Making Sense of Techno-Economic Assessment & Life Cycle Assessment Studies for CO₂ Utilization (Version 2):

A guide on how to commission, understand, and derive decisions from TEA and LCA studies









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List of abbreviations

AACE	Association for the Advancement of Cost Engineering			
AHP	Analytic Hierarchy Process			
CAPEX	Capital Expenditure			
CCU	Carbon Capture and Utilization			
EC	European Commission			
EIT Climate-KIC	European Institute of Innovation and Technology			
	Climate-Knowledge and Innovation Community			
GCI	Global CO ₂ Initiative			
GHG	Greenhouse Gas			
ISO	International Organization for Standardization			
LCA	Life-Cycle Assessment			
MCDA	Multi-Criteria Decision Analysis			
MCDM	Multi-Criteria Decision Making			
NETL	National Energy Technology Laboratory			
NGO	Non-Governmental Organization			
OPEX	Operational Expenditure			
PEM	Polymer Electrolyte Membrane			
R&D	Research and Development			
SA	Sensitivity Analysis			
TEA	Techno-Economic Assessment			
TRL	Technology Readiness Level			
UA	Uncertainty Analysis			
WSM	Weighted Sum Method			

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Introduction

Carbon capture and utilization (CCU) or CO_2 utilization technologies attract researchers, policy makers, and industry actors in search of sustainable solutions for industrial processes. This increasing interest can be explained by the fact that these processes comprise the capturing of CO_2 – the most relevant greenhouse gas (GHG) – from the air or industrial point sources, and promote its use as a feedstock for the production of goods. CCU processes are expected to contribute to the greenhouse gas neutrality targets of several industrial sectors and the development of a circular economy. Therefore, understanding the environmental impacts and economics of CO_2 utilization routes is essential for decision makers from relevant fields, such as technology developers, entrepreneurs, funding agencies, policy makers, administrators and more. A deep understanding of the specific implications of CO_2 utilization technologies is needed to make decisions in line with sustainability strategies, and to discard inappropriate solutions.

The 'Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO2 Utilization'1 (henceforth TEA and LCA Guidelines) published by the Global CO₂ Initiative (GCI) in October 2018, represent a milestone in the harmonization of Life Cycle Assessment (LCA) and Techno-Economic Assessment (TEA) for evaluating CCU technologies. Henceforth, we refer to this document as TEA and LCA Guidelines. The TEA and LCA Guidelines provide a guide to overcoming methodological discrepancies that lead to confusion among practitioners, concerning how to conduct assessments, and which often lead to contradictory results.^{2 3} Documents with a similar focus have also been published by the National Energy Technology Laboratory (NETL).4 The success of the GCI publication and the demand for such guidelines is evidenced by the strong response that the authors registered in the months following its publication: more than 2,000 copies of the TEA and LCA Guidelines have been distributed in digital form or hard copy, and a growing community of practitioners, and decision makers from science, industry, and public administration are learning how to generate robust and comparable assessments when evaluating CCU technologies. In addition to the guidelines and the present report, the same research group has recently released five illustrative worked examples⁵ to support the application of the TEA and LCA Guidelines, and three accompanying peerreviewed articles.⁶ At the same time, policy officers at national and international levels have frequently signaled the urgency of further developing these tools, to enable evaluation of innovative technologies as a basis for decision making in funding and policy design (e.g., the EU Innovation Fund). Despite the urgent need to address planetary climate change, the development and diffusion of new technologies often takes considerable time. Consequently, leveraging the current momentum amongst all involved actors that CCU has achieved to date is paramount and is an opportunity that must not be missed.

¹ Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO₂ Utilization, 2018. GCI. Available at: https://www.globalco2initiative.org/2018/09/06/the-global-co2-initiative-at-the-university-of-michigan-publishes-valuable-toolkit-to-assess-co2-utilization-technology/.

² Artz, J., Müller, T.E., Thenert, K., et al., 2018. Sustainable Conversion of Carbon Dioxide: An Integrated Review of Catalysis and Life Cycle Assessment. Chem. Rev. 118:2, 434–504. Doi: 10.1021/acs.chemrev.7b00435.

³ Zimmermann, A.W., Schomäker, R., 2017. Assessing Early-Stage CO₂ utilization Technologies − Comparing Apples and Oranges? Energy Technology, 5:6, 850 − 860.

⁴ Carbon dioxide utilization life cycle analysis guidance for the U.S. doe office of fossil energy, NETL. August 30, 2019. Available at: https://www.netl.doe.gov/energy-analysis/details?id=3732.

⁵ A list of all worked examples already published is available at: https://www.globalco2initiative.org/research/techno-economic-assessment-and-life-cycle-assessment-toolkit/.

⁶ Müller, L.J., Kätelhön, A., Bachmann, M., et al., 2020. A Guideline for Life Cycle Assessment of Carbon Capture and Utilization. Frontiers in Energy Research, 8:15. Doi: 10.3389/fenrg.2020.00015; Zimmermann, A., Wunderlich, J., Müller, L.J., et al., 2020. Techno-Economic Assessment Guidelines for CO₂ Utilization. Frontiers in Energy Research, 8:5. Doi: 10.3389/fenrg.2020.00005; Sick, V., Armstrong, K., Cooney, G., et al., 2019. The Need for and Path to Harmonized Life Cycle Assessment and Techno-Economic Assessment for Carbon Dioxide Capture and Utilization. Energy Technology, 1901034. Doi: 10.1002/ente.201901034.

Despite demands for aligned assessment methods from the industrial and policy spheres,⁷ there are evident challenges in dealing with the practical application of such methods in commissioning, reading, and interpreting LCA and TEA studies. There is also a risk of insufficient transfer into policy or other decision-making processes, in cases where the involved actors do not possess disciplinary expertise in the relevant methodology.

About this report

This report provides guidance to decision makers in all types of public and private organizations involved in the planning and development of CCU. It is prepared within the scope of the *CO2nsistent* project funded by the Global CO2 Initiative and EIT Climate-KIC, and is based on the published *TEA* and *LCA* Guidelines. This report provides user-centered guidance on how to commission and understand TEA and LCA studies for CCU, and how to determine whether existing studies are eligible to be used in a decision making process. Another primary goal of this report is to ensure that disciplinary expertise is effectively taken up by decision makers and all potential audiences.

The remainder of this document is structured in two parts. Part A introduces the reader to the concept of TEA and LCA studies: What types of input can such assessments provide for decision making? What are the limitations of their explanatory power? This part focuses on the goal and scope definition for such studies, and on other aspects that are particularly relevant for decision making such as uncertainty analysis, sensitivity analysis, and Multi-Criteria Decision Analysis. The document presents how the decision maker (or commissioner) and the assessment practitioner can jointly set the various assessment phases. These terms are explained in the boxes below. The approach and main components of TEA and LCA studies are described, with the specific goal of making the most sensitive disciplinary concepts clear and comprehensible to all audiences.

Decision maker and Commissioner

Decision makers are actors from the policy or corporate fields who make decisions based on the results and interpretation of existing TEA and LCA studies, or based on new studies that they commission (which we term the Commissioner in this report).

The Commissioner can be any organization or individual that commissions a TEA or LCA study.

Practitioner

Practitioners are experts with sufficient technical background and experience to conduct TEA and LCA studies autonomously. They may work in academia, industry, or NGOs, as well as for governmental, research, or funding organizations.

⁷ Towards a Common Understanding of LCA and TEA for CO₂ Utilization Technologies, IASS 2020. Workshop Report. Brussels, October 2, 2019. Available at:

https://publications.iass-potsdam.de/rest/items/item 6000025 1/component/file 6000026/content.

⁸ The CO₂nsistent Project is a US-European initiative funded by the GCI and the EIT Climate-KIC engaged in further developing TEA and LCA for CO₂ utilization technologies. More information is available at: https://www.globalco2initiative.org/research/co2nsistent-project/.

Part B provides two case studies. The first is an example of how to commission a new TEA or LCA study to answer the research question of the decision maker. The second example focuses on the steps needed to evaluate if existing TEA or LCA studies can answer specific research questions posed by the decision maker. These worked examples were created in accordance with the decision trees presented in part C of this document.

Part C consists of practical tools to guide actors interested in commissioning TEA and LCA studies, and to support decision makers when evaluating and assessing TEA and LCA studies submitted by third parties. A series of consecutive steps, displayed as decision trees, provide support for checking the completeness of key aspects and requirements of TEA and LCA studies.

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PART A Understanding TEA and LCA for CCU

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A.1 Introduction

This section introduces the reader to the concept of TEA and LCA studies. After a general overview of TEA and LCA approaches, the step-wise process for defining the scope of such studies is discussed. Additionally, guidance is given on how to interpret and contextualize TEA and LCA results.

A.1.1 What kinds of information do TEA and LCA provide?

TEA and LCA are tools to assess the economic and environmental impacts of products or processes. TEA provides robust estimates of the technical and economic performance of a product, and presents best indications of expected profitability for potential investors.⁹

A.1.1.1 TEA

TEA results provide information on the economics of a given product or process associated with a specific location and time period, their accuracy, and variability in time due to, e.g., technological developments or future scenario conditions. Commonly used indicators include Total Costs of Production per unit of product: e.g., €2020/tonne¹0 of methanol (if used as a chemical feedstock), €/tonne of cement; or in Euros per unit of energy: e.g., energy content of methanol (if used as a fuel), electricity, etc. Through a complete TEA it is possible to evaluate if an innovative product or process is economically feasible under the conditions/scenarios considered, which processes or steps are technological or economic 'hotspots',¹¹¹ and how performance relates to competing options.

A.1.1.2 LCA

LCA is a standardized method to assess the environmental impacts of products or processes by taking into account all stages of the life cycle, from raw material extraction until final waste disposal. The LCA results indicate different environmental impacts, such as GHG emissions, air pollutant emissions, human toxicity, acidification of soil or water, etc. This holistic view of LCA avoids shifting environmental burdens between life-cycle stages, or between different environmental impacts. For example, a new product or process may reduce GHG emissions, while on the other hand its raw material extraction may lead to increased soil acidification. GHG emissions estimated via LCA are expressed as Kg CO₂ equivalents (eq.) per tonne of product, or as Kg CO₂ eq. per Mw of energy produced, etc., depending on the output of the product or process investigated. Standards for LCA defined by the International Organization for Standardization (ISO) are ISO 14040 and ISO14044.

Both TEA and LCA are conducted under specific assumptions and scenarios (e.g., with regard to the share of renewable, energy supplied or energy prices), and are usually compared with new technologies or alternatives already established in the market. To determine whether the assessed product or process is economically (TEA) or environmentally (LCA) preferable compared with other options, a benchmark has to be identified. In most cases, a new assessment is made against currently available conventional products, applying quantifiable indicators. A comparison between two or more innovative products or processes is also possible. This general approach is shown in Figure 1. In rare cases where it is difficult to identify an appropriate benchmark, statements about attributes such as carbon neutrality can still be made, since they do not necessarily require a reference product.

⁹ European Commission - Joint Research Centre, *ILCD Handbook - General guide for Life Cycle Assessment - Detailed guidance*. Luxembourg, 2010; SETIS ERKC, 2016. Techno-economic assessment. Available at: https://setis.ec.europa.eu/energy-research/techno-economic-assessment.

¹⁰ Time and location are often important in TEAs. They are usually shown as indices of the currency, e.g., €_{2020.}

¹¹ The term "hotspot" relates to processes that have a high impact on the TEA results, and that therefore must be more closely and thoroughly investigated.

TEA and LCA also help to identify the main drivers to ameliorate environmental and economic impacts: iteration between the practitioner and the commissioner/investor can be fruitful to identify action plans, and improve the environmental performance or the economics of a product or process. However, insufficient knowledge presents a limitation to the quality of TEA and LCA, for example due to the early developmental state of a product or process, or due to high uncertainty when determining external factors such as energy demand.

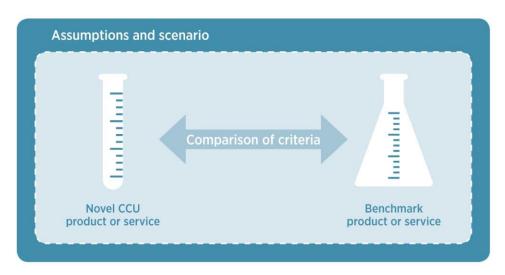


Figure 1: The main goal of TEA and LCA is to enable comparisons between a novel product and its conventional counterpart

A.1.2 Life cycle interpretation and temporary storage of CO₂

CCU technologies consume CO_2 to produce value-added products. Thus, intuitively, CCU technologies may be thought of as technologies with zero or even negative emissions. Nevertheless, this cannot be taken for granted, for example because of the high amount of energy usually needed to convert CO_2 into valuable products.¹² ¹³ Therefore, LCA can provide the information necessary for assessing the real emissions implications of these technologies. These attributes may be decisive in a policy-making context as well as for industrial purposes (TEA and LCA Guidelines v.2, Section C.7.1).

Table 1 describes the necessary conditions that a given technology must fulfil to be categorized as carbon neutral, carbon negative, or GHG emission reducing¹⁴ (for technology/product comparisons).

In order to provide evidence for the carbon emissions status of CCU technologies, a cradle-to-grave assessment is required (section A.4.4). Therefore, the assessment methodologies shall include the carbon sources and storage aspects of the use and end-of-life phases. For demonstrating carbon reduction through replacement of a conventional product or process, a gate-to-gate analysis might be sufficient, under the precondition that all other phases of the life cycle are identical (section A.4.4).

¹² See references: 2 and 3.

¹³ Von der Assen, N., Jung, J., Bardow, A. Life-cycle assessment of carbon dioxide capture and utilization: avoiding the pitfalls. Energy and Environmental Science, 9, 2013. Doi: 10.1039/C3EE41151F.

¹⁴ Please note that in the TEA and LCA Guidelines the definition "Carbon reducing" is occasionally used instead of "GHG emission reducing".

Table 1: Classification of CCU concepts according to GHG emissions [Based on Section C.7.1 of the TEA and LCA Guidelines v.2]

Carbon neutral	Carbon negative	GHG emission reducing (or carbon reducing) ¹⁵ for comparative studies
GHG emissions are zero over the entire life cycle	GHG emissions are lower than the amount of CO ₂ fixed	GHG emissions over the entire life cycle are less than in the benchmark process. Such outcomes therefore make a net contribution (compared with the current benchmark) to mitigating climate change
CO2 is captured from the atmosphere (via biogenic point sources or direct air capture) and released at the end-of-life or CO2 is captured from fossil point sources, and is sequestered or permanently stored in the product; and All other GHG emissions are zero (or minimal) over the entire life cycle	CO ₂ is captured from the atmosphere (via biogenic point sources or direct air capture) and CO ₂ is sequestered or permanently stored in the product and The overall life-cycle GHG emissions are lower than the amount of CO ₂ fixed	Regardless of CO ₂ sources (via biogenic point source, direct air capture, or fossilfueled plant), GHG emissions are lower than those exhibited by the competing conventional process, under the same system boundaries

Key messages for decision making:

- When commissioning a study or deriving conclusions from existing studies, keep in mind that only a cradle-to-grave analysis can provide evidence of carbon neutrality or negative emissions through CCU.
- > Emission reductions due to replacement of technology can be demonstrated in gate-to-gate approaches under certain conditions, and shall be interpreted as a less harmful solution rather than as a negative emission.

A.1.3 TEA and LCA in Multi-Criteria Decision Making

Many decisions based on TEA and LCA will need to take into account multiple underlying dimensions. Multicriteria Decision Analysis (MCDA), and subsequently Multi-criteria Decision Making (MCDM), are methods that allow the evaluation of trade-offs, and thus support decisions involving multiple dimensions or criteria. These methods allow systematic evaluation of economic, social, and environmental criteria (including competing priorities), and the interdependencies among them. Therefore, such approaches may inform policy makers and other stakeholders of feasible alternatives, and aid the decision-making process by clearly and comprehensively presenting complex and interlinked data, impacts, and trade-offs. This information is of particular relevance for policy decisions, as they impact multiple sectors of society.

Several methods might be considered for applying MCDA/MCDM to TEA and LCA analyses of CCU. TEA and LCA Guidelines v.2, Section B.7.4). When commissioning a study, such analyses can be included as requirements of the reporting and conclusions sections, to be undertaken by the practitioner. When using existing studies as inputs for a commissioned analysis, it is again crucial to ensure that all studies are

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¹⁵ See: reference 14.

consistent in scope and thus provide comparable data. For further reading, please refer to the worked example on MCDA¹⁶ or visit section A.7.

If the commissioner of a study wishes to use TEA and LCA outputs in a MCDM process, it might be helpful to integrate additional societal aspects when commissioning a study, so that practitioners can provide the relevant information as part of the final report, or already consider these factors in their conclusions. Such data may include, for example, the cost of CO₂ abated, the number of jobs created or maintained, or the reductions in fossil imports.

Key messages for decision making:

- When commissioning a study, MCDA can be requested by the commissioner at an early stage, to ensure that the practitioner will include this additional phase in the reporting and conclusions sections.
- When using existing studies as the input basis for such methods, it is again crucial to ensure that the scopes of the eligible studies are consistent and thus provide comparable data.

A.2 How is a TEA or LCA structured?

TEA and LCA studies consist of four main operational phases:17

- Definition of "goal and scope";
- "Inventory" compilation (collection and quality control of relevant data);
- Calculation of "indicators";
- "Interpretation" of the results.
- "Reporting".18

A similar approach was first published in the ISO 14040 and 14044 for standardization of the LCA methodology. The ISO approach to LCA has been adapted in the TEA and LCA Guidelines for the needs of TEA practitioners, as there is not yet an ISO standard for TEA. This general framework for both TEA and LCA is shown in Figure 2.

The goal and scope of the TEA or LCA study lay the basis for the entire assessment: They specify the details of the research questions, and therefore define how the study needs to be set up. The goal of the study is first proposed by the commissioner, while the final definitions of the goal and scope should be a shared effort, since their preparation requires the commissioner to understand the operational phases and their importance. The following sections provide guidance in this respect. Once agreed with the commissioner, all further phases are carried out by the practitioner according to the study's defined goal and scope. In the inventory phase, all relevant data are collected, usually with contributions from external entities, published data, or process measurements. Confidentiality of corporate data such as production costs and market prices can come at the expense of transparency and credibility of TEA and LCA results. To overcome this challenge a close relationship with data providers, a large panorama of data sources and anonymization of

¹⁶ Multi-Attributional Decision Making in LCA and TEA for CCU: An Introduction to Approaches and a Worked Example, 2021. Available at: https://deepblue.lib.umich.edu/handle/2027.42/167009.

¹⁷ European Committee for Standardization. ISO 14040: *Environmental Management – Life Cycle Assessment.* - *Principles and Framework.* 2006 ed. Beuth Verlag GmbH, Berlin; 13.020.10.

¹⁸ The ISO Standard comprises only four phases, and places reporting within "interpretation." Nevertheless, due to its crucial importance and the attention that needs to be given to this phase, the TEA and LCA Guidelines v.2 introduce reporting separately, as fifth phase.

information are suggested. During the calculation of indicators, the results of the impact assessment are obtained. Following this path, the interpretation phase is carried out alongside the other phases, to evaluate the consistency and robustness of the derived outcomes. Consequently, the interpretation phase can result in modifications or even necessitate repeating a prior phase. In the reporting phase, the practitioner must again pay specific attention to the goal and scope of the study, to ensure that the commissioner is provided with the necessary information and interpretation required to meet the agreed goal and scope.

This report provides guidance for decision makers on how to make sense of LCAs and TEAs in the crucial phases of their involvement during: *Goal and Scope Definition*, when the commissioner, together with the practitioner, sets the scene for the study by defining the targets; and in the Reporting phase, when the commissioner needs to understand the results and derive conclusions concerning the initial goal.

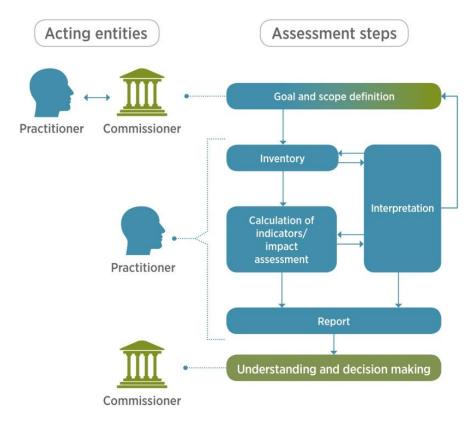


Figure 2: General framework for TEA and LCA studies and their acting entities [adapted from ISO¹⁹]

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¹⁹ See reference: 17.

A.3 Goal and research question: What do I want to achieve with the TFA or LCA?

As a starting point for every TEA and LCA study, the goal needs to be defined. The underlying goal, which may be specified by one or more research questions, determines the design of the assessment and its outcome. The goal and research questions are developed by of actors the group commissioning carrying out the reflecting assessment, their specific objectives. Actors may come from the fields of policy making, research and development, industry, or elsewhere.

For example, an objective of the *research & development* sector is to identify foreseeable barriers to, and drivers of, a given technology, or to compare different existing technologies (e.g., *what prices for CO₂ allowances are needed for selected technologies to break even?*).

In contrast, from a corporate perspective, the objective could be to analyze alternative investment opportunities, by investigating how a CCU technology or product will perform against current and/or upcoming benchmarks. Since the underlying question is the starting point for the practitioner to make important methodological choices such as defining the system boundaries (section A.4.4), a precise and feasible definition of the initial research question is of major importance.

EXAMPLE: Problem definition

A funding agency has the ability to fund research on how to lower emissions from the chemical industry. A literature review revealed that methanol is not only a widely used base chemical, but could also be produced from CO₂ instead of fossil resources. In order to derive a decision, the following question has to be answered: Is this solution environmentally beneficial?

Reminder: This and the following examples are based on the methanol worked example published by CO₂nsistent project (see: Footnote 6)

EXAMPLE: Research question

What would be the environmental consequences (with a focus on global warming impacts) of using methanol as a chemical feedstock, synthesized via hydrogenation of CO₂, compared to methanol synthesis from natural gas?

EXAMPLE: Technology description

An expert suggests the following process: CO_2 is captured via membrane capture from a cement plant; H_2 is produced via Polymer Electrolyte Membrane (PEM) electrolysis; subsequently, methanol is produced via thermochemical synthesis.

Figure 3 shows examples of such underlying questions. Here, the questions on the left aim to investigate the possible effects of specific CCU technologies compared to conventional processes, while the two questions on the right forecast future opportunities. To answer these questions, the assessments need to be tailored differently, and based on specifically defined assumptions and conditions. Therefore, it is often impossible for a single study to answer research questions that were not explicitly defined in the initial phase, or to compare assessment results that have been developed under different research questions, even if they evaluate the same product or process. To avoid difficulties or bias when deriving decisions based on pre-existing results, the underlying goals and approaches adopted by the practitioner should be clearly requested by, and communicated to, the commissioner.

To best define your goal, these questions should be asked: What problem do I want to tackle?" or "What question do I need to answer to take a sound decision? Hence, it is key to consider the following points to define the goal of your research:

- Context of the study: comparison to what (benchmark), location, time horizon and involved partners;
- Intended use and reasons of the study;
- Target audience;
- Commissioners and authors of the study;
- Known limitations of the study.

EXAMPLE: Goal definition

The goal of the study is to assess the environmental impacts of Methanol production as a chemical feedstock in Germany in the year 2020, using CO₂ captured from a cement plant and comparing it to methanol synthesized via conventional steam methane reforming. The study is intended to support the decision makings of the funding agency, is commissioned by the agency itself and performed by the Technical University Berlin. The goal of the study is limited to the current state of the technology and not suited to assess future developments of this technology.

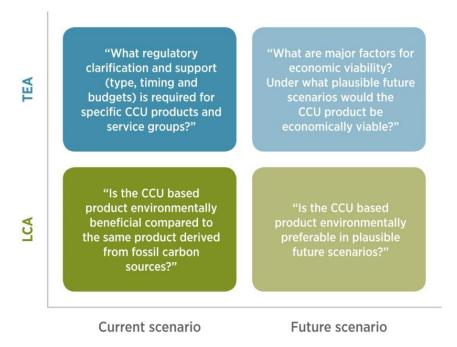


Figure 3: Examples for research questions for the assessment of CCU technologies [adapted from the TEA and LCA Guidelines v.2]

Key messages for decision making:

- When commissioning a study, propose clear goals (to be adapted if necessary) and demand that the assessment be structured accordingly. Discuss with the practitioner the levels of certainty and accuracy of the anticipated results.
- When basing your decision on existing studies, be aware of their underlying goals and research questions. Do they match the specific needs of your decision-making processes?

A.4 Scope selection: How to address the goals

Once the goal of the assessment is defined as described above, the next step is to define its scope. The scope of a TEA or LCA determines which aspects of a product or process will be assessed. The scope definition is subdivided into several tasks that need to be completed to set up a study. The major activities for scope selection are described further in the following sections (Figure 4):

- Selecting the subject of analysis (product systems and their functions);
- Selecting comparison metrics for the subject (defining functional units and reference flows);
- Specification of elements needed, and boundary selection (defining the unit processes²⁰ and system boundaries);
- Selecting systems for comparison (benchmark systems);
- And understanding the maturity of the product system (technology maturity). (Please note that
 this can also be performed as an earlier step, depending on the practitioner/commissioner or the
 technology evaluated).

The decision on whether the commissioner or the practitioner defines the TEA or LCA scope will differ according to each individual case. Generally speaking, the phases explained in the following section will have to be undertaken by the practitioner and communicated to the commissioner, to ensure that the study is aligned with the specific needs of both actors. For existing TEA or LCA studies, it is important to be aware of how the scope has been defined, since this largely influences the results and might therefore limit the information that can be extracted from the results.

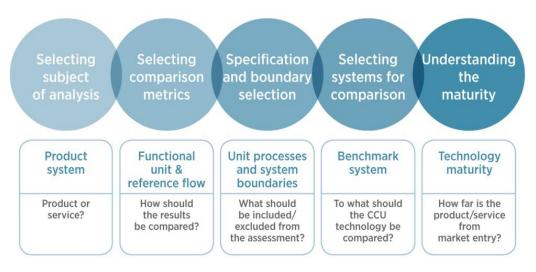


Figure 4: Major phases in scope definition for TEA and LCA studies of CCU technologies

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²⁰ Unit processes are usually defined as system elements in TEAs.

A.4.1 Selecting the subject of analysis

To select the subject of analysis of a TEA or LCA study, the product system has to be defined. This refers to all the processes required to provide a product or service across one or multiple stages of the life cycle (e.g., the production, application, use, and disposal of a product). Before defining the product system for

an analysis, the market segment and application of the product or process need to be clear, since TEA and LCA are typically based on a single or multiple applications defined by the goals of the assessment. This is crucial, since choosing a certain application will very likely impact different stages of the life cycle. This approach is described in Table 2. Therefore, if an investigated application differs from that chosen by the commissioner, the assessment outcomes could be meaningless for the underlying goals.

EXAMPLE: Product system

Methanol can be used as a fuel or as feedstock in the chemical industry for products such as polymers, formic acid, and acetic acid. In line with the research question, the selected application is "Base chemical for the chemical industry."

EXAMPLE: CCU application

<u>Fossil fuel</u>: Synthesized non-fossil methanol could potentially be burned in conventional combustion engines. In order to assess the impacts of this application, the use phase would have to be assessed in detail because methanol has different properties than conventional fuels.

<u>Chemical product</u>: Synthesized non-fossil methanol could directly replace methanol from fossil sources, with no differences or assessment of the use phase. (Choosing the appropriate subject of the analysis matters!).

Table 2: Examples for defining the application of a CCU product or service

The product or process has one or few applications	The product or process has a large number of applications			
One relevant application should be defined (e.g., fuels for transportation, polyols for foam)	Choice 1: no specific application is considered The product or process itself should serve as the application (e.g., methanol or carbonate aggregates)	Choice 2: Multiple applications are considered in parallel: If multiple applications can be investigated in parallel, define the 'application-mix' (e.g., for multiple ash sources for CO ₂ mineralization, the application mix could be based on a yearly average of all ash sources used)	Choice 3: Only one application is considered If only one of the multiple applications can be carried out at a time, it is sufficient to include only one application in the assessment	

Key messages for decision making:

- When commissioning a study, ensure that the selected product system is in line with your goal and that appropriate unit processes are specified.
- When deriving decisions based on existing TEA or LCA studies, it is important to validate that the applied product system was appropriately chosen: Does the CCU product or process contribute to a small or large number of applications? In the case of multiple applications, which ones are most relevant for deriving your decision?

A.4.2 Selecting comparison metrics for the subject

Based on the selected application and market segment (section A.4.1), it is essential to choose common metrics that allow meaningful comparison. This operation is fulfilled through definition of functional units and reference flows.

A functional unit quantifies the technical performance of a product or process, and must be defined unambiguously to ensure meaningful comparison with alternatives. Functional units can be defined by mass, volume, or energy according to the applications chosen. The functional unit also serves as a reference system to ensure that comparisons between systems serve equal functions (TEA and LCA Guidelines, Sections B.4.2 and C.4.1).

The reference flow is the relevant output in a given system that is required to fulfil the function expressed by the functional unit, e.g., the amount of paint (reference flow) required to cover a defined area at a defined opacity (functional unit). Since product systems can also serve more than one function (e.g., a combined heat and power system provides both electricity and heat), functional units might contain more than one reference flow that pertains to the scope of the assessment (TEA and LCA Guidelines v.2, Sections B.4.2 and C.4.1). Another case involving multiple reference flows concerns product systems with multiple inputs and outputs (e.g., co-products, water streams, etc.) that may or may not be functions of the system product. As many CCU product or process are characterized by multifunctionality, this aspect needs particular attention when setting up studies.

Figure 5 shows a schematic overview of a generic product system. Its elements are explained in more detail in the following sections.

EXAMPLE: Comparison of product system

If we aim to utilize CO₂ emissions from a cement plant, our overall product system must also include the cement plant. Our system will therefore have two output streams: produced methanol and produced cement.

EXAMPLE: Functional unit

The functional unit for the assessment must be aligned with the chosen application. Here, methanol is seen as feedstock for the chemical industry. As CO_2 -based methanol is the same chemical species as that derived from fossil fuels, it can be compared on a mass basis. The cement that our product system produced can also be compared on a mass basis.

EXAMPLE: Reference flow

The reference flows are the produced methanol and cement: 1 tonne of methanol feedstock and 1.96 tonne of cement, which are produced from specific input quantities.

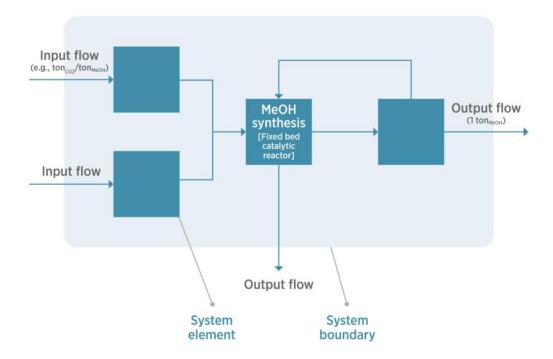


Figure 5: An exemplary product system, with its elements, boundaries, and input/output flows

A.4.3 Defining functional units for TEA and LCA studies

The definition of functional units and reference flows for TEA and LCA studies of CCU technologies involves several steps. The decision tree shown in Figure 6 enables the commissioner and practitioner to comprehensively undertake these steps one by one, or to understand why certain decisions were taken in existing studies (TEA and LCA Guidelines, Sections B.4.2.2 and C.4.1.1).

Prior to this process, the first fundamental step is to differentiate CCU pertaining to energy storage systems from other applications, since the former can usually only be assessed as part of a larger system (Figure 6). In case the latter is investigated, two major scenarios need to be distinguished:

- 1. The CCU chemical composition or structure of the product or process is identical to the conventional one (in this case, we term the product or process a substitute), or
- 2. The CCU chemical composition or structure of the product/service differs from the conventional one (in this second case, we term the product or process a non-substitute).

In the last step, the intended use of the product or process (i.e., fuel vs. chemical/material/others) must be defined.

Defining reference flows and functional units for CCU energy storage systems can be more challenging, as here the functional unit needs to be defined in consideration of the service delivered by the object being assessed. To appraise new energy storage systems, this should be compared to scenarios where no storage is contemplated.

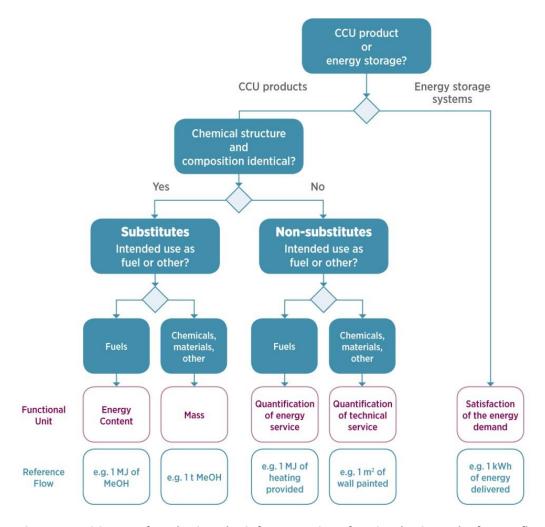


Figure 6: Decision tree for selecting a basis for comparison, functional units, and reference flows

For product or process where **multiple applications have to be considered**, we recommend selecting the functional unit based on the most important among all the applications. In such cases, the results of the study should only be compared to other studies if the same application (and therefore functional unit) is investigated. A better option would be to conduct individual studies of each specific application.

Key messages for decision making:

- When commissioning TEA and LCA studies, special attention needs to be given to the definition of the functional unit if the chemical structure of conventional products differs.
- When comparing existing TEA or LCA studies, or consulting the results of an LCA and TEA applied to the same product or process, ensure that the functional units are consistent.

A.4.4 Specification of elements needed, and boundary selection

The elements constituting the product systems and describing key activities are called **unit processes** (TEA and LCA Guidelines v.2, Sections B.4.3.1 and C.4.2.1). According to the goal of the study, they can be defined at very different levels, ranging from processes (e.g., feedstock mining, production phase, use phase) to unit operations (e.g., CO_2 capture and compression, distillation), or even unit equipment (e.g., pump, reactor vessel). Each unit process should serve as an accounting unit for inventory, calculation, interpretation, and reporting. The practitioner defines the unit processes for the specific object being assessed.

The **system boundaries** set the limits of the product system, and must be selected in line with the overall goal of the assessment, as defined by the commissioner. During their life cycle, products undergo different stages: from feedstock extraction to production phase, and use phase, until the end-of-life (disposal). With regard to the research question and goal of the study, as well as the attributes of the assessment object, not all of these phases always need to be considered and analyzed in order to produce reliable results. Furthermore, a lack of data may also justify the exclusion of a certain phase, if this is in line with the defined goals. Generally, three different approaches may be distinguished, depending on how many of the upstream (i.e., before the use-phase) and downstream (i.e., after the use-phase) processes of the production phase are included in the assessment (Figure 7).

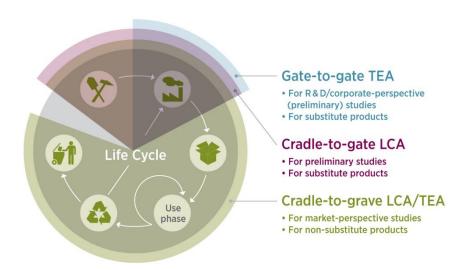


Figure 7: Scope of TEA and LCA in the product life cycle [adapted from TEA and LCA Guidelines]

A.4.4.1 Gate-to-gate assessment

This considers the production phase only, and is mostly applied in TEAs with a focus on analyzing costs, revenues, and technical performance. The system boundaries are therefore set around the activities strictly operated by the company (within the company's 'gates'). Upstream and downstream activities are excluded from the analysis. This approach is also viable for comparing product or process that are chemically identical, with identical upstream and downstream processes. Here, only the process within the 'gates' differs and is thus relevant for a comparison. Nevertheless, it should be noted that the CCU upstream is usually different from the benchmark one, as conventional technologies do not use CO₂ as feedstock. This implies relevant limitation to apply gate-to-gate boundaries to LCA.

A.4.4.2 Cradle-to-gate assessment

This is mostly applied in LCA rather than TEA, and the system boundaries here cover the product system from extraction of raw materials (i.e., upstream phase) to the factory gate. This approach is viable for comparing applications that create products which are chemically identical, with identical downstream

processes but different material inputs or other upstream processes. Here, since the respective useand end-of-life phases of the technologies being compared are exactly the same, they can be excluded from the assessment. Moreover, this approach can be applied when no specific

EXAMPLE: System boundaries

Since the life cycles of both the produced methanol and the cement are identical to conventional products, a cradle-to-gate assessment will be sufficient.

application of the product is of particular interest (in case numerous applications exist), or in early stage of development when the potential application is unknown. Note that if gate-to-gate TEAs include the costs of raw material inputs, they also cover the upstream costs and can thus be considered as fitting with a cradle-to-gate LCA.

A.4.4.3 Cradle-to-grave assessment

This approach considers the entire product life cycle, including all the phases from raw material extraction until end-of life, and is usually only applied in LCA. It is applicable to non-substitute product or process with differences in their entire life cycle. Cradle-to-grave TEAs are not commonly performed from the corporate perspective, but they can be necessary to align TEA and LCA studies or to assess the full costs to society, which may be relevant for policy makers. In order to classify CCU as carbon neutral, negative or GHG emission reducing (see Table 1), a cradle-to-grave perspective is a prerequisite.

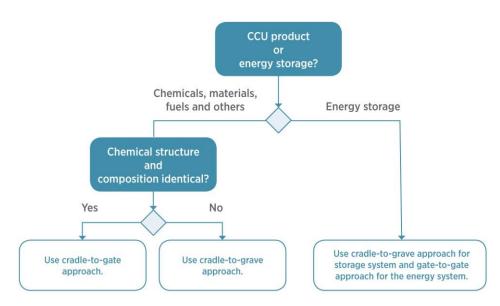


Figure 8: Decision-making process concerning system boundaries for LCA [adapted from TEA and LCA Guidelines v.2]

For comparison of an energy storage system, the system boundaries shall cover the entire energy system and the entire life cycle of the energy storage. See Figure 8 for guidance on deciding which LCA system boundaries must be applied.

Due to potential data scarcity, and in order to reduce the workload, TEA and LCA studies may require cutoffs of input/output flows and unit processes when defining the product system. A cut-off means considering only flows and processes that substantially affect the results, while omitting those for which minor effects are foreseeable. In these cases, the cut-off criteria and the level of completeness shall be clearly described in the scope definition.

Key messages for decision making:

- > TEAs and LCAs produced from a corporate perspective tend to use a gate-to-gate analysis, as this is the major focus of a company. When deriving decisions from existing studies, ensure that the scope does not allow for shifting of emissions or other negative effects.
- ➤ It is not good practice for an LCA to be tailored or based on a corporate perspective, as this contravenes the basic principles of LCA. Other methods, such as the GHG protocols, describe such assessments.
- When commissioning a study, the system boundaries must be clearly stated, explained, and justified according to the research questions and goal of the study. Moreover, their choice needs to guarantee comparability with the benchmark, and among comparable product or process.

A.4.5 Selecting systems for comparison

To assess and analyze how the CCU product performs against a conventional product or process with the same application (i.e., is the CCU product beneficial for the climate compared with the existing technology?), the two have to be compared. The system of the conventional product or process is therefore defined as the **benchmark system** (i.e., best-in-class benchmark) and its product as the **benchmark product**.

A.4.5.1 How to define benchmarks for TEA and LCA studies

The appropriate benchmark product has to be selected based on the product application and the assessment goal. An important factor here is to distinguish between direct substitutes and non-substitutes (TEA and LCA Guidelines, Sections B.4.4 and C.3.1).

These are defined according to whether the innovative CCU application does/does not have exactly the same performance as a conventional one. The former case (direct substitute in Figure 6) is true if the conventional and CCU chemical or fuel products have identical chemical structures and composition. In the case of energy storage systems, the conventional and CCU service must have the same characteristics (unfortunately, this is often not possible). In these cases, the service that is currently the most common or best in its class shall be selected as the benchmark. Applications that might be relevant in the future shall also be considered. The term non-substitute refers to product or process that provide the same application but with different performance. Non-substitutes make an exhaustive and comprehensive comparison more challenging.

A single CCU product or process can be used in multiple applications in different sectors (e.g., methanol may be used as a feedstock in the chemical industry, or else as a vehicle fuel). Cross-sectoral analysis

facilitates the identification of these additional applications (e.g., comparing its use as a chemical or fuel), which must then be assessed and compared against each other. In such cases, a specific benchmark needs to be defined for every application.

EXAMPLE: Benchmark definition

The benchmark for our selected technology must be the conventional production of methanol. Here, one of the most common technologies is steam methane reforming, which is therefore selected as the benchmark.

Key messages for decision making:

- If a direct substitute does not exist, an exhaustive and comprehensive comparison becomes more challenging and requires greater elaboration.
- When using existing TEA or LCA studies to answer your research question, the key metrics must be properly analyzed and comparisons must be performed against the appropriate benchmark.
- When analyzing the results of studies, it is important to look at the underlying benchmark, as this can determine whether or not the assessed technology will be beneficial. For example, methanol produced from CO₂ might be more environmentally sustainable than fossil-based production processes, but not when compared to other technologies.

A.4.6 Understanding the maturity of the product system

The technological maturity of products or processes must be investigated to define the overall maturity of a product system (TEA and LCA Guidelines v.2, Sections B.4.5.2 and C.3.1). Technology maturity describes the stage of development of a product or process according to three major categories: applied research, development, and deployment. A more detailed tool for defining technology maturity is 'technology readiness level' (TRL). Figure 9 shows TRLs as applied by the European Commission.



Figure 9: Technology readiness levels (TRL) and definitions, as used by the European Commission [adapted from EC 2014²¹]

The development stage of the assessed technology has important implications for the general availability and reliability of data. During the course of developing a new technology, practitioners gain additional data and greater certainty. Thus, compared with high-TRL options, assessments of low-TRL technologies are more reliant on assumptions, resulting in greater uncertainty. This matter has been illustrated by the Association for the Advancement of Cost Engineering (AACE) in relation to capital cost estimations, and at its core is also true for TEAs and LCAs in general (Figure 10).

The technology maturity of each product system and unit process must be determined. The overall maturity of the product system is equal to the unit process with the lowest maturity. Consequently, a high level of uncertainty needs to be taken into account by the commissioner when interpreting results derived from technologies with low maturity. TEA and LCA currently lack a common understanding of how to assess low-

²¹ European Commission, 2014. *Technology Readiness levels (TRL)*. Available at: https://ec.europa.eu/research/participants/data/ref/h2020/wp/2014_2015/annexes/h2020-wp1415-annex-g-trl_en.pdf.

TRL technologies, and the CO₂nsistent project will provide assessment guidelines for low-TRL technologies in its final publication (TEA and LCA Guidelines v.2, due in 2022).

When commissioning a study, potential data deficits must be considered. If in the course of the assessment the practitioner identifies that required data for maturity categorization do not exist, are not available, or are of insufficient quality, the goal of the study might need to be critically reviewed. Technology maturity can also be relevant when selecting the appropriate indicators (TEA and LCA Guidelines v.2, Section B.4.5.2).

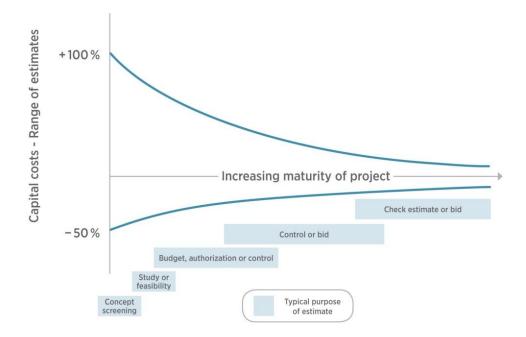


Figure 10: Variation of the accuracy of capital cost estimations through the course of a project. The capital cost "0 %" represents the final cost [adapted from Christensen et al., 2019²²]

Key messages for decision making:

- > The technology maturity of a product or process is of major importance for the assessment. When comparing technologies at different TRLs, keep in mind that in TEA and LCA options with higher TRL have, accordingly, higher level of certainty.
- Technologies with low TRL will typically require more time before their eventual deployment.
 When deriving decisions, it is crucial to envision each option at the time and location of its full-scale deployment.

²² Christensen, P., Dysert, L.R., Hollmann, J.K., 2019. *Cost Estimate Classification System – As Applied in Engineering, Procurement, and Construction for the Process Industries*. AACE International Recommended Practice No. 18R-97.

A.5 Understanding TEA and LCA results

The outputs and conclusions of TEA and LCA studies constitute the scientific basis for subsequent decisions. While the practitioner usually provides an interpretation of the results for the commissioner (Figure 2), it is of primary importance that the commissioner or the decision maker develop an understanding of the various parameters, in order to examine the consistency, completeness, and reliability of these studies; to thereby evaluate their overall significance (interpretation of results); and, consequently, to make well-founded, substantiated decisions based on these conclusions. Prerequisites for this process are the scope definition for newly commissioned studies, or analysis of the original study scope when making utilizing existing studies, as described above.

In this section, we elaborate on the following: **sensitivity analysis** and **uncertainty analysis** as ways of assessing uncertainties in TEA and LCA; and the life cycle interpretation of CCU applications. While such assessments are undertaken by the practitioner, an understanding of how to read the results will facilitate sound decision making by the commissioner.

A.5.1 Uncertainty and Sensitivity Analysis

Uncertainty analysis (UA) and sensitivity analysis (SA) are performed by the practitioner in order to:

- Increase the reliability, credibility, and robustness of conclusions; and
- Identify the most influential input variables among the calculated indicators.

Uncertainty and sensitivity analyses allow the commissioner or decision makers to understand the levels of uncertainty inherent in the results, and to determine the influence of uncertain assumptions on the results of existing or commissioned studies (TEA and LCA Guidelines v.2, Sections B.7.2 and C.7.2).

UA allows practitioners to analyze (and in the best cases, to quantify) the ranges of uncertainties contained in the model outputs (which depend on uncertainties in the input data). It functions as a quality test for the whole model and seeks to avoid misleading interpretations. SA shows how sensitive the model outputs are to variations in one or more input variables. UA and SA are complementary, as the latter reveals how the uncertainty of the output is constructed. Factors characterized by low sensitivity and low uncertainty do not require further investigation. Conversely, high priority should be given to verifying the reliability of results that show both high uncertainty and high sensitivity to change.

A.5.1.1 What kinds of uncertainty may arise?

There are three main sources of uncertainty:

- Uncertainties in input variables (e.g., interest rates or reaction yields) due to imprecise measurements or low accuracy of inventory data;
- Uncertainties in model structure and processes, such as imprecise inter-relations among unit processes, system boundaries, selection of processes, etc.;
- Uncertainties related to contexts and scenarios, and due to methodological choices such as determination of functional units or allocation criteria.

To understand the different kinds of uncertainty than can arise from these sources, the distinction between uncertainty and variability has to be clear. This distinction can be illustrated in the choice of assumptions used for model parameters (e.g., interest rate, reaction yield). Here, uncertainty refers to the "lack of knowledge of the precise parameter" (Rubin 2012²³), while variability refers to the range of values that this

²³ Rubin, E. S. (2012). *Understanding the pitfalls of CCS cost estimates*. International Journal of Greenhouse Gas Control, 10, 181-190. Doi: 10.1016/j.ijggc.2012.06.004.

parameter "may take on" (e.g., different interest rates in different countries). Often, the term uncertainty is used to encompass both lack of certainty and large potential variability.

The following paragraphs provide a short overview of methods for assessing UA and SA. Given the complexity of these topics, for further insight, please refer to the TEA and LCA Guidelines.

A.5.1.2 Uncertainty analysis methods

Different methods of UA are available, depending on the categories of uncertainty described above. **Monte Carlo Analysis** (particularly common in LCAs for modelling the effect of the uncertainty of input variables) describes the statistical distribution of possible output data generated by iteratively selecting input parameters within their ranges (if parameter ranges exist and are characterized).

Probability density plots generated by Monte Carlo Analysis in the best-case show decision makers the ranges described by all potential output data on the x-axis, while the likelihood of obtaining each of these individual outputs is shown on the y-axis. The example in Figure 11 shows results that are 'normally' distributed, with the data described by a bell-shaped curve. The results of a Monte Carlo Analysis can be conveyed in a simplified way by reporting the mean values of all results, defined as the "most" expected output data of the LCA or TEA study. The standard deviation of the data set can be used to provide a mathematical indication of how 'spread-out' the output data are. A small standard deviation indicates a pronounced bell-shaped curve, where most of the results are positioned close to the mean value. A large standard deviation indicates instead a flattened bell-curve, where the results are more widely distributed across the entire range of results. In the latter case, the TEA or LCA results are more uncertain (Figure 11). Here, it should be noted that Monte Carlo Analysis always bears a certain amount of bias resulting from the underlying choices, which require practitioners to define the statistical behaviors of all parameters. Hence, results should not be viewed as always displaying the true distribution of values. While for variable parameters this is easily manageable, for uncertain input parameters this is more difficult. Hence, if the underlying conditions/assumptions of a Monte Carlo simulation are not clearly disclosed, decision makers should refrain from using probability plots as the sole basis for decisions.

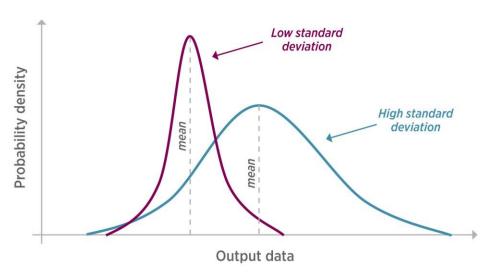


Figure 11: Bell-shaped curves representing two normal distributions of Monte-Carlo analyses

Qualitative uncertainty analysis can be used as an alternative or complementary method when analyzing data from different sources, or when there are insufficient reliable data for statistical analysis (a common

case under low-TRL conditions). Qualitative methods such as 'pedigree analysis' can be helpful in qualifying whether an assumption within the model calculation was made with high or low certainty.²⁴

A.5.1.3 Sensitivity analysis methods

The goal of sensitivity analysis is to determine the extent to which uncertainty in parameter values impacts the model's output. The objectives of these methods usually include ranking those input parameters to which the output display the highest sensitivity, identifying the direction of the relationship (i.e., positive or negative²⁵), and determining the nature of the relationship (e.g., linear, non-linear, etc.). Sensitivity analyses can be broadly categorized as employing either local or global methods. In local sensitivity analyses, only one input parameter (e.g., interest rate, yield of reaction, or electricity grid emissions) is varied at a time, while global methods use Monte Carlo simulations as the basis, where multiple input parameters in the model are varied simultaneously.

Local sensitivity analysis includes *one-at-a-time* and *one-way* methods. Both can be utilized by decision makers to grasp the input—output relationships among uncertain parameters in a presented LCA or TEA study. The outputs of both methods are shown in Figure 12.

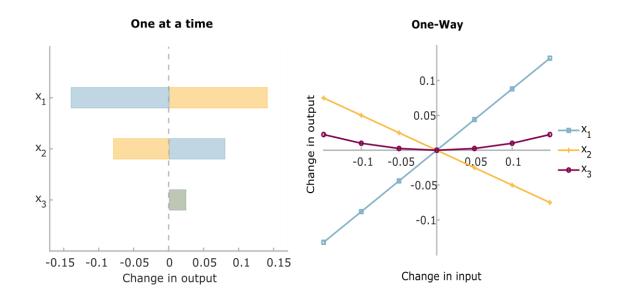


Figure 12: Visual representation of one-at-a time sensitivity analysis via tornado diagram (left) and one-way sensitivity analysis as spider diagram (right).

One-at-a-time (OAT) sensitivity analyses are usually displayed using tornado diagrams. Tornado diagrams show the impact that each variable (i.e., the bars in Figure 12) has on the outputs, when the maximum and minimum values characterizing each variable are selected. Larger range (i.e., longer bar) indicates that the output is more sensitive to variations in the parameter value. Additionally, the nature of the relationship is visualized using colors (i.e., in Figure 12, yellow on the right side indicates a positive relationship). In the example shown in Figure 12, input X_1 has the highest impact on the output, followed by X_2 ; the results show a positive relationship for X_1 , whereas X_2 has a negative relationship to the output.

²⁴ Guidance Note for Lead Authors of the IPCC Fifth Assessment Report on Consistent Treatment of Uncertainties. IPCC Cross-Working Group Meeting on Consistent Treatment of Uncertainties, Jasper Ridge, CA, USA 6 – 7 July 2010. IPCC. Available at: https://www.ipcc.ch/site/assets/uploads/2017/08/AR5 Uncertainty Guidance Note.pdf.

²⁵ A positive relationship means that input and output value move in the same direction: An increase (or decrease) in an input value (e.g., electricity price) leads to a corresponding increase (or decrease) in the model output (e.g., total costs of production). In a negative relationship the input and output move in opposite directions (i.e., an increase in an input value leads to a decrease in the output value).

One-way sensitivity analyses commonly use spider diagrams, which show the sensitivity of the outputs when varying each single variable: a steeper slope indicates stronger sensitivity of the output data to variations in the selected input parameter. Accordingly, the direction of the slope shows indicates whether a positive or negative relationship is present. Spider diagrams also show if the relationship between the input parameter and the output data is linear (i.e., a straight line on the graph) or not (described by non-linear curves such as exponential, logarithmic, etc.). In the Figure 12 example, both X_1 and X_2 have a linear effect on the output, whereas X_3 exerts a non-linear influence.

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Global sensitivity analysis uses statistical methods such as rank correlation, variance-based indices, or density-based indices to derive an impact ranking of parameters that have effects on the model outputs. As the interpretation of these methods can become rather complex (e.g., for a correct interpretation of the results, the underlying assumptions and theories of the statistical analysis methods need to be known), decision makers should not take decisions without consulting a practitioner for correct interpretation. Overall, it must be pointed out that rankings derived via these methods become more reliable with increasing maturity of a given technology, and as more information is gained about the probabilities of the estimated inputs. Given the complexities of interpreting the outputs of some methods, scatter plot analysis can therefore be recommended for decision makers, since it does not require detailed statistical knowledge. Scatter plots can be used to visually determine input—output relationships. For this, an output sample generated by Monte Carlo simulation is plotted against the values of each of the input variables (X_1 , X_2 , and X_3). The strength, direction, and nature of the relationships can be observed visually, where a strong relationship will lead to a smaller variance in the sample (i.e., closer clustering of the scatter cloud) (Figure 13). In the Figure 13 example, for X_1 the model shows the highest sensitivity with a linear positive relationship.

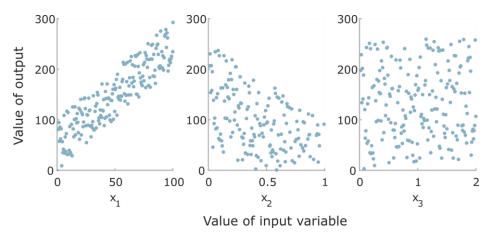


Figure 13: Example of three scatter plots derived from Monte Carlo simulation.

Key messages for decision making:

- > Sensitivity analyses used in TEA or LCA studies showcase those parameters that have the greatest influence on the results. When deriving decisions, it is essential to verify whether factors that have high sensitivity are expected to change or might be influenced by particular decisions. When conducting sensitivity analyses, practitioners are recommended to cross-check whether foreseeable changes would influence the outcome of the decision-making process.
- Outcomes of global sensitivity analyses are helpful for estimating the certainty levels of LCA or TEA underlying data, on which decisions will be based. Furthermore, such analyses can provide decision makers with insights into the likelihood of underlying conditions deviating in future from the most likely scenario currently predicted by the TEA or LCA, and the potential implications of such changes for the future accuracy and applicability of the present TEA or LCA results.

A.6 Reporting – How to communicate TEA and LCA results for CCU

Assessment results and their interpretation must be reported fully, transparently, and accurately by the practitioner in a format that is appropriate for the target audience. The following aspects should be considered when seeking the advice of practitioners or when commissioning TEA or LCA studies for CCU applications:

- The report shall include the goal and scope of the study, results, limitations, conclusions, and recommendations, a clear executive summary (addressing decision makers), and a technical summary with tables²⁶ to enable the reader to easily access the data used in the assessment.
- The data sources shall be explicitly stated, to guarantee reproducibility and full traceability for the reader, as long as this does not conflict with commercially sensitive considerations.²⁷
- The report should also include details of the practitioners (and their background) that carried out the analysis, and the review process that has been undertaken.
- It is paramount to clearly state that the CO₂ utilized to produce a certain product or process does not necessarily correspond to the amount of CO₂ avoided (when compared to the reference scenario), which is instead determined by the LCA. This distinction is important, as these values can be very different and any resulting ambiguity can lead to misinterpretation.
- Careful consideration of energy requirements is often an important aspect in CCU processes, due
 to the necessity of using low-carbon or renewable energy to avoid additional environmental
 impacts. The report should state how the modelling process considered the potential intermittency
 of future energy scenarios based on renewable energy.

Key message for decision making:

When commissioning a study, it is crucial to specify a reporting format that is suitable for verifying whether the TEA or LCA results can be used to answer the research question from the presented data.

 $^{^{\}rm 26}$ For examples see Section B.9.3 of the TEA and LCA Guidelines v.2.

²⁷ European Commission - Joint Research Centre, ILCD Handbook – *General guide for Life Cycle Assessment* - *Detailed guidance*. Luxembourg, 2010.

A.7 Multi-Criteria Decision Analysis: Taking Decisions in Complex Systems

An aspect of particular importance for decision making is to understand the trade-offs implied by different choices. TEA and LCA are two independent assessment methods that are utilized for different goals: evaluating the environmental impact and determining the costs of a given technology. They are fundamental to understanding whether a specific technology or service plays a tangible role in reducing GHG emissions, and whether this is economically feasible and likely to attract investment. In order to asses all aspects of a technology, TEA and LCA results must be put together to identify and evaluate existing trade-offs, contributing to comprehensive understanding of a particular CCU technology.

Taking decisions (e.g., investment, funding, or R&D) in the field of developing new technologies is a complex exercise. This is particularly true for CCU technologies, where multiple perspectives encompassing environmental, economic, and social aspects have to be taken into account, and benefits from these decisions are expected or required. Hence, in most cases, such decisions cannot be easily derived from a single indicator. Here, Multi-criteria decision analysis (MCDA) can ease this process and provide guidance on how to conduct decisional processes in complex systems. These decisions are based on results from TEA and LCA, which can be used to compare technologies or products among a set of alternatives and to define their performance (e.g., identify the most cost-effective processes for obtaining a required chemical while being also minimizing environmental harm. Independently of how closely the studies are aligned, environmental and techno-economic analyses of each alternative might still not clearly indicate which technology or product should be selected. For example, one option may greatly reduce environmental downsides and risks but have poor techno-economic performance, or vice versa. The same can occur within the environmental or techno-economic field where, for each impact category, technologies can perform differently and not provide a straightforward indication of which is (or could be) the best choice (e.g., CO₂ emission reductions could come at the expenses of increased freshwater consumption). This complexity is increased by the fact that performances are based on the specific circumstances outlined for each study; Consequently, their evaluation can change according to the needs and priorities of the commissioner (i.e., decision maker), and scenario settings (e.g., regional peculiarities and period of the analysis). Simultaneously assessing a multitude of decision criteria can reach a level of complexity that makes the management of all relevant data unfeasible, with the risk of underestimating or mishandling parts of the information (e.g., a decision may be taken based on only part of the results). Another obstacle for decision making is the subjective perception of product or technology performances against impact categories. Although study results provide quantitative estimations, their position on a value scale often differs according to each individual's beliefs and values, thereby creating a complex decision-making environment exacerbated by balancing trade-offs and uncertainty. Questions that must be answered by stakeholder groups with different interests and background may therefore need qualified and structured decisional processes.²⁸

EXAMPLE: The following question might be addressed with the support of MCDA: Methanol can be produced via three different techniques: conventional methods (i.e., steam reforming of natural gas), via biogenic CO_2 and green hydrogen, or via direct air capture and blue hydrogen (i.e., steam reforming of natural gas, with capture and storage of CO_2 emissions). For each option, aligned TEA and LCA have been performed and results are available. While one production process is by far the cheapest, the others have better environmental performances but in different impact categories. Which criteria should the decision maker prioritize, and how? To what extent should each criterion then impact the final decision?

²⁸ McDaniels, T.L., Gregory, R.S., Fields D. 1999. *Democratizing risk management: Successful public involvement in local water management decisions*. Risk Analysis 19:497–510.

In the context of TEA and LCA, some of the questions that a decision maker may have to face include: Shall I give priority to environmental or economic aspects? Which performance parameter is more important for my goals, and why? How can I take into account the variability of each of these elements in time, or their regional dependencies? How can I ensure that all the decision criteria are properly weighted and sufficiently considered?

MCDA theory and its applications represent a viable solution that decision makers have applied in many fields when seeking to thoroughly acknowledge all information provided by analytical investigations and to systematically scrutinize all available options to arrive at the most appropriate decision. Through MCDA it is possible to appraise a finite set of alternative solutions and rank them based on the level of satisfaction they achieve against specific criteria. MCDA methods present structured and formalized tools that have been used for decades and an have been applied to a multitude of case studies and disciplines.^{29,30} The advantages of MCDA are as follows:

- Avoid loss of information (e.g., relative to specific criteria) that typically occur when complex systems are simplified through unorganized processes;
- Systematically catalogize the importance of the different decisional criteria on a value scale;
- Help decision makers to deal with the inherent trade-offs between criteria;
- Take into account the different (subjective!) values assigned among the stakeholders to each decisional criterion;
- Take into account potential constraints in the alternatives. This is the case when only some options belong to the "acceptable" set of choices;
- Systematically compute input uncertainties, and evaluate their effects on results (e.g., via application of Monte Carlo simulation methods);
- Include probability distribution of risks (e.g., via application of Bayesian theory)

Here, we want to outline notions that help the decision maker to understand if and when MCDA can be applied to respond to their specific goals. Following this introduction, we therefore present the relevant MCDA conceptual and operationalization steps and provide basic guidance on how the decision maker can set and run their own MCDA tool.

A.7.1 MCDA: the operationalization steps

Different MCDA frameworks exist. Selecting one that best addresses the study goal depends primarily on the data available and the nature of the question that the decision maker is facing: Some methods rank a finite set of available options, some identify the best option, others differentiate acceptable versus unacceptable alternatives, and so on. After choosing which MCDA framework best applies to the research question, the steps presented in the following outline the basic structure for operationalization.

A.7.1.1 Formulate your objective

What is the research question that must be answered? Will your decision be based on performance appraisal on different criteria? Is it already clear which criteria are relevant, and which are not? Can MCDA techniques provide a supporting tool to specifically answer your research question? Accurately describe the

EXAMPLE: Purchase of a new car. Which propulsion system shall my new car have? Which people will contribute to the decision (e.g., family members)?

²⁹ Saaty, T., 1980. *The Analytic Hierarchy Process*, Mcgraw Hill, New York.

³⁰ Roy, B., 2005. *Paradigms and challenges*, in: Figueira, J., Greco, S., Ehrgott, M. (Eds.), *Multiple Criteria Decision Analysis: State of the Art Surveys*. Springer Science+Business Media, New York, pp. 3–24.

choice you need to make, which constraints exist, and which experts should be included in the group of decision makers.

A.7.1.2 What are the alternatives?

Define the available array of finite options/alternatives that you can choose from, or that you have identified based on your constraints (i.e., among the existing technologies available for your specific goal).

EXAMPLE: Four propulsion systems are considered by prospective purchasers: gasoline, natural gas, full electric, and hybrid electric. Diesel cars were excluded at this early stage due to predicted restrictions on their use in cities (technically, this is a constraint that the decision maker has set in their decision process).

This should comprise all the alternatives (or a selection of them) available in your specific case. The greater the numbers of alternatives and decision criteria, the more articulate and complex your analysis will be.

A.7.1.3 Define the criteria

The decision maker is required to select criteria that reflect the values relevant for making the decision. Criteria may also be categorized under different levels (e.g.., 1st level: environment, economic, etc.; 2nd level: impact on ground water, impact on air, climate impact, etc.; 3rd level: heavy metals, oxygen depletion, organic pollutant, etc.). It is important to mention that for decisions involving larger numbers of stakeholders, the process of identifying and quantifying preferences is more complex and time-consuming. Despite bringing several advantages, such processes can also be susceptible to pitfalls that have to be addressed or avoided.³¹

EXAMPLE: After a discussion with family members, the decision criteria that that will guide the purchasers are:

Economic criteria: selling price, fuel cost (costs/km); Environmental criteria: carbon footprint (CO_{2e}/km);

Others: delivery date.

A.7.1.4 Weight the criteria

Not all criteria are equally relevant, and the decision maker must assign each criteria a "level of importance" based on their goal and perceptions. The most common MCDA method is known as the weighted sum method (WSM).³² Here, the importance of each criterion is indicated by assigning each one a relative numerical value or ranking, i.e., if two criteria have the same number, their importance is equal. These values are normally given as fractions of one (or in percent), and their sum must equal 1 (or 100%). Criteria ranking can be highly subjective and can change over time. Here again, methods must be found for dealing with different opinions among a group of stakeholders.

EXAMPLE: Each family member has differing preferences about the importance of each criterion. One way to account for each standpoint might be to average the values for each criterion. Example for the criteria "selling price":

Father: 40% Mother: 30% Son: 15% Daughter: 10% Average: 24%

A.7.1.5 "Score" the criteria

For each criterion, a score must be given. This is assigned based on the performance that each alternative

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³¹ See Reference: 28.

³² Chauvy, R., Lepore, R., Fortemps, P., De Weireld, G., 2020. *Comparison of multi-criteria decision-analysis methods for selecting carbon dioxide utilization products*. Sustainable Production and Consumption 24, 194-210.

"scores" relative to each single criterion. Here, the decision maker must choose a reference scale to apply (e.g., 1=very poor, 2=poor, 3=acceptable, 4=good, 5=excellent). The scoring system is chosen by the decision maker based on how many "levels" of performance they identify, or the level of accuracy required for reporting, or a predefined scale. Different scoring is expected by stakeholders: each of them may have a different opinion on "how good or how bad" is the performance of alternative A when assessed using criterion X (e.g., A certain level of groundwater pollution may be manageable for some but unacceptable

for others). This relates to individual perceptions, values, and expert assessments.

EXAMPLE: Family members must assign a performance score for each option and criterion. Again, opinions may differ. In such cases, averaging systems or agreement must be pursued. The resulting matrix could look like this:

Criteria	Selling price	Fuel cost	Carbon footprint	Date of delivery
Weighted criteria	24%	10%	30%	15%
Gasoline	5	2	4	1
Natural gas	4	5	3	4
Full electric	1	3	1	5
Hybrid	3	1	4	4

A.7.1.6 Compute data and results

Through a combination of criteria scoring and weighting, at this stage the decision maker can calculate the overall score of each alternative against the chosen criteria. Such results are in numerical form and can also be summed up to obtain the overall priority score for each option under consideration.

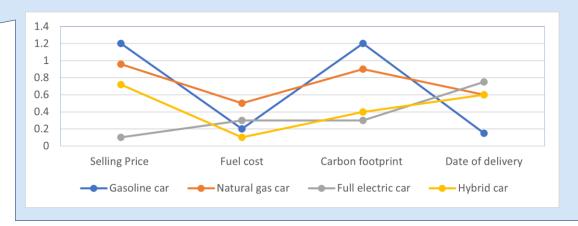
EXAMPLE: Each score has to be multiplied by the weighted criteria. A MCDA on which type of family car to purchase might look like this:

Scoring	Selling price overall score	Fuel cost overall score	Carbon footprint overall score	Date of delivery overall score	Total score
Gasoline	1.20	0.20	1.20	0.15	2.75
Natural gas	0.96	0.50	0.90	0.60	2.96
Full electric	0.10	0.30	0.30	0.75	1.45
Hybrid	0.72	0.10	0.40	0.60	1.82

A.7.1.7 Evaluation and decision

None of the outputs indicates a perfect or unimprovable solution to our original question, but provide a systematic framework to assess overall alternative performances based on the stakeholder priorities and preferences. The results can be plotted on diagrams to visualize the pros and cons of each choice, and to evaluate these trade-offs. From this point forward, stakeholders should aim to reach consensus on the preferred solution to the initial question. At this point, stakeholders should aim at sharing the same solution of the initial question.

EXAMPLE: The results might be visualized as in the following diagram: This clearly demonstrates how the gasoline car has very high performance (the bests among all choices) in 2 of 4 criteria, but very poor in the others. In contrast, a natural gas-powered car shows good but not outstanding performances for all criteria. If date of delivery is a decision constraint, the fully electric car should be purchased. However, if the best total score is chosen as a decisional indicator, the natural gas car is the winner (total score: 2.96 – see table at step 6). In this case, a hybrid car does not seem appropriate for the family's needs.



A.7.2 Analytic Hierarchy Process (AHP)

Among all MCDAs, the Analytic Hierarchy Process (AHP) is considered best suited to supporting decision making in contexts with low or medium complexity.³³ This method is applied across a multitude of fields, and is particularly simple to set and operate with little or no experience in MCDA. It does not require large amounts of data, and is easy to scale. AHP is based on the assumption that humans are much better at evaluating preferences between two alternatives, rather than a simultaneous comparison of multiple choices. To weight the criteria, the decision maker must define the relation of criteria importance (i.e., weighed criteria) via comparisons in a pairwise manner. This is operated via a scale from 1 (e.g., criterion A is of equal importance to criterion B) to 9 (e.g., criterion A is much more important than criterion B), and the respective reciprocating values (fractions of 1). All values generated by these pairwise comparisons are compiled in a matrix form showing all relations among criteria. The matrix presented in Table 3 is based on the example used in the introduction to this chapter.

Table 3. Example matrix of an AHP pairwise comparison of criteria relative to the example presented in the introduction of this chapter.

		In relation to	n relation to					
	Criterion	Selling price	Fuel cost	Carbon footprint	Date of delivery			
	Selling price	1	6	1/2	4			
e of	Fuel cost	1/6	1	1/7	1/3			
importance	Carbon footprint	2	7	1	5			
impo	Date of delivery	1/4	3	1/5	1			

³³ Dodgson, J.S., Spackman, M., Pearman, A., Phillips, L.D., 2009. Multi-criteria analysis: a manual, vol. 11, n. 1-3.

In the next step, the decision maker must evaluate the performance of each possible alternative (i.e., weighted alternatives) against individual criteria, again in a pairwise comparison. This will generate as many matrixes as the number of criteria. Combination of normalized weighted criteria and alternatives will generate a series of values that, once integrated, will provide an overall weighted total score for each alternative, with higher score indicating stronger preference. The AHP method allows the ranking of criteria at different levels (i.e., criteria, sub-criteria, etc.), and the pairwise comparisons of criteria (and performances) are run only among criteria at the same level. Several online tools introduce the topic of AHP and provide step-by-step guidance for the process. These are suited to aid decision making (also in the field of CCU) for any case that does not present particular complexity.

A.7.3 Links to AHP online tools:

http://www.healthstrategy.com/ahp/ahp.htm

https://comcastsamples.github.io/ahp-tool/

A.7.4 AHP explained:

https://www.passagetechnology.com/what-is-the-analytic-hierarchy-process

https://kids.frontiersin.org/articles/10.3389/frym.2020.00078

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PART B

Case study for commissioning and evaluating LCA & TEA

SUPPORTED BY













B.1 How to commission and evaluate TEA or LCA studies

In this chapter, we provide an explanatory case study on how to commission or evaluate TEA and/or LCA studies, based on the decision trees presented in section B (Reference Tree, Case A, Case B1). While these trees present the sequence of steps to be followed and are generally applicable, in the following pages we present an example of how to apply them to a specific case and under specific circumstances. Taking a technology as reference, all steps will be addressed following the theory presented in Part A of this report, and according to the level of knowledge available. The CO₂ utilization technology chosen for this case study is called CO₂ mineralization. Before addressing the steps pertaining to commissioning a new study or evaluating an existing one, in the next section we introduce the technology, to clarify beforehand what this process entails and which products are included. This is fundamental to enable the reader to better understand the analysis conducted in the following pages, and to be aware of the types of missteps or inaccuracies may occur in LCA or TEA studies.

B.1.1 The mineralization technology

In the field of CO_2 utilization, the transformation of CO_2 in a stable mineral is often called CO_2 mineralization. CO_2 mineralization concepts are of particular interest for decarbonizing the cement industry. Here, captured CO_2 reacts with minerals containing calcium oxides or magnesium oxides (e.g., present in rocks containing magnesium-rich silicate minerals) to produce solid carbonates that remain stable over geological timescales (i.e., >1000 years). Therefore, the implementation of mineralization technology in a cement plant could make significant contributions to reducing CO_2 emissions. Moreover, studies demonstrate that the resulting mineralized materials can be mixed with cement to improve its techno-physical properties, thereby substituting for and reducing demand for cement's main ingredient of clinker. Since clinker production is highly energy intensive and releases large volumes of CO_2 from its limestone feedstock (via a process called calcination), this process is responsible for the majority of the total CO_2 emitted by the cement industry. CCE hence reduces the amount of clinker needed to produce cement, and can reduce the overall climate impact of a cement plant. A concept of how to integrate CO_2 mineralization into the cement industry is shown in Figure 13.

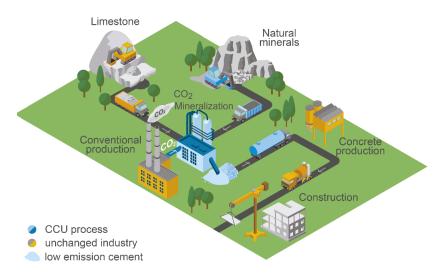


Figure 13: Envisioned integration of CO₂ mineralization into the cement industry (adapted from Olfe-Kräutlein et al., 2021).³⁴ Original illustration designed by Wernerwerke, Cordes + Werner GbR ©2021.

³⁴ Olfe-Kräutlein, B., Strunge, T., Chanin, A. 2021. *Push or Pull? Policy Barriers and Incentives to the Development and Deployment of CO2 Utilization, in Particular CO2 Mineralization*. Frontiers in Energy Research, 9 (522). Doi: 10.3389/fenrg.2021.742709.

Here, the CCU process is located directly adjacent to the cement plant. It produces carbonates that capture CO₂ emitted from the cement plant, which also simultaneously replace a proportion of the clinker required to produce more cement. In this case, two products are formed, one carbonate-rich and the other silicarich. For replacing cement, the silica-rich product of CO₂ mineralization is envisioned, while the carbonate-rich product will have to be stored. A process suggested for this type of application is called direct carbonation (or more precisely direct aqueous carbonation), where magnesium-rich silicates are first activated via a pre-treatment step, and are therefore carbonated in a pressurized reactor, where they are mixed with water and captured CO₂. The silicate-rich and carbonate-rich products are then separated in a post-treatment step.

B.1.2 Research guestion definition (see also Reference Tree, Part C)

A company or governmental agency is interested in investing in or funding emission reduction technologies that are applicable to cement production. To this end, they want to investigate the potential emission reduction that could be achieved by introducing CO₂ mineralization processes to a conventional process (here we refer specifically to the technology presented in the previous paragraph and Figure 13). At the same time, it is also of particular interest for the company or agency to understand how the adoption of such technology would influence total production costs. Thus, the decision maker at the company or agency wished to establish, with the greatest certainty, the potential emissions reductions, and costs, to evaluate the pros and cons of such potential investment or funding choices. Based on capital expenditures (CAPEX) and operational expenditures (OPEX), the company or agency will be able to assess the cement costs of this innovative production process, and consequentially its market profitability. For this specific case, two research questions can be defined:

Does the implementation of CO_2 mineralization in the cement industry reduce total greenhouse gas (GHG) emissions of cement production under current conditions? If so, by how much and at what cost?

A literature review reveals that no studies have been conducted on the potential for this specific technology to reduce GHG emissions and under current circumstances. However, the decision maker identified a handful of TEA studies that might be suitable for answering the economic part of the research question. At this point, the decision maker must decide whether to proceed by commissioning new studies or else attempting to use existing results (if identified). Based on the conditions encountered, the decision maker opts to commission a new LCA study to answer the research question (reference tree, Case A), while aiming to use an existing TEA study to assess the economics of such technology (reference tree, Case B1).

B.2 Commissioning an LCA study for CO₂ mineralization in the cement industry

When commissioning a new LCA study on the CO₂ mineralization technology described previously, the decision maker (also defined as commissioner in this case) should follow the schematic shown in the decision tree, Case A, Part C. The following paragraphs go through those steps in relation to the case study.

B.2.1 Step 1 – Definition and communication of the research question and study goal (Section A.2 and A.3)

The commissioner communicates the research question to the practitioner, to jointly define the goal of the study. Following Part A.3 the decision maker defines the goal of the study, stating the context of the study, the intended use, the target audience, the authors, as well as the limitations. The commissioner and practitioner thereby jointly define the study goal as follows: The goal of the study is to assess the reduction in GHG emissions achievable by capturing CO₂ from the cement plant to permanently store it via mineralization, and reusing part of this resulting product as a cement additive (in the same fashion explained in the description of the mineralization process at the beginning of this chapter). Potential emission reductions must be measured using conventional cement production pathways as benchmarks. The study is intended to support the investment decision of the funding company or agency. The LCA is commissioned by company or agency name and is performed by Organization XY/practitioner XY in collaboration with the commissioner. The goal of the study is limited to the current state of the technology, and is not suitable for assessing future developments of this technology.

B.2.2 Step 2 — Understanding, evaluating, and reflecting the proposed scope definition with the practitioner (Section A.4)

Once the study goal has been jointly defined, the practitioner proposes a scope definition to the decision maker including: Product system, Functional unit and Reference Flow, Unit process and System boundaries, Benchmark, and Technology maturity). The same practitioner revises these choices, and highlights to the practitioner any contested points or issues that have been identified.

As subject of analysis, the practitioner proposes the service of storing CO_2 via mineralization in the cement industry. Based on this choice, the functional unit and reference flow selected are kg of CO_2 stored per tonne of cement. The system boundaries suggested by the practitioner include CO_2 mineralization and storage, but not the processes of the conventional cement plant, and its CO_2 capture (Figure 14). The conventional system of cement production is proposed for comparative purposes. The practitioner rates the overall TRL of the process from 4 to 5 based on a literature review, implying that some unit processes are still under development and the related data quality could be poor.

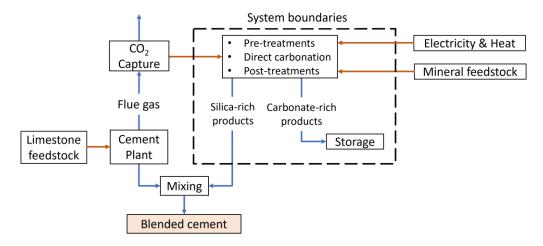


Figure 14. Example of unit processes of the study and incorrect system boundaries.

B.2.3 Step 3 – Checking and revising by the decision maker

At this stage the decision maker evaluates whether the scope definition proposed by the practitioner appears appropriate to answer the research goal. Such evaluation must be conducted with reference to sections A.4.1 to A.4.6, and Case A (Part C) of this report.

Consequently, the decision maker concludes that the subject of analysis (service for storing CO_2 via mineralization), as proposed by the practitioner, does not fit the initial research question; and considers that the subject of analysis should focus on a product rather than a service (see also Table 2, Part A). This also leads to re-evaluation of the functional unit and reference flows (see also Figure 6, Part A): kg of CO_{2eq} emitted per 1 tonne of blended cement (Note, CO_{2eq} refers to all GHG emissions, which are measured in CO_{2eq}). To reach this conclusion, we must point out that although the chemical composition of the final blended cement is not identical to conventional cement, they are assumed to be equivalent since they fulfil the same service. Moreover, the cement production and CO_2 capture system are not included within the proposed system boundary, thereby leading to inaccurate results since the CO_2 capture system requires energy and hence is itself a source of GHG emissions. An expansion of the system boundaries is therefore proposed in order to include these processes (Figure 15).

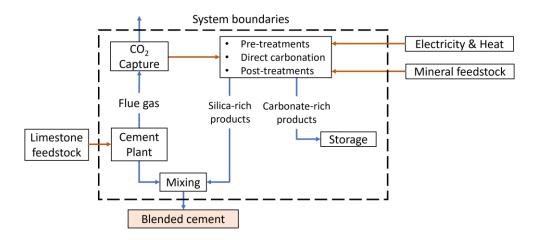


Figure 15. Revised unit processes of the study and system boundaries.

The practitioner agrees to the amendments and will revise the scope accordingly, then propose a new scope for the study (Table 3).

Table 3: Final scope definition for the case study.

Subject of analysis: Product system (Section A.4.1)	Selecting comparison metrics: Functional unit and reference flow (Sections A.4.2 and A.4.3)	Specifications of required elements and boundary selection: Unit processes and system boundaries (Section A.4.4)	Selecting systems for comparison (Benchmark) (Section A.4.5)	Understanding the maturity of the product system (Section A.4.6)
Product: cement	Kilograms of CO _{2eq} emitted per tonne of blended cement.	CO ₂ mineralization (pre- treatments, direct carbonation, post- treatments), storage, CO ₂ capture, cement plant, mixing (See Figure 15)	Conventional cement production	Overall TRL of the process: between 4 and 5

Since all the decision maker's recommendations have been thoroughly addressed, they accept the proposed scope definition, thereby allowing the LCA exercise to progress to the next step. From this point onwards, these steps will be mainly conducted by the practitioner as they pertain to their own technical skills.

B.2.4 Step 4 – Understanding the results and reporting

Once the practitioner has finished the study, the results are presented to the commissioner for final discussion (See Final Step in the Reference tree, Part C). The results of the case study are shown in Table 4, where they are compared with cement produced via the conventional process. The negative sign shown for CO_2 storage indicates that 117.4 Kg CO_2 eq. per tonne of blended cement are not emitted but instead stored as carbonate-rich minerals for each tonne of blended cement produced. This process – but not the overall production process, that is the results of all processes combined – is an example of negative emissions. Thanks to this amount of CO_2 being sequestered rather than emitted to the atmosphere, the total emissions generated by the case study are 25% lower than for conventional cement production (640.5 vs. 852 Kg CO_2 eq./tonne of blended cement).

Table 4: Results from carbon footprint calculation of carbonated mineral (values adapted from Ostovari et al., 2020).³⁵

				kgCO₂eq./t blended cement		
				Conventional		
Mineral feedstock	3.5	No.				
Pre-treatment		28.5	_	Negative values:		
CO ₂ mineralization	Direct carbonation	16.7	10.7		assessments, emissions	
	Post-treatment	2.9		values can be presented as negative. T		
Plant construction		4.0	understand whether such values result			
Capture		20.7		overall negative emissions, the scope of		
Storage		- 117.4	analysis must be properly defined.			
Cement		681.6		852		
Sum	640.5 852					
Carbon footprint reduct	25%		-			
(compared with conven	tional cement)					

 $^{^{35}}$ Ostovari, H., Sternberg, A., Bardow, A., 2020. *Rock 'n' use of CO*₂: *carbon footprint of carbon capture and utilization by mineralization*. Sustainable Energy & Fuels. Doi: 10.1039/D0SE00190B.

B.3 Evaluating existing TEA studies

B.3.1 Initial screening of literature

Through initial screening of existing TEA studies for CO₂ mineralization, the decision maker identifies five studies that might help answer the research question stated above. For the initial screening, the decision maker performs a literature review of article titles and abstracts, to select a reasonable number of studies suitable for further investigation (we recommend a maximum of 10 studies for this step). Although this may appear to be a complex task for some, the simple strategy at this step is to select potentially suitable studies that will go undergo more detailed investigation, as explained as subsequently. In this case, the following five studies were selected (5):

Table 5: Selection of existing TEA studies for CO₂ mineralization.

	Study 1	Study 2	Study 3	Study 4	Study 5
Titles	Business case for	CO₂ utilization in	Emission	Classification of	Techno-economic
	CO₂ mineralization	the cement industry	reduction	CO ₂	assessment of ex-situ
	in cement	– overview and	technologies in	mineralization	mineralization as a
		perspectives for	hard to abate	pathways and	negative-emission
		2045	sectors	related costs	technology
1					

B.3.2 Step 1 – Comparison of the subject of analysis

At this point, the five studies must undergo more detailed investigation (i.e., are they really suitable for answering the research question?) following sections A.4.1 and reference tree Case B1. The first selection criterium pertains to the subject of analysis. Following the research question "How much does the implementation of CO₂ mineralization in the cement industry costs under current conditions?" the decision maker selects the same subject of analysis as defined for the LCA study (see above): CO₂ mineralization integrated into a conventional cement plant to produce blended cement. Comparing the subjects of analysis among the five selected TEA studies (Table 1) shows that study 1 and study 3 have subjects of analysis that fit the current research question, so they appear to be feasible for the current purpose. Additionally, study 2 has the same subject of analysis but also investigates other options. Here, the decision maker must check that the results for each application are reported separately, so that it is possible to select only those data that are of interest. Study 4 and 5, meanwhile, assess a slightly different subject of analysis: In study 4 a coal-fired power plant was used as a CO₂ source, while study 5 examined direct air capture. Therefore, neither study matches the decision maker's selected subject of analyzing the integration of a CO₂ mineralization plant into conventional cement production. The subject of analysis must be appropriate, and hence studies 4 and 5 must be excluded (Table 4).

B.3.3 Step 2 – Comparison metrics for the subject

As a second step the comparison metrics needs to be assessed. Following sections A.4.2. and A.4.3 and in particular the decision tree presented (Figure 6, Part A), the decision maker concludes that the assessment focuses on a CCU product material that will have different chemical properties from conventional cement (i.e., cement is replaced with carbonated minerals), and hence the functional unit is defined over the quantification of technical service / performance of the product (i.e., blended cement). Here the reference flow shall therefore be 1 tonne of blended cement (using the carbonated minerals), with the same performance as 1 tonne of conventional cement. As a comparison metric, the decision maker is interested in the production costs of the new product. Therefore, the ideal comparison metrics for the research question is total production cost measured in €/t_{blended cement}, which is true for studies 1 and 2. Study 3, meanwhile, applies a different metric, using the CO₂ storage as a service. To use study 3, the decision maker must consult a TEA practitioner to evaluate whether the values used in that study can be adapted to the current purposes; otherwise, study 3 must be excluded from further evaluation (Table 5).

Table 1: Comparison of subject of analysis: selected TEA studies.

	Study 1	Study 2	Study 3	Study 4	Study 5
Titles	Business case for CO ₂ mineralization in cement	CO ₂ utilization in the cement industry – overview and perspectives for 2045	Emission reduction technologies in hard to abate sectors	Classification of CO ₂ mineralization pathways and related costs	Techno- economic assessment of ex-situ mineralization as
			Sections	related costs	a negative- emission technology
Subject	Conventional	Conventional cement plant	Conventional	Coal-fired	Direct air
of	cement plant	equipped with post-	cement plant	power plant	capture plant
analysis	equipped with	combustion CO ₂ capture	equipped with	equipped with	with CO ₂
	post-combustion	and multiple utilization or	post-	post-	mineralization
	CO ₂ capture and	storage options:	combustion CO ₂	combustion CO ₂	plant to produce
	CO ₂ mineralization	a) CO ₂ mineralization b) Geological storage c) Methanol production from CO ₂	capture and CO ₂ mineralization	capture and CO ₂ mineralization	a cement additive
				X	X

Studies covering multiple applications:

If the study covers multiple applications, the decision maker must check if the values of interest are reported separately, or if they can be derived.

Wrong subject of analysis:

If studies cover a different subject of analysis, they shall not be used to derive a decision, as results are very likely not applicable to other cases.

Table 2: Comparison of metrics used in selected TEA studies.

	Study 1	Study 2	Study 3	Study 4 Study 5
Titles	Business case for CO ₂ mineralization in cement	CO ₂ utilization in the cement industry – overview and perspectives for 2045	Emission reduction technologies in hard to abate sectors	Classification of CO ₂ mineralization pathways and related costs Techno-economic assessment of ex-situ mineralization as a negative-emission technology
Functional unit and	Total cost of product:	Total cost of product:	Levelized cost of storage:	Inappropriate functional unit and reference flow: A study with inappropriate
reference flow	€/tblended cement	€/tblended cement	€/tco2 stored	functional unit cannot be re-used in the present context, as it might lead to incorrect conclusions. Here, we suggest consulting a TEA practitioner, who can assess whether data can be adapted from an existing study.

B.3.4 Step 3 — System elements and boundary selection

As a third step the decision maker must assess the system elements used in each of the candidate studies. Similarly to the LCA study presented previously, the decision maker selects cement production, CO₂ post-combustion capture, mineral pre-treatment, CO₂ direct carbonation, and post-treatment as the system elements. Studies 1 and 2 both fit the system elements and system boundaries selected by the decision maker (Table 6).

Table 3: Comparison of system elements and boundaries of selected TEA studies.

	Study 1	Study 2	Study 3	Study 5	
Titles	Business case for CO₂ mineralization in cement	CO₂ utilization in the cement industry – overview and perspectives for 2045	Emission reduction technologies in hard to abate sectors	Classification of CO ₂ mineralization pathways and related costs	Techno-economic assessment of ex- situ mineralization as a negative- emission technology
Specification of system elements	 Cement production CO₂ capture Mineral pretreatment CO₂ mineralization Posttreatment 	 Cement production CO₂ capture Mineral pretreatment CO₂ mineralization Post-treatment 	Care mus assessed uncomm system	in a TEA/LCA on to find stud element (e.g.	e system elements a study. It is not lies that exclude a a., CO ₂ capture) s' goal and scope.

B.3.5 Step 4 – System for comparison

As system for comparison, the decision maker chooses conventional cement production, as the research question aims to compare the innovative CO₂ mineralization process with the **conventional way to produce cement.** Both study 1 and study 2 feature this as the benchmark, hence it might be feasible to use them in deriving the current decision (Table 7).

Table 4: Systems for comparison of selected TEA studies.

	Study 1	Study 2	Study 3	Study 4	Study 5
Titles	Business case for CO ₂	CO₂ utilization in	Emission	Classification	Techno-economic
	mineralization in	the cement	reduction	of CO2	assessment of ex-situ
	cement	industry –	technologies	mineralization	mineralization as a
		overview and	in hard to	pathways and	negative-emission
		perspectives for	abate	related costs	technology
		2045	sectors		
System for	Conventional cement	Conventional			
comparison	production	cement production			
		/			

B.3.6 Step 5 – Selected scenario

The final step of the comparison is to investigate the selected scenario. As the research question states, "How much does the implementation of CO₂ mineralization in the cement industry costs under <u>current</u> <u>conditions</u>?" **the scenario must contain the current conditions,** while future or past scenarios will not suffice for the decision maker to derive a decision. Hence, the decision maker must reject study 2, which bases its analysis on the future scenario for the year 2045 (Table 8).

Table 5: Comparison of the assessed scenarios of selected TEA studies.

	Study 1	Study 2		Study 3	Study 4	Study 5		
Titles	Business case for CO ₂ mineralization in cement	CO ₂ utilization in the cement industry – overview and perspectives for 2045	Emission reduction technologies in hard to abate sectors		Classification of CO2 mineralization pathways and related costs	Techno-economic assessment of ex-situ mineralization as a negative-emission technology		
Selected scenario	Estimated costs under current conditions as a European average	Estimated costs for the year 2045 in France		Future and past scenarios: Studies that use different scenarios to those chosen by the decision maker also have differing assumptions, and so their calculated values can also differ greatly. Hence, they shall not be used further by the decision maker.				

The decision maker finds that study 1 fits the intended research question. In this example, we proposed five potential studies that deserved further investigation, of which only one was appropriate for answering the proposed research question. In a different case, where no suitable study can be identified after the five-step analysis, we suggest searching the literature for other prior studies. After selecting additional candidate studies, the evaluation steps 2 to 5 should then be repeated.

B.3.7 Step 6 – Understanding the results and reporting

The decision maker reads study 1 in detail and finds an appropriate summary table (here presented in Error! Reference source not found.). Through a detailed analysis of the presented results, the decision maker finds the desired estimated production costs of blended cement with integrated CO_2 mineralization. Here, two values are presented: the production cost in regard to the functional unit is $76 \ \text{€/t}_{blended\ cement}$ without taking CO_2 certificates into account. With an assumed CO_2 certificate price of $40\ \text{€/t}_{CO2}$, the specific cost of production is reported as $101\ \text{€/t}_{blended\ cement}$. According to the results for the benchmark presented in the study, conventional cement has production costs of $63\ \text{€/t}_{cement}$ without taking CO_2 certificates into account, and $97\ \text{€/t}_{cement}$ with a CO_2 certificate. Hence, the research question "How much does the implementation of CO_2 mineralization in the cement industry costs under current conditions?" can be answered as follows: The implementation of CO_2 mineralization in the cement industry will increase the price cost of cement production by $13\ \text{€/t}_{blended\ cement}$ without taking CO_2 certificates into account; alternatively, when considering CO_2 certificates, cement production costs increases by $4\ \text{€/t}_{blended\ cement}$ under current conditions.

Table 6: TEA results adapted from Strunge et al. (in press).36

			Description	Value	Unit	1	
	Capital costs (CAPEX)	5					
			Pre-treatment	17.13	M€	-	
Breakdown of costs	into sub-		Carbonation - reactors	24.64	M€	-	
categories: In TEA stu process units may l			Carbonation - compressors and pumps	10.47	M€		
down into more	specific		Carbonation - heat exchangers	3.85	M€	-	
subcategories, or be	presented		Post-treatment	6.80	M€]	
in aggregate.			Post-combustion capture	27.79	M€	Capital expenditures: In	
	Annualized CAPEX			7.75	M€/a	TEA studies, capital expenditures are often	
Operational	Variable OPEX					reported as a one-time	
expenditures:	Fixed OPEX		Utilities	12.33	M€/a	payment during construction, and broken	
OPEX are often			Mineral feedstock	4.21	M€/a	down over the lifetime of	
broken down into			Water and additives	1.77	M€/a	the plant (here	
two categories,			Conventional cement	68.54	M€/a	annualized CAPEX).	
variable and fixed,			Transport	4.22	M€/a		
with the former				4.93	M€/a		
only taking place during operations.	Total production			103.79	M€/a	Different levels of detail: It is not uncommon to	
	costs Specific			76.32	€/t _{blended}	see different levels of	
production				75.52	cement	detail for different	
	costs					process units. Here,	
	CO₂ certificates (40€/t _{CO2}) Specific production costs with CO₂ allowances		1	34.00	M€/a	cement is considered as a feedstock for the carbonation facility, and	
				101.32	€/t _{blended} cement	is therefore not included in CAPEX, as the cement plant will be retrofitted.	

Multiple scenarios or indicators presented: Often, multiple scenarios or indicators are reported. Here, the calculation is presented once without taking CO₂ certificates into account, and once with a CO₂ certificate price of 40€/tco2.

³⁶ Strunge, T., Renforth, P., Van der Spek, M., (in press). Towards a business case for CO2 mineralisation in the cement industry. Communications Earth & Environment. Doi: 10.21203/rs.3.rs-478558/v1.

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PART C

Step-by-step guide to commissioning and evaluating TEA & LCA

SUPPORTED BY













C.1 Introduction

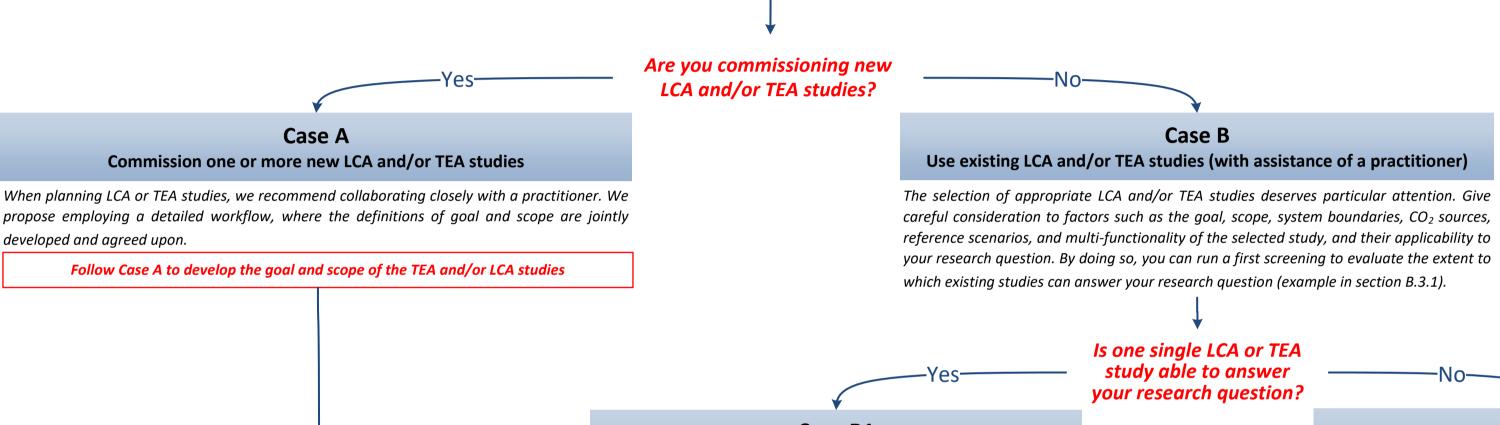
In this section we present a tool, based on decision trees, that guides the reader in making decisions based on the results of LCA and TEA studies. This section is tailored to actors interested in both commissioning new CCU studies and assessing existing studies. We propose key questions, to be answered using the supporting information provided in Part A of this document. We recommend that decision makers answer the proposed CCU-related questions and ultimately derive their own corporate or political decisions. The next page presents an initial decision tree (henceforth: reference tree) for beginning this process: the decision maker will be asked to evaluate whether a new study must be commissioned to answer their research question (Case A), or if one (Case B1) or several (Case B2) existing LCA/TEA studies can be used for this purpose. Once this decision is made, the reference tree indicates the process, decision trees, and check lists to be followed in Cases A, B1, or B2. An example on how to apply these decision trees for both commissioning and evaluating TEA and LCA is given in the case study presented in Part B.

Reference tree Start Research question Define your research question, based on the CCU product or service you want to examine and the decision you need to make (section A.3)

methodology suits your needs (for this, we recommend utilizing Part A of this report with the assistance of an experienced practitioner).

Evaluate your resources and decide whether to commission a new LCA and/or TEA study or use published studies. As a first step, check whether a study fitting your research question and goal already exists in the literature, and if its

If any doubt arises regarding compatibility issues, as a general rule we recommend commissioning a new study (or more, e.g., if both LCA and TEA are required) to ensure that the results are tailored to your specific research question and that any potential bias is avoided.



Case B1 Use one existing LCA or TEA study

To assess whether the study you have chosen fits your purposes and is therefore applicable to your goals, we recommend closely inspecting the goal and scope definitions (example in sections B.3.2 to B.3.5). This will clarify whether the existing study fits your research question, and whether its results can be applied (or need to be adjusted) to derive your decision.

Follow Case B1 to identify if the study is aligned with, and applicable to, your purposes

Case B2

Use and compare multiple existing LCA and/or TEA studies

To assess whether the study you have chosen fits your purposes and is therefore applicable to your goals, we recommend closely inspecting the goal and scope definitions (example in sections B.3.2 to B.3.5). This will clarify whether the existing study fits your research question, and whether its results can be applied (or need to be adjusted) to derive your decision. As a second step, it is also necessary to evaluate whether the scope

As a second step, it is also necessary to evaluate whether the scope definitions of your selected studies are similar and, consequently, whether their results are comparable.

Follow Case B1 to identify if each study is aligned with, and applicable to, your purposes

- AND -

Follow Case B2 to evaluate the comparability of your selected studies

Final step Understanding the results and reporting

- Assess TEA/LCA results: Do they allow you to answer your research question? Can you identify any crucial aspect that makes the results unsuitable for your needs?
- Are you aware of what was omitted from the assessment scope, and why?
- Are the level of technological maturity and its implications for your decision known? (See also Part E of the TEA and LCA Guidelines v.2)
- Are you aware of the overall limitations/uncertainties of the study? To make sound decisions, please carefully investigate the uncertainty and sensitivity analyses of the results, as they determine how 'flexible' you can be with your decision (section A.5.1);
- Are you aware of the assumptions and scenarios (e.g., year and location) that were used in the assessment? For LCA in particular, be aware of the carbon emission classification of the service or product (carbon-neutral, negative, or reducing?);
- In the report, include a summary and state clearly the goal and scope of the study, to facilitate future comparisons. Also be aware of your study's target audience, and tailor the report language and terminology accordingly;
- When using LCA and TEA studies applied to the same product or service, be aware of their level of integration (e.g., are the same boundaries and assumptions applied?). (See also Part D of the TEA and LCA Guidelines v.2).
- To properly present the results of the studies, the practitioner has to report them to the decision maker following the indication in sections A.6, and examples in B.2.4 and B.3.7.

Decision making

Decision making requires the understanding of the tradeoffs implied by different choices. When dealing with multiple indicators (such as results from TEA and LCA studies), we recommend to apply tools to support the decision making process. One of these is the Multi-Criteria Decision Analysis presented in sections A.7.

Case A Commissioning a new LCA or TEA study (example in section B.2)

Definition and communication of the research question and study goal (sections A.2 and A.3)

The commissioner communicates the research question to the practitioner, to jointly define the goal of the study (example in section B.2.1).



Practitioner

Based on the goal definition, the practitioner proposes and communicates the scope definition to the commissioner, to answer the proposed research question (example in section B.2.2).

Understanding, evaluating, and reflecting the proposed scope definition with the practitioner (section A.4)

Select the subject of analysis Product system (section A.4.1)

In order to select the product system of the product or service you are investigating, all required processes have to be defined. In the case of multiple applications, a mix of applications relevant to your decision should be selected.

Selecting comparison metrics Functional unit and reference flow (sections A.4.2 and A.4.3)

The functional unit and reference flow need to be carefully defined according to the product or service under analysis, and must be aligned to the research questions.

Specification of required elements and boundary selection Unit processes and system boundaries

(section A.4.4)

To reduce complexity, it is important to check whether and which unit processes might be excluded from the assessment. This assessment must consider how the study may be applied to future scenarios (e.g., due to policy changes or technological developments). You can evaluate these aspects together with the practitioner.

Selecting systems for comparison Benchmark (section A.4.5)

The benchmarks selected by the practitioner and commissioner may differ. In order to align your expectations, discuss with the practitioner any doubts and/or potential alternatives you can envisage.

Understanding the maturity of the product system Technology maturity (section A.4.6)

The technological maturity of each unit process must be determined in order to assign an overall TRL to the product system. High uncertainty for low-TRL technologies, or due to poor data quality, has to be carefully taken into account.

Revision of scope definition



Iterative

Practitioner

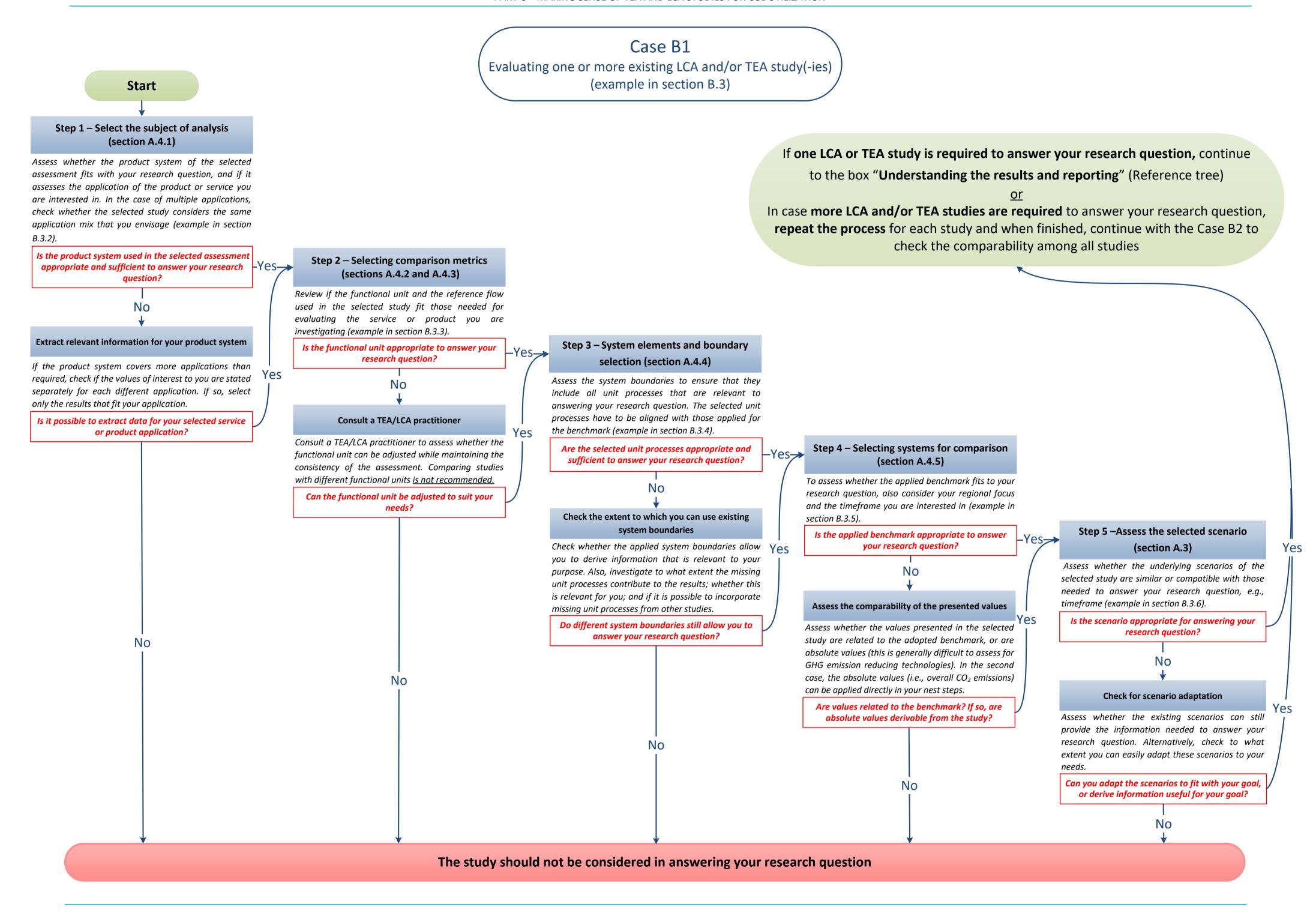
The practitioner carries out the remaining steps of the LCA and/or TEA study(-ies).

Do you agree on the scope definition proposed by the practitioner? Is it appropriate for best answering the research goal?

Continue to the box "Understanding the results and reporting" (Reference tree)

Practitioner

The practitioner revises the scope definition to address any contested points highlighted by the commissioner (example in section B.2.3).



Case B2

Checklist: Comparing multiple studies

Start

Evaluate the comparability of the studies

After following Case B1 for each study, please verify their respective comparability. The following checklist will guide you in this assessment, selecting a study of your preference as your reference study

How to use the Checklist table: If you answer "Identical" mark the corresponding box and move to the next question. If you answer "Partially similar" or "Different," follow the recommendations indicated in the column on the right hand side to evaluate, with the support of a practitioner, whether you can move to the next question or else have to discard the study under evaluation. If you marked all boxes as "identical" then answer the final question with "Yes".

Question			Comments/recommendations		
How simil studies?	ar are the goals	of the two	If the two studies have "partially similar" or "different" goals, it is very likely that their comparison can only have limited significance (section A.3). In this case, it is not recommended to use the		
Identical	Partially similar	Different	study under evaluation.		
	milar are the ns in the two studio		If the two studies consider the same product application, the product systems must also be consistent with each other (section A.4.1). If the product applications are not identical (i.e., the		
Identical	Partially similar	Different	answer is "partially similar" or "different"), it is not recommended to use the study under evaluation.		
How similar are the functional units and reference flows used?		al units and	While comparing two studies, the same functional units or reference flows must be applied (sections A.4.2 and A.4.3. If the answer is "partially similar", check with the practitioner whether it is possible to convert the functional unit and/or the reference flow to that of the reference		
Identical	Partially similar	Different	product or service. If the units are entirely different it is not recommended to use the study und evaluation.		
	How similar are the unit processes and system boundaries applied in the two studies?		In case "partially similar" or "different" unit processes are considered (section A.4.4), evalual whether the missing unit process significantly influences the results, and if it can be incorporate from other studies. Should the influence be high and integration not possible, it is not possible.		
Identical	Partially similar	Different	recommended to use the study under evaluation.		
	ar are the benchma two studies?	ark systems	This is especially relevant when the values of interest are expressed in relation to the benchmark (section A.4.5). If "partially similar" or "different" benchmarks are used, evaluate if it is possible to		
Identical	Partially similar	Different	align the benchmark to the reference study. If not, it is not recommended to use the study under evaluation.		
	How similar is technology maturity in the two studies?		If the levels of technological maturity are "partially similar" or "different", try to assess if and how this can affect the comparison (section A.4.6). Based on this assessment, decide whether using the study under evaluation can still be recommended.		
Identical	Partially similar	Different	the study under evaluation can still be recommended.		
scenarios	How similar are the underlying scenarios used (e.g., electricity grid mix, year, cost assumptions etc.)		Different underlying scenarios may imply different results despite assessing the same technology. In cases where the two studies under comparison employ "partially similar" or "different' scenarios, check how this affects the final results, and whether you can adapt the scenarios. If the		
Identical	Partially similar	Different	scenarios cannot be adapted, it is not recommended to use the study under evaluation.		

Is the evaluated study comparable to your reference study?

—N

Include this study in your analysis, and compare the following LCA or TEA studies to your reference study using the same checklist

When completed, move to the next step

Exclude this study from your analysis, and proceed to compare the next candidate study against your reference study, following the same checklist

When completed, move to the next step

Continue to the box "Understanding the results and reporting" (Reference tree)

