COMBINED TECHNOLOGIES FOR WATER, ENERGY AND SOLUTE RECOVERY FROM INDUSTRIAL PROCESS STREAMS

# Deliverable 4.1

## Report on the Main Methodological Choices

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[1] **R**=Document, report; **DEM**=Demonstrator, pilot, prototype; **DEC**=website, patent fillings, videos, etc.; **DMP**=Data Management Plan

[2] **PU**=Public, **SEN**=Sensitive

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# Acronyms

| | |
|---|---|
| **ALCA** | Attributional Life Cycle Assessment |
| **CAPEX** | Capital expenditure |
| **CLCA** | Consequential Life Cycle Assessment |
| **DC** | Direct costs |
| **EBITDA** | Earnings before interests, taxes, depreciation and amortisation |
| **f** | Factor for cost estimation models |
| **FCOP** | Fixed costs of production |
| **FU** | Functional unit |
| **IC** | Indirect costs |
| **ILO** | International Labour Organization |
| **IP** | Impact Pathway |
| **ISO** | International Organization for Standardization |
| **LCA** | Life Cycle Assessment |
| **LCI** | Life Cycle Inventory |
| **LCIA** | Life Cycle Impact Assessment |
| **LCC** | Life Cycle Costing |
| **LCSA** | Life Cycle Sustainability Assessment |
| **PC** | Purchase cost |
| **OPEX** | Operational expenditure |
| **PRP** | Performance Reference Point |
| **PSILCA** | Product Social Impact Life Cycle Assessment |
| **SETAC** | Society of Environmental Toxicology and Chemistry |
| **S-LCA** | Social-Life Cycle Assessment |
| **TEA** | Techno-Economic Assessment |
| **TRL** | Technology Readiness Level |
| **UN** | United Nations |
| **UNEP** | United Nations Environment Programme |

| | |
|---|---|
| **VCOP** | Variable costs of production |
| **WHO** | World Health Organization |
| **WW** | Wastewater |

# Executive Summary

This document **outlines the methodological roadmap for the sustainability and circularity assessment of the CORNERSTONE project technologies, which focus on water, energy and solute recovery**. Life Cycle Sustainability Assessment (LCSA) comprises Life Cycle Assessment (LCA), Life Cycle Costing (LCC) and Social – Life Cycle Assessment (S-LCA) methodologies that respectively address the environmental, economic and social pillars of sustainability. An exploration of the main guidelines for Life Cycle Sustainability Assessment (LCSA) are presented in this deliverable with the aim of defining a solid basis for future analyses. The contents of the document provide an overview for each sustainability pillar following the triple bottom line approach, diving both into generalities and key aspects.

**The Life Cycle Assessment (LCA) framework is presented first as the main methodology to address the environmental performance of the technologies**. A brief mapping of relevant industrial standards and guidelines in coherence with sectorial needs and sustainability assessment goals is presented in this document. The two main LCA standards widely used throughout by industry and academia practitioners, ISO 14040:2006 and ISO 14044:2006, are referred to and used as a basis to introduce key concepts such as goal and scope definition aligned with the foreseen targets of the project. Key aspects of LCA such as the functional unit definition when addressing multifunctional systems are explored, alongside the potential strategies for solving this multifunctionality and the two main LCA approaches for conducting the assessments. Moreover, the exploration of other methodological particularities including databases, marginal suppliers and impact assessment method is presented as well. The assessment of the water footprint according to the ISO 14046:2014 will also be included. The latest method AWARE (2.0 or later) will be utilised.

Life Cycle Costing (LCC) through the **Techno-Economic Analysis (TEA) approach is presented as the main strategy for evaluating the cost-effectiveness and economic competitiveness of CORNERSTONE technologies**. The structure of the TEA model is summarised, showcasing the categorisation of main cost components and tentative models for their estimation. Relevant economic indicators corresponding to different criteria are summarised, to evaluate the economic potential of water, energy and solute recovery systems in future assessments.

Social sustainability analyses will follow the **Social Life Cycle Assessment (S-LCA) approach, a novel methodology that builds upon the life cycle thinking bases of LCA**. The main target of this methodology is to identify the most critical impacts of a system in different stakeholder groups. Specificities related to the workflow, the use of Product Impact Life Cycle Assessment (PSILCA) and the creation of site-specific case studies are discussed in the report.

# 1. Introduction

Water management innovations that address water and resource recovery are essential strategies within the context of Circular Economy [1], [2]. Coupling research and pilot-scale implementation efforts with continuous sustainability assessment could ensure that these water recovery solutions align with European Union goals, as well as specific sectorial needs [3], [4], [5].

Life Cycle Sustainability Assessment (LCSA) presents a compendium of holistic and systematic approaches that allows the assessment of products, services and organisations. LCSA includes Life Cycle Assessment (LCA), Life Cycle Costing (LCC) and Social – Life Cycle Assessment (S-LCA) methodologies that respectively address the environmental, economic and social pillars of sustainability. When conducted in a complementary and coherent manner, these frameworks provide the possibility to evaluate the environmental performance of a system, combined with its economic costing and the identification of the main social impacts and vulnerable stakeholders.

Sustainability assessment tools are conducted by following industrial standards, guidelines and other reference documents that serve as a basis for a variety of applications. In the field of innovative water recovery technologies, these frameworks provide an added value, supporting the identification of hotspots and main technological improvements towards future technological transferability. The latter is of particular interest in low Technology Readiness Level (TRL) and pilot-scale applications.

While the LCA framework is a widely implemented tool for environmental assessment, it is also employed as a reference for evaluating other dimensions of sustainability through LCC and S-LCA. The framework is an iterative process that consists of four main intertwined steps shown in Figure 1. These steps are summarised as follows [6]:

1. **Goal and scope definition.** This initial step frames the assessment, which includes defining the specific objective of the analysis. In addition, the product system to be studied, its system boundaries and the functional unit (FU) are described within the scope definition. FU details the specific function of a product system, which could refer to the quantity of a product.

2. **Life Cycle Inventory (LCI).** This data compilation phase includes the identification and collation of data required and estimations for quantifying all the energy and mass flows. In addition, other relevant information for obtaining the economic and social performance through LCC and S-LCA is collected.

3. **Life Cycle Impact Assessment (LCIA).** The impacts derived from the collected data in the LCI phase are estimated through the combination of databases and impact assessment methods. The latter encompasses characterisation factors, which allow the calculation of impacts from the input LCI data.

4. **Interpretation.** This transversal phase targets a systematic assessment based on several elements such as identification of possible issues, verification of results and completeness of the evaluation. The main objective is to draw the final conclusions, limitations and recommendations for the study.

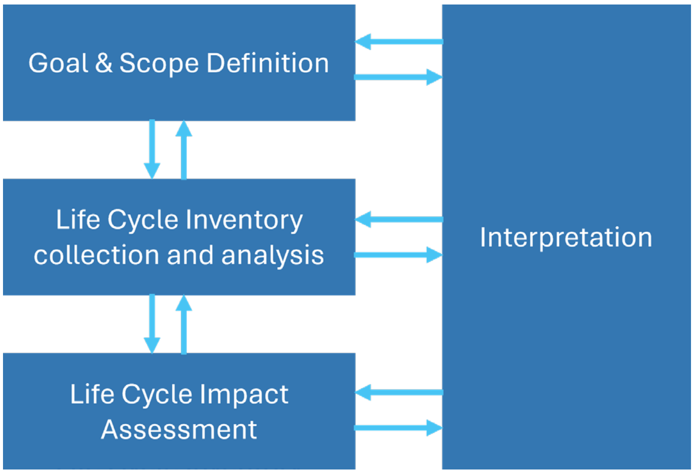


**Figure 1. Scheme of LCA methodology based on ISO 14040:2006.**

## 1.1. Goal and scope of the deliverable

This deliverable aims to define the basic methodological approaches and guidelines for the development of environmental, economic and social assessments of the different technologies of CORNERSTONE project. Methodological particularities and preferences for the LCA, LCC and S-LCA are highlighted throughout the document, setting the bases for future assessments and providing a framework to address the potential challenges that could emerge during the process. Furthermore, the guidance seeks to provide a framework for evaluating the water, energy and solute recovery potential whilst addressing the potential impacts of emerging and innovative technologies. Therefore, the subsequent sections delve into key aspects including the following:

- Basic guidelines and standards for each of the assessments
- Definition of goal and aim
- Functional unit and scope
- Databases and indicators
- Other methodological choices

The basic guidelines provide a starting point for the LCSA according to recognised and standardised methodologies, in alignment with the general preferences of the scientific and industrial sectors. In addition, the guidance provides a flexible framework that could be adapted in alignment with i) particularities of the emerging technologies towards improved water management strategies and ii) any new consensus that could emerge during the execution of the project.

# 2. Overall vision of CORNERSTONE

## 2.1. Project overview

The CORNERSTONE project aims to develop novel recovery technologies from industrial wastewater streams promoting circular economy principles and enhanced water management strategies. Six different technological modules will comprise the systems proposed within this EU funded project, as shown in Figure 2. The main objective is to achieve water recycling combined with energy and solute recovery, integrating the innovative technologies into existing treatment plants.

The integration of CORNERSTONE technologies is foreseen for three demonstration sites: steel, pulp & paper and chemical industries. The following itemisation summarises these three sites [7]:

- **Steel industry**. Waste heat recovery with non-clogging heat exchanger is the core strategy for this demonstrator. Furthermore, the conceptual design includes coupling the **recovered heat** into membrane distillation for a sustainable production of **high-purity water**.

- **Pulp & paper industry**. An integration of several key modules is the base for the pulp & paper pilot train. The technological train will target heat exchanging combined with technologies such as nanofiltration, membrane distillation, electrodialysis and membrane crystallisation. The demonstration concept aims at integrating **water, energy and material recovery** following circular economy principles.

- **Chemical industry**. Anaerobic biological treatment comprises the main strategy for chemical industry wastewater streams, addressing pretreatment options for inhibitory and recalcitrant compounds. This system seeks **biogas valorisation as an energy source or as a feedstock** for subsequent chemical processes, aligned with carbon neutrality and decarbonisation goals.

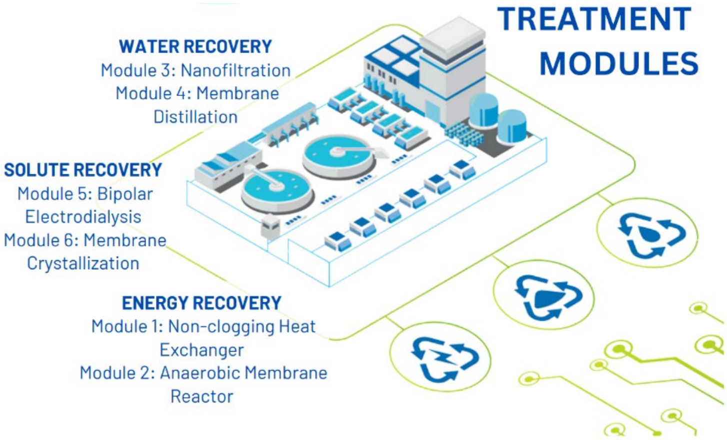


**Figure 2. Overview of the CORNERSTONE project technological modules.**

## 2.2. Conceptual scheme and scope definition

CORNERSTONE systems encompass a diversity of technologies for achieving recovery and reuse of valuable streams within industrial settings. The conceptual diagram for these integrated processes is shown in Figure 3, which depicts two distinct options for outputs. On the one hand, the combined recovery of water, energy and compounds in the multi-product system is displayed. On the other hand, the representation also emphasizes wastewater treatment as the main service provided from implementing CORNERTONE systems. These two particularities are considered among the methodological approach due to their relationship with specific modelling decisions. Moreover, they will be deciding factors throughout the execution of the assessments in the project.

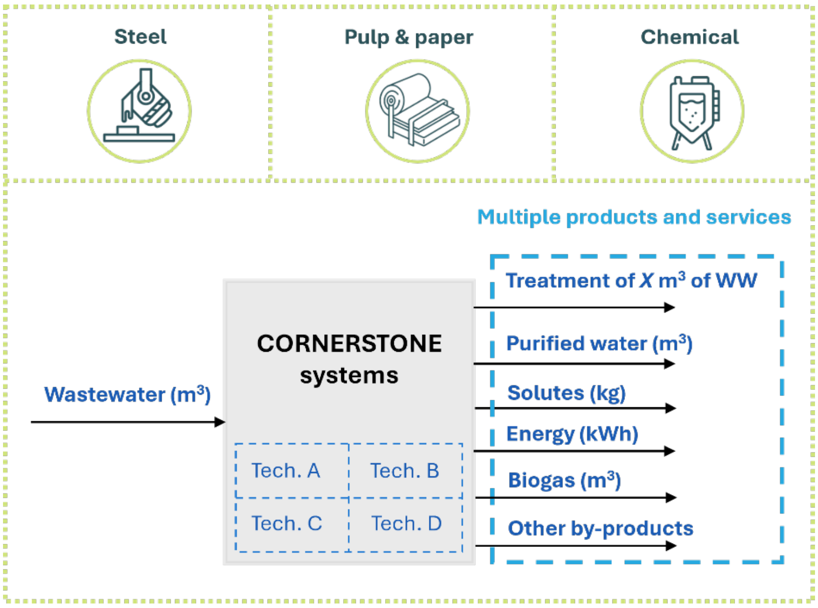


**Figure 3. Conceptual scheme for the main products and services from CORNERSTONE systems.**

An expanded CORNERSTONE diagram is illustrated in Figure 4. This depiction allows the identification of different analysis levels following a bottom-up approach for the construction of the assessments. The boundary for **level one** is defined by a specific process of the proposed system, for instance a *gate-to-gate* analysis of a single technological module comprised within the final technological train of operations. **Level two** includes additional modules as supporting operations to that of level 1, forming a line level-subprocess. Lastly, **level three** describes the final coupling of all technological modules for each CORNERSTONE system. Each level of analysis will be developed further during the project execution, including an individual diagram complemented with the expected mass and energy flows accordingly.

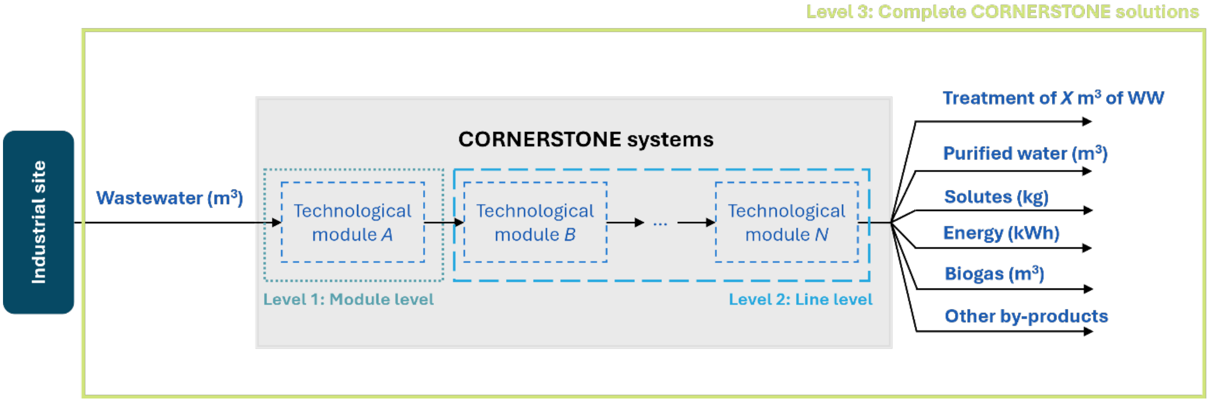


**Figure 4. Levels of analysis for CORNERSTONE systems. WW: Wastewater.**

# 3. Life Cycle Sustainability Assessment: Coherence throughout the framework

## 3.1. Goal and target audience

The main results and outcomes from the Life Cycle Sustainability Assessments (LCSA) might target different audiences. Environmental, economic and social analyses of CORNERSTONE technologies and systems could be directed towards one or more of the following interested parties:

- Internal consortium partners
- Research groups
- Consultants in the water sector
- International non-profit organisations
- Local communities
- Water basin stakeholders
- Private corporations and industries
- Policymakers

Aligned with the specific interests of each interested party, the valuable information to be obtained from future assessments will vary depending on the nature of their decision-making. This aspect is considered throughout the methodological guidance developed in the document, especially since it potentially determines the aim & scope definition, specific methodological choices, indicator selection, among others. For instance, the target information for a research group may differ from that of market consultancies and private industries. Table 1 summarises a selection of examples for different audience groups and their corresponding main interests from the assessments.

**Table 1. Audience group and target information examples for sustainability assessments**

| Audience group | Target information |
|---|---|
| **Researcher or technology developer** | Environmental and economic hotspots. |
| **International non-profit organisation** | Water recovery potential and high-risk stakeholder groups. |
| **Consultants in the water sector** | Payback period of the projected plant or avoided burdens. |
| **Private corporations and industries** | Greenhouse gas emission reduction or economic margin of the projected plant. Comparison of various plant designs. |
| **Policymakers** | Consequences of adopting novel technologies and their future performance aligned with decarbonisation targets. |

## 3.2. Functional unit, system boundaries and multifunctionality

The technological schemes proposed in CORNERSTONE potentially provide several product outputs and services, as presented in Figure 3. This particularity of CORNERSTONE systems is referred to as **multifunctional systems** [8]. Multifunctionality is a relevant aspect to consider when defining key methodological decisions for the assessments. One of these critical decisions is the functional unit (FU) selection, meaning the desired function of the system, which will be further developed in the **Functional unit and reference flows** section.

System boundaries define the different unit processes to be considered in the assessments for a given scheme. The delimitation of the system and its related functional unit shall be maintained throughout the analyses, maintaining coherence between the environmental performance, cost-effectiveness and social impact results. For instance, the *gate-to-gate* carbon footprint for treating 1 $m^3$ of wastewater in each demonstration site is to be accompanied by the cost per $m^3$ of implementing such wastewater technological train and its potential social impacts. Accordingly, the definition of scenarios related to the chosen functional unit and their analysis in the three sustainability dimensions must maintain this alignment.

## 3.3. Geographical coverage

The parameters for evaluating the three sustainability dimensions potentially depend on the geographical definition for their future implementation. The European Union (EU-27) defines the geographical coverage for the CORNERSTONE systems. Thus, regionalisation of the required database processes and contour conditions will be placed in Europe. Average EU conditions could be selected for initial assessments and screening purposes, whereas an adaptation to specific regions will be considered for the three demonstration sites. The latter facilitates better result interpretation and alignment of the assessments.

# 4. Life Cycle Assessment (LCA)

## 4.1. Methodological compass

The present chapter aims to define a baseline methodological compass for the environmental performance assessments of the different CORNERSTONE technologies. The guidelines herein presented target the identification of water recovery potential in enhanced water management strategies, potentially coupled with energy or solute recovery. Furthermore, the methodological aspects explained in the following subsections will define the roadmap for future analyses, including the three integrated case studies.

One of the essential aspects to consider within the methodological LCA framework is the availability of recognised reference documents and industrial standards, since these frame the main requirements and suggestions to conduct comparable and valid assessments. The following section presents an overview of the main relevant standards and guidelines that align with the CORNERSTONE project objectives.

## 4.2. LCA standards and guidelines

The compilation of reference documents included the identification of relevant standards from the International Organisation for Standardisation (ISO), as well as useful guidelines that support methodological decisions and modelling considerations. These documents provide valuable specifications that align with the different industrial sectors within CORNERSTONE.

The references presented in this section also support important modelling considerations to account for multiple products (e.g. purified water, energy carriers and recovered solutes) or services (e.g. wastewater treatment). Moreover, additional documents included in the compilation provide resourceful insights to guide the assessments following a market approach.

### 4.2.1. Industrial standards

- **ISO 14040:2006** Environmental management — Life cycle assessment — Principles and framework [6]
- **ISO 14044:2006** Environmental management — Life cycle assessment — Requirements and guidelines [9]
- **ISO 14067:2018** Greenhouse gases — Carbon footprint of products — Requirements and guidelines for quantification [10]
- **ISO 14046:2014** Environmental management – Water footprint – Principles, requirements and guidelines [11]

### 4.2.2. Guidelines

- **International Reference Life Cycle Data System (ILCD) Handbook** – General guide for life cycle assessment – detailed guidance [12]
- **Together for Sustainability PCF Guideline** – The Product Carbon Footprint Guideline for the Chemical Industry [13]
- **Global Guidance Principles for Life Cycle Assessment Databases** – A Basis for Greener Processes and Products [14]

### 4.2.3. Other references & information sources

- Market information in life cycle assessment [15]
- Marginal Production Technologies for Life Cycle Inventories [16]
- Consequential LCA initiative [17]

## 4.3. Goal and scope definition

LCA frameworks identify the **goal and scope definition as the first step for the environmental performance evaluation of a system**. This delimitation establishes the basis for *what* is being analysed and *why*, which includes specifications regarding the life cycle stages and the processes considered within the modelling. Moreover, since CORNERSTONE project focuses in developing a variety of technologies, it is important to define the specific goal for each system under study.

LCA generally focuses on obtaining the environmental performance of a product system through a set of quantitative indicators or impact categories. Nonetheless, it is recommended to perform a more detailed and explicit goal definition aligning with the particularities of the process or set of processes included in the system under analysis. According to some authors, the goal definition potentially determines the overall conceptualisation of the assessment as well as key methodological choices [18]. The following sections explore this perspective, providing an overview of possible goals, the applicable LCA approach and corresponding criteria for different cases. The detailed definition of a specific goal encompasses the identification of i) the product system under analysis and ii) the reason for the assessment. This relates to the following aspects:

- **Product or process oriented**: affects the data collection phase, the definition of FU and the approach for multifunctionality resolution.
- **Objective/reason for LCA**: which could include accountability, hotspot mapping or consequential approach.

### 4.3.1. Product-oriented or process-oriented

The distinction between product-oriented and process-oriented LCAs has been presented previously in the literature [18], [19]. The process-oriented approach presents a focus towards the process itself, the transformation operations involved and a systematic understanding of the by-products' role in the environmental performance. For instance, this approach could be suitable for optimising a given production or treatment process. On the other hand, product-oriented assessments aim at identifying the share of impacts associated to one specific product obtained from the system. This methodological choice affects the functional unit definition. Furthermore, the latter is ultimately related to the goal definition and will subsequently impact the choice of allocation procedure to address multifunctional systems.

### 4.3.2. Objective identification

LCA typically relates to a combination of objectives, which could include the following:

- Account of impacts
- Identification of main environmental drivers or hotspots
- Technological improvement insights
- Consequential analysis

Accountability of impacts typically relates to quantifying the environmental burdens of producing or consuming a given product, such as consuming 1 kWh of energy recovered from anaerobic digestion systems or producing 1 kg of solutes using CORNERSTONE technologies. For these cases, Attributional LCA (ALCA) approach allows the identification of impacts attributed to the corresponding systems. Alternatively, Consequential LCA (CLCA) targets the quantification of environmental impacts that arise from making a decision, including the implementation of a specific production process. For example, the consequences of increasing the demand for 1 kWh of energy produced from anaerobic digestion plants in the market, and its related burdens. The consequences reflected in the assessment could include effects such as changes in consumption patterns in other value chains, even at a global level.

For the identification of main drivers and hotspots, both ALCA and CLCA could be employed since the background processes are specific to each approach. Their respective supply chains would underline the key flows that define process hotspots in both alternatives. ALCA conceptualisation and the assimilation of its results may be more accessible to a wider range of audience groups and stakeholders. For this reason, it will be potentially considered the primary approach for the assessments. Nonetheless, the CLCA will also be explored for CORNERSTONE systems. Further details about the approaches are presented in the **Approach and multifunctionality resolution** section.

## 4.4. Functional unit and reference flows

ISO 14040:2006 standard defines the FU as the "*quantified performance of a product system for use as a reference unit*". Therefore, the input and output flows of a system are defined using the FU as a reference. Regarding the reference flow, ISO standards define it as the "*measure of the outputs from processes in a given product system required to fulfil the function expressed by the functional unit".* The understanding of these two concepts is important to frame the assessment and avoid confusion when conceptualising the LCA itself.

Coherently with the stated concepts, there is a close interlinkage between the three elements –goal, FU and reference flow–. The definition of FU is intrinsically related to the desired goal whilst the reference flow is defined by the function of the system and its magnitude. Therefore, the concepts are specific to the system under analysis, aligning with the specific technologies and unit operations to be evaluated. For the CORNERSTONE systems, a selection of possible FU is detailed below:

a. The treatment of ***X* m$^3$ of wastewater**

b. The production of ***X* m$^3$ of biogas**

c. The production of ***X* m$^3$ of purified water**

d. The recovery of ***X* kg of solutes**

e. An **extended FU** that includes all the functionalities of a given system (e.g. purification of 1 m3 of water with the recovery of *X* kg of solutes or *Y* kWh of energy)

Figure 5 depicts three of the examples mentioned above. The extended FU illustrates a process-oriented approach which aims at understanding the process, the role of by-products and the burdens attributed throughout the system. On the contrary, the FUs corresponding to producing a certain mass of biogas or a certain mass of recovered solutes align more to a product-oriented LCA approach, focusing on determining the impacts associated with each specific product.

## 4.5. Approach and multifunctionality resolution

The selection of an LCA approach is directly related to the selected method to address multifunctionality in a system, meaning the strategy to distinguish impacts for a process involving more than one product or service. In addition, the approach determines aspects such as the background processes selection and the applicable suppliers for the analysis. Information on background processes in LCA is included in the **Database and background processes** section.

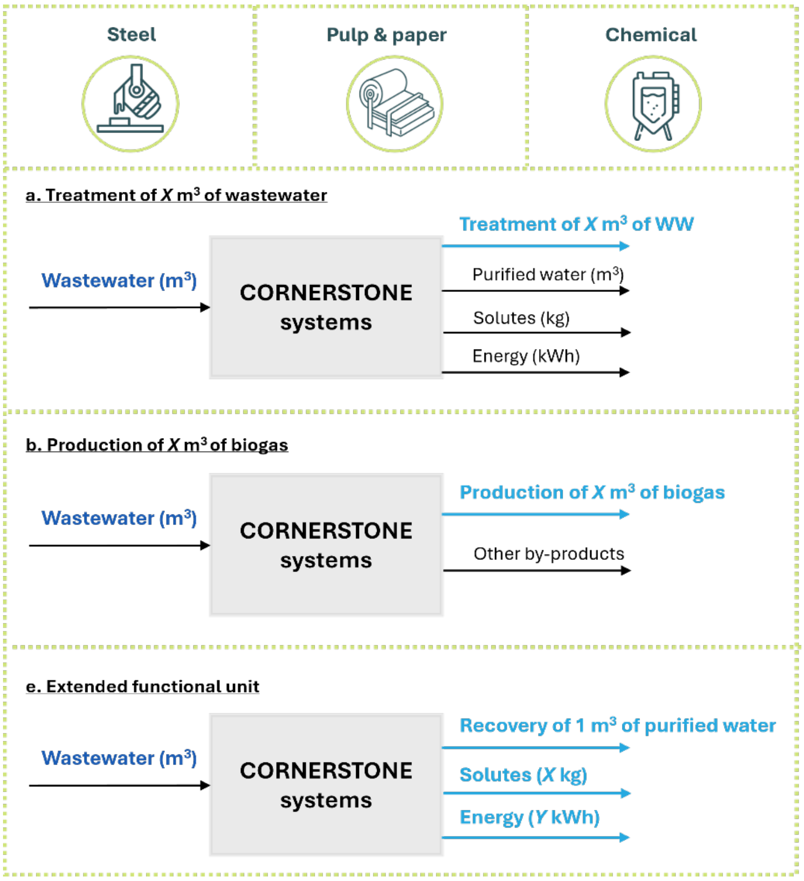


**Figure 5. Conceptualisation of CORNERSTONE system schemes and functional unit examples. Functional units are shown in bold and light blue colour.**

Table 2 summarises the two LCA approaches and relates them to the default method for multifunctionality resolution and the reference database for background processes. In general terms, ALCA is widely used for accountability, while CLCA is suitable for determining the consequences of a decision. It is important to note two main aspects related to ALCA and CLCA. Firstly, preferences emerge throughout the LCA standards and guidelines for a certain approach and for the suggested hierarchy for multifunctionality resolution. For instance, the ILCD suggests ALCA instead of CLCA for eco-design purposes. Secondly, ALCA and CLCA could be performed in a complementary manner with the objective of increasing the robustness of results and conclusions and providing a wider overview of the system.

As mentioned previously, each approach defines important parameters within the modelling such as i) the method for multifunctionality resolution and ii) the selection of the technologies that provide a requested service or product from background processes. Regarding multifunctionality resolution, ALCA is usually associated with allocation as the default method when assessing systems with various outputs. On the other hand, the substitution approach is more appropriate for CLCA. Nonetheless, it is important to consider that LCA standards and guidelines may present different hierarchies for multifunctionality resolution. Finally, as for the identification of the suppliers, ALCA typically requires average or regionalised market mixes for suppliers, while CLCA implements a mix of marginal suppliers.

The section dedicated to **Development of marginal mixes** expands on the concept referring to marginal suppliers and the methodologies to identify these providers.

**Table 2. Definition of LCA approaches and suggested methodological decisions**

| Approach | General goal | Background processes database | Definition of suppliers | Multifunctionality resolution | Acronym |
|---|---|---|---|---|---|
| **Attributional** | Accountability for the environmental impacts of a product or a service | Ecoinvent cut-off | Average or regionalised market mixes | Subdivision, system expansion, allocation by partitioning or the method suggested in the preferred standard or guideline | ALCA |
| **Consequential** | Consequences on global impacts influenced by the demand for a product or an activity | Ecoinvent consequential | Marginal suppliers' mixes | Substitution | CLCA |

## 4.6. Database and background processes

Background processes in LCA are necessary to model a system that interacts with input flows obtained from processes that are not specific to the studied system. These refer for instance to materials, energy carriers or services purchased in a market, such as electricity supply. The background system is typically incorporated in the assessments through Life Cycle Inventory databases, containing information for average industry data representative of country-specific or world region supply [8].

The background processes for CORNERSTONE assessments will be modelled using Ecoinvent databases (v3.10 or later) [20]. With the aim of covering the two LCA approaches mentioned previously, both the cut-off and consequential versions of the Ecoinvent database will be used for ALCA & CLCA respectively.

## 4.7. Development of marginal mixes

One difference between the ALCA and CLCA is the criteria used to define the supplier, thus the background processes selection. In ALCA, the suppliers are defined based on a shared contribution to the product supply in the market. However, in the case of CLCA, the supplier follows the marginal criteria. That is the definition of the technology that could fulfil the increase in the demand for a certain product or service. Therefore, the sum of marginal suppliers forms the marginal mixes.

For the present case studies, the different suppliers of water, solutes and energy should be carefully identified following some of the proposed methodologies in the literature [16] or novel ones based on the previous existing methods.

In the case of the CLCA, different methodologies will be used for the identification of different marginal suppliers. Among the methodologies found, the following ones will be used as a reference:

- Marginal Production Technologies for Life Cycle Inventories [16]
- International Life Cycle Data system handbook [12]

## 4.8. Life Cycle Impact Assessment

The elementary exchanges in the form of natural resources and/or emissions for a system are reflected as potential environmental impacts using an impact assessment method. This results in the Life Cycle Impact Assessment of a given product or process.

The Environmental Footprint (EF) midpoint impact method v3.1 is the selected method for the environmental assessment of CORNERSTONE technologies. EF v3.1 aligns with the recommendations and guidelines established by the European Commission [21], [22], hence contributing to a harmonised presentation of results. Table 3 summarises a holistic selection of impact categories from the EF v3.1. It is relevant to include a wide range of categories to represent the potential impacts in ecosystems, resources and human health. These categories are coherent with the needs of the industrial sectors of interest.

**Table 3. Summary of impact categories and corresponding units from the EF midpoint impact method**

| Abbreviations | Impact category | Units |
|---|---|---|
| **Ac** | Acidification | mol H+-Eq |
| **CC** | Climate change | kg $CO_2$-Eq |
| **ETX-f** | Ecotoxicity: freshwater | CTUe |
| **ER-nr** | Energy resources: non-renewable | MJ, net calorific value |
| **EU-f** | Eutrophication: freshwater | kg P-Eq |
| **EU-m** | Eutrophication: marine | kg N-Eq |
| **EU-t** | Eutrophication: terrestrial | mol N-Eq |
| **HT-c** | Human toxicity: carcinogenic | CTUh |
| **HT-nc** | Human toxicity: non-carcinogenic | CTUh |
| **IR-hh** | Ionising radiation-human health | kBq U235-Eq |
| **LU** | Land use | dimensionless |
| **MR: m** | Material resources: metals/minerals | kg Sb-Eq |
| **OD** | Ozone depletion | kg CFC-11-Eq |
| **PM** | Particulate matter formation | disease incidence |
| **PCOF** | Photochemical oxidant formation: human health | kg NMVOC-Eq |
| **WU** | Water use | $m^3$ world Eq deprived |

## 4.9. Water accounting in LCA

Depending on the selected impact assessment method, LCA methodology typically comprises impacts related to water provision supply chains, water use and intertwined water-related effects including eutrophication and acidification. Nonetheless, an extended and holistic approach for water footprint could provide valuable insights for the technologies developed within CORNERSTONE. However, there are different concepts behind water accountability approaches. On the one hand, the established Water Footprint method is ruled by ISO 14046:2014; and on the other hand, additional methods such as Available Water Remaining (AWARE).

### 4.9.1. Water footprint (ISO 14046)

ISO 14046 provides a comprehensive, science-based framework for measuring and managing the water footprint, helping organizations to contribute to global sustainability and responsible resource management. Coherently with the LCA structure, it defines the direct and indirect water consumption and balances from both the foreground technologies and the upstream processes of the value-chain [11], [23]. It can be measured with different impact methods, including the latest method AWARE.

### 4.9.2. Available Water Remaining (AWARE)

AWARE is a methodology that emerged from the Water Use in Life Cycle Assessment (WULCA) working group, addressing the need for a harmonised method accounting for water use impact in environmental analyses. This methodology includes both the impacts on the water resource itself and the subsequent effects in water availability for humans and ecosystems [24].

The main goal of AWARE is to depict water scarcity, interpreted as the potential of water deprivation for either humans or ecosystems. To this end, the method subtracts the water demand (accounting both human-related and ecosystem demands) from the total water availability per region. The result is then normalised to the world average value and inverted [24].

Water availability in the most recent version of AWARE (AWARE2.0) builds upon a global hydrological model, incorporating recent hydrological data and improving calculations for watersheds according to seasonal flow patterns. Moreover, availability estimations include an improved representation for large river deltas and an approximation for inland sinks as well. As for the human demand, the requirements include the irrigation, domestic, manufacturing, electricity and livestock sectors [25].

The use of AWARE in Life Cycle Impact Assessment can provide spatial resolution, due to the country aggregations included within its methodology. The holistic approach of AWARE combined with its regionalisation features can be potentially explored for the three demonstration sites throughout the CORNERSTONE project execution.

# 5. Life Cycle Cost (LCC)

## 5.1. Role of LCC & Techno-Economic Analysis (TEA)

Life Cycle Costing (LCC) is an approach that represents the economic pillar in LCSA, providing insights related to the costs and performance of a given technology or process. Within the context of conventional LCC, Techno-Economic Analysis (TEA) presents a modelling framework accounting for investments and internal costs allowing the evaluation of economic functionalities through different indicators. Conducting an economic assessment could fulfil different purposes including budgeting, planning tools, hotspot identification, investment evaluation and decision-making support for different stakeholder groups [26].

Aligned with environmental assessments, implementing techno-economics and LCC in the early stages of development presents diverse benefits for emerging technologies. The proper goal delimitation accompanied by a suitable selection of cost components and economic indicators could address the challenges related to low-TRL processes. Furthermore, considering these aspects in the conceptualisation of the analysis also supports the transferability potential evaluation towards future industrial application.

## 5.2. Techno-economic modelling

TEA modelling presents an approach for determining the economic performance of processes based on investment and manufacturing costs. This assessment follows the structure and guidelines of LCA, building upon its different phases and maintaining coherence regarding functional unit definition, system boundaries and data collection. Consequently, the data and estimations for LCI serve as the basis for one cost component considered within TEA.

Project costing frameworks provide cost categorisation guidelines for TEAs that include investments for equipment acquisition, operative costs, consumables, and waste treatment, among others [27], [28]. Table 4 summarises the typical cost breakdown for conducting economic analyses, alongside their calculation model proposal. The categorisation displays capital expenditures (CAPEX) and operational expenditures (OPEX), which represent the two main components to consider when assessing the economic sustainability of CORNERSTONE systems. CAPEX accounts for the initial investment efforts for procuring main process equipment while considering additional inputs required for installation, conditioning and setting up the equipment itself. On the other hand, OPEX represents an annual expense that accounts for both variable and fixed production costs. Complementary components dedicated to working capital and start-up & validation costs are considered as well.

**Table 4. Cost component breakdown and calculation model for techno-economic analysis**

| Cost component breakdown | | | Calculation models |
|---|---|---|---|
| **CAPEX** | **1. Direct costs (DC)** | Purchase cost of equipment (PC) | Consortium partners & literature cost data |
| | | Complementary costs related to installation of main equipment (e.g. piping, instrumentation, insulation, electrical works) | $f_a \cdot PC$ |
| | **2. Indirect costs (IC)** | Engineering, construction, contractor's fee & contingencies | $f_b \cdot PC$ |
| **Working capital** | | | OPEX for a given operation timeframe |
| **Startup and validation costs** | | | $f_c \cdot (DC + IC)$ |
| **OPEX** | **1. Variable costs of production (VCOP)** | Raw materials, input chemicals, utilities (e.g. steam, electricity, cooling water), consumables & waste treatment | Based on LCI, literature & other data |
| | **2. Fixed costs of production (FCOP)** | Maintenance, insurance, property taxes, overhead expenses, labour costs and laboratory & quality analyses | $f_d \cdot PC$,<br>$f_e \cdot (DC + IC)$ &<br>Other estimations |

## 5.3. Economic evaluation and indicators

TEA modelling provides the base for conducting cash flow analysis and obtaining economic indicators of interest according to the established goals and perspectives for CORNERSTONE systems. Table 5 summarises a selection of relevant indicators to be considered for economic assessments. Most economic criteria can be fulfilled directly from the cost categorisation within the TEA model shown in Table 4. Nonetheless, it is important to account for price variation throughout the years, as well as inflation and interest rates aligned with the recommendations of the JRC for the economic analysis used in the frame of the Best Available Techniques guidelines and Industrial Emissions directive [29].

**Table 5. Economic criteria and related indicators for TEA**

| Criterion | Indicators |
|---|---|
| **Operational effort** | Operational expenditure (OPEX) |
| **Investment effort** | Capital expenditure (CAPEX) |
| **Break-even point** | Payback period |
| **Product margin** | Market-derived margin for a product, internal-company margin |
| **Product volume** | The market volume for a product, internal-company demand |
| **Profitability** | Revenues, EBITDA[1], Net present value, Internal rate of return |
| **Profit or total cost per FU** | Total annualised cost in € per FU. FU examples: $m^3$ of wastewater, kg of recovered compound or kWh of recovered energy. |

[1]EBITDA: Earnings before interests, taxes, depreciation and amortisation.

Economic indicators related to profitability and cost per unit (net present value, internal rate of return and total annualised cost) account for the time value of money. This concept refers to discounting monetary values of upcoming years to represent the "*present value*" at the start of the project. The latter is achieved by incorporating a discounting rate into the calculations, representing the cost of capital which is calculated based on interest rates and equity financing [27], [28].

# 6. Social–Life Cycle Assessment

## 6.1. Introduction to S-LCA

Social Life Cycle Assessment (S-LCA) is part of the Life Cycle Sustainability Assessment methodologies. It focuses on assessing the social pillar of sustainability by measuring the social impacts of products or services across their life cycle, from raw material extraction to disposal [30]. The first formal publication on the subject was authored by O'Brien et al. in 1996 [31], aiming to establish a methodology for evaluating social impacts in a manner consistent with environmental LCA principles. Since then, considerable progress has been made towards developing a scientifically robust S-LCA framework for assessing the social implications throughout the life cycle of products and services. Presently, the S-LCA community is focused on advancing towards the formal standardisation of the methodology [32]. Such a standard would support informed decision-making, enhance understanding, and promote human dignity and well-being by improving the social and socioeconomic performance of product, process and service life cycle. However, this remains an ongoing challenge for the scientific community.

In line with its foundational principles and its connection to LCA, the current ISO standards for LCA—ISO 14040:2006 and ISO 14044:2006—serve as key references for S-LCA as well. There are two approaches to social impacts in S-LCA [30], [33]. The first is the Impact Pathway (IP) approach, which is more quantitative and models the cause-effect relationships between social indicators and potential impacts, similar to environmental LCA. It uses data and characterization models to estimate social consequences. The second is the Performance Reference Point (PRP) approach, which is more qualitative or semi-quantitative. It assesses social performance by comparing it to established norms, standards, or stakeholder expectations, making it useful for identifying social risks and hotspots. This approach is widely used for analysing social impacts at the company level [34]. These approaches can be used separately or together, depending on the assessment's goals. Combining both approaches offers a more comprehensive and balanced analysis. They enhance the robustness of the assessment by integrating, on one hand, a general assessment of the social impacts generated in the supply chain, identifying critical social hotspots and countries most affected and, on the other hand, the specific social performance of the companies in a site-specific social context of the country.

An attempt at standardisation was the development of the UNEP/SETAC Guidelines for the Social Life Cycle Assessment of Products, published in 2009 and updated in 2020 [30], which were also complemented by Methodological Sheets for implementation [35]. In these documents, a series of indicators are proposed for assessing various sub-categories associated with stakeholders, including workers, local communities, consumers and society at large. Another important contribution to S-LCA has been the development of databases with specific assessment methods to generically assess social hotspots of products and services, such as the Product Social Impact Life Cycle Assessment (PSILCA) [36], that can be used in LCA software as SimaPro and OpenLCA.

## 6.2. Workflow for S-LCA

The S-LCA for the CORNERSTONE systems will adopt a dual-method approach. First, a general assessment of social impacts is carried out using the PSILCA database for the three demonstration sites, Steel in Germany, Pulp & Paper in France, and the Chemical Industry in Germany. This aligns with the IP approach, offering a broad view of social impacts across the supply chains, particularly concerning the volume of wastewater generated. Complementing this, a PRP approach is applied for a more detailed, case-specific analysis. This second method focuses on the direct social impacts associated with the operations of the companies at each site, taking into account the specific impacts during the production phase.

## 6.3. S-LCA Impact Pathway using PSILCA

For conducting the S-LCA Impact Pathway, the current study employs the PSILCA v.3 database within the OpenLCA software [37]. This setup enables the analysis of social impacts linked to products and their components throughout their life cycle, drawing on diverse data sources. Developed by GreenDelta, PSILCA is integrated into the open-source OpenLCA tool and offers transparent, regularly updated data on social issues across nearly 15,000 sectors and commodities. It includes 55 indicators—both qualitative and quantitative. Depending on the study's objectives, these indicators can be expressed in either raw values or working hours [38]. In this case, the analysis uses the "working hours" variable, which reflects the labour time required to generate one US dollar of output in a given sector.

PSILCA is built upon the EORA multi-regional input-output database, which encompasses 189 countries and approximately 15,000 sectors, categorized into industries and commodities. EORA models economic exchanges through input-output tables that represent the flow of goods and services within an economic system over a specific time frame. In PSILCA, the reference unit is one US dollar of economic output.

The assessment of CORNERSTONE technologies will be conducted using homologue PSILCA sectors producing the inputs needed for each technology, considering it in economic terms. The same inventory data from the LCA and LCC will be used for the PSILCA processes. This will be achieved by modelling the quantities of the inputs in the foreground processes as monetary flows directed to the background processes within PSILCA.

Choosing the right indicators is a key challenge in S-LCA. PSILCA provides a wide range of indicators that address various social dimensions, following the structure of the UNEP/SETAC Guidelines [30]. In the CORNESTONE project,  55 indicators are organized into 17 subcategories that reflect essential social and socioeconomic concerns and are grouped under four main stakeholder categories: workers, local communities, society, and value chain actors (see Table 6).

Data sources include international organizations (e.g., the World Bank, ILO, WHO, UN), government and private databases, public records on health and safety violations, and case studies conducted by GreenDelta [37]. The indicators are measured in terms of "medium-risk hours," which estimate the average likelihood of a social issue occurring. PSILCA assesses indicators in an ordinal negative social risk scale that goes from no risk to very high risk and a positive social opportunity scale from low to high opportunity. The characterisation factors are provided in PSILCA by the Social Impacts Weighting method [37].

**Table 6. Social indicators considered in PSILCA by impact subcategory and stakeholder category**

| CATEGORY | SUBCATEGORY | INDICATOR |
|---|---|---|
| **Local Community** | Environmental Footprints | Embodied agricultural area footprints |
| | | Embodied biodiversity footprints |
| | | Embodied forest area footprints |
| | | Embodied water footprints |
| | | GHG Footprints |
| | Access to material resources | Biomass consumption |
| | | Certified environmental management system |
| | | Fossil fuel consumption |
| | | Industrial water depletion |
| | | Minerals consumption |
| | Migration | International migrant stock |
| | | International migrant workers (in the sector/ site) |
| | | Migration flows |
| | | Net migration |
| | Respect for indigenous rights | Indigenous rights |
| | | Risk of conflicts |
| | Safe and healthy living conditions | Drinking water coverage |
| | | Pollution |
| | | Sanitation coverage |
| **Workers** | Child labour | Child Labour, female |
| | | Child Labour, male |
| | | Child Labour, total |
| | Fair Salary | Fair Salary |
| | Discrimination | Gender wage gap |
| | | Women in the sectoral labour force |
| | | Men in the sectoral labour force |
| | Health and Safety | DALYs due to indoor and outdoor air and water pollution |
| | | Fatal accidents |
| | | Non-fatal accidents |

| | | |
|---|---|---|
| | | Safety measures |
| | | Violations of employment laws and regulations |
| | | Workers affected by natural disasters |
| | Forced Labour | Frequency of forced labour |
| | | Goods produced by forced labour |
| | | Trafficking in persons |
| | Freedom of association and collective bargaining | Association and bargaining rights |
| | | Trade unionism |
| | Social benefits, legal issues | Social security expenditures |
| | Working time | Weekly hours of work per employee |
| **Value Chain Actors** | Fair competition | Anti-competitive behaviour or violation of anti-trust and monopoly legislation |
| | Promoting social responsibility | Promoting social responsibility |
| | Corruption | Active involvement of enterprises in corruption and bribery |
| | | Public sector corruption |
| **Society** | Contribution to economic development | Contribution of the sector to economic development |
| | | Expenditures on education |
| | | Illiteracy, female |
| | | Illiteracy, male |
| | | Illiteracy, total |
| | | Unemployment |
| | | Value added (total) |
| | | Youth illiteracy, female |
| | | Youth illiteracy, male |
| | | Youth illiteracy, total |
| | Health and Safety | Health expenditure |
| | | Life expectancy at birth |

## 6.4. Towards a case-specific S-LCA

Secondly, a detailed evaluation of the social impacts of the companies involved in the CORNERSTONE project will be conducted using the PRF approach. This analysis will rely on a survey-based methodology targeting the companies that are implementing wastewater reuse technologies. The process begins with the selection of relevant social indicators and subcategories, guided by the UNEP/SETAC Guidelines, specially tailored to the context of the CORNESTONE industries.

The selection of indicators and sub-categories will follow a single materiality assessment approach [39], which focuses on identifying the most relevant social issues from the perspective of the companies involved. This process will begin with a comprehensive review of existing literature on social challenges affecting the sectors represented in the CORNESTONE project. To complement this, interviews with representatives will be conducted to gather insights into their specific situation. The result of this process will be a prioritised list of key social subcategories relevant to each company and sector. Based on these findings, customized questionnaires will be developed to gather primary social data directly from the companies, forming the basis for the case-specific S-LCA.

Indicators will be evaluated using a scoring system based on reference scales, allowing for the measurement of social performance and the degree of compliance with recognized social standards. Moreover, the information obtained will be adapted and used to complement the data in PSILCA.

Social aspects analysed will include working conditions, occupational health and safety, respect for workers' rights, corporate responsibility with suppliers, social commitment to the local community and compliance with government regulations, among others.

These indicators will be aligned with PSILCA indicators assessed previously to contribute to the harmonization and comprehensive understanding of critical social impacts.

# 7. Uncertainty Mitigation in LCSA

LSCA in low-TRL and pilot-scale applications is potentially prone to uncertainty due to diverse sources such as considerations and assumptions within the models. Modelling choices, parameter selection and data limitations could play a relevant role in uncertainty throughout the assessments. Table 7 summarises a selection of the main uncertainty sources that could emerge during the environmental, economic and social analyses, aligned with the categorisation presented in the literature [40], [41].

**Table 7. Identification of potential uncertainty sources for LSCA models**

<table>
<tr><th>Category</th><th>Uncertainty source</th><th>Examples</th></tr>
<tr><td rowspan="2">Parameter or data uncertainty</td><td>Inventory data estimations and data availability</td><td>• Raw material, electricity and energy flows<br>• Productivities, water recovery yield, conversion factors and scaling-up factors<br>• Lifespans<br>• Other relevant parameters</td></tr>
<tr><td>Temporal variability</td><td>• Definition of future prices for raw materials, electricity, etc<br>• Resource availability in the market<br>• Other economic parameters (e.g. plant lifetime, interest rates, discount rate)</td></tr>
<tr><td rowspan="2">Scenario uncertainty</td><td>Methodological choices</td><td>• Functional unit definition<br>• Attributional or consequential-based modelling decisions (e.g. providers and suppliers, multifunctionality resolution approach)<br>• System boundaries limitation and excluded processes</td></tr>
<tr><td>Geographical coverage</td><td>• European mix (EU-27) or European market group<br>• Site-specific parameters, suppliers, and locations for the models</td></tr>
</table>

Different strategies have been proposed to provide tools for reducing and managing uncertainties in sustainability assessments [42]. Based on the specific needs of CORNERSTONE technologies, the following options potentially provide resourceful strategies to deal with uncertainty during the execution phase of the assessments:

- **Scenario analysis.** Scenarios are useful to determine the consequences of a situation that may continue in the future. For instance, different scenarios could address a set of diverse suppliers for raw materials, or a change in one of the technologies involved in the system under study.
- **Sensitivity analysis.** This method is based on performing a set of iterations changing the value of key figures and assumptions in the models within specific limits, executing the variations in the parameters one by one. The objective is to evaluate the overall effect in impact assessment results, obtaining more representative data with each iteration. This approach contributes to result and conclusion robustness, as well as to facilitate the identification of critical points for further assessments.
- **Monte Carlo simulation.** This approach is a numerical calculation method based on probability and statistics. The underlying concept is to generate first random values for the variables of interest, then the assessment results are statistically analysed. Monte Carlo results are presented as probability distributions; thus, its accuracy increases with the number of iterations.

# 8. Conclusion

This deliverable addressed the strategical overview for sustainability and circularity assessment of CORNERSTONE systems. The basic methodological choices for the Life Cycle Sustainability Assessment were established for its three main frameworks: LCA, LCC and S-LCA.

Key aspects and considerations were included regarding the different sustainability disciplines, framing future assessments towards the evaluation of water reuse and energy and resource recovery strategies. In this sense, the report established the methodological compass for obtaining the environmental, economic and social performance of the different systems throughout the execution of the project. Furthermore, the different goals and perspectives that could be explored through LCA, LCC and S-LCA were included, alongside the complementary approaches to conduct the evaluations.

The establishment of mechanisms to address potential uncertainties related to diverse sources including inventories, up-scaling and temporal and geographic variabilities were defined. Scenario analyses, sensitivity analysis and Monte Carlo simulation were presented among the main techniques or tools to address uncertainty sources in the modelling of the three LCSA disciplines.

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