (SS2.1)	Sensor measuring Nitrogen (SS2.1) from Nitrogen (SS2.1) in the process N.E.
		Carbon dioxide (SS2.2)	Sensor measuring Carbon dioxide (SS2.2) from Carbon dioxide (SS2.2) in the process N.E.
		Oxygen (SS2.2)	Sensor measuring Oxygen (SS2.2) from Oxygen (SS2.2) in the process N.E.
		Suspended solids	Sensor measuring Suspended solids from Suspended solids in the process N.E.
		Ammonia	Sensor measuring Ammonia from Ammonia in the process N.E.
		Chemical oxygen demand	Sensor measuring Chemical oxygen demand from Chemical oxygen demand in the process N.E.

Figure F 1 - Description of Processes tab for case study A.

2. Life Cycle Inventory

Description of Processes

Options 1

		Flow	Data collection from
Inputs	SS1 - Option 1	C12H22O11	Sensor measuring C12H22O11 from C12H22O11 in the process SS1
		H2O	Sensor measuring H2O from H2O in the process SS1
		(NH4)2SO4	Sensor measuring (NH4)2SO4 from (NH4)2SO4 in the process SS1
		KH2PO4	Sensor measuring KH2PO4 from KH2PO4 in the process SS1
		MgSO4	Sensor measuring MgSO4 from MgSO4 in the process SS1
		CH4N2O	Sensor measuring CH4N2O from CH4N2O in the process SS1
		H2O	Sensor measuring H2O from H2O in the process SS1
		Water	Sensor measuring Water from Water in the process SS1
		Seed fermenter	Sensor measuring Electricity from Seed fermenter in the process SS1
		Production fermenter	Sensor measuring Electricity from Production fermenter in the process SS1
		Compressors	Sensor measuring Electricity from Compressors in the process SS1
		Pumps	Sensor measuring Electricity from Pumps in the process SS1
		Agitation of vessels	Sensor measuring Electricity from Agitation of vessels in the process SS1
		Steam	Sensor measuring Steam from Steam in the process SS1
	SS2 - Option 1	NaCl (0.5 M)	Sensor measuring NaCl (0.5 M) from NaCl (0.5 M) in the process SS2
		TRIS HCl	Sensor measuring TRIS HCl from TRIS HCl in the process SS2
		NaCl (0.1 M)	Sensor measuring NaCl (0.1 M) from NaCl (0.1 M) in the process SS2
		NaOH (0.5 M)	Sensor measuring NaOH (0.5 M) from NaOH (0.5 M) in the process SS2
		H2O	Sensor measuring H2O from H2O in the process SS2
		Water	Sensor measuring Water from Water in the process SS2
		H2O (CIP)	Sensor measuring H2O from H2O (CIP) in the process SS2
		NaOH (CIP)	Sensor measuring NaOH (0.5 M) from NaOH (CIP) in the process SS2
		HNO3(CIP)	Sensor measuring HNO3(CIP) from HNO3(CIP) in the process SS2
		Agitation of vessels	Sensor measuring Electricity from Agitation of vessels in the process SS2
		Pumps	Sensor measuring Electricity from Pumps in the process SS2
		Filters	Sensor measuring Electricity from Filters in the process SS2
Outputs	A. Stage - Option 1	Beta-Galactosidase	Sensor measuring Beta-Galactosidase (output) from Beta-Galactosidase in the process A. Stage
		Nitrogen	Sensor measuring Nitrogen (output) from Nitrogen in the process A. Stage
		Oxygen	Sensor measuring Oxygen (output) from Oxygen in the process A. Stage
		Carbon dioxide	Sensor measuring Carbon dioxide (output) from Carbon dioxide in the process A. Stage
		Carbon monoxide	Sensor measuring Carbon monoxide (output) from Carbon monoxide in the process A. Stage
		Carbon dioxide	Sensor measuring Carbon dioxide (output) from Carbon dioxide in the process A. Stage
		Methane	Sensor measuring Methane (output) from Methane in the process A. Stage
		Nitrogen oxides	Sensor measuring Nitrogen oxides (output) from Nitrogen oxides in the process A. Stage
		Dinitrogen oxide	Sensor measuring Dinitrogen oxide (output) from Dinitrogen oxide in the process A. Stage
		Sulfur dioxide	Sensor measuring Sulfur dioxide (output) from Sulfur dioxide in the process A. Stage
		Amino acids	Sensor measuring Amino acids (output) from Amino acids in the process A. Stage
		Beta-Galactosidase	Sensor measuring Beta-Galactosidase (output) from Beta-Galactosidase in the process A. Stage
		Lactose	Sensor measuring Lactose (output) from Lactose in the process A. Stage
		Proteins	Sensor measuring Proteins (output) from Proteins in the process A. Stage
		Water	Sensor measuring Water (ouput) from Water in the process A. Stage
		Salts	Sensor measuring Salts (output) from Salts in the process A. Stage
		Sodium chloride	Sensor measuring Sodium chloride (output) from Sodium chloride in the process A. Stage
		TRIS HCl	Sensor measuring TRIS HCl (output) from TRIS HCl in the process A. Stage
		Sodium hydroxide	Sensor measuring Sodium hydroxide (output) from Sodium hydroxide in the process A. Stage
		Water	Sensor measuring Water (ouput) from Water in the process A. Stage
		Sodium hydroxide	Sensor measuring Sodium hydroxide (output) from Sodium hydroxide in the process A. Stage
		Nitric acid	Sensor measuring Nitric acid (output) from Nitric acid in the process A. Stage
		Biomass	Sensor measuring Biomass (output) from Biomass in the process A. Stage
		Debris	Sensor measuring Debris (output) from Debris in the process A. Stage

Figure F 2 - Description of Processes tab for case study B.