Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization

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Foreword from CO_2 Sciences

Climate change is one of the largest challenges of our time. One of the major causes of anthropogenic climate change, carbon dioxide, also leads to ocean acidification. Left unaddressed, these two challenges will alter ecosystems and fundamentally change life, as we know it. Under the auspices of the UN Framework Convention on Climate Change and through the Paris Agreement, there is a commitment to keep global temperature increase to well below two degrees Celsius. This will require a variety of strategies including increased renewable power generation and broad scale electrification, increased energy efficiency, and carbon-negative technologies.

We believe that Life Cycle Assessment (LCA) is necessary to prove that a technology could contribute to the mitigation of environmental impacts and that Techno-Economic Assessment (TEA) will show how the technology could be competitively delivered in the market. Together they are a valuable toolkit for promoting carbon capture and utilization (CCU) technology development.

The work presented here was made possible through the vision of the Chairman of the Global CO_2 Initiative, Bernard David, and the expertise of the CEO of CO_2 Sciences Inc., Issam Dairanieh.

The Global CO_2 Initiative was launched during the 2016 meeting of the World Economic Forum with the goal of catalyzing innovative research in CO_2 utilization. Beginning in July of 2018, the Initiative will continue its work as *The Global CO_2 Initiative at the University of Michigan*.

Development of standardized CO_2 Life Cycle and Techno-economic Assessment Guidelines was commissioned by CO_2 Sciences, Inc., with the support of 3M, EIT Climate-KIC, CO_2 Value Europe, Emissions Reduction Alberta, Grantham Foundation for the Protection of the Environment, R. K. Mellon Foundation, Cynthia and George Mitchell Foundation, National Institute of Clean and Low Carbon Energy, Praxair, Inc., XPrize and generous individuals who are committed to action to address climate change.

Global CO2 Initiative@UM, August 2018

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List of abbreviations

ANOVA	Analysis of variance
BDF	Block flow diagram
CAPEX	Capital Cost
CAPM	Capital asset pricing model
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
CEPCI	Chemical Engineering Plant Cost Index
CO_2	Carbon dioxide
COGM	Cost of goods manufactured
COGS	Cost of goods sold
ETS	Emission trading system
EU	European Union
FCI	Fixed capital investment
FOAK	First of a kind
GWP	Global warming potential
H_2	Hydrogen
IRR	Internal rate of return
ISBL	Inside battery limits
ISO	International standardization organization
LCA	Life cycle assessment
LCC	Life cycle costing
LCI	Life cycle inventory
LCOE	Levelized cost of electricity
LHV	Lower heating value
MADM	Multiple attribute decision making
MCDA	Multicriteria decision analysis
MODM	Multiple objective decision making
NGO	Non-Governmental Organisation
NOAK	Nth of a kind
NOX	Nitrous Oxides
NPV	Net present value
OPEX	Operational Cost
OSBL	Outside/off-site battery limits
P&ID	Piping and instrumentation diagram
PEM	Proton exchange membrane
PFD	Process flow diagram
R&D	Research and Development
ROI	Return on investment
SA	Sensitivity analysis
SI-UNITS	International System of Units
SMR	Steam methane reforming
TCI	Total
TEA	Techno-economic assessment
TRL	Technology readiness level
UA	Uncertainty analysis
US DOE	United States Department of Energy
USD	United States Dollars
WACC	Weighted average cost of capital

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PART A
General Assessment Principles

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Contents Part A

A.1 Introduction

In times of climate change, research on CO_2 utilization is gaining momentum in industry, academia and policy leading to a vast number of promising technologies, for example in the fields of CO_2 derived chemicals, fuels and minerals [1], [2]. The term "promising technology", however, reflects a subjective opinion on commercial and environmental viability but does not represent a systematic evaluation. Consequently, techno-economic assessment (TEA) and life cycle assessment (LCA) are essential methodologies for guiding research and development towards commercialization [2]. TEA is a methodology framework to analyze the technical and economic performance of a process, product or service; whilst LCA is a methodology to account for the environmental impacts of a product or service throughout its entire life cycle.

The methods applied to perform TEA and LCA especially at different technology maturity stages and for selected indicators, are currently lacking standardization in academia and industry across most CO_2 utilization fields *(e.g. there is no CCU protocol for LCA derived from the ISO approach)*. Hence, 'apples-to-apples' comparisons of different technologies remain difficult [3]. Most CO_2 utilization technologies are currently in early stages of development and only some have entered demonstration plant stage; however, many more are expected to come. While the investments needed for the demonstration phase will increase, these funds need to be allocated based on transparent, comparative and rational assessment methods. Therefore, in particular, from the view of funding agencies, but also for improved communication with external stakeholders, industry and academia, there is an increasing need to adopt guidelines for standardized TEA and LCA of CO_2 utilization.

This project aims at developing such a standardized approach (guidelines) for both TEA and LCA for CO_2 utilization. These guidelines are intended to substantially reduce ambiguity in methodological choices and enhance the transparency and comparability of both TEA and LCA results. The primary aim is to make CCU assessments more systematic, transparent and comparable. The guidelines are developed based on an extensive literature study and the input of two expert workshops, allowing for a close participation of the CCU community. The final project deliverables are TEA and LCA guidelines and three worked examples illustrating their use.

The projects are carried out by four partners, IASS Potsdam, RWTH Aachen, The University of Sheffield and TU Berlin and are supported by CO_2 Sciences and EIT Climate KIC. The fruitful discussions with all contributors, reviewers and with colleagues from the MIT Energy Initiative are thankfully acknowledged.

A.2 How to read this document

A.2.1 Structure of this document

The document consists of three parts, part A, **'General Assessment Principles'** that introduces both TEA and LCA, part B, the **TEA guidelines** and part C, the **LCA guidelines**. As these guidelines follow a commercial and product-oriented approach, the TEA part is presented first. This order can however be reversed by the practitioner depending on individual needs. The document parts are marked and color-coded on the top of each page. The guidelines are accompanied by worked examples that are presented in a separate document.

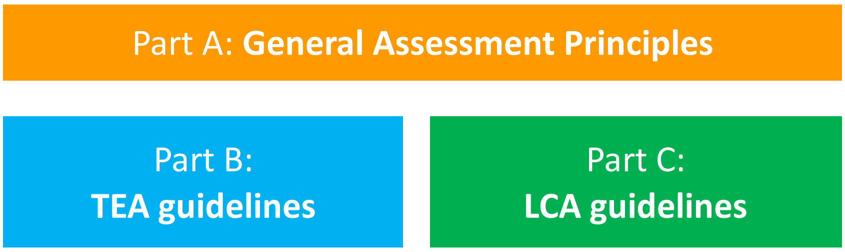

Figure 1. Structure of the TEA & LCA Guideline document

A.2.2 Scope of this document

A thorough review of published TEAs and LCAs for CCU technologies has identified a number of methodological choices and pitfalls *(e.g. setting system boundaries for multifunctionality, selecting comparable indicators, identifying the Technology Readiness Level, selecting CO_2 prices, calculating OpEx and CapEx, integrating LCA and TEA)*. These difficulties lead to wide differences in current TEA and LCA practice in the field of CCU, potentially misleading decision makers.

The TEA and LCA guidelines are built upon existing LCA ISO standards and guidelines as well as commonly applied assessment concepts and a collection of best practices. The guidelines target CCU-specific challenges for methodology and provide recommendations how to address these challenges in a way that ensures comparability and transparency of the results. Detailed worked examples to provide clarity on how to apply the guidelines are published alongside this document. In general, each chapter or sub-chapter consists of an introduction, a 'how to....' Section (for TEA only), clarifying CCU examples, further reading and the recommended guidelines for that topic.

Regarding LCA, this document aims to provide short and concise guidance on CCU-specific assessments challenges complementing existing ISO standards and guidelines. Therefore, and unlike in TEA, general issues of LCA are omitted if these issues are not specific to LCA on CCU. However, since readers might be new to the concept of LCA, we provide a short introduction to each step of a LCA study and further reading is recommended.

A.2.3 Intended audience

The intended audience for this document are practitioners that want to learn how to create comprehensible and consistent techno-economic assessments and life cycle assessments in the CCU field. These practitioners may come from academia, industry or government and may work in technology assessment and technology research and development, or funding, they may be part of the CCU community, the TEA community or the LCA community. Readers of TEA and LCA, such as investors, policy makers or funding decision makers are not the intended audience for these TEA and LCA guidelines, but may use this document to understand the challenges and pitfalls for TEA and LCA.

A.2.4 Limitations of this document

These guidelines have been developed to enable consistent and comparable LCA and TEA studies for CCU. They are not intended to serve as an assessment standard or rulebook. Instead they are meant to help practitioners to conduct sound assessments efficiently, avoid common mistakes and to derive meaningful results that can be compared to other studies. This document serves as an addition to conventional existing standards (in particular for LCA) and literature and does not replace any chemical engineering, economics or project planning principles. However, since the guidelines aim to enhance the comparability and transparency of studies, the LCA guidelines are more restrictive than the general ISO-framework. In some cases, there may be need to add further tasks to the ones discussed in this guideline since they are important to a specific study. Such additions are not excluded by the present guideline. However, the guidelines provide a consistent methodological core for conducting all LCA and TEA CCU studies.

This document is intended as the first step of a longer framework development process. TEA and LCA remain two separate approaches in this document as is common in current assessment practice in academic literature and industry. However, a combined approach is in strong demand to include trade-offs in decision making. The integration of TEA and LCA into one singular study is a next major development step that is subject to future work. This document provides some initial guidance to those who wish to carry out an integrated TEA & LCA study, however many facets of the integration process are still to be determined.

A.2.5 The guidelines

The guidelines for TEA are presented in part B of this document and LCA in part C. At the end of each guideline chapter there is a box listing rules that these guidelines recommend. The box contains three categories, shall, should and may:

- Shall: these rules are the minimum requirements that are recommended to achieve a standardized TEA/LCA for CCU. Every TEA/LCA produced using these guidelines must cover these basic rules. All rules in this category have to be addressed.
- Should: these rules cover a recommended level of analysis and should be applied to produce a TEA/LCA of greater depth.
- May: use of these rules produces the greatest detail of TEA/LCA. These rules may not be applicable in all studies and should be applied as determined by the practitioner.

If specific guidelines from this work are referenced in the TEA or LCA report, they can be addressed by guideline topic or number, as for example "[Guideline Topic] shall 2" or "A.X should 3".

Table 1. Guideline template table

Guideline A.X - [Guideline Topic]	
Shall	1) Shall Guideline 1 2) Shall Guideline 2
Should	1) Should Guideline 1 2) Should Guideline 2
May	1) May Guideline 1 2) May Guideline 2

A.3 Carbon Capture and Utilization

A.3.1 Introduction

Carbon capture and utilization (CCU) is the capture of carbon dioxide (CO_2) from flue gas or the atmosphere and the subsequent conversion of CO_2 into value added products (see Figure 2). CCU has already shown its potential to reduce environmental impacts such as greenhouse gas (GHG) emissions and fossil depletion in comparison to conventional technologies. However, CCU alone cannot mitigate climate change since the amount of potentially convertible CO_2 to chemicals, fuels and materials is much lower than emitted CO_2 today [1]. Furthermore, many CO_2-based products lie thermodynamically uphill, or in other words, many CO_2-based products have a higher Gibbs enthalpy of formation than CO_2 and thus, energy is required to chemically reduce the CO_2. Other CCU technologies such as mineralization processes have lower Gibbs enthalpy of formation and thus, no energy is required to convert the CO_2. However, those processes often have slow kinetics and require energy intensive preparation of reactants *(e.g. grinding of olivine and other minerals)*. Therefore, environmental benefits and economic viability of CCU technologies often depend on the setting *(e.g. availability of electricity with a low-carbon footprint and low prices)*.

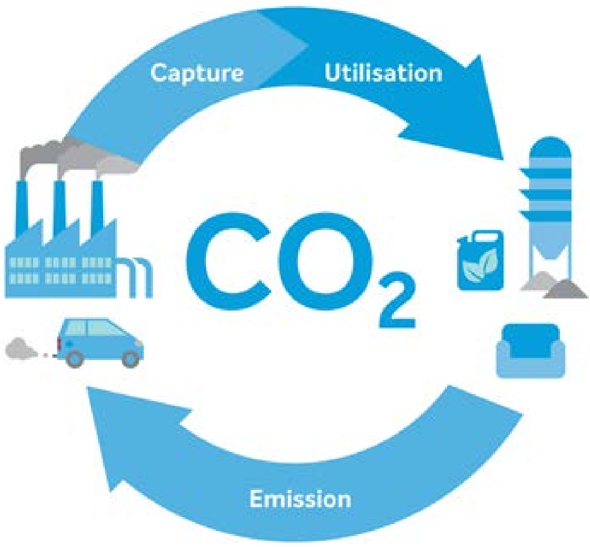

Figure 2. The CO_2 utilization cycle, taken from ***[1]***

Interest in CCU has increased in the last decade with sharply rising scientific publications in the field. Many applied research institutes and established industrial companies as well as start-ups from around the world are developing CCU products, aiming for market solutions. Some projects have already entered the market *(e.g. CRI's Vulcanol, Covestro's Cardyon, Carbon8's C8Agg)*. A 2016 market study for CCU products projected an annual revenue of up to 800 billion US Dollars through 2030, relating an annual uptake of up to 7 billion tonnes of CO_2 [4]. CCU markets can be categorized in two groups: niche markets (smaller volumes but high margins) such as plastics, chemicals or carbon fibres, and bulk markets (large volume but low margins) such as concrete, asphalt and fuels; through their large volumes, bulk markets can also provide a large potential for emissions mitigation.

The high current interest and positive future projections for CCU are based on several, potential economic and environmental advantages:

- CCU can provide an economical carbon feedstock, partially or fully replacing other, more expensive carbon feedstock.
- CCU can open doors to new synthesis routes for existing products or even for new products and can thereby open new markets (for example see [5]).
- CCU can provide solutions for chemicals, fuels, materials, waste treatment and the mitigation of industrial CO_2 emissions, for integrating renewable electricity into the chemicals and transportation sectors and overall for industrial symbiosis and circular economy.
- CCU can reduce the complexity of chemical reaction pathways (for example see [5]–[7]).
- CCU can increase process efficiency and decrease input price volatility.
- CCU can potentially reduce environmental impacts beyond climate change as demonstrated for CO_2-based fuels that reduce NOx and soot emissions (for example see [6]).
- CCU technologies can even be carbon-negative if combined or integrated with CO_2 sequestration *(e.g. through mineralization)*.

On the other hand, CCU also faces several potential challenges:

- The vast majority of CCU processes have a high energy demand or require 'high energy' co-reactants, that can increase operating cost and environmental impacts.
- CCU processes often require new plants, many include high pressure processes, that increase capital cost.
- CCU mostly focusses on low-margin, large-volume industrial markets requiring substantial investments.
- CCU addresses the chemical, fuels and materials industries with high cost for adapting existing processes and very slow product adaption rates (slow uptake in the market).
- Reduction of environmental impacts is one important criterion for commercialisation of CCU. If a CCU technology cannot reduce environmental impacts, a successful commercialisation as a measure to mitigate emission is unlikely.

Since both the economic and environmental benefits of CCU technologies are important criteria to guide future research and deployment, comprehensive assessments are required. A commonly accepted method for a comprehensive environmental assessment is life cycle assessment (LCA) and for technical feasibility and economic viability is techno-economic assessment (TEA).

A.3.2 Classification of CCU technologies

In this guidance, CCU technologies are classified according to differences of compared products or services and their intended application. A classification is not mandatory for LCA or TEA studies. However, the classification can help to solve methodological choices *(e.g., the definition of the functional unit)*. Since products or services are classified by their intended application, the same product or service might fall into different classes *(e.g. methanol can serve as chemical intermediate and as fuel)*. The following CCU classes are defined:

- CO_2-based products
    - with identical chemical structure and composition to their reference/benchmark, *(e.g. chemicals or intermediates such as syngas, ethylene, methanol, oxalic acid, formic acid, dimethyl carbonate).*
    - with different chemical structure and composition to their conventional reference/benchmark, *(e.g. materials such as thermosets, foams, elastomers, mineral aggregates, bricks, carbon nanotubes)*.
- CO_2-based fuels

  - with identical chemical structure and composition to their reference/benchmark counterparts *(e.g. methane).*
  - with different chemical structure and composition to their reference/benchmark counterparts *(e.g. CO_2-based methanol vs reference/benchmark gasoline for use as a drop-in fuel).*
- Energy storage systems *(e.g. CO_2-based methane that is stored and subsequently used for dispatchable electricity production).*

The guidelines and best practices presented in this document can also be applied to technologies not belonging to the CCU classes presented above, however application should be carried out cautiously.

A.3.3 Further Reading

- General introduction
  - TU-Berlin report for the general public: "CO_2 utilization today"[1]
  - Styring et al.'s book on various conversion pathways: "Carbon Dioxide Utilization"[8]
  - Artz et al.'s review on chemical conversion of CO_2 and environmental assessment:[5]
- Future potential and developments of CCU
  - Global CO_2 initiative's study: "Global Roadmap for Implementing CO_2 Utilization"[4]
  - Ecofys study: "Implications of the Reuse of Captured CO_2 for European Climate Action Policies Final Report"[9]
  - Global CCS Institute study: "Accelerating the update of CCS: Industrial Use of Captured Carbon Dioxide"[10]
  - Mission Innovation report on priority research directions: "Accelerating Breakthrough Innovation in Carbon Capture, Utilization and Storage"[2]
  - Dechema study on future of the chemical industry: "Low Carbon Energy and Feedstock for the European Chemical Industry"[11]

A.4 Technology maturity

A.4.1 Introduction

The term ‘technology maturity’ describes the stage of development of a system element or product system (for definitions of system elements and product systems see TEA and LCA guidelines). The selection of assessment methods and indicators depends on the technology maturity. As CCU products include a broad variety of new technologies, technology maturity needs to be identified and described in a systematic and comprehensible way while conducting a TEA or LCA.

Technology maturity can be subdivided in the three major phases of applied research, development and deployment. For a more detailed analysis, the concept of Technology Readiness Levels (TRLs) can be used. The major maturity phases can be associated with distinct TRLs. Commonly used general TRL concepts relevant for CCU are the US Department of Energy TRL description [12] and the European Commission Horizon2020 program TRL description [13]. However, specific TRL descriptions for the chemical and process industries are lacking at the moment. This has proven to make assigning TRLs difficult and subjective for TEA practitioners [14], especially in the case of CCU. Table 2 combines the general TRL concepts from US DoE and EU Horizon 2020 and adapts them for the chemical and process industries (a table with further details can be found in the TEA Guideline Annex).

*Table 2. Characterizing Technology Readiness Levels for the Chemical Industry (excerpt from **[15]**)*

TRL	Phase	Title	Description
1	**Research**	*Idea*	Basic principles observed and reported, opportunities identified, basic research translated into possible applications
2		*Concept*	Technology concept and application formulated, patent research conducted
3		*Proof of concept*	Applied laboratory research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)
4	**Development**	*Preliminary process development*	Concept validated in laboratory environment, scale-up preparation started
5		*Detail process development*	Shortcut process models found, simple property data analyzed, simulation of process and pilot plant using bench scale information
6		*Pilot trials*	Pilot plant constructed and operated with low rate production, products tested in application
7	**Deployment**	*Demonstration & full-scale engineering*	Parameter and performance of pilot plant optimized, (optional) demo plant constructed and operating, equipment specification incl. components conferrable to full-scale production
8		*Construction and start-up*	Products and processes integrated in organizational structure (hardware and software), full-scale plant constructed
9		*Continuous operation*	Full-scale plant audited (site acceptance test), turn-key plant, production operated over the full range of expected conditions in industrial scale and environment, performance guarantee enforceable

Applied research is conducted mainly in TRLs 1-3 but often expands into later TRLs; please note that in Table 2, basic research is seen prior to the TRL phases as it is not driven by economic targets. Deriving ideas from basic research that can be exploited economically (ideation) is seen as the start, TRL 1. Systematic development is started in TRL 4 and is mainly carried out until TRL 6, but it can be carried out until plant commissioning in TRL 8. Deployment is started with detailed planning of a full-scale plant at TRL 7 and completed with running production at TRL 9.

Once a TRL is assigned for a system element and product system, the maturity also clarifies what data can theoretically be available for the TEA practitioner. If this data does not exist, is not available or lacks quality, the maturity assignment of the product system in focus needs to be critically reviewed or repeated.

A.4.2 Identifying technology maturity for CCU product systems

A.4.2.1 General steps for identifying technology maturity

Defining technology maturity helps to systematically explore the interplay of a study's goal and scope, or of what is known about a product system and what questions could be answered; especially providing indication on data availability and study limitations. Therefore, technology maturity shall be defined in each assessment.

Technology maturity is specific for each product system as well as for each system element (TEA) or unit process (LCA). The technology maturity shall therefore be defined first for each system element or unit process individually and second for the overall product system. The maturity of the product system shall equal the lowest maturity of the system elements / unit processes. *(e.g. when the systems elements H_2 generation and CO_2 capture are at deployment stage, the CO_2 separation is at development stage, and the CO_2 utilising reaction is at the research stage, the overall CCU product system is defined as at the research stage)*. While any maturity concept can be used, the concept and its criteria shall be clearly documented. For better transparency and comparability, it is recommended that the TRL-concept should be used to identify technology maturity. Furthermore, the used TRL concept *(e.g. EU Horizon 2020, US DoE)* and its definitions should be clearly referenced or added to the report.

A.4.2.2 Common CCU challenges in identifying technology maturity

In many CCU TEA studies, the maturity of product systems is derived from similar product systems that are either already on the market or at high technology maturity. However, the maturity of a system element cannot be simply derived from other product systems, unless their data is available for the TEA study. Furthermore, the system elements of the similar product system can be different and might not necessarily match the product system in focus. It is therefore necessary to rate technology maturity for all system elements based on the data available for the actual process that is currently in research, development or deployment (R,D&D). System elements that are not in focus of the R,D&D and therefore not implemented in earlier stages can be excluded from maturity rating.

A.4.2.3 Further Reading

- US Department of Energy, “Technology Readiness Assessment Guide,” 2011 [12].
- European Association of Research Technology Organisations, “The TRL Scale as a Research & Innovation Policy Tool, EARTO Recommendations,” 2014 [14].
- HORIZON 2020 – WORK PROGRAMME 2014-2015, General Annexes, G. Technology readiness levels (TRL) [13].

A.4.2.4 Guidelines

Guideline A.1 - Technology maturity	
Shall	1) Technology maturity shall be defined in each assessment - first for each system element and second for the overall product system 2) The maturity of the overall product system shall equal the lowest maturity of the individual system elements 3) The maturity concept and its criteria shall be clearly documented
Should	1) The TRL-concept should be used to identify technology maturity 2) The TRL-concept and its definitions should be clearly referenced or added to the report

A.5 Integrating LCA and TEA

A.5.1 Introduction

The decision to implement new CO_2 utilization technologies usually takes into account all three, technological, economic and environmental criteria. TEA generally aims to examine technological feasibility and economic profitability while LCA in general aims to compare environmental impact reductions of technologies. Hence by integrating TEA and LCA results, solutions can be found that balance economic and environmental factors.

Both TEA and LCA support decision making by providing interpreted indicators for criteria (TEA) or impacts (LCA). By aligning or integrating the assessments, for example by choosing the same goal and functional unit for the study, combined interpretation of LCA and TEA results becomes possible. However, if an LCA and TEA are interpreted in combination without being properly aligned, difficulties of interpretation and unreliable conclusions might be a consequence. For this reason, an approach for aligning CCU TEA and LCA is suggested below. Once the aligned studies have been carried out, combined environmental and economic indicators can be calculated and Multi-Criteria Decision Analysis (MCDA) applied. MCDA enables trade-offs between economic and environmental impacts to be balanced to find the optimal outcome. For example, increasing process temperature could lead to improved economics but worsen environmental impacts, therefore MCDA assists in determining the optimal temperature which balances both impacts. Integrating LCA and TEA studies is complex and can encompass many aspects [16]–[18]. This is an evolving area of study, therefore many aspects of methodology have yet to be defined. As such, we do not seek to provide a concrete methodology or guidelines for undertaking such studies here, but highlight key issues and provide initial guidance that could help the practitioner avoid pitfalls.

A.5.2 Types of study

There are different levels to which TEA and LCA studies can be integrated. Table 3 lists approaches which can be taken to unite TEA and LCA. If the studies are or were carried out independently on the same system with different goals, non-aligned scopes and varying inventories, only a 'Qualitative Integration' remains possible (type 1). Here, only qualitative conclusions can be reached based on observed hot-spots as the data is not identical. This approach may be sufficient for early TRL systems, as little to no alignment between TEA and LCA assessments is necessary, which reduces the assessment effort. In such early TRL cases, large uncertainties are typically present, which limit the recommendations that integrated assessments can give. 'Alignment and Combined Indicators' (type 2) is next on the step towards a completely integrated study, here two separate studies are carried out but with aligned scope and inventory. Initially the studies will have individual goals to ascertain environmental and techno-economic indicators. Once these initial TEA and LCA are completed and conclusions have been drawn, a further goal based on combined indicators can be applied, combined indicators calculated and combined sensitivity analysis performed. This can also be taken further by applying multi-criteria decision analysis. A 'Fully Integrated' study (type 3) would consist of a joint TEA and LCA, where combined indicators are chosen. Here a single goal of the study would encompass both environmental and economic factors. The interpretation phase would involve multi-criteria decision analysis to find viable solutions. This chapter discusses type 1 and type 2 of integration and provides guidance for alignment. Type 3 is not discussed here as this is outside the scope of this project.

Table 3. Approaches for integrating TEA and LCA

Type	Description	Content	What to do
1	Qualitative integration	Two separate, not aligned studies but using same product system. System boundaries for LCA and TEA can differ depending on requirements.	Only qualitative comparison of hot-spots
2	Alignment & combined indicators Integration (partial integration)	Two separate but aligned studies (regarding scope) with separate inventories, resulting in combined indicators and combined sensitivity analysis also can include MCDA	Combined indicators, sensitivity analysis
3	Full integration	One study with one inventory with TEA/LCA indicators as well as combined indicators, normalization and MCDA	(not discussed here)

A.5.3 Alignment

In order to integrate the results from an TEA and LCA, it is essential for each study that the goal and scope are identical and the inventory data is as similar as possible, otherwise the combined outcomes will be incorrect. Ideally, one combined inventory will serve both TEA and LCA. However, LCA requires more and different types of data than TEA. It needs to be reported, if varying data is used for TEA and LCA.

System boundaries for the studies and the method of solving multi-functionality must match, in other words if systems expansion is applied in LCA, it must be applied in TEA (see section below for an explanation of system boundaries in integration). Therefore, careful planning is necessary before either study is commenced to ensure compatibility and to avoid integration problems.

When starting, the following should be the same in both studies:

- Scope definition including:
    - Functional unit
    - System boundaries of the study *(e.g. both cradle-to-gate)*
    - Method of solving multi-functionality (sub-division, system expansion, substitution or allocation using underlying physical or other relationship)
    - Time and geographical representation of the study
- Inventory, in particular, processes and data used, including electricity supply
- Scenarios applied (needed if combined indicators shall also be calculated for the scenarios)

In the case of aligning the goals, there can be one overall goal for the integrated study and individual goals for TEA and LCA. It is not necessary to just have one all-encompassing goal. For example,

- TEA goal: What is the technical viability and economic performance of methanol production via CO_2 hydrogenation within a renewable power to liquid context in Germany?
- LCA goal: To compare the environmental consequences of producing methanol for use as a chemical feedstock in Germany, synthesized via two routes: the hydrogenation of CO_2 captured from a cement plant vs. methanol synthesized using the conventional steam methane reforming process from natural gas.
- Integrated goal: How can a methanol production plant via CO_2 hydrogenation using wind energy in Germany be optimized to maximize technologic, economic and environmental performance?

A.5.4 Multi-functionality and system boundaries

TEA aims to assess the technical feasibility and the economic viability of production and sales mostly from the perspective of the acting entity (as described in this guideline). LCA aims to calculate environmental impacts of a production system with all its functions (as defined in the goal and scope). TEA does not usually deal with up-stream multi-functionality in the same way as LCA. It is not common practice within TEA to apply system expansion (for discussion of system expansion see part C, LCA guideline chapter 4.3.2) including upstream and downstream processes or functions in the functional unit. For example, if the study analyses a CCU plant with a cement plant as the CO_2 source and system expansion is applied in LCA, upstream processes such as cement production would be included into the system boundaries, leading to the inclusion of multiple functions, so called 'basket of functions', such as cement and the CCU product(s) into one single functional unit. Whereas in a common TEA, the production of cement would not be included in the system boundaries but just the CO_2 input flow *(e.g. by calculating the costs of CO_2 capture from the CO_2 source or by assuming CO_2 costs via a market price for CO_2)*. While system expansion can be applied when conducting TEA, it can cause complications involving the detailed modelling and data collection for the CO_2 providing process which may not be known in detail.

For multifunctional product systems, the 'alignment and combined indicators' approach (type 2) is recommended; meaning conducting two independent TEA and LCA studies (in accordance to the presented guidelines) followed by a separate integration study. This ensures that the most appropriate approaches are applied to the TEA and LCA (see hierarchy in the LCA guideline chapter 4.3.2). Differences in boundaries and methods for multifunctional product systems must be resolved before conducting the integrated study using combined indicators. To do so, the system boundaries can be redrawn if necessary, scopes aligned and aspects of analysis conducted again to allow integration, once the independent studies are completed. It should be noted that this approach is time-consuming, as aspects of the analysis may have to be repeated. However, areas or inputs of importance such as hot-spots, which were identified in the individual studies' sensitivity analyses, can be used to determine how the multi-criteria decision analysis (MCDA) is conducted in the integrated study.

A.5.4.1 Burden Sharing

Integrating LCA and TEA results for CCU is an evolving field with many theories on burden sharing. In the first instance, when integrating LCA and TEA, one simple approach is to assign all burdens to the CCU technology. In this way, all carbon capture costs and environmental impacts associated with CO_2 are assigned to the CCU process and are not shared with the CO_2 producer. Similarly, allocation via cut off can be applied, drawing the system boundary at the point where the CO_2 enters the system whilst including the capture technology inside the system, which results in gate-to-gate system boundaries. This approach negates the need to include the CO_2 producer *(e.g. cement/steel plant)* inside the boundaries and therefore the system will be limited to the functions provided by the CCU process itself. Applying allocation via cut-off in this way simplifies the integration but also reduces the completeness of the studies because the impacts of producing CO_2, which could be significant, are not included. Therefore, if this approach is used, it should be clearly documented by including a diagram of the system and explaining how and why the boundaries have been set. Burden sharing is particularly important if carbon taxes or credits are to be taken into account in the analysis. This area is still under much discussion and at this time clear guidance cannot be given to the practitioner as to how to definitively share burdens. Therefore, it is essential to clearly explain the approaches used.

A.5.5 System elements

The guidelines recommend analyzing and reporting results by system elements (TEA) or unit processes (LCA) as well as by the overall product system, which allows for easy identification of hot-spots and areas for improvements; this approach is particularly valuable when the LCA and TEA studies are to be integrated. In integrating studies, trade-offs will often be analyzed *(e.g. if process temperature is increased to raise the yield, profit might increase but also environmental impacts).* If the system is broken down into system elements (TEA) or unit processes (LCA), this type of analysis can become more straight forward and clearer in reporting.

A.5.6 Calculating combined economic and environmental indicators

Indicators which combine results from the TEA and LCA such as abatement costs are commonly used to analyze economic and environmental efficiency, hence, they are of particular interest for CCU options. These combined indicators become especially important when comparing alternative scenarios. In the following an example for a combined indicator is provided: abatement cost of CO_2 emissions c_{abated} (or also described as cost of CO_2 avoided). Similar methodology can be applied to calculate other combined enviro-economic indicators. Although, combined indicators for CCU are often based on greenhouse gas emission other environmental indicators should be included in the combined analysis to broaden the scope from carbon foot printing to encompass multiple LCA indicators.

A.5.6.1 Example of a combined indicator calculation

An example of a combined indicator is the abatement cost. This can only be calculated if the CCU process has lower greenhouse gas emissions than the benchmark, otherwise no emissions are abated and the indicator is meaningless. The abatement cost of CO_2 c_{abated}, can be calculated using the specific production costs of the CCU and benchmark plants (c_{CCU} and c_{ref}) and the specific environmental impacts of the CCU and reference/benchmark plant (ei_{CCU} and ei_{ref}). All values relate to the same system boundary and are set with respect to a single functional unit which is used consistently in both the techno-economic and the environmental parts of the analysis.

$$c_{abated} = \frac{c_{CCU} - c_{ref}}{ei_{ref} - ei_{CCU}}, \qquad \{for\ all\ ei_{ref} - ei_{CCU} > 0\}$$

The lower the abatement cost, the higher the economic efficiency of the CCU technology with respect to emission savings. Negative abatement costs indicate that greenhouse gas emissions can be abated by reducing production costs overall; positive abatement costs indicate either that the CCU technology may need market incentives or that the CO_2-based product needs to achieve a premium price over the conventional product. It should be noted that a negative abatement cost does not serve as an indicator of environmental viability, as other impact categories such as human toxicity or eco-toxicity have to be taken into account to avoid shifting environmental impacts from one impact category to another (‘burden shifting’). By comparing the abatement cost of technology options, e.g., via marginal abatement cost curves, a merit order of measures to prevent environmental impacts can be drawn-up.

While abatement costs are specific to the functional unit, the abatement of the overall plant can also be calculated to analyze the significance of the abatement. In the example below, the amount of greenhouse gas emissions abated, GHG_{abated}, is calculated using the CCU plant output, $m_{CCU,output}$ (which can be represented by the annual production, or as approximation by the plant capacity and a load factor; this does not apply for multiple products), and the difference in specific greenhouse gas emissions between the reference and CCU plants:

$$GHG_{abated} = m_{CCU,output} \cdot (GHG_{ref} - GHG_{CCU})$$

In addition, the abatement potential of a technology can be estimated by assuming a total global market penetration. Subsequently, the comparison of this abatement potential to Socolov's stabilization wedges (reduction of one Gt CO_2-eq. per year) can reveal if the technology can significantly contribute to climate change protection [19]. However, this comparison is only of a qualitative, informative nature as unforeseen changes during scale-up might occur.

A.5.7 Interpretation of integrated studies

A.5.7.1 Introduction

Once a partial or fully integrated TEA and LCA (type 2 or type 3) have been completed, multi-criteria analysis can be conducted to evaluate the interdependency of the most influential technology barriers, cost drivers and environmental impacts to determine the most beneficial outcome based on the goals of the study. Furthermore, additional relevant combined indicators, for example the cost of CO_2 abated/tonne of product can be calculated as boundaries and scope are aligned. The integration of the studies should consider numerous environmental impacts, not just the Global Warming Potential (CO_2eq.), to ensure that trade-offs across environmental categories are included in the analysis. The analysis can be either quantitative or qualitative depending on the approach used.

A.5.7.2 Common hot-spots to consider

Identifying hotspots can benefit the analysis. Here, a hot-spot is process or an input that has a significant influence on the technical, economic or environmental performance of the plant or process. Common hot-spots in CCU generally include carbon capture, electricity source and price, hydrogen production, preparation of materials (particularly in mineralization) product separation and even end-of-life phases. When performing an integrated study, hot-spots can be identified in either the TEA or LCA and then varied to analyze the respective technical, economic and environmental effects. This is achieved by varying the hot-spot parameters in the process design and conducting further assessment to analyze the magnitude of the effects.

A.5.7.3 Multi-criteria decision analysis (MCDA)

MCDA is a form of integrated evaluation. A single criteria approach is normally aimed at identifying the most efficient options at a maximum technical performance and profitability (TEA) or the best environmental improvement (LCA). By having a dual or multi-criteria approach, technical, economic and environmental factors can be considered simultaneously. This is necessary if an integrated study (TEA and LCA) is performed. The integration of the TEA and LCA studies can follow the same principles as multi-criteria analysis within one field of assessment: this means that criteria of both assessment fields should be carefully selected to reflect performance in meeting the objective and processed via rigorous TEA and LCA. Both, Multiple Objective Decision Making (MODM) and Multiple Attribute Decision Making (MADM) can be applied. Further detail on MCDA can be found in the part B, TEA guidelines, chapter 7.4.

MODM provides a group of solutions when multiple goals (objectives) are in focus and can be used to display feasible and non-feasible regions. Typically, the optimization methods involve conflicting techno-economic and environmental objective functions such as energy efficiency, investment costs and emission rates *(e.g. investment in SO_X emission reduction technologies is costly but environmentally necessary)*.

MADM is used to rank, classify or select alternatives with regards to criteria. MADM techniques are classified under outranking, interactive, multi-attribute utility theory (MAUT), and multi-attribute value theory (MAVT).[20]–[22] MADM is used when a single goal (objective) is in focus and a wide range of criteria (attributes) have to be considered when making the decision. These criteria can be either qualitatively or quantitatively evaluated, *(e.g. CO_2 emissions could be rated on a relative, ordinal scale on low/medium/high)* or in terms of actual emission rates to the atmosphere. MADM methods are integrative evaluation methods in the sense that they combine information about the performance of the process with respect to the criteria (scoring) or with subjective judgements about the relative importance of the evaluation criteria in the particular decision-making context (weighting).[23] For instance, in the case of aggregates production from CO_2, environmental benefits can be considered of higher significance compared to economic criteria due to effective waste disposal and permanent CO_2 storage.

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PART B
TEA
Guidelines

SUPPORTED BY

Contents Part B

B.1 Introduction to techno-economic assessment

Techno-Economic Assessment (TEA) is a methodology framework to analyze the technical and economic performance of a process, product or service. TEA "includes studies on the economic impact of research, development, demonstration and deployment of technologies"[1], uncovering the cost of manufacturing and market opportunities. TEA is different to Life Cycle Costing (LCC) mainly in its integration of cost, revenue and technical criteria as well as its general focus on the production phase and on the producer or investor.

In this guideline, TEA has been subdivided in the following phases: goal and scope, inventory, calculation of indicators and interpretation (see Figure 1). The goal provides guidance for the overall study, the scope defines what aspects are included and how the comparison is being conducted, the inventory collects all relevant data and the calculation of indicators produces results. While each phase is carried out, the consistency and robustness of its outcomes are evaluated and if necessary modifications are recommended in the interpretation phase, which is carried out in parallel. As TEA is an iterative process, practitioners might have to go back to a prior phase to modify the assessment if recommended by interpretation. Finally, goal, scope, inventory and results and their interpretation are summarized in a TEA report (see Figure 1).

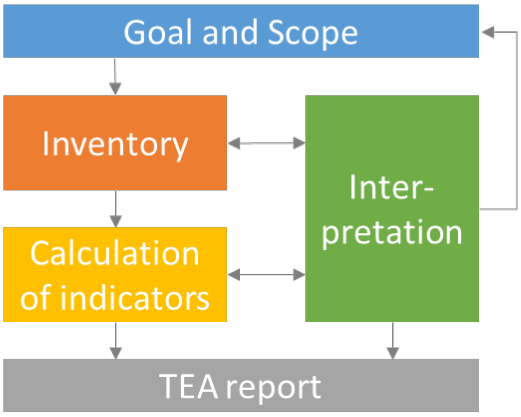

Figure 1. Phases of techno-economic assessment

Assessment and decision-making are two different steps and need to be considered separately. The results of the TEA support finding the next steps in technology development or identifying business cases and are a valuable tool for decision making and monitoring in various fields such as research, product or process development, investment and funding, policy and regulation [1]. TEA can provide decision support for single as well as for a combination of products. In this document, 'services' will also be referred to as 'product'. TEA is strongly interlinked with technical development activities such as chemical process design. Strictly speaking, TEA is based on information provided by process design and feeds back recommendations for process design, it does not include technical development activities. At the same time, TEA is conducted in close interaction and in parallel with research, development and deployment to reduce development effort and time to market.

It should be noted that specific TEA results require specific assumptions, making the study context-specific study for example to location, time horizon or access of information. Furthermore, TEA provides results for questions regarding technology and economics, while leaving out environmental impact or social aspects. TEA can support decision making in a project-specific and technology as well as economic context, such as R&D support or investment decision making. Applying TEA results in a generalized context, such as for global policy making, can be limited and should be carried out cautiously.

B.2 How to read this document

B.2.1 Scope of this document

A thorough review of published TEAs for CCU technologies has identified a number of methodological challenges and pitfalls *(e.g. setting system boundaries for multifunctionality, selecting comparable indicators, identifying the Technology Readiness Level, selecting CO_2 prices, calculating OpEx and CapEx, integrating LCA and TEA)*. This leads to differences in current TEA practice which can be confusing and misleading to readers and decision makers. This document and its attachments summarize and extend commonly applied assessment concepts, provide a collection of best practices and show three detailed worked examples to provide guidance in conducting assessments for CCU. Based on a comprehensive literature review to identify best practice and common pitfalls as well as workshops with leading practitioners, the guideline aims to provide specific guidance on TEA challenges of CCU, as well as an overview of standard TEA practice. In general, each chapter or sub-chapter consists of an introduction, a 'how to....' section, some CCU examples, further reading and the recommended guidelines for that topic.

B.2.2 Linking TEA and LCA

The link between techno-economic and life cycle assessment (LCA) is strong for many industries, and especially for CCU. All CCU processes aim to synthesize products in an economically viable way and most with lower environmental impacts, therefore both LCA and TEA are needed to assess the viability of a process. Subsequently, the structure proposed here in part follows the methodological structure of a LCA as presented in ISO standards 14040 and 14044 and the ILCD handbooks. By applying good TEA practice concepts as well as introducing concepts used in LCA and LCC, these guidelines aim for a systematic and transparent assessment as well as for a better integration of TEA and LCA or LCC studies. It is also envisaged that the TEA guidelines will benefit the CCU community by improving the understanding of the results of both analyses, allowing for better comparisons of the results among different studies. Consequently, each chapter covers specific techno-economic aspects and, if applicable, how these are linked to LCA principles.

B.2.3 The guidelines

At the end of each chapter there is a box listing rules that these guidelines recommend. The box contains three categories, shall, should and may:

- **Shall**: these rules are the **minimum requirements** that are recommended to achieve a standardized TEA for CCU. Every TEA produced using these guidelines must cover these basic rules and all rules in this category have to be addressed.
- **Should**: these rules cover a **recommended level of analysis** and should be applied to produce a TEA of greater depth.
- **May**: use of these rules produces the **greatest detail** of TEA. These rules may not be applicable in all studies and should be applied as determined by the practitioner.

If specific guidelines from this work are referenced in the TEA or LCA report, they can be addressed by guideline topic or number, as for example “[Guideline Topic] shall 2” or “B.X should 3”.

Table 1. Guideline template table

Guideline B.X - [Guideline topic]	
Shall	1) Guideline 1 2) Guideline 2
Should	1) Guideline 1 2) Guideline 2
May	1) Guideline 1 2) Guideline 2

B.3 Goal

B.3.1 Introduction to techno-economic assessment goals

The first step for a TEA is to identify the goal, which will set the scope for the study. The goal addresses techno-economic questions, such as the cost or profitability of a new technology, product, plant or project, often for a specific audience *(e.g. assessment of a CCU reaction concept for a funding agency, assessment of a CCU plant concept for industry managers, assessment of CCU technology options for policy makers)*. The goal definition is decisive for all other phases as it guides the detailed aspects of the scope definition and both together frame all following phases of the study. The TEA goal also interacts with the subsequent phase of inventory creation. On the one hand, different goals lead to different comparisons, with varying data requirements and inventory creation efforts. On the other hand, the inventory also impacts the goal, especially if data is not available.

It is important to note that the assessment goal is specific to the individual study and the practitioner's view. Even when focusing on the same product system, the assessment goal can vary between studies depending on the scope and size of the project, the technology maturity, the region or time horizon. For example, when assessing lab-scale technologies, the goal for an early research project at a university or a company might be to identify a general, technical viability and overall economic potential. Whereas the goal for an industrial implementation project involving several companies and authorities might be to calculate project-specific costs and risks, involving multiple factors for the purpose of budgeting, pricing and contract negotiation or even litigation.

If the available inventory makes the pursuit of the original goal impossible, either the goal needs to be revised in a way that it can be accomplished with the available inventory and remains meaningful at the same time or the study needs to be discontinued.

B.3.2 Perspectives and principles of assessment goals

B.3.2.1 Introduction

CCU literature analysis shows that comparisons between the studies are challenging[2], especially when comparing technologies of varying disciplines, markets and technology maturities *(e.g. comparing research-stage photocatalytic water splitting concepts with early market stage PEM electrolysis or mature market stage steam methane reforming processes)*. Stating the goal in the proposed way as described below may be uncommon for TEAs today, however it will be useful as it facilitates comparing different technologies, products and markets as it is necessary for CCU.

B.3.2.2 How to define TEA goals for CCU

Plausible process concepts
First and foremost, all assessments need to be based on process concepts that are technologically plausible, meaning for example that proposed concepts do not violate the first and second law of thermodynamics. Before the assessment, a 'sanity check', for example checking mass and energy balances, needs to be conducted by the TEA practitioner.

Perspectives of assessment goals
As a range of stakeholders are involved in the research, development and deployment of CCU products, TEAs for CCU are typically conducted from three different perspectives: R&D, corporate and market. Each perspective involves a different group of stakeholders and poses its own specific questions, relevant for defining the assessment goal (see Table 2).

When comparing product applications *(e.g. is it more profitable to use methanol as a chemical or as a fuel? Is it more land-efficient to use algae for food or fuel?)*, the assessment needs to first be carried out by each application individually before a comparison can be carried out.

Table 2. Common TEA perspectives, questions and goal examples

Common perspectives	Description	Common goal related questions	Goal examples
R&D-perspective	Assessment of specific project(s) in research or development; either identification of major barriers and drivers (hot-spots) for a single project or comparison of various projects	• What are major cost and value drivers? • What product performance characteristics have to be met? • What aspects need to be worked on (next)? • How does the current development state rank amongst alternatives? • Should we fund CCU research and development of project X?	• *(Scientific) assessment of economic potential of product or technology* • *Planning of next R&D steps or priorities* • *Funding program decision making*
Corporation-perspective	Analysis of projects in development and deployment; assessment as investment alternatives and comparison to existing processes; use of detailed process data is common	• How does the CCU product perform against current and upcoming benchmarks? • Is the CCU product in a future scenario economically viable? • How does the investment in a CCU product deployment / demonstration project / full-scale plant compare to alternatives?	• *Business case of new CCU plant* • *Economic due diligence for investment in CCU start-up*
Market-perspective	Analysis of projects in development and deployment stages; focus on supply chains, effects of economic policy, the best use of resources or the best way of obtaining a specific utility	• What are current states, favorable conditions, best practices and necessary actions for regional CCU value chains? • What regulatory clarification and support (type, timing and budgets) is required for specific CCU products and services groups?	• *Local CO_2 supply chains* • *National CO_2 regulations* • *Comparing multiple product applications, comparing best resource use of CO_2, H_2, electricity*

Principles of goal definition

Following the principles of LCA, goals of TEAs shall state clearly and unambiguously:

- the study context, especially comparison to what, location, time horizon, scale and involved partners
- the intended application and reasons for carrying out the study *(e.g. decision support for R&D funding allocation, investment decisions or policy and regulation; methodological studies)*
- target audience *(e.g. R&D experts, funding agencies, investors, corporate management, policy makers, NGOs, journalists, the public)*
- commissioners and authors of study *(e.g. funding organisation, university, company, individual)*
- limitations in the usability from assumptions or methods *(e.g. time, location or specific use cases of the products)*

B.3.2.3 Further reading

Goal concepts and definitions of LCA are described briefly in ISO 14044:2006[3] and in more detail in the ILCD Handbook – these can be easily related to TEA studies.[4]

B.3.2.4 Guidelines

Guideline B. 1 - Goal definition	
Shall	1) State the study context (especially comparison to what, location, time horizon, scale and involved partners) 2) State the intended application and reasons for the study 3) State the target audience for the study 4) State commissioners and authors of the study 5) State limitations in the usability from assumptions or methods
Should	1) State the intended TEA perspectives (R&D, corporation, market)
May	

B.3.3 Assessment scenarios

B.3.3.1 Introduction

Scenario analysis is the process of considering scenarios for evaluating potential future events. Scenarios are alternative, though not equally likely states of the world, that represent plausible conditions under different assumptions; whether or not the scenario is plausible depends on the study context. Scenarios and scenario analysis present a creative and flexible approach to support coordinated decision making with long-term consequences. The practitioner can design the scenario according to his or her need. However, scenarios are not forecasts, predictions or representations of the most likely future conditions; they are not based on empirical evidence. The insights from scenario analysis are limited by the underlying hypothesis and bias. This is why when using scenario analysis, practitioners should analyze and communicate uncertainty clearly to stakeholders [5], [6].

A common scenario for setting the baseline of analysis is the “base case” scenario, a potential future where current trends continue to exist *(e.g. absence of carbon pricing)*. Additional scenarios to the base case should test limits of an unknown future and question the base case scenario *(e.g. presence of carbon tax, low carbon technology subsidies or tax benefits, cap and trade scheme with low or high prices)*; the most surprising scenarios can end up providing insightful information. Various processes of creating scenarios are described in literature, some can be found in the further reading (see B.3.3.3). First and foremost, scenarios have to be created distinct and physically but also economically plausible. The combination of qualitative and quantitative techniques and close involvement with stakeholders help to create more robust, diverse and relevant scenarios. As each new scenario can create additional insight but also leads to additional effort, the creation of three to five scenarios is recommended in the literature; the final number is subject to the practitioner’s judgement. To make more efficient use of research time and budgets, practitioners are encouraged to report, discuss and share scenario data more openly [5], [6].

B.3.3.2 How to define scenarios for CCU assessments

As TEA studies are supporting decision making with long-term implications, especially for CCU products that often require substantial investments, scenario analysis is a useful approach. TEA scenarios can either be defined in the initial goal phase or when having reached the interpretation phase where key data for improvement is identified and the study goal can be refined in another iteration (also see iterative approach in inventory B.5.2 and interpretation B.7.2).

If scenario analysis is applied, all scenarios used for analysis shall be distinct and physically as well as economically plausible. Scenarios used should alter factors accounting for dynamic changes *(e.g. analysis of various competing technology developments or consequences of large-scale technology adoptions, analysis of different potential states in future markets and regulation or societal acceptance)*. The base case scenario shall serve as a baseline for analysis extending current trends in terms of technology performance, sales prices and volumes as well as policies and acceptance. Scenarios shall be developed in interaction with the stakeholders of the study, to ensure they remain relevant to the audience. Scenario assumptions and data should be provided at open access to facilitate future work. The analysis and reporting of uncertainty for each scenario is important and is further described in the interpretation and reporting chapters (see B.7.2 and B.8.2.6).

If TEA and LCA are integrated, the same set of scenarios shall be used. The LCA guidelines offer four scenarios (status quo, low decarbonized, high decarbonized, full decarbonized), which can serve as a helpful starting point for scenario definition (see LCA guidelines, Annex 10.1).

B.3.3.3 Further reading

- Guidance on scenario development and planning: Liu et al (2008),[7], Mahmoud et al. (2009),[5], and Amer et al (2013), [6].

B.3.3.4 Guidelines

Guideline B. 2 - Assessment scenarios		
Shall	1)	Scenarios used shall be distinct and physically as well as economically plausible
	2)	Scenarios used should alter factors accounting for dynamic changes
	3)	The base case scenario shall serve as a baseline for analysis extending current trends
	4)	Scenarios used shall be developed in interaction with the stakeholders of the study
	5)	If TEA and LCA are integrated, the same set of scenarios shall be used
Should	1)	Scenario assumptions and data should be provided at open access
May		

B.4 Scope

B.4.1 Introduction to scope

Building on the goal, the assessment scope describes what aspects of a product will be assessed and how it will be compared to competing solutions. The scope concept used in these TEA guidelines is based on LCA methodology but adapted and extended to the economic perspective. The TEA guidelines introduce the functional unit concept for TEA, as well as a maturity-based selection approach for indicators and methods.

Major activities in the TEA scope phase are identifying the subject of analysis (product system) and how it is compared to other systems (functional unit), further specifying the system (system elements), defining what is included and excluded from the assessment (system boundaries), selecting systems for comparison (benchmark systems), understanding how far the technologies are from market-entry (technology maturity) and what measures are used for comparison (assessment indicators). From the assessment scope, the requirements for the inventory phase, for example for data quality, but also for the reporting phase are derived [3], [4].

CCU-specific challenges in the scope phase are that many CCU products provide a similar but not identical performance compared to benchmarks products *(e.g. in the case of materials a varying molecular structure leads to different behavior compared to conventional solutions, providing a sufficient or possibly even improved performance in a certain application)*. This is why in many cases CCU researchers and developers try to match the CCU product's performance to the existing standards, aiming on an at least similar or even improved performance. Moreover, CCU products can provide several applications for different markets, for example as a building block for chemicals or for fuels or as electricity storage, requiring cross-sector analysis.

To enable the future integration of TEA and LCA, key terms product system and functional unit will be adopted from ISO 14040 and the ILCD handbook and further defined in the next chapters.

B.4.2 Product systems and functional units

B.4.2.1 Introduction

For the purpose of this document, the term ‘product’ describes goods, services, events or a combination of the prior that are object of analysis for the TEA study *(e.g. coating for outdoor walls)*. Each product can have multiple applications, meaning the purpose or value proposition *(e.g. purpose for outdoor walls coating can be weather protective or decorative)*. Based on the assessment goal, the relevant applications of a product system are selected. This selection depends on the number of applications and their dependency on each other. Applications can be further defined by market segments *(e.g. graffiti art or home renovation)*.

The term 'product system' refers to all processes required to provide the product involving one or multiple processes across one or multiple stages of the life cycle *(e.g. the production, application, use and disposal of coating for outdoor walls)*. The product system can have one or multiple output flows, also called co-products or by-products.

The ‘basis of comparison’ and the ‘functional unit’ describe the qualitative and quantitative aspects of the product’s performance to make it comparable for different alternatives, covering the “what”, how much”, “how well” and “for how long” *(e.g. decorative coating for home renovation of 1 m^2 outdoor wall at 90% opacity over 10 years)*. The ‘reference flow’ describes the flow to which all other input and output flows are set into relation with *(e.g. 25l bucket of paint, mass of paint required for renovation of one average residential house)*. Note that for a product system with multiple output flows, a functional unit can also have multiple reference flows. The basis of comparison and the functional unit are derived based on the product application. All three, basis of comparison, functional unit and reference flow, enable a systematic comparison.[4]

Further description on these concepts common for LCA can be found in further reading. Please note that in LCA the term 'function' is used for both, products and product systems; in LCA, 'multifunctionality' can mean that a product has multiple applications or that a product system has multiple outputs.

B.4.2.2 How to define CCU product systems and functional units

CCU product systems and their functions

In general, the product application shall be defined according to the study goal and documented clearly in the assessment report. Potentially, CCU products can provide applications other than similar, conventional products *(e.g. carbonation of mineral slags serves the function of waste treatment but also creates aggregates for cement)*. Cross-sectoral analysis facilitates the identification of these additional applications of CCU products that contribute to industrial symbiosis. If desired, multiple applications may be assessed and compared against each other *(e.g. comparing the use as chemical or as fuel)*, following the guidelines for each application individually.

Also for CCU products, the definition of product applications depends on how many applications exist. For products with a small number of applications, one relevant application should be defined *(e.g. fuels for transportation, polyols for foams)*. For base chemicals, materials or other products with a large number of applications or where the application cannot be specified, the product itself should serve as the application *(e.g. methanol, or carbonate aggregates).* In this case, it is important to include a detailed description of the product *(e.g. molecular structure and properties)* to increase transparency and comparability of the study. Furthermore, the definition of product applications is subject to their dependency. If multiple applications can be carried out in parallel (either by itself or in combination), a relevant 'application-mix' should be defined *(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).* If only one of multiple applications can be carried out at a time, including only one application in the assessment is sufficient *(e.g. polyols for flexible or rigid foams, energy storage for household-scale or grid-scale)*.

The product applications should be defined specific to the market segment as it is recommended to compare products with equal performance, such as comparing high-quality products to other high-quality products. Comparing products with different performances is possible in TEA but requires a good understanding of price-performance correlations *(e.g. market segments: low carbon footprint, commodities and specialities)*. As the customers and users are in the focus of corporate-perspective TEAs, they should additionally include a description of at least one customer group and their needs, which helps to understand the customer priorities for an application and facilitates product research, development and deployment. Customer needs can be classified into essential, desirable and useful.[8] Fulfilling all essential user needs is obligatory for customer acceptance. Fulfilling desirable user needs can provide a competitive advantage. Examples of CCU product system functions and market segments are listed in Table 3.

Table 3. Examples of CCU product system functions and segments (not exhaustive)

CCU Class	CO_2-based fuels	CO_2-based chemical products	CO_2-based material products	CO_2-avoidance
Product system function	Fuels for efficient and clean transportation	Methanol for chemical production	Polyols for flexible foams Waste treatment for industrial ashes	Lowering CO_2 emissions of another process (e.g. cement or steel)
Market segment	Fuels with low NO_x/soot emissions or heavy duty vehicles	Chemicals with low carbon footprint	High-quality flexible foams for mattresses Low-quality aggregates for low cost concrete	Large-scale CO_2 avoidance for steel plants Small-scale CO_2 avoidance for biogas plants

Functional units and reference flows

Defining the functional unit shall be conducted by the good judgement of the practitioner and needs to be convenient for the TEA. The definition of functional units in CCU depends on product properties and the number of applications. For chemical, material, fuel or energy storage products with the same chemical structure, composition or characteristics as benchmark products ('substitutes') the functional unit shall be defined on a mass or energy basis. For products with a large number of applications or unspecified applications *(e.g. base chemicals, materials, fuels)*, the functional unit may be defined as the output of a conventional plant, however scale that was used to generate the data needs to be consistent with the scale of the plant *(e.g. annual output of 1,600,000 t methanol per year for 10 years).*

For products with a structure or characteristics different to benchmark products ('non-substitutes'), the functional unit shall be derived from the product performance *(e.g. compare performance of new, structurally different material to existing materials, compare performance of new power storage device with different characteristics to existing solutions)*. The reference flow can be expressed either in a functional unit oriented way *(e.g. 1 kg of polyol)* or in a product oriented way *(e.g. per mattress)*.[4] If the TEA study is conducted together with an LCA, the functional unit shall be consistent for both studies. For examples see Table 4.

Table 4. Examples of CCU substitutes, basis of comparison, functional units and reference flows

Properties **CCU Class**	**Substitutes** Chemical products	 Material products	 Fuels	 Energy storage systems	**Non-substitutes** All
Basis for comparison	Mass	Material performance	Energy	Storage performance	Service or performance provided
Functional unit	*e.g. mass, plant output*	*e.g. mass, plant output*	*e.g. energy, mass, plant output*	*e.g. energy, plant output*	Compare performance of new to existing solutions
Reference flow	*e.g. 1 t methanol, 1,6 Mt/a plant output*	*e.g. 1 t concrete, 50 kt/a plant output*	*e.g. 1 MJ of H_2, 2,5 Mt/a diesel output*	*e.g. storing 1 MJ of electricity, 80 MWh battery*	*e.g. 1 t, 1 MJ, output of conventional plant*

B.4.2.3 Further Reading

The concept of function is described briefly in ISO 14044:2006,[3] and in more detail in the ILCD Handbook.[4]

B.4.2.4 Guidelines

Guideline B. 3 - Definition of product systems and functional units	
Shall	1) The product application shall be defined by the good judgement of the practitioner following these principles: a. For products with the same structure, composition or characteristics as benchmark products, the functional unit shall be defined on a mass or energy basis b. For products with a structure or characteristics different to benchmark products, the functional unit shall be derived from the product performance 2) If the TEA study is conducted together with an LCA, the functional unit shall be consistent for both studies
Should	1) The definition of the product application should further follow these principles: a. For products with a small number of applications, one relevant application should be defined; for a large number of applications, the product itself should serve as the application b. If multiple applications can be carried out in parallel, a relevant application-mix should be defined c. The product application should be defined specific to market segments 2) Corporate-perspective TEAs should include a description of at least one customer group and their needs
May	1) The definition of the product application may further follow these principles a. Multiple product applications may be assessed and compared against each other, following the guidelines for each application individually b. For products with a large number or unspecified applications, the functional unit may describe the output of a conventional plant

B.4.3 Product system elements and boundaries

B.4.3.1 Introduction

For the purpose of this document, the term 'system element' describes a key activity of the product system that can be a unit process, a unit operation or an equipment. The identification of system elements facilitates the definition of system boundaries, the structuring of the inventory and interpretation as well as the reporting of results. For example, for interpretation, the most crucial system elements can be identified by sensitivity analysis and uncertainty analysis, or for reporting, results can be reported for each element individually, making TEA studies more transparent.

The 'system boundary' defines the limits of the product system and describes which system elements belong to it. Material and energy flows crossing the system boundary are referred to as 'input flows' and 'output flows' (see Figure 2)[4]. A product system can have one or multiple input or output flows *(e.g. co-products or by-products, waste streams, various feedstocks for algae, various inputs for waste treatment)*, the latter are often referred to multifunctional product systems or 'multifunctionality'. System boundaries can be defined for product systems and benchmark systems and are derived from the assessment goal and product functions. System boundaries allow for a transparent and process-based comparison of the product and benchmark systems. System boundaries set the basis for reviewing what's included in a TEA study and for comparing different TEA studies with each other. It is crucial that system boundaries are consistent throughout the study.

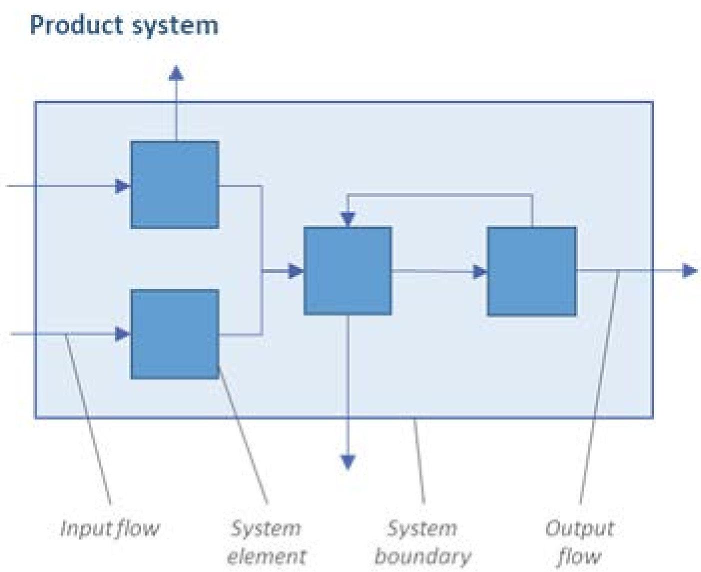

Figure 2. An exemplary product system with its elements, boundaries, input and output flows

B.4.3.2 How to define elements and boundaries for CCU product systems

Deriving CCU system elements

When defining system elements, choosing an appropriate level of detail is crucial. Process units shall be used as basis for system elements *(e.g. electrolysis, CO_2 capture, methanol synthesis)*. If required by the assessment goal, the system elements may be further refined as unit operations *(e.g. reaction, distillation, adsorption, membrane filtration)* or even unit equipment *(e.g. pump, reactor vessel, rectification column).*

The assessment should not only be carried out for the overall product system in an overall manner, but for each system element individually, meaning that each system element should serve as the accounting unit for inventory, calculation, interpretation and reporting. Recommendations for future improvement at the system element level should be included where relevant. For example, if the product system contains an electrolyzer (system element), the relevant energy and mass flows and cost should be collected, calculated, interpreted and reported for the individual electrolyzer unit and a break-even cost and operating hours could be calculated.

Deriving CCU system boundaries

Overall, the system boundaries shall be consistent with the TEA goal and perspective. The TEA system boundaries can be derived from two points of views: from the perspective of the study and from whether the product is a substitute.

TEAs with an R&D or corporate perspective typically focus on product development and market introduction, which is why they tend to draw the system boundaries around the activities of a real or imaginary company (gate-to-gate). This resembles the cradle-to-gate approach in LCA, where all impacts from resource extraction to the factory gate are taken into account (see LCA guidelines, chapter 4.2.1); in the case of TEA one could argue that the resource extraction impacts are represented by the input prices. TEAs with a market perspective can, however, draw the system boundaries around a whole value chain involving multiple companies or also governmental organizations, potentially spanning from resource extraction ('cradle') and upstream processing to downstream processing, use phase and disposal ('grave'). Such cradle-to grave system boundaries are suited to analyze the full cost for society, but also the benefits for and the power of each player in the value chain. Such cradle-to-grave system boundaries are especially relevant for policy-maker audiences.

Furthermore, the system boundaries need to be consistent with product properties. For substitutes, the use and disposal phases are likely to be the same as in benchmark systems; a gate-to-gate approach is therefore sufficient. In other cases, where the structures do not match with benchmark products (non-substitutes), any TEA assessment with gate-to-gate boundaries should include price-performance correlations to benchmark products that need to be available in sufficient quality. If these correlations are not available, the boundaries should be extended to properly account the technologic and economic implications for further processing steps, use or disposal phases to cradle-to-grave (also see LCA guideline, chapter C.4.2.1).

While cradle-to-grave boundaries are currently not common practice for TEA, they may be used to align a TEA study with an LCA study; cradle-to-grave boundaries may also be used if required by TEA audience or goal. If the intention is to integrate economic and environmental assessment, the system boundaries shall be derived from the LCA boundaries guidelines (especially in the case of multifunctional processes); also see Figure 3 for different boundary possibilities.

The approach of Life Cycle Costing (LCC) can be helpful when extending the boundaries to cradle-to-grave [9]–[11]. However, some challenges remain for using LCC: a large freedom of approaches and the low importance of profit. The large possible variety of LCC approaches leads to a reduced comparability of the resulting studies; for example, LCC can take a customer, producer, investor or governmental perspective and can focus on a project life cycle or a product life cycle. Especially for research and development-stage CO_2 utilization, a product or process-based approach is however recommended. A related challenge from a TEA perspective is LCC's strong cost focus, leaving not only technical feasibility aside, but also revenue and thereby all profit related indicators or criteria – the major driving force of all business and investment decisions. Recent discussions of integrating LCC and LCA exist, which could be helpful when addressing an integrated techno-economic-environmental assessment study with cradle-to-grave boundaries (see [11]–[14]).

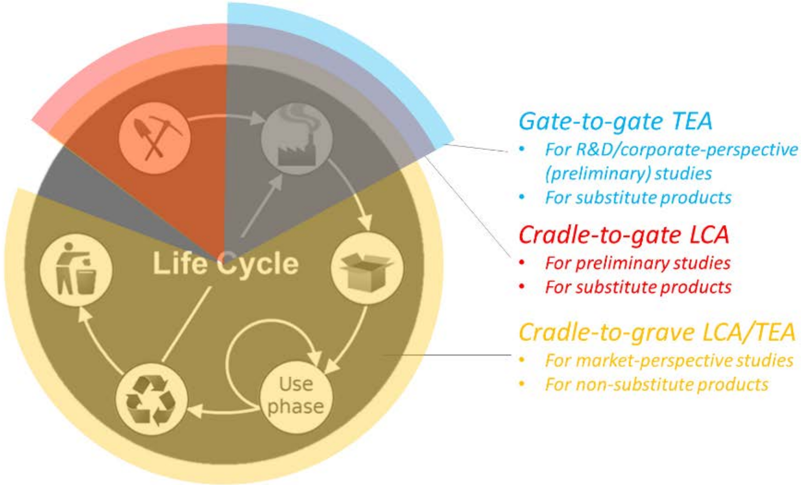

Figure 3. The scope of TEA and LCA in the product life cycle, adapted from [15]

Including or excluding CCU upstream processes in system boundaries

A common question for CCU product systems is to whether include or exclude CO_2 capture, separation and transport processes. Other common important upstream processes can be H_2 production, electricity production and many more. For examples see Table 13 in the Annex (list is not exhaustive).

The decision whether to include or exclude a process upstream or downstream shall be made for each process individually and shall not be taken to improve results, but based on the assessment goal, material and energy flows as well as on data requirements and potentially the audience or stakeholder perspective. If TEA and LCA studies are conducted in parallel, CO_2 capture, separation and transportation shall be included in system boundaries (see LCA guidelines chapter 4.2); other upstream processes shall follow the LCA principles. In the case of an independent TEA, an upstream process shall be included in the system boundary, if it is within the focus of the assessment goal, if it is required for linking other system elements, *(e.g. steel plant flue gas emission is linked by flue gas treatment to a CO_2 utilizing process)*, or if it significantly contributes to uncertainty of the results.

Following the iterative approach in data collection (see chapter B.5.2), it might be that an upstream process is excluded at first, but added to the analysis later, when their strong contribution to uncertainty becomes apparent. If an upstream process is excluded from the final system boundaries, the practitioner shall include an explanation of the reasoning. The exclusion of upstream processes in TEA does not mean that the economic impacts are not accounted for, but that process-specific technical and economic data is replaced by average or generic data. Therefore, the exclusion of upstream processes cannot result in input flows with zero cost, as it is unlikely that CO_2 or H_2 or electricity are provided without charge. For example, if CO_2 can be economically used, they gain in value for the CO_2 consumer and the emitter will demand compensation; if CO_2 emissions are fiscally penalized, they create an additional burden for the emitter, and the CO_2 consumer will demand compensation for consumption.

Multifunctional product systems

For product systems with multiple functions, relationships and dependencies between functions should be taken into account. When applications are dependent on each other and have to be carried out at the same time, it is necessary to include all dependent functions in the assessment *(e.g. by-products of water electrolysis – both, hydrogen and oxygen, need to be included; side products of a chemical reaction – all outputs need to be included).* Multifunctionality can be challenging if the outputs of the product and benchmark systems do not match. Multifunctionality is crucial for TEA studies individually and when TEA studies are integrated with LCA studies, especially for setting the system boundaries and creating the inventory (see TEA Guideline chapter B.5.3.2 and LCA Guideline, chapter 4.3).

Presentation of system elements and boundaries

Product systems, their elements and boundaries shall be presented in a graphical scheme (see Figure 2 or worked examples). Furthermore, the required specifications for all input flows shall be described, including mass flows and their composition, energy flows, temperature and pressure.

B.4.3.3 Further Reading

Principles of Life Cycle Costing are described in the following publications:

- Standards: ISO 15686-5 [11], ISO 15663, DIN EN60300-3-3, VDI Guideline 2284, VDMA Unit Sheet 34160
- Book: Life-cycle costing: a Code of Practice (98 pp.), SETAC Press [13]

B.4.3.4 Guidelines

Guideline B. 4 - Definition of system elements and system boundaries		
Shall	1)	Product systems, elements and boundaries shall be presented in a graphical scheme and specifications for all input flows shall be described
	2)	Process units shall be used as basis for system elements
	3)	TEAs for CCU shall at least comprise the key production steps of a real or imaginary company (gate-to-gate)
	4)	The system boundaries shall be derived from the assessment goal and shall be consistent throughout the study
	5)	The decision whether to include or exclude a key process upstream or downstream should be made for each process individually and key processes shall not be included or excluded to improve results
Should	1)	System elements should serve as the unit for accounting and recommendations
	2)	For non-substitute products, any gate-to-gate assessment should either include price-performance correlations or should be extended at least to the use phase
	3)	Key CCU processes, such as CO_2 capture, separation and transport, should be included in the assessment
	4)	For product systems with multiple functions, function dependencies should be taken into account
May	1)	Wide boundaries may be used to align a TEA study with a LCA study or if required by audience or goal

B.4.4 Benchmark systems

B.4.4.1 Introduction

The term ‘benchmark product’ describes products other than the one in focus, providing the same application; the product systems of benchmark products are further referred to as ‘benchmark systems’. The term ‘benchmark’ has further meanings: it is used to describe a benchmark product with the best evaluation result (here referred to as ‘best in class’ benchmark product) or it is used for describing a characteristic, preferably quantitative variable of a benchmark product (here referred to as ‘benchmark value’).

The term ‘substitute’ describes a product not only that provides the same application as the benchmark product, but also the same performance, which requires an identical, chemical structure and composition for chemical or fuel products and the same characteristics for energy storage systems. The term ‘non-substitute’ is used for products that potentially provide the same application but with a different performance.

B.4.4.2 How to define benchmark systems for CCU products

Benchmark product systems can have varying technologies *(e.g. CCU fuels can be produced in thermochemical, electrochemical, biochemical or photochemical pathways)* and belong either to existing technology regimes *(e.g. CCU methanol compared to conventional methanol)* or to new ones *(e.g. transport by CCU fuel vehicles compared to transport by battery electric vehicles)*. Essential for identifying and selecting relevant benchmark products is a good understanding of the product application (see B.4.2).

Benchmark products (and services) and their benchmark systems shall be selected according to application and assessment goal. The defined customer needs should be used to identify whether the product achieves utility for the customer and where it might have a competitive advantage. The currently most common or best in class products shall be selected as benchmark products; one or multiple products can be selected *(e.g. comparing a CCU material with three materials available on the market).* In addition, benchmark products that might be relevant in the future should be additionally included in the assessment *(e.g. extending the prior comparison by two promising future material concepts)*. Please note that if the time horizon of the assessment goal is in the future, learning curves and improvements have to be included for the product as well as the benchmark systems (see B.5.3.2 and B.6.3.2).

B.4.4.3 Further Reading

Principles and concepts for chemical product design can be found in [8]. Approaches on challenges in marketing such as market segmentation or identification of benchmarks are for example explained in detail in [16].

B.4.4.4 Guidelines

Guideline B. 5 - Definition of benchmark systems		
Shall	1)	Benchmark products and benchmark systems shall be selected according to the product application and assessment goal
	2)	The currently most common or best in class products shall be selected; multiple benchmark products can be included
Should	1)	Customer needs should be used to identify utility and competitive advantage
	2)	Benchmark products that are likely to become relevant in the future should be included

B.4.5 Assessment indicators

B.4.5.1 Introduction

In the following, ‘criterion’ is referred to as a parameter in decision making *(e.g. profitability)*, ‘indicator’ is referred to as a representative measure for a criterion *(e.g. net present value)*, whereas ‘method’ is referred to as the way of generating an indicator *(e.g. equation for net present value)*. The choice of criteria, indicators and corresponding methods for a TEA study is derived from the goal of the study and from the maturity of the product system.

In TEAs, comparison of product systems and decision making are typically based on multiple criteria and indicator types in the area of technology and economics (‘techno-economic’) *(e.g. energy efficiency of a process, NPV of a new plant, price per km driven, cost of kWh stored, cost per tonne CO_2 used).* Please note that the combination of environmental and economic criteria is also possible, but requires an integration of TEA and LCA. Enviro-economic criteria and indicators are discussed in Section A: wrapping section.

Both, an internal company and external market view need to be included in a TEA *(e.g. considering the internal processing cost as well as the sales price defined by the external market)*; analyzing product systems purely on an internal cost basis is not sufficient. While a range of economic criteria exists (for examples see

Table 5), profitability is an economic criterion that uses aggregated indicators *(e.g. net present value)*, that combine other economic criteria such as cost and revenue.

B.4.5.2 How to select assessment indicators for CCU TEAs

Common indicators for TEAs in CCU

TEA results are difficult to compare as practitioners use indicators of their particular interest, leading to the effect that studies do not have a common indicator basis. This lack of indicator standardization was demonstrated for CCU TEAs, where a large set of different indicators is currently used to evaluate the same criterion and different methods are applied to derive the same indicator, representing a major obstacle for evaluating and comparing CCU technologies [2]. Example criteria and indicators are shown in Table 5.

Table 5. List of example criteria and indicators

Area	Criterion	Indicator examples
Technical	Energy demand	*Heat demand, cooling demand, electricity demand, primary energy demand*
	Energy efficiency	*Lower heating value efficiency, higher heating value efficiency, energy/exergy efficiency, CO_2 capture penalty*
	Mass demand	*Mass demand of individual inputs, mass of CO_2 converted*
	Mass efficiency	*Atom economy, yield, percentage of CO_2 converted*
Economic	Processing effort	*Operational expenditure (OpEx)*
	Investment effort	*Capital expenditure (CapEx)*
	Product margin	*Market-derived margin for product, company-internal margin*
	Product volume	*Market volume for product, company-internal demand*
	Resource availability	*Market volume for feedstocks, company-internal availability of resources, number of suppliers*
	Profitability	*Profit, net present value, internal rate of return*
	Profit/cost per functional unit	*Cost per kg benchmark product equivalent, cost per km, cost per MJ stored*
Techno-economic	Technology maturity	*Technology Readiness Level (TRL) regarding market introduction (Horizon2020 definition), company internal maturity rating*

As many TEAs apply TRL, OpEx and CapEx, using varying definition and equations for calculation, these three indicators and their methodological approaches are covered in the guidelines (for TRL see section A, chapter 4), for CapEx and OpEx see in sub-chapters B.6.3 and B.6.4). Further methods for calculating indicators are not presented as the preferences for criteria, indicators and corresponding methods largely vary between organizations and the final choice depends on assessment goal, available data and experience of the TEA practitioner. An overview of calculation methods can be found in the recommended literature listed in further readings. Indicators and methods can be selected from the list presented above, or from the pool of indicators used in similar TEA studies.

Selecting indicators based on assessment goals

The selected indicators shall be compliant with the assessment goal. Suitable indicators deliver information necessary for answering the questions posed *(e.g. select cost and revenue indicators for a corporate-perspective TEA)* and are accessible for the intended audience of the study *(e.g. detailed, technical indicators for researchers, aggregated indicators for politicians)*. As the goals for CCU TEAs relate to technical and economic questions, indicators from both fields should be included in the assessment. Depending on the assessment goal, either multiple indicators, or aggregated indicators may be selected to represent one criterion. Please note that aggregated indicators have to be used with caution if they require normalization and weighing. Weights reflect subjective choices based on quantitative or qualitative criteria (see B.6.6).

Selecting indicators based on technical maturity

The selected indicators and respective calculation methods shall be compliant with data availability, which is associated with technology maturity. Technology maturity *(e.g. TRL)* can provide an indication whether data is available and whether estimation methods can be used or have to be avoided *(e.g. approximated or measured energy demand for OpEx)*. With increasing maturity from research, development to deployment phases, process and economic data becomes more reliable and representative and estimation methods increase in quality *(e.g. energy demand can be estimated from reaction data at early maturity for a first indication, from simulated process data at mid-maturity for a more detailed indication, and from measured process data at high maturity for highly detailed indication).* For technical criteria and indicators, the level of technical and process detail increases with increasing maturity, for economic indicators the understanding of product, cost and market improves during development. Depending on the maturity simpler or more complex indicators can be chosen *(e.g. simpler relative profit vs. more complex dynamic net present value)*. Both technical and economic analysis become more and more reliable and representative as maturation progresses.

A TRL scale listing specifications for the chemical and industries is introduced in part A, chapter A.4.1 and presented in more detail in part B, Table 14 in the TEA guideline Annex. The use of economic indicators depending on the TRL scale from Table 14 is further discussed here. In the early research stage, the use of quantitative indicators is not meaningful; instead qualitative evaluation can be conducted, for example multi-criteria rankings [17], [18]. In later research stages, theoretical stoichiometry or laboratory experiments determine the mass balance, which makes the calculation of a static profit from product sales (revenue) and associated costs possible; costs can already include material and other cost items. Starting from early-stage process development, OpEx and CapEx can be included in the economic assessment. To allocate the overall CapEx to the product, it is divided by the project life time or recovery period and capacity [19]. Furthermore, the annual (static) profit of the product system can be calculated from the specific profit *(e.g. €/kg)* and the annual addressable market volume that is identified in market analysis. In addition, CapEx can be allocated to this sales volume. Starting from mid-stage development, first dynamic profitability calculations can be carried out. Starting from later-stage development, various technical options and market (entry) scenarios can be examined with dynamic calculations (for more detail see [20], for further discussion regarding indicator calculation see B.6.3 and B.6.4).

Indicators can either exclude or include changes over time, further called static and dynamic indicators. In the research phase, static indicators *(e.g. relative profit, static return on investment, static payback time)* are recommended as they do not require detailed data and are easy to calculate. However, they only provide a first indication and not an in-depth analysis. In the development phase, the market view is completed with the external projected sales volume in order to calculate an absolute profit. Furthermore, the product definition is accurate enough for the prediction of future revenues; dynamic economic indicators can be used. Plant optimizations or changes in capacity planning can be evaluated. In the deployment phase, dynamic indicators can be used at an even greater level of detail. Assessment can be refined to complex simulations of future economic activities prior to building a full-scale plant. At TRL 9, cost and profitability checks are carried out in conventional accounting.

B.4.5.3 Further reading

Cost estimates and profitability analysis in the chemical industry:

- Peters & Timmerhaus (2003) [21]

- Sinnot & Towler (2009) [22]
- Turton (2012) [18]

Selection of economic indicators in research and development:

- Sugiyama et al. (2008) [23]
- Patel et al. (2012) [24]
- Otto et al. (2015) [25]
- Buchner et al. (2018) [20]

The use of indicators in CCU TEAs:

- Zimmermann, Schomäcker (2017) [2]
- NETL, "Cost and Performance Metrics Used to Assess Carbon Utilization and Storage Technologies" (2014) [26]

B.4.5.4 Guidelines

Guideline B. 6 - Assessment indicators and methods		
Shall	1)	Selected indicators shall be compliant with the assessment goal
	2)	Selected indicators and calculation methods shall be compliant with data availability, which is associated with technology maturity
Should	1)	Both, technical and economic fields should be included in the assessment
May	1)	Aggregated indicators may be selected but have to be used with caution

B.4.6 Consistency and reproducibility

It has been observed that consistency and reproducibility are challenging for CCU TEAs and therefore it is suggested to follow the criteria of the ILCD handbook [4] with minor adaptions. These criteria have to be met during the scope, inventory and calculation phase.

B.4.6.1 Guidelines

Guideline B. 7 - Consistency and reproducibility		
Shall	1)	Apply methods and assumptions in a sufficiently consistent way to all processes, parameters and flows of the analyzed systems, including benchmark systems
	2)	Apply sufficiently consistent data regarding accuracy, precision and completeness
	3)	Document any inconsistencies. If significant, the inconsistencies shall lead to the adaption of the goal or shall be taken into account for interpretation and reporting
	4)	All selected methods for calculating indicators shall be described clearly, including why they were chosen
	5)	Document methods, and method selection a) *For public reports:* in an appropriate and transparent way that would enable another TEA practitioner to sufficiently reproduce the assessment and results b) *For confidential reports:* in a separate, confidential file that shall be made available to the critical reviewers under confidentiality
Should	1)	Apply system boundaries, methods and assumptions in a sufficiently consistent way so that results can be related to other studies by another TEA practitioner
	2)	Begin the documentation from the project start; documentation should be guided by reporting needs
May	1)	The assessment may include suggested ways or techniques to avoid pitfalls in assessment procedures

B.5 Inventory

B.5.1 Introduction to inventory

A substantial part of the work required for carrying out a TEA study is the creation of an inventory. The general approach to establish the inventory for product and benchmark systems covers five interlinked phases: quality requirements of data to be collected are defined, relevant processes are identified, technical data is collected, economic data is collected and data is documented (see Figure 4).

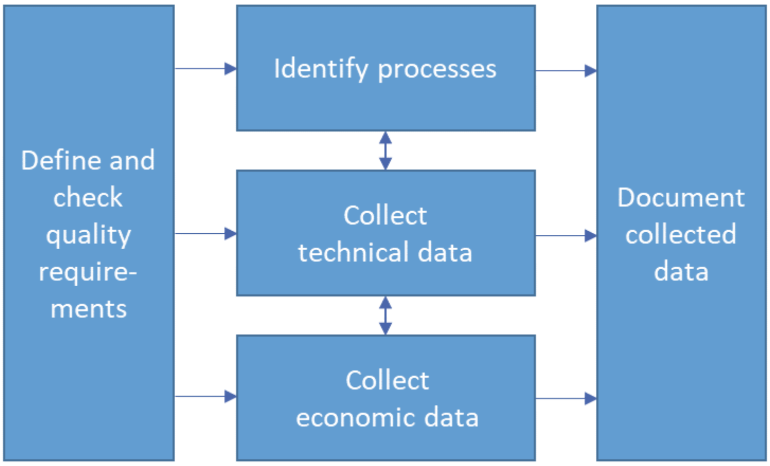

Figure 4. Five phases of TEA inventory creation

The identification of relevant system elements and their level of detail regarding flows and associated equipment is defined in the goal and scope phases. The existing process design as depicted by engineers in block flow diagrams (BFD), process flow diagrams (PFD) or piping and instrumentation diagrams (P&ID) provides information for the underlying processes. If TEA is conducted in parallel or following an LCA, technical data collected for the Life cycle inventory (LCI) might be useful for the TEA inventory. However, the level of required quality and detail of data for each system element might vary between LCA and TEA as determined varying goal and scope of assessment.

If data gaps remain in the inventory, they need to be filled by estimation otherwise indicators cannot be calculated. However, following an iterative approach, the setting of suitable quality requirements for each data set to be collected can help to reduce the effort as will be described in the following chapter B.5.2.2. Deriving economic data for the inputs CO_2 and other key inputs will be discussed in more detail within this chapter.

As a result, the inventory summarizes all relevant technical as well as economic parameters and assumptions of the product and benchmark systems, such as equipment, material and energy flows, transport or waste and their assigned prices and market volumes. Additionally, information about the context (temporal, regional, economic) of the studied scenario are collected and documented transparently to describe specific conditions of market, value chain and their limitations. The description of the specific context is highly important to ensure meaningful comparisons among studies.

B.5.2 Types of data and interim quality control

B.5.2.1 Introduction

Interim quality control helps to ensure consistency and reproducibility in the TEA study (see B.4.5 It is conducted in parallel to data collection and saves time and effort by verifying whether the required data quality is already achieved while collecting it. Data quality requirements and principles of data documentation have to be clear before collecting data. Consideration of the technology maturity is important to understand which data is available for TEA or needs to be estimated, as required by the selected assessment indicators. Different types of data (process-specific, average, generic) and their data sources (primary, secondary) exist. An iterative approach serves to selectively collect high quality data.

Types of data and sources

Different types and sources of data exist that are relevant for TEA as indicated by assessment goal [4]. The following three major types of data exist for TEA:

- ***Process-specific data***, measured data obtained from a known process (product-specific) or from partners within the supply chain providing access to their proprietary data, not derived from industry average *(e.g. published energy use of a real process, material prices from own supplier quotes, measured input flows or energy efficiencies and other technical process data documented in patents etc.)*
- ***Average data***, data reflecting industry average on the basis of reported measured data comprising several processes *(e.g. average CO_2 capture cost from data bases or literature reviews, average contents of typical steel plant flue gas streams, average transportation cost within a certain region etc.)*
- ***Generic data,*** data that has not been measured from an existing process but is calculated to reflect a typical scenario based on different assumptions such as stoichiometry, data from similar processes or expert knowledge *(e.g. simulated process data based on or validated by a similar water electrolysis unit, energy demand based on reaction enthalpies etc.)*

Each type of data described above can be collected either from a primary or from a secondary source:

- ***Primary sources,*** direct access to the original data is provided *(e.g. via process measurements, quotes from suppliers, descriptive examples provided in patents of respective process etc.)*
- ***Secondary sources***, access to data is provided via an intermediary source and data is not based on measurements of the respective process *(e.g. via similar patents, process engineering models, data bases etc.)*

B.5.2.2 How to control data quality?

Defining and checking data quality requirements

First, quality requirements shall be defined for each data point to be collected according to the assessment goal. Second, data quality shall be checked and documented during data collection. The aim is to substantially reduce time and effort by collecting high quality data sets only when these contribute sensitively to the TEA result.

Goal and scope define which system elements are included and at which level of detail each process needs to be analyzed. The required quality of the data generally increases with higher level of detail of the system element *(e.g. data for system elements only assessed at the level of a unit equipment generally requires higher quality than data only describing in- and outputs of a unit process)*.

Applying sensitivity analysis and uncertainty analysis

A standardized way of evaluating, how much influence a single data point has on the TEA result, meaning whether a certain parameter and its variations contribute quantitatively to the calculated indicator *(e.g. operational expenditures)*, is a sensitivity analysis, which is generally part of the interpretation phase (see detailed description in B.7.2). Running sensitivity analysis early on and in parallel to the inventory collection helps ensuring that data is collected in sufficient quality where needed. Data quality itself can also be evaluated in parallel by conducting uncertainty analysis (see detailed description in B.7.2). Requirements for data quality are defined by goal and scope and are strongly connected to the results of the sensitivity analysis, generally linking high sensitivity with high quality demand. Therefore, both analyses should be applied to characterize each parameter along the inventory collection, as is required for the iterative approach which will be explained in the next chapter.

Iterative approach for choosing relevant data types and sources

The practitioner should aim at collecting all relevant data available, which results from the corresponding technology maturity. At the same time focusing collection effort primarily on data with high quantitative contribution to the TEA results. Multiple iterations of data collection aim to reduce the overall effort by helping to identify and increase quality of significant data points only.

In each iteration, data types and sources should be chosen according to the quality requirements. In the first iteration, all data points are collected at lower effort allowing low data quality with the goal to identify the data points with high quantitative contribution. In the second and following iterations, the quality requirements and collection effort for these data points are raised *(e.g. to check the sensitivity of a CCU polymer TEA towards propylene oxide as input, a price obtained from open internet platforms could be sufficient as indication; in case of high sensitivity a second price could be obtained from a commercial price database; third, prices and predictions could be obtained from a market study including supplier price quotes)*. If data quality cannot be improved to a satisfactory level, the practitioner might not be able to answer the questions posed in the goal. Thus, assessment goal and scope should either be adjusted according to data availability, or the TEA study needs to be discontinued.

In general, with increasing maturity of the assessed process more process-specific and primary data should be used, as this data increasingly represents the projected process at the deployment stage. However, generic or average data from secondary sources should be used where sufficiently representative:

- Average or generic data from secondary sources that is readily available might be sufficiently representative in the first iteration of data collection to identify significant data points *(e.g. CO_2 capture cost or H_2 production cost derived from published studies on similar processes, Methanol cost from databases reflecting industry average, experience-based estimates etc.)*.
- Average or generic data from secondary sources might be sufficiently specific for unit processes that are not in the core of process development *(e.g. process units such as water treatment, flue gas treatment, transportation of goods etc.)*.
- Generic or average data from secondary or primary sources might be more representative over longer periods *(e.g. for costs that vary considerably over the years)*.
- Average data from secondary sources might be more relevant for market-perspective TEA *(e.g. price quotes from the producer might be primary data points with a high quality regarding a specific novel production process, however this technology specific price data might not be representative for your scenario if an average over multiple suppliers or mature technologies has to be accounted for)*

Data availability as a challenge in data collection

The technology maturity of a product system gives an indication, whether certain data points can be collected directly at high quality or need to be estimated to represent a plant ready for implementation. Incomplete data sets need to be sufficiently completed by estimation before these can be used for assessment. Based on the available data from the present technology maturity, the projected plant (TRL 9) is estimated. Data estimation to overcome large maturity gaps is especially relevant for CCU, where many new product systems at early technologic maturity are proposed and detailed economic data such as plant cost or market volumes are often unavailable *(e.g. at research and development, specific data regarding the process design and related costs is not sufficiently available; cost estimation methods enable the practitioner to fill data gaps to estimate the cost for a full-scale plant, which can further be distinguished between first of a kind, not including learning curves, or n^{th} of kind, including learning curves)*. Applying suitable cost estimation methods at early technology maturity poses a major challenge when assessing scale-up process models. In case there are no highly similar plants that provide reliable data, plant costs potentially need to be estimated in a bottom-up approach. A general overview of cost estimation methods and harmonization approaches required for calculation of TEA indicators will be presented in chapter B.6.

Confidentiality as challenge in data collection

Particularly in academic TEAs, practitioners face the problem of acquiring cost and market price data which are confidential to the technology providers or users, thus often causing incomplete data sets. Additionally, if industrial performance data and cost data is published, the underlying assumptions are often not clearly stated. This causes problems in transparency and credibility to the TEA practitioner, especially for more mature technologies.

The following recommendations facilitate data acquisition if confidential industry inputs are required by academia:

- Workshops with industry experts to comment on academic research and gather qualitative and quantitative input
- Collection and averaging of confidential data from several entities
- Providing relative relationships of data points instead of absolute data values
- Collection, anonymization and provision of data by a trustworthy third-party
- Selected exchange or publication of basic results of industrial process design and simulations

B.5.2.3 Further reading

Principles on selecting data types and a description of interim quality control and its elements is included in the ILCD Handbook [4].

B.5.2.4 Guidelines

Guideline B. 8 - Interim quality control and approximations	
Shall	1) Define quality requirements for each collected data set according to the assessment goal by applying sensitivity and uncertainty analyses of data points 2) Check and document data quality during data collection 3) Clearly state problems with acquisition of confidential data
Should	1) Conduct multiple iterations of data collection focusing on data with high quantitative contribution to the TEA results identified by sensitivity analysis to reduce overall effort; In each iteration, chose types of data and sources according to quality requirements 2) Use readily available generic or average data from secondary sources where sufficiently representative 3) Use process-specific and primary data with increasing maturity of the assessed process

B.5.3 Collecting data

B.5.3.1 Introduction

The collection of technical and economic data may be done in parallel or in consecutive steps. Economic information in form of costs and prices are related to collected or estimated technical flow data as well as equipment. Apart from cost data, market data such as sales volume and selling price are vitally important and are derived from market analysis.

As described, TEA and process design are strongly interlinked, as one motivation of TEA is to guide improvement of the whole process and single system elements. This means that by conducting a thorough TEA including sensitivity analysis the potential of improvement of single system elements can be identified, which is then fed back to process design for further development. A scenario analysis can serve to evaluate the potential impact of such identified future technology improvements regarding the overall economic benefit. A collection of data for each identified system element and the detailed documentation is required for analysis of single system elements to support further process design.

B.5.3.2 How to collect data in CCU projects

Technical data are obtained from process design with the level of detail being defined by the identified system elements *(e.g. material and energy flows, waste flows, equipment etc.)*. Collection of technical data includes all relevant technical process conditions as well as theoretical thermodynamic limitations of conversion steps to enable a transparent and meaningful assessment. Flow sheets, equipment lists and documentation of technical parameters are essential parts of technical data collection (see B.5.6).

Economic data such as prices or market volumes and cost for equipment can be obtained from a variety of sources and need to be related to the technical data *(e.g. price quotes for a reactor vessel from suppliers, country-specific wages from public databases or proprietary databases, sales platforms, cost of high-pressure steam based on expert estimates, literature values from similar published processes etc.)*. The acquisition of input and especially equipment prices poses the risk of non-standardized names, requiring the practitioner to carefully understand the process design to identify the right price *(e.g. different names for same items or, on the contrary, same name for different items)*. Other economic parameters which are relevant for cost estimation of a projected plant highly depend on the specific scenario *(e.g. considering the difference in location of original cost data and location of studied scenario)*. An example list of such parameters can be found in B.5.6.2. A more detailed explanation of the use and application of important economic parameters can be found in the calculation of indicators part (see chapter B.6). For processes of lower maturity overall uncertainty is generally higher and a detailed definition of certain parameters, such as cost of capital assumed when financing a plant, is less meaningful than for processes of higher maturity, where higher reliability of certain parameters is required. Note, that prices for material and energy flows can vary substantially depending on where these are sourced from, as should be clearly stated in the investigated scenario. In case of highly integrated plant infrastructure, company internal prices might be relevant, in other cases average market prices serve as good estimate. However, in general there are no free feedstocks and costs of some kind have to be accounted for.

When collecting technical and economic data from different sources, harmonization of the data points is required. If data might be time dependent due to expected technical development, price fluctuations or inflation/deflation, then the data should be selected from same years or should be adapted to the same year if possible and any other underlying assumption should be aligned. Also when selecting technical parameters, uniformity of the underlying information has to be maintained *(e.g. deciding on continuous use of lower heating value or higher heating value etc.)*.

Cost estimation methods

Generally, three main cost areas can be listed [20], [21], [27]:

- **Capital expenditures (CapEx):** Costs related to non-consumable parts *(e.g. investment into the production plant equipment, engineering cost, working capital)*
- **Operational expenditures (OpEx):** Costs for ongoing operation/providing a chemical product *(e.g. costs of all material and energy flows, labor cost)*
- **General expenses:** Costs that cannot be specifically allocated to a manufacturing operation *(e.g. cost for administration, marketing & sales or general research)*

Cost estimation methods need to be applied to calculate potential cost data of a projected plant, where real data is not yet available. The choice of the cost estimation method depends on data availability and requirements. Suitable methods can be found in widely accepted process design and economic assessment literature [18], [21], [22]. Additional information on methodological approaches to estimate cost data as part of CapEx and OpEx are described in chapters B.6.3 and B.6.4.

Sales prices and market volume

Besides collecting cost data from a process plant point of view, the estimation of sales prices and market volumes are essential for understanding profitability. Sales price and market volumes are derived from market analysis and are closely linked to the benchmark products.

For deriving sales prices of substitutes, a value-based pricing approach is recommended, meaning that the price of a product is set primarily based on the perceived value of the product or service to the customer. Prices for products usually are not static but are subject to certain dynamics, which need to be analyzed to understand profitability of new processes. Hence, a statement whether an average price or specific prices are selected is required. The sales price of substitutes can be derived from quotes of benchmark products. If these are not available, a cost-plus pricing approach can serve as an approximation. This means that the practitioner bases the price on all related costs of the product adding a constant amount as profit. Alternatively, and if available, the cost and assumed profit of a benchmark product can serve to estimate a price. However, this approach does not take into account the market value of the product. The sales price of non-substitutes can be derived from a market-specific price-performance ratio of benchmark products, if such is available. This ratio is defined by the performance and prices of benchmarks and the sales price is related to the performance of the product system.

The market volume for substitutes can be derived from the market volume of benchmark products. However, estimating the market volume for non-substitutes can be challenging. Market volumes of any known benchmark product can be used to derive the market volume of non-substitutes. Further limitations such as regions *(e.g. European Union, California, Port of Rotterdam)* or addressable market segments *(e.g. eco-savvy customers, high performance application)* or market growth rates may be added to the identification of market volumes.

Potential sources of secondary cost data

Table 6 lists some public as well as restricted sources for the collection of statistical and industrial cost data. Commonly, information from a variety of sources has to be combined in order to get the desired data point.

Table 6. Example sources of secondary and primary cost data

Source	Cost type	Region	Access
Euro-Stat Prodcom database	Statistical data on manufactured goods	EU member states	Open
U.S. Bureau of Labor publications	Cost of operating labor	US	Open
IHS Markit	Industry price data, market studies , business news	Worldwide and country-specific	Restricted
ICIS	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
Platts	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
Argus Media	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
Alibaba	Industry price data	China	Open
US Energy Information Administration (EIA)	Energy and energy carrier prices	US	Open
UN Comtrade Database	Customs/trade data	Worldwide and country-specific	Open
Zauba Technologies & Data Services	Customs/trade data	India	Open/Restricted
Alphasights	Expert interviews	Worldwide	Restricted

Description of technical and economic context

The consideration of temporal and regional context *(e.g. value chain characteristics)* as well as resulting limitations is necessary for the collection of meaningful economic inventory and the alignment to the predefined scope of the study (see B.4). Assumptions about market conditions, up and downstream processes defined by boundaries of the study and contextually specific parameters shall be justified by also describing and assessing expected risks and limitations, both for the base case scenario and any additional scenario *(e.g. regional requirements and restrictions, supply chain mechanisms and availability, time frame, scale and production capacity, availability of required investment etc.)*. A purely generic TEA not focusing on specific market conditions might result in non-representative results.

It should be assessed if sufficient access to the local value chain for both input material as well as product sales can be achieved. If prices or market volumes are estimated based on similar studies, a reasonable overlap between temporal and geographical conditions is required to not underestimate given limitations. Besides project specific risks regarding feedstock, also governmental regulations might strongly vary between locations and impact the feasibility of the TEA project *(e.g. subsidies on feedstock, taxes, site regulation etc)*.

Multifunctionality

Product systems can have multiple inputs or outputs. In LCA literature this can be a case of "multifunctionality" which is especially challenging when comparing product systems with different outputs. How to address multifunctionality in TEA depends on the perspective of the study and whether the TEA study is integrated with an LCA study or not.

If a TEA study is conducted independently of an LCA study, then indicators are often calculated for the whole product system and an accounting for individual functions may not be necessary, depending on the goal of the study. For some TEA studies, especially with a corporate perspective, the allocation of cost to each product function however might be a key question. If a TEA study is conducted together with an LCA study and integration of both studies is aimed for, solving multifunctionality shall follow the principles from LCA (see Wrapping Document A.5, and LCA guideline, chapter C.4.3). If TEA is not integrated with LCA, allocation can follow any principle that ensures meaningful results for the particular product system. A common approach for TEA is economic allocation. This means that the full cost of the studied product system can be allocated to each product function after deriving each product value either based on external sales prices from market or from company internal prices used for flows between business units *(e.g. derive relative CapEx of an electrolyzer for oxygen and hydrogen by the relation of the gases sales prices)*. However, economic allocation is challenging in case of highly uncertain prices and therefore needs careful consideration *(e.g. for intermediates without specific market value, for non-substitute products or for novel future products and processes)*.

B.5.3.3 Further reading

Additional information on types and acquisition of technical data from process design as well as widely accepted methods to acquire economic data can be found in basic process design literature, such as Peters & Timmerhaus (2003), Sinnot & Towler (2014), Turton et al. (2012), Smith (2016) [18], [21], [22], [27].

B.5.3.4 Guidelines

Guideline B. 9 - Collecting data	
Shall	1) Plan and prepare data collection according to data requirements, selected methods and indicators and overall assessment goal 2) The level of detail of the technical data shall follow the identified processes along the system elements 3) Describe temporal and geographic context of the TEA project including description of limitations and risks of location-specific market conditions and value chain 4) Relate technical and economic data to functional unit and reference flow where possible 5) If both LCA and TEA studies are integrated, then the same method for solving multifunctionality shall be applied
May	1) Allocation of cost may follow economic allocation 2) Add regions or addressable market segments or market growth rates to the identification of market volumes

B.5.4 Deriving a CO_2 price

B.5.4.1 Introduction

For many CCU-TEA studies, the price of CO_2 is a decisive factor for profitability, which is why calculation or estimation of CO_2 prices needs to be planned and executed carefully. Different approaches to derive the CO_2 price are reported in literature, calling for a clear documentation regarding CO_2 sources and purity, cost type or dependencies on location and regulation.

Typical pitfalls the TEA practitioner needs to avoid when selecting CO_2 prices in TEA of CCU are:

- Assuming zero cost for CO_2
- Assuming emission trading price or emissions tax as CO_2 price
- Assuming cost of CO_2 avoided instead of cost of CO_2 capture (for definitions see following paragraph “Cost of CO_2 capture and cost of CO_2 avoided”)

Cost of CO_2 capture and cost of CO_2 avoided

In the following, the terms ‘cost of CO_2 captured’ and ‘cost of CO_2 avoided’ are discussed in more detail.

The amount of CO_2 captured states the amount of CO_2 emissions that are separated and available for further processing in a plant with CO_2 capture. Cost of CO_2 captured relates all resulting cost of the capture process to the amount of CO_2 captured *(e.g. cost/$t_{CO2\ captured}$)*. The costs include all operational and capital expenditures of capturing CO_2 from flue gas or air over the whole life time of the unit. The cost of CO_2 capture shall be reported, otherwise a statement that this information is not available has to be included.

In contrast, ‘CO_2 emissions avoided’ states the difference in overall CO_2 emissions between a system with CO_2 capture and the reference system without CO_2 capture, including the additional emissions caused by the capture process, transport and potentially storage or production processes. The cost of CO_2 avoided (also being referred to as "CO_2 abatement cost") relates all resulting cost of the capture, transport and storage or production processes to the CO_2 emissions avoided *(e.g. cost/$t_{CO2\ avoided}$)*. The ‘cost of CO_2 avoided’ is a widely used measure from the field of CO_2 capture and storage (CCS). Note that, the capture and reference plant both provide the same functional unit, for example the amount of product. In literature, cost of CO_2 avoided is commonly used to report the capture portion only, effects of transport and storage are often excluded [28]. However, the IPCC recommends the calculation for the full system, including capture, transport and storage. In case of CCU systems, this full approach increases assessment complexity, as both the CCU system as well as the reference system would have to include the corresponding production processes for the desired product in the system boundaries. As defined by LCA (see LCA guidelines, part C), system expansion would be required, adding the benchmark process of the CO_2 utilization process to the overall reference system. Both ways of reporting CO_2 avoidance cost (capture only or full system) usually result in different values. Hence, the practitioner is required to carefully analyze any found information on cost for CO_2 avoided.

Generally the cost of CO_2 avoided tends to be higher than the cost of CO_2 capture as the capture requires additional energy, leading to increased emissions and thereby decreasing the potential emissions reduction [29]. To obtain results for overall CO_2 emissions, a life cycle assessment approach is required, underlining the strong linkage between LCA and TEA. The use of the CO_2 abatement cost as a combined enviro-economic indicator is further explained in the Wrapping Document, part A. If data for cost of CO_2 capture is not available, data for cost of CO_2 avoided may serve as a conservative approximation for the CO_2 price, when detailed documentation of the underlying assumptions is provided.

B.5.4.2 How to derive a CO_2 price

The CO_2 price and its calculation or estimation strongly depend on the system elements in the product system, meaning whether CO_2 source, capture process, purification, compression or transport are included or excluded from the assessment boundaries. If the CO_2 capture process is within the system boundaries, the cost of CO_2 capture shall be calculated by estimating required capital and operational expenditures of the system elements associated to capture, purification, compression and transport. Otherwise a suitable market price for CO_2 should be assumed. In order to find a suitable market price, it is recommended to consider nearby plants that have adequate CO_2 emission streams and consider average costs for capturing, compressing and transporting CO_2 at these plants. In case of highly pure CO_2 streams ready for use, capture is not relevant, and compression and transport are cost driving. Please note, only if no information about capture cost is available, commercial price quotes for CO_2 from industrial gas businesses may be used as conservative indication for the upper price limit.

Deriving CO_2 costs from literature

Generally, when considering published data on CO_2 costs, careful consideration of all underlying technologic constraints and assumptions made in the original publication is required, documenting not transparent or missing information *(e.g. assumptions regarding type and source of energy, statements whether costs of capture are for a single system element or for the full process etc.)*. Valuable information on CO_2 cost can be retrieved from academic literature studies as well as industrial and public sources. Depending on the scope of the TEA, focus can be on reports on specific emitting sources and capture technology or on aggregated reviews across multiple studies to estimate average costs. Information from renown (inter-)governmental or industrial organizations dealing with climate issues is relevant to complete data gaps and to validate any estimated data. Furthermore, such literature has higher chance to be updated in certain time intervals, thus providing information on how technology classes have matured in terms of cost performance. Information regarding current and future political instruments relevant for CCU technologies are also being discussed in above mentioned sources as well as in governmental media such as reports provided by political bodies.

When investigating literature about CO_2 cost data, both the research fields carbon capture and utilization (CCU) and carbon capture and storage (CCS) should be included. Note, that in literature both cost of CO_2 capture as well as cost of CO_2 avoided could be reported. Recommendations on how to deal with each cost type is provided in a dedicated paragraph further below. Following information sources are recommended to be included in the search:

- **Academic literature studies on CCU and CCS**:
    - Specific technology studies: Increasingly providing detailed data on CO_2 costs specific to CO_2 emitting source, capture technology, time frame, and location
    - Literature reviews: Listing, analyzing and comparing reported data on CO_2 cost from specific technology studies and studies on policy aspects effecting cost

    - Scientific conference and workshop contributions: Recent or so far unpublished data is potentially being introduced at scientific conferences or in reports of dedicated workshops
- **Literature from (inter-)governmental or industrial organizations dealing with climate issues:**
    - International Energy Agency *(e.g. IEAGHG Technical Workshop publications)*
    - Intergovernmental Panel on Climate Change *(e.g. Carbon Dioxide Capture and storage reports)*
    - Global CCS institute *(e.g. The Global Status of CCS annual report)*
    - Zero Emissions Platform - EU *(e.g. The costs of CO_2 capture report)*
    - National Energy Technology Laboratory - US *(e.g. carbon storage publications)*
    - United Nations Industrial Development Organization *(e.g. CCS – Roadmap)*
    - Other CCU based research projects and platforms

CO_2 emitting sources and costs

The CO_2 cost generally differs depending on the selected CO_2 source due to the varying CO_2 purity and purification effort of the stream. Careful investigation of the suitability of the available or assumed source is critical for the quality of the inventory. While some CCU production processes require high purity CO_2 streams as an input, others require less pure CO_2 streams. Since purification requires additional efforts, it has important impacts on costs, and CO_2 should therefore be considered in the lowest amount of purity that is technically necessary.

Many industrial CO_2 emitting sources exist, such as power plants, cement plants, steel plants, ammonia plants (see Table 7). Depending on sector and time as well as capture technology and final stream purity, reported CO_2 capture costs range between 5 USD and 180 USD per tonne of CO_2, or even higher for some sectors [28]–[31]. The open access database "EU Eurostats Prodcom" reports an average EU-28 market value for CO_2 of 0.078 EURO per kg of CO_2 in 2016 (division of the overall annual financial value of traded carbon dioxide by the annual sold volume in the EU-28 states in 2016) [32]. Any technology specific cost data presented in this document would outdate fast due to technology development. However, technology specific literature and review studies provide information on cost ranges for orientation. It needs to be emphasized, that before selecting any cost data from literature, careful consideration of the described source, underlying technology and publication date is required to align the information to goal and scope of the TEA. A selection of the most common CO_2 sources is presented in the following Table 7.

Table 7. Examples for CO_2 emitting sources to illustrate the span of different sectors potentially providing CO_2 streams of different purities

CO_2 emitting source *(according to producing sector)*
Power Sector (Coal, Lignite, Natural Gas)
Cement
Ammonia
Hydrogen
Iron and steel
Oil refineries
Ethylene production
Ethylene oxide production
Bioenergy
Aluminium production
Pulp and Paper

If goal and scope define a certain location, a location-specific CO_2 price shall be derived, otherwise a location-average CO_2 price is sufficient. Location-specific CO_2 prices are usually relevant for product systems including source type, capture and transport of CO_2 in the system boundaries, thus requiring data of locally available CO_2 emission sources. Location-average CO_2 prices are usually relevant for product systems excluding the specific source, capture process and transport of CO_2 from system boundaries, thus requiring data of averaged CO_2 cost from regionally relevant sources with average assumptions about transport cost.

A statement about the local proximity of the CO_2 source to the plant investigated for utilization should be made regarding potential transport cost. In most cases transport of CO_2 is connected to relatively high costs, especially if there is no dedicated infrastructure, such as a pipeline system, in place. Most likely, transport cost of CO_2 will decrease with growing proximity of the capture to the utilization plant. Further options that may be considered if there is no information available for capture from common emission sources are whether CO_2 will be purchased and delivered by an industrial gas selling company or whether direct air capture is applied.

Regulation and CO_2 price

This guide refrains from recommending the use of regulatory adjustments or cost lowering mechanisms in the base case of each TEA. Although specific examples of such mechanisms exist *(e.g. emission-trading-systems (ETS), carbon tax, global net emissions reduction scenarios from scientific models etc.)*, large regional differences as well as potential short-term future political decisions add to high underlying complexity. Including these mechanisms in the base case would decrease comparability between TEAs on CCU, which is therefore not recommended.

Instead, these may be considered for additional scenarios to the base case. Applying sensitivity analysis and uncertainty analysis on the effect of these mechanisms on the economic performance of the CCU process potentially reflects future development needs. Any assumptions made need to be justified in a temporal and regional context and carefully documented.

Steps for documenting the CO_2 price

As described above, boundaries defined in goal and scope indicate whether data shall be derived from process development or from literature reports on emitting sources and resulting CO_2 capture costs. In case of literature values, the choice of emission source should not be based on the lowest CO_2 price available without critically reviewing the underlying sources and capture processes, as these might cause higher environmental burdens compared to alternatives. In case of reported ranges of CO_2 costs for a specific source or capture technology, analysis is required regarding harmonization of underlying values and development state of reported technologies. For other scenarios than the base case the CO_2 price may be approximated by CO_2 avoidance cost or the CO_2 price may be adjusted by regulatory mechanisms such as emissions trading and emissions taxes or other CO_2 related subsidies or penalties.

The following underlying technological and economic information shall be documented:

- Process-specific or average prices
- For average prices: chosen CO_2 cost type (cost of CO_2 capture or cost of CO_2 avoided)
- Process specific capture technology
- CO_2 purity in obtained stream
- Captured stream flow rates
- CO_2 flow conditions (pressure, temperature) before capture and after capture and compression
- Capture technology base case and additional scenarios
- Regional restriction, reference year and applied transformation factors
- Inclusion of compression, transport and storage cost
- Underlying cost estimation methods and economic assumptions for CapEx and OpEx

B.5.4.3 Further Reading

An overview about CO_2 emitting sources and reported CO_2 capture cost as well as cost of CO_2 avoided is provided by Naims (2016), Zero Emission Platform (2011), Leeson et al. (2017) [29]–[31].

An extensive amount of literature exists on carbon capture technologies. Broader overviews of available and emerging capture technologies are provided by Smit et al. (2014), Wilcox (2012), Lackner et al. (2012), de Coninck et. al (2014) [33]–[36].

B.5.4.4 Guidelines

Guideline B. 10 - Deriving a CO_2 price	
Shall	1) Relate the CO_2 price to the assessment scope, especially to emission source and CO_2 capture technology 2) The CO_2 price in the base case shall represent cost of capture, compression and transport or a market price, at which CO_2 can be procured in adequate purity 3) Derive location-specific CO_2 price if goal and scope state a certain location, otherwise a location-average CO_2 price is sufficient 4) If assessment scope includes CO_2 source, capture, compression and transport the CO_2 price shall a. be calculated based on the full process b. be location-specific 5) If assessment scope excludes CO_2 source, capture and compression, the CO_2 price shall a. be collected either from a supplier quote or b. be estimated by considering a nearby CO_2 emitting plant flue gas stream with capture, purification, compression and transport 6) Document technological and economic assumptions 7) Report cost of capture and include statement if information is not available 8) Check and harmonize selected cost data or cost ranges from literature to ensure the use of adequate assumptions, such as same units, same year, appropriate scales, underlying boundary conditions etc.
Should	1) Select CO_2 source by considering CO_2 in the lowest purity and level of compression that is technically necessary and where transport requirements can be fulfilled 2) Consider local proximity of CO_2 source to utilization plant regarding transport costs
May	1) Apply regulatory adjustments (e.g. ETS) or cost-lowering mechanisms for additional scenarios other than the base case

B.5.5 Other key CCU inputs

B.5.5.1 Introduction

There is a considerable range of different key inputs for CCU technologies, besides CO_2, which will partly be introduced in the following chapters. Some typical CCU key inputs are electricity, hydrogen, mineral sources, fly ash, catalysts, fossil hydrocarbons, or microorganisms and culture media for bioconversion. There is no ranking of importance among the described inputs, as the practitioner collects the inventory according to the underlying process design and required data quality.

B.5.5.2 Hydrogen as input

For many CCU studies assessing the production of methane, synthesis gas as well as higher-value chemicals such as methanol, the price of H_2 is a decisive factor for profitability, which is why calculation or estimation of H_2 prices needs to be planned and executed carefully. Being strongly connected to energy input, H_2 generation can have both substantial economic and environmental impacts. When selecting the H_2

generation process, environmental trade-offs need to be considered and "green" H_2 generation should be favored by process design. For transparency, H_2 generation should be described systematically and in detail.

Typical pitfalls the TEA practitioner needs to avoid when deriving H_2 prices in TEA of CCU are:

- Assuming, unintentionally, an inexpensive hydrogen source with severe impacts in life cycle assessment, which results in an increase of overall CO_2 emission in the CCU process *(e.g. choosing an inexpensive, but high carbon emission hydrogen source)*
- Assuming free or negative electricity prices in the base case scenario
- Assuming H_2 from intermittent (dynamic) electricity sources without including impacts in the technologic feasibility or economic potential *(e.g, OpEx versus CapEx trade-off at different loads)*
- Assuming H_2 production scales for particular technologies, that are economically or technologically not feasible
- Assuming as base case an optimistic future scenario of H_2 generation

Present and future H_2 generation routes

Hydrogen is an essential input for the chemical and petrochemical industry today and can be produced by various processes, currently mainly from fossil raw materials. Production costs and therefore also the H_2 price significantly differ from process to process. Depending on the regional concentration of industrial sites, hydrogen production can either be located onsite or offsite. The user can produce hydrogen onsite for direct application either in dedicated plants as captive H_2, or as a by-product from other processes. Merchant H_2 is produced offsite by a H_2 supplier. An overview of current and future H_2 production technologies and estimated production costs can be found in technology roadmaps, such as provided by the International Energy Agency (IEA) [37]. The currently predominant H_2 generation processes are listed below (see Table 8).

Table 8. Hydrogen generation routes

H_2 generation route	Global market share 2014 [38]	Market
Steam methane reforming (SMR) large-scale	49%	mature
Partial oxidation or reforming of other hydrocarbons	29%	mature
Gasification of coal and biomass	18%	mature
Electrolysis of water - Alkaline	4%	mature
Electrolysis of water - Proton Exchange Membrane (PEM)	-	early

Additionally, many potential hydrogen generation technologies are under development, broadening the potential mid and long term portfolio, for example:[37], [39]

- Small-scale steam methane reforming
- Solid oxide electrolysis
- Photocatalytic water splitting (artificial leaf)
- Solar high temperature thermochemical cycles
- Methane pyrolysis
- Biohydrogen production (from bioderived liquids and microbial conversion)

The required energy for producing H_2 (calculated from the heat of formation) from fossil sources, biomass or water differs considerably, being much lower for hydrocarbons than that for water electrolysis.[40] This makes energy a major cost driver, especially for novel technologies. Although the use of electrolysis is increasing, especially with future efforts to shift towards renewable energies, it is likely that industrial hydrogen production will continue to be mainly based on hydrocarbons in the near future as energy prices and prices for hydrocarbons are currently strongly correlated. This statement does not take into account the level of environmental pollution caused by these technologies, making it crucial to consider environmentally friendly alternatives as H_2 source.

Besides local feedstock and electricity prices, main cost drivers for hydrogen production processes in terms of capital investment depend heavily on the pursued plant capacity and whether scale effects *(e.g. for SMR)* or modular systems *(e.g. for electrolysis)* are assumed. Depending on the distance to the H_2-source and given the infrastructure at CCU-plant, also transport and storage costs need to be considered.

Steps for deriving the H_2 price

In this document, no specific prices for hydrogen will be stated, as data will outdate fast due to technology development and dependency on input prices. In B.5.5.6 references to publications providing cost information for H_2 production technologies are provided.

Similar to the CO_2 price, the H_2 price shall represent cost of production or a market price. It is of high interest to consider the need for transportation and storage of H_2, as energy for compression and safety measurements for storage shall be reflected in the attributed costs. H_2 production and related processes *(e.g. separation, transport and storage)* should be included in system boundaries if economically significant *(e.g. in case of large demand of merchant hydrogen from offsite production)*. An analysis of local conditions is necessary to adequately provide information about prices, especially due to governmental regulations, and availability of the feedstocks needed for the multiple potential production technologies.

- If H_2 production is included in system boundaries, the H_2 price shall be calculated based on the full location-specific process
- If H_2 production is excluded from system boundaries, the H_2 price shall be collected either from a supplier quote or a location-average estimate, specific to the production route.
- H_2 transport and storage shall be represented in the H_2 price, independent of inclusion in system boundaries.

For the base case scenario, a current, mature H_2 generation process shall be selected. In additional scenarios, future, low-carbon-footprint H_2 generation processes should also be considered for cost estimation. Scale and maturity of the selected H_2 generation process shall be documented and discussed. Technological parameters *(e.g. process type, efficiency and operating time)* and parameters regarding energy sources and electricity prices *(e.g. cost type, time and location)* shall be clearly documented.

H_2 price from water electrolysis is strongly dependent on the price of electricity and on the selected type of electricity. If grid electricity mix is selected, cost calculation shall be based on an electricity spot price and H_2 generation utilization factor. If a specific electricity technology is selected *(e.g. for wind (onshore / offshore), photovoltaic, solar-thermal, nuclear, and other major low-carbon electricity generation technologies)*, cost calculation shall be based on intermittent energy supply or levelized cost of electricity (LCOE). The price of H_2 from Steam Methane Reforming is dependent on methane price, therefore cost calculation may be based either on methane spot or contract prices.

B.5.5.3 Consumption of electricity

Depending on the type of technology, the consumption of electricity might contribute significantly to the economic performance of the process. Some technologies contain energy intensive mechanical process steps, others require electricity as input for chemical conversion steps in the CCU process. TEA helps to identify where electricity is a cost driver *(e.g. by applying sensitivity analysis)*.

Electricity can be produced on-site or be acquired from the grid. The system boundaries defined by goal and scope then define, whether electricity production is included as system element and needs to be assessed based on process design or whether electricity is outside the boundaries and can be estimated via market price. The electricity price depends on multiple factors which need to be carefully defined and justified, such as location, production technology or mix thereof, type of electricity (intermittent or general supply), required infrastructure, taxes or subsidies. The importance of electricity for hydrogen production via electrolysis is discussed in chapter B.5.5.2

With CCU technologies bearing the potential of CO_2-emission reductions, also the choice of electricity source becomes vital in many CCU studies. Electricity from renewable resources is of particular interest as carbon neutral energy production can be achieved. However, the insufficient local availability as well as considerable production costs are current limitations. For reasons of comparability, the locally available electricity grid mix should be considered in the TEA, either in the base case or in an additional scenario. A clear documentation of the contained energy sources regarding both fossil energy carriers as well as renewable sources needs to be provided.

The prediction of future prices for electricity is highly challenging due to the complexity caused by differences in production costs after technology development or fluctuation of feedstock prices. However, there are extensive literature as well as publicly available sources listing current and local electricity prices as provided by the market and according to different technologies, that present spot prices or average prices and allow for deriving cost trends. Such information sources are for example:

- Eurostat - Energy database (European Commission statistics)
- US Energy Information Administration (EIA)

Note, that electricity cannot be provided entirely for free, as costs of production need to be accounted for. This means that the required capital expenditures *(e.g. wind turbines, solar-panels, other equipment etc.)* needs to be included in the cost. Therefore, any electricity price assumed in the base case should not be zero, whereas in additional scenarios, any price and its influence can be analyzed by sensitivity analysis.

B.5.5.4 Inputs for mineralization

For mineralization technologies, there are generally two main sources of feedstock: mined minerals (*e.g. olivine, serpentine*) and mineral wastes (*e.g. fly ash and steel slags*). Additionally, there are a number of technologies that use CO_2 for carbon curing, meaning the mixing of CO_2 into wet concrete while it is mixed to form limestone particles supporting the concrete. All pre-steps necessary to prepare the feedstock for use in the CCU process are potential cost drivers and of high relevance for technical and economic inventory collection. The required purity of the CO_2 input stream can be low as the presence of impurities such as NO_x has no effect on the carbonation reaction. Costs for additional inputs such has acids and bases as well as the disposal of resulting waste after carbonate formation need to be accounted for. The value and the market volume of the resulting carbonate products has to be carefully investigated within the temporal and regional context.

Main cost drivers for technologies requiring mined minerals are extraction of the mineral, transportation to the CCU plant, as well as further processing by energy intensive grinding and milling of the raw material to obtain the required particle size. Therefore, when collecting inventory, local proximity as well as quality of the raw material from the mining site should be considered. Transport and energy demand can be cost drivers and should be evaluated by sensitivity analysis.

For mineralization technologies utilizing waste material from industrial processes, transportation from the source as well as storage and further preparation steps are potential cost drivers. In addition, choosing CCU as alternative treatment of industrial waste might provide an economic incentive when certain country-dependent governmental regulations are in place, such as tax reliefs or other tailored subsidies. Part of inventory collection therefore is the investigation of the local regulatory context for the treatment of industrial mineral waste by CCU. Financial rewards of this kind can have a major effect on the overall cost performance of the process making it economically viable.

B.5.5.5 Further inputs

Fossil based organic starting material

If additional inputs in form of fossil based organic compounds are required for CCU technologies applying chemical conversion (*e.g. synthesis of polycarbonates via reaction of CO_2 and propylene oxide*), then the following considerations should be part of inventory collection. Prices of fossil based organic compounds are strongly dependent on the market of fossil resources, which is reflected by global crude oil and natural gas prices. Generally, there is the trend, that the closer the chemical is to the crude oil resource within the value chain, the closer will also be the market price. However, demand-supply relationships might result in deviating prices and always need to be considered as well. Also, the future availability of such fossil based organic compounds is depending the regional availability of their fossil resources, which can be subject to physical scarcity and political restriction. Hence, for collection of economic inventory, volatilities in price and risks concerning availability of sources shall be accounted for. Especially when looking at long term strategies for the assessed CCU process, potential scarcity of resources can have a major impact on profitability. Sources and methods for raw material price estimation are further discussed in chapter B.6.4. Any assumptions and justifications for fossil-based feedstock should be carefully documented.

Catalysts for chemical conversions

Metal-based catalysts (heterogeneous or homogeneous) are of major importance for many CCU technologies applying chemical conversion. At the same time these can be among the main cost drivers of the CCU process. Catalysts enable the activation of the chemical reactants and are critical for an economically feasible conversion. The design of suitable catalysts and the technical development of processes for the catalytic conversion are crucial research activities. The catalyst material production can be highly cost intensive, especially if it requires rare metals, expensive ligands or advanced carrier material. When collecting inventory, the catalyst input needs to be carefully considered, especially if future market prices are difficult to predict. This can be the case if large amounts of catalyst material are required that are not yet available in the market or are subject to strong price fluctuations. Furthermore, catalyst prices can be dependent on the maturity of novel production pathways as well as the necessity of entire new production facilities that would need to be built based on specific supply contracts. For cost estimation approaches see also B.6.4 Depending on the recycling rate of the catalyst material, also the make-up cost for replacement of the catalyst after a predefined period of time needs to be considered. Any risks arising from limited procurement options of rare metals in the regional and global market need to be evaluated regarding the time frame defined in the scope phase.

Algae production for CCU

The use of algae to convert CO_2 from atmosphere and flue gases into chemical products (*e.g. bio-oils, proteins, polysaccharides, fuels*) is a promising technology field. Being a biological conversion process, certain material and utility inputs are required, such as photosynthetic microorganisms, CO_2, water, nutrients and light. The management of the culture medium and the subsequent harvesting process to efficiently separate biomass from the culture medium currently are among the main cost drivers. The input water needs to be considered regarding its composition (purified water or waste water) as well as its temporal and regional availability. Other important parameters are light (sunlight or artificial) for biological conversion, required energy for dewatering processes, the use of waste heat from flue gas, as well as suitable bioreactor equipment for algae growth and processing.

B.5.5.6 Further reading

Hydrogen: The following publications are recommended for further reading about Hydrogen:

- H_2 price estimation of different production routes: Secure Sustainable Together, Technology Roadmap. (2015),[38] Hart et al. (2015).[39]
- A general overview about H_2 production technologies can be found in Häussinger et al., Ullmann's Encyclopaedia of Industrial Chemistry (2011).[40]
- Information regarding conversion efficiency, life time, maturity and future predictions can be found in IHS Markit - Hydrogen Handbook (2015).[41]

Mineralization inputs: Information about current developments: Pan et al. (2015).[42]

Algae production for CCU: Following reviews about technology development and future predictions: Barros et al. (2015),[43] Cheah et al. (2015),[44] Milano et al. (2016).[45]

B.5.5.7 Guidelines

Guideline B. 11 - Other key inputs for CCU technologies	
Shall	<u>**Hydrogen as input**</u> 1) H_2 price shall represent a market price or cost of production 2) H_2 compression, transport and local storage shall be represented in the H_2 price independent of system boundaries 3) Inclusion of H_2 production in boundaries: Calculate H_2 price based on the full location-specific process 4) Exclusion of H_2 production in boundaries: a) Collect H_2 price either from supplier quote or b) collect from a location-average estimate depending on the production route 5) Include a current, mature hydrogen generation process in the base case, instead of an optimistic future technology, unless process design describes future technologies in their current development stage and sufficient documentation is provided 6) Document and discuss scale and maturity of selected H_2 generation process regarding current and future technological and economic viability 7) Clearly document technological parameters and parameters regarding energy sources and electricity prices impacting the hydrogen production costs 8) Route-specific price inputs for electrolysis: a) Grid electricity mix: cost calculation shall be based on electricity spot price and H_2 generation utilization factor b) Specific electricity technology: cost calculation shall be based on intermittent energy supply or LCOE <u>**Electricity**</u> 9) Inclusion of electricity production process in investigated boundaries: Calculate electricity price based on the full location-specific process regarding CapEx and OpEx 10) Exclusion of electricity production process in investigated boundaries: a) Collect electricity price either from supplier quote or b) collect from a location-average estimate (market price) depending on the production route or the mix thereof 11) If electricity from renewable sources is selected, then discuss availability and document temporal and regional context
Should	<u>**Hydrogen as input**</u> 1) Include scenarios of future, low-carbon-footprint H_2 generation processes <u>**Electricity as input**</u> 2) Consider electricity from grid mix either in base case or in a scenario

3) Any electricity price in the base case should not be considered zero

Mineralization

4) Assess and document all mechanical pre-steps to prepare the mineral feedstock for conversion as well as proximity to the feedstock
5) In case of treating industrial waste, consider potential existing regulatory mechanisms rewarding waste treatment via CCU in inventory

Further inputs

6) For fossil-based compounds, investigate the price-dependency on fossil feedstock, price volatility and long-term availability and put into local and temporal context of the study
7) For metal catalysts, investigate make-up costs and any risks regarding future supply of rare metals

B.5.6 Documentation of data collection

B.5.6.1 Introduction

Documentation of all collected and estimated data as well as of all underlying technical and economic assumptions needs to be ensured to enable quick and transparent comparisons of important parameters. A description of the temporal, geographic and economic context of the study and the collected data is a vital part of documentation. In a separate table important economic parameters and assumptions are listed, preferably being easily accessible in the final TEA report. Where possible, data should be related to functional unit and reference flow. A TEA flow diagram is an option to document important technical and economic data along the data collection process.

B.5.6.2 How to ensure documentation

Documenting technical data and assumptions

Technical conditions and assumptions for material and energy flows as well as equipment should be documented along the data collection to prepare for the reporting *(e.g. temperature, pressure, purities and compositions of input / output material, energy types and contents, assumed efficiencies of conversion, underlying reference values, assumptions for waste treatment, recycling and recovery, transportation, type of equipment regarding dimension, durability and lifetime)*. All flows shall be documented in relation to the functional unit. If available any results from sensitivity and uncertainty analysis conducted along the data collection shall be documented as well including a statement of data quality. An independent documentation of measured or estimated data for each system element enables a subsequent analysis to support further process development and improvement, which is one major goal of TEA in research and development.

In terms of overall process performance, any underlying thermodynamic limits of chemical conversions should be discussed and documented. This is particularly important if novel technologies are assessed, that have not been optimized yet to the level of mature benchmarks. An overestimation of efficiencies needs to be prevented, which makes a transparent documentation of technical assumptions necessary.

All collected technical data needs to be documented in a suitable format. The required content varies depending on the assessed process as well as the practitioner's demand. Any chosen documentation format should list all technical parameters and underlying assumptions made for each system element in a way that *overview is ensured and comparisons are facilitated. An example of a tabulated list of technical parameters is provided in Table 15 the annex.*

Any parameter having specific characteristics and limitations regarding regional and temporal context shall be described and documented. Additionally, all varied parameters for the different scenarios should be transparently documented along the base case parameters.

Documenting economic data and assumptions

Relevant parameters, decisions and assumptions concerning economic data collection shall be documented along the data collection process *(e.g. market entry strategy, time of depreciation, interest rate, exchange rates, inflation index, reference values, data sources, operating hours, location, base year, lifetime, tax rate, debt-equity-share, units and conversion, transformation of data to the reference time and locations such as CEPCI Index and Richardson International Construction Factors Manual™)*. Both, the base year and the location of the studied scenario are particularly relevant for comparison of the study and should be explicitly stated, preferably early at the beginning of a case study.

Highly important is the documentation of the temporal and regional context of the project including a justification of project specific economic parameters such as scale and production capacity, supply chain mechanisms or availability of required investment. The uniqueness of the underlying value chain and how it is reflected by the specific data shall be described. A statement of potential limitations of the studied scenario regarding market conditions and underlying value chain shall be documented to enable a comparison to other studies. When documenting economic data, it should be stated for which of the analyzed scenarios these are relevant.

For reasons of transparency, all economic parameters and assumptions regarding the context of the study should be collectively displayed in a list which should be easily accessible either in the beginning of the study or in the annex of each analysis. All assumptions underlying the economic parameters need to be properly documented and justified by including an explanation and reference to the study context. The specific needs of different practitioners vary and not all economic parameters are relevant. For illustration, an example list of main economic parameters is provided in Table 9.

Table 9. Example list of economic parameters and assumptions to be documented (needs to be adapted to the specific TEA study)

Example economic parameters		**Explanation/ reference to context of the study**
Base year	Year	…
Location	-	
Location index for capital investment	-	
Currency	-	
Plant capacity	t/a	
Project lifetime	Years	
Operating time	Hours/year	
Construction period	Years	
Tax rate	%	
Equity/Debt ratio	%/%	
Debt payment	Years	
Return on Equity	%	
Cost of capital	%	
Salvage value	Currency	
Depreciation method	-	
Depreciation period	Years	
Material and utilities prices		
Assumptions for market entry		…
Temporal and regional context		
Market limitations		
Other parameters		

TEA flow diagram

A TEA flow diagram may be derived for documentation of important technical and economic data, serving as a summary diagram of the assessed system elements. The TEA flow diagram can differ from technical flow diagrams depicting the process design as it includes only relevant information for TEA. The different system elements may be represented at different levels of detail *(e.g. electrolysis as black box, methanol synthesis as PFD)*. In addition, relevant economic data may be included for description of energy and material flows along the depicted system elements. The TEA flow diagram is a useful tool for the TEA practitioner to focus on the system elements which are relevant within the system boundaries and to enable a visualization of the main technical and economic parameters required for assessment. Optionally the TEA flow diagram could be limited to a graphical representation of only the most significant parameters as defined along the iterative approach. This way, potential hot spots along the process steps can be visualized.

Uniformity of scientific units

Transparency and comparability of different TEA-results strongly depend on the consistent use of scientific units. Technical parameters should therefore be documented in SI-Units (International System of Units/Système International) within the metric system, due to their broad acceptance and clear definitions. In case non-SI-units are being used, their common understanding shall be assured by providing a clear documentation and unit definition.

B.5.6.3 Guidelines

Guideline B. 12 - Documentation in data collection		
Shall	1)	Document economic parameters, decisions and assumptions as well as specific temporal and regional context of the value chain including market limitations of the studied scenario
	2)	Document parameters in SI-units or in other common units by clearly documenting a unit definition
Should	1)	Document all technical data and approximations by each system element in a way to prepare for the reporting phase, including a discussion of underlying thermodynamic limits of the conversion steps
	2)	Collectively display economic data in a separate list which is easily accessible either in the beginning or in the annex of each report
	3)	Document technical and economic data based on the functional unit and reference flow
May	1)	Integrate important technical and economic data in a TEA flow diagram

B.6 Calculation of indicators

B.6.1 Introduction to calculation of indicators

In the goal and scope phase indicators that are suitable for assessment are selected. In the inventory phase data needed for their calculation are collected and documented. The actual calculation of assessment indicators forms a separate phase and explained in this chapter. The results represent the projected technical performance or economic impacts in the market or within an economic entity and serve as a basis for subsequent interpretation.

At first, this chapter presents best practices in assessment indicator calculation. Capital expenditure (CapEx) and operational expenditure (OpEx) are intermediate indicators that are either directly interpreted compared to values of the same indicator or aggregated in further calculations, especially in all profitability indicators *(e.g. net present value)* or in enviro-economic indicators *(e.g. CapEx / t_{CO2e})*. The importance of CapEx and OpEx in CCU is acknowledged in separate sections of this chapter by proposing methodology approaches. CapEx and OpEx are inputs to the calculation of profitability indicators, which are outlined in a separate section as they are desired especially for decision-making in business-driven contexts. As CCU technologies cover a large range of chemistry fields *(e.g. thermochemical, biochemical, electrochemical, photochemical etc.)* and include projects at varying technology maturity, normalization and weighting of results might be useful but has to be conducted carefully.

B.6.2 Best practices in indicator calculation

B.6.2.1 Introduction

Some TEAs for CCU technologies include calculations of assessment indicators that are difficult to comprehend for an external readership. Best practices in indicator calculation can tackle this issue and help practitioners to set up calculations that are more easily understood and reproducible by their readership.

B.6.2.2 How to approach indicator calculation

While each practitioner conducts the calculation according to her or his needs, some general principles need to be kept in mind. Transparency and reproducibility are major challenges for all calculations. In order to ensure transparent calculation, assumptions and data shall be listed in SI-units or other common units and in separate documents from indicators and equations *(e.g. in a separate spreadsheet or database)*. For calculation, data and equations shall be linked, so that calculations can be repeated, and results should be stored in a separate file *(e.g. spreadsheet)*. Calculations shall be conducted for the overall product system as well as for each system element individually, allowing better comparability and analysis of system element alternatives *(e.g. inclusion or exclusion of CO_2 capture, H_2 products)*. Levels of detail of calculation can vary between system elements according to data requirements *(e.g. black box or detailed process)*. While analysis of costs or technical performance can be conducted for each system element, analysis of market price or volume can prove difficult for intermediates and thus impede calculation of aggregated indicators, especially profitability indicators, for the respective system element. If required data turns out to be missing and cannot be estimated in the inventory phase, remaining data gaps shall be documented.

B.6.2.3 Guidelines

Guideline B. 13 - Best practices in indicator calculation	
Shall	1) In indicator calculation files, list required data and assumptions, indicators, their formulas and results in a structured and transparent way 2) Store data and assumptions in a separate file or spreadsheet from indicators and their formulas 3) Make use of SI-units or common units 4) Link data and assumptions to calculations (repeatability) 5) Document remaining data gaps 6) Conduct calculations for the overall system but also for single system elements individually
Should	1) Store results in a separate file or spreadsheet from data and assumptions as well as indicators and their formulas

B.6.3 Estimation of capital expenditure

B.6.3.1 Introduction

Capital expenditure (CapEx) refers to the initial investment needed for "designing, constructing, installing [and commissioning] a plant and the associated modifications needed to prepare the plant site".[22] While it is an important economic indicator (see scope chapter B.4.5) and can be a crucial part of CCU technologies' costs, sound capital expenditure estimation is difficult for the following reasons:

- CCU projects are often in the research and development phases, when realistic CapEx estimation is difficult because process development does not yet offer a detailed data basis.
- CCU projects belong to different fields of technology. A variety of methods for CapEx estimation is available; however, from literature it is not always evident which methods are best applied for what detail and quality of input data.

For these reasons, a brief general methodology overview is presented in this chapter. In the next chapter, guidance applicable for CCU projects of how to estimate CapEx is presented (see B.6.3.2).

CapEx can be structured into fixed capital investment (FCI) and other cost items such as working capital, start-up expenses and contingencies. FCI comprises the core plant (inside battery limits, ISBL) and the infrastructure that is needed to connect the core plant to the outside world (outside battery limits or off-site, OSBL). Both ISBL and OSBL contain physical cost items (direct cost) *(e.g. equipment cost, piping)* as well as intangible cost items (indirect cost) *(e.g. construction supervision, insurance)*.

In general, methods for the estimation of CapEx vary regarding their data used. Frameworks for CapEx estimation methodology are widely adopted in chemical engineering and are referred to in this guideline as they facilitate choice of methods. The AACE International Cost Estimate Classification System [46] presents the most common framework. The following clusters of methods estimating FCI or ISBL cost were identified:

- 'Short methods' consider one or few characteristic parameters as inputs and return cost. Short methods often include cost-capacity curves or scales of operation factors (see [47], [48]).
- 'Parametric techniques' conclude cost from process characteristics and related parameters; most are based on the number of significant process steps and other characteristic process parameters (see [49], [50] for low detail methods, see [51], [52] for high detail methods).
- 'Factored methods' apply factors to equipment cost and return other direct or indirect cost items. Some authors apply one, global factor to cumulative equipment cost to calculate ISBL (see [53], [54]), while others estimate single cost items via detailed factors that are individually adapted to single components (see [55]–[57]).

- ‘Unit cost line items’ derive cost from rigorous design and offers or detailed single equipment cost calculation. Items surrounding the main equipment are calculated in the same way or estimated in great detail with item-specific methods by scenario-specific adaptions of detailed factors for single equipment.
- ‘Cost transformation’ describes the adoption or transfer of similar plant's CapEx to a projected plant, usually based on capacity or other significant plant parameters *(e.g. by using the popular six-tenths power rule*[58], [59] *or adaptions*[60]*)*. The same logic can be applied for scaling of equipment or transformation of location *(e.g. via factors* [22]*)* and date *(e.g. CEPCI index)*.

B.6.3.2 How to estimate capital expenditure

General CapEx estimation framework

Table 10 provides an overview of cost estimation methodology and serves as an orientation for the selection of adequate methods; the table is based on the AACE International Recommended Practice 18R-97 [61] and includes types of methods as described above.

Table 10. Capital expenditure estimation methodology in research, development and deployment phases

Phases	Research	Development	Deployment
AACE Estimate Classes	5 and 4	4 and 3	2 and 1
Typical methods adapted from AACE	• short methods • parametric techniques (low detail) • factored methods • cost transformation	• component factored methods • parametric techniques (high detail) • inclusion of unit cost line items • cost transformation	• unit cost line items (high detail or based on design quantities) • still undefined items: detail component factored methods (or “forced detail”)

Method selection

Data collection and estimation method selection should follow the iterative approach (see B.5.3.2). In this context, this means the use of rough estimation, especially with short methods in a first iteration. Then, the parameters that the CapEx is most sensitive to are identified (see B.7.2.2) and more accurate methods are selected. This means that while the most accurate estimates possible are preferred in general, more simple methodology can be applied. Methods selected shall comply with goal and scope of the TEA *(e.g. with the addressee’s accuracy demands)*. As in one plant system elements with different maturity can exist, a combination of different methods might be necessary for the calculation of a complete CapEx.

Overall, methods should be as precise as possible (exploiting best available data) but only be as precise as available data permits (indicated by technology maturity) to lead to the most accurate overall cost possible and subsequently best decision basis. Two exceptions can be made, if properly justified:

- If equipment specifications are needed for a complete estimate but cannot be derived from technical development at the point of assessment, they may be assumed for economic calculations only ("forced detail"). In this case, strict separation of technical development and assumptions for economic calculations is necessary in order not to force into a certain pathway for future development.
- If CapEx is judged to be of minor importance compared to OpEx, accuracy demands of the CapEx estimate may be lowered.

CapEx estimation methods that are accepted in literature should be used. Other methods *(e.g. company internal techniques, recently published methods)* can be helpful; however, reasons for their application and explanation of the calculation shall be given as they are uncommon and can thus be difficult to comprehend for external readers. Highest level of care and accuracy of estimations is needed in deployment phases which prepare realizing cash flows *(e.g. procurement of equipment)*. For estimating CapEx, cost transformation should be applied if the degree of similarity and quality of available data is judged to be sufficient by an experienced practitioner.

Especially for larger plants, OSBL cost can contribute a major share to the overall CapEx estimate. In early to mid-maturity stages, OSBL cost are often estimated in total as a factor applied to ISBL cost. For high maturity stages, detailed estimation of OSBL cost becomes necessary. Descriptions of methods for OSBL component estimation are not covered in these guidelines as they involve further disciplines such as civil engineering. Including experts from these respective fields is necessary for a complete CapEx estimation in high maturity stages.

Challenges in CapEx estimation for CCU technologies

For CCU plants, it often is not clear what are inside (ISBL) and what are off-site (OSBL) facilities. For example, energy and utilities supply can either be seen as core plant function or outside world connection (grid). Thus, ISBL and OSBL components should be stated clearly; different scaling and usually increasing OSBL to ISBL ratio with increasing plant size have to be considered.

Cost estimation methods, especially parametric techniques, are typically based on company experience with fossil resource-based processes. In addition, methods emphasize individual technology parameters differently, leading partly to under- or overestimation. For CCU, CapEx estimation should be conducted critically using multiple methods in parallel to help understanding the economic composition of a plant and identifying key cost drivers. Please keep in mind that CapEx estimates at early technology maturity have large uncertainty, which needs to be reflected in the interpretation (see B.7).

When applying cost transformation for CCU plants, the scaling exponent should reflect how the costs of the main components change with the scale of the estimated plant compared to a reference plant. While costs of some typical system elements in CCU plants scale via the area *(e.g. PEM electrolysis)*, leading to an exponent close to 1, others scale via volume with an exponent of roughly 0.67 *(e.g. storage vessels)*. Furthermore, CCU plants often include non-standardized equipment which does not follow the scale effects underlying a lot of methods. In this case, short methods and some parametric techniques tend to underestimate CapEx.

Contingency

By choice of project management, costs for unforeseeable events and circumstances may be included in the estimation of CapEx as “contingency” cost. Contingency can mean the following:[18], [21], [22], [62]–[64]

- Allowance: specific, known but undefined items *(e.g. currency exchange rate fluctuations, estimation errors, metal price changes)*
- General contingency: unknown items that are unlikely and unforeseeable, force majeure *(e.g. natural disaster or labor strike)*
- Management reserves: changes in scope *(e.g. changes in end product specification, plant location, building date)*

There is no commonly accepted understanding in literature of what items are included in contingency estimations and how these are performed. The idea of contingency is to reduce the probability of overrunning the budget by adding reserves to a base estimate.

Contingency can be calculated in deterministic or probabilistic approaches. Deterministic methods apply a single factor to the base estimate or parametric calculation for different events and are preferred in early phases. Factors are derived from expert judgements or institution-specific guidelines.[65], [66] Probabilistic techniques use either expected values of cost impacts of a range of potential events [67] or probability distribution functions (PDF) of FCI. In the latter case, contingency is the amount that needs to be added in order to provide a desired certainty not to overrun the budget [68] and commonly excludes general contingency and management reserves.

In early to mid-maturity stages, the value of the upper estimation error of FCI can be chosen as a contingency factor. Allowance decreases with technology maturation since the technology is better understood and estimates can rely on more exact methods. Management reserves will decrease with better understanding of the scope defining market and scenario that a plant will be situated in which usually goes along with increasing technology maturity. External threats (force majeure) which determine general contingency are not directly affected by technology maturation. Overall contingency below 10% of FCI is not recommended.[18], [21], [22]

Learning curve effects

As current CCU projects tend to create new kinds of plants, learning curve effects are of great importance for estimating CCU plant cost. The first plant can have significantly higher CapEx than following plants of the same kind. The following two types are therefore distinguished:

- ‘First of a kind' (FOAK): none or only a few similar pioneering plants exist and learning rates are not yet achieved
- 'Nth of a kind' (NOAK): several plants exist that are using the same or similar technologies and learning rates can be estimated

If desired by goal and scope, a FOAK plant may be converted into a representative NOAK plant by including learning curve effects, as it is described in literature [69]–[72]. When applying CapEx learning curve effects, great caution is required to make sure that the converted estimate still represents the inventory in a realistic way, meaning that items motivating the reduction have to be stated *(e.g. single equipment that is expected to drastically improve due to research in near future)*. In addition, the expectation that the market volume supports multiple plants needs to be justified. Furthermore, it has to be considered that learning curve effects can also apply to benchmark systems, which is especially important when directly comparing CapEx to other systems or calculating profitability.

B.6.3.3 Further Reading

Similar to the to the AACE International Cost Estimate Classification System [61], cost estimation frameworks and groups of methods are presented by several authors [20], [60], [73]–[77]. The most prominent methods for CapEx estimation are described in detail in general literature for process design (with economic objective), for example in [18], [21], [22] [78], [79]. Some authors interchangeably use the terms such as "functional unit" (in a different sense than in LCA) or "significant process step" for parts that a process or plant consists of. Detailed information about contingency estimation is for example presented in the AACE International recommended practices: 41R-08, 42R-08, 43R-08, 44R-08 [65]–[68].

B.6.3.4 Guidelines

Guideline B. 14 - Estimation of Capital Expenditure	
Shall	1) Select methods that comply with goal and scope of TEA 2) State and consider assumptions, requirements, adjacent estimates 3) Give motivation and explanation for use of uncommon methods
Should	1) Select methods that are as accurate as possible, following the iterative approach 2) Use methods accepted in literature 3) Use multiple cost estimation methods 4) Apply cost transformation if high quality data of similar plants is available 5) Calculate only ISBL independently from OSBL in early-maturity stages 6) Estimate OSBL independent of ISBL as soon as site is selected 7) Estimate all CapEx items independently before building the plant 8) State ISBL and OSBL components and reflect how their main components scale in transformation exponents for mid and high-maturity stages
May	1) Use 'forced detail' with great caution, no development feedback 2) Lower accuracy demands if CapEx is judged to be of minor overall importance 3) Consider learning curves in order to estimate NOAK plant CapEx 4) Contingency may be included in a CapEx estimate in order to reduce the probability of overrunning the projected budget

B.6.4 Estimation of operational expenditure

B.6.4.1 Introduction

Operational expenditure (OpEx) can be divided into variable costs and fixed costs. Variable costs depend directly on the amount of product produced *(e.g. raw materials, energy, utilities, waste disposal)* [22], [27]. On the contrary, fixed costs do not directly depend on the amount of product produced *(e.g. labor, supervision, direct salary overhead, property taxes, insurance, general plant overhead)* but can indirectly be influenced by it, for example *via* the plant size [18]. Variable OpEx can be further divided into costs for raw materials, energy and utilities, and other items.

Operational expenditure is an important economic indicator (see scope chapter B.4.5). Especially for high-volume products that compete on price-sensitive markets, accurate estimation of operational expenditure is particularly important. Often, CCU technologies require a substantial amount of energy. The energy can be either provided directly *(e.g. electricity, light, heat)* or through energy-rich co-educts *(e.g.* H_2*, epoxides)*, making reliable data for these inputs a crucial factor.

A 'cost increment' is understood as an amount of money that covers an assigned cost item (mostly per functional unit) *(e.g. adding 0.10 €/kg as an estimate for energy cost)*. 'Factored estimation' describes the procedure of multiplying a cost item with a factor for the estimation of another cost item *(e.g. assuming 0.01*FCI as the annual cost for property taxes)*.

B.6.4.2 How to estimate operational expenditure

General OpEx estimation framework

The methodology selected for OpEx calculation shall comply with goal and scope of the TEA *(e.g. with the addressee's accuracy demands)*. Furthermore, institution-specific assumptions, requirements and adjacent estimates necessary for OpEx estimation shall be stated and considered *(e.g. company internal estimation and budget authorization frameworks)*. Similar to the estimation of CapEx, the most accurate estimates possible for OpEx are preferred; however, less accurate methodology might be applied in order to reduce estimation effort if goal and scope definition allow it. Table 11 shows proposed OpEx estimation methodology as well as required data and sources along technology maturation phases of research, development and deployment.

Table 11. Proposed methodology for operational expenditure estimation

Phase	Research	Development	Deployment
Material	• Based on stoichiometry, measured mass flows or design/simulation	• Based on measured mass flows or design/simulation	• Based on measured mass flows or design/simulation
Energy, utilities & other variable OpEx	• Based on measured energy flows or design/simulation • Factored estimation (based on material cost) • Cost increments from similar plants	• Based on measured energy flows or design/simulation • Cost increments from similar plants	• Based on measured energy flows or design/simulation
Fixed OpEx	• Simple factored estimation • Cost increments from similar plants	• Detailed factored estimation • Cost increments from similar plants	• Detailed factored estimation • Separate calculation of fixed OpEx items
General expenses & freight	• Factored approach	• Factored approach or company-specific	• Company specific
Main price data and sources	• Price data: market-average • Sources: few, secondary	• Price data: market-average • Sources: multiple, secondary	• Price data: process-specific • Sources: few, primary (supplier quotes)

Variable OpEx: Raw material cost

The cost for raw materials are based on the mass balance. In early research stages, which rely on concepts rather than tangible results, material demand is estimated according to the reaction stoichiometry or conceptual design. In late research and all following stages, the mass balance for the OpEx estimate is based on the actual mass flows from the conducted process *(e.g. laboratory experiments, pilot trials, plant operation)*. Mass balances of system elements that are not yet built, are determined following process design *(e.g. with process simulation)*.

Raw material prices can be obtained from primary or secondary sources (see B.5.2). Using specific raw material prices from suppliers is preferable but often challenging, especially for development projects without trustworthy relationships to suppliers or in early stages with unknown trade conditions.

Variable OpEx: energy, utility and other cost

The cost for energy and utilities are based on the energy balance. The energy balance is based on the measured consumption in the conducted process *(e.g. laboratory experiments, pilot trials, plant operation)*. Energy balances of system elements that are not yet built are determined following process design *(e.g. with process simulations)*. In research in development phases in general, assuming cost increments for energy or utilities or other variable OpEx from similar plants should be considered, if data at a substantial degree of similarity and quality are available. In addition, variable OpEx estimation may be facilitated, in the research phase in particular, but also up to development stages if properly justified:

- If the energy cost is judged to be of minor importance, energy cost may be estimated as a share of the total raw material cost.

- If the utility or other variable cost are judged to be of minor importance, utility or other variable cost may be estimated as a share of the total energy cost.

Energy prices can be obtained from data bases similar to raw material prices. For plant integration into existing sites where utility supply might already exist, prices are subject to offers from site operators. For greenfield projects, facilities producing and delivering energy or utilities to the core plant have to be estimated in the same way as the core plant. In this respect, other variable costs such as waste disposal are approached in the same way.

Fixed OpEx

In general, fixed OpEx can be adapted from similar plant's data, estimated via factors or specific correlations or also projected in detail. Factors for fixed OpEx estimation are either directly applied to CapEx or to major OpEx items. A variety of estimation factors and typical OpEx items are available from literature [18], [20]–[22], [80], [81].

In the research and development phase, a factored approach should be used, once the FCI estimate is available. Factors shall be adapted to the projected scenario with care *(e.g. increase of maintenance factor for plants with increased operating pressure or safety demands)*. Alternatively, cost increments from similar plants should be considered, given the high degree of similarity and data quality needs up to later development stages. No quantitative approach for judging degrees of similarity of plants in order to deduce appropriate cost increments is available. For absolute values for cost increments or factors applied to other cost items no general rules can be given here, since they are technology-specific and can vary considerably. This issue is left to the practitioner's expertise, experience, good judgement and careful consideration of the company's and technology's specific characteristics. Prior to plant commissioning, all major fixed OpEx items should be calculated in detail, or estimated separately following methods based on specific literature.

General expenses & Freight

The relevant cost on the market are represented by the cost of goods sold (COGS). COGS are obtained by adding general expenses and potential freight or delivery costs to the cost of goods manufactured (COGM), which consists of CapEx and OpEx. Freight can make up for a large share of COGS in CCU; if so, a detailed calculation becomes necessary. For the estimation of general expenses, a factored approach is often chosen in research phases, whereas in more advanced phases of development and deployment, company-specific values can be added. Freight can make up for a large share of COGS in CCU; if so, a detailed calculation becomes necessary. No guidance can be given here because freight costs are unique for each product and related sales activity.

Price data and sources

In the research and development phases, average market prices should be used as a starting point. With increasing maturity, OpEx estimates should be based on price data from an increasing number of sources; meaning that single sources are be substituted by multiple sources *(e.g. by commercial market studies that are based on multiple sources or even multiple studies)* and scenario-specific data where possible. In the late developing phase and deployment phase, date- and location-specific prices should be additionally considered. In the deployment phase, process-specific data and primary sources, such as supplier quotes should be used. If supplier quotes are not available or for minor cost items, the use of secondary, average data such as from commercial market studies can be used, but trade conditions *(e.g. Incoterms)* have to be accounted for.

OpEx estimation is largely dependent on increment and factor values, as well as on similarity of plants. No general rules for increment or factor values can be given here, since they are technology-specific and can vary considerably. Furthermore, no quantitative approach for judging degrees of similarity of plants is available. These issues are left to the practitioner's careful consideration and judgement of the company-specific and technology-specific characteristics.

B.6.4.3 Further reading

Cost items and values for factored estimation as well as correlations for single cost items of fixed OpEx are available from literature (often including general expenses) [18], [20]–[22], [80], [82], [83]. The estimation of operating labor demand is particularly important since it is used as basis in factored estimation, methods for estimating labor hours and cost are available in literature [18], [22], [78]. For price collection for variable OpEx, no textbook approach is at hand; adequate data collection is left to the practitioner's experience, creativity and good judgement.

B.6.4.4 Guidelines

Guideline B. 15 - Estimation of operational expenditure	
Shall	1) Select methods that comply with goal and scope of TEA 2) State institution-specific assumptions, requirements, adjacent estimates 3) Carefully adapt factors to the projected scenario for fixed OpEx
Should	<u>Estimation methodology</u> 1) In research and development, consider data from similar plants for cost increments for energy, utility and other variable OpEx as well as for fixed OpEx 2) In late research stage, as soon as fixed capital investment is available, use factored estimation for fixed OpEx 3) In deployment, calculate or detail estimate all cost items separately prior to plant commissioning for fixed OpEx <u>Price data and sources</u> 4) Increase number of sources along technology maturity 5) In research and development, use market-average price data 6) In late development and deployment, include date and location specific prices 7) In deployment, use process-specific data and primary sources
May	1) Estimate less important cost items *via* factors applied to other variable OpEx items for energy, utility and other variable OpEx

B.6.5 Calculation of profitability indicators

B.6.5.1 Introduction

For interpretation and decision-making in business-driven contexts, profitability indicators present the most important basis. TEA is a comparison of alternatives: Cost estimation is directly followed by an interpretation if used as an instrument for the comparison of process options that do not have different market implications. In most TEAs, adding a market view to the internal company view on cost becomes necessary in order to calculate indicators that are suitable for profit-oriented stakeholders. In addition to quantitative profitability indicators, there are economic factors that are difficult to translate into monetary measures *(e.g. availability of qualified personnel*[78]*)* and therefore left to qualitative evaluation.

For this guideline, profitability indicators are specified as "calculated values of investments, representing monetary gains or losses in comparison to an alternative investment"[20]. Profitability indicators reveal if, how much and when money can be earned with an economic activity scenario [84].

Two types of profitability indicators can be distinguished: static and dynamic [85]. Static indicators consider only one period or an average of multiple periods. The general alternative action in static calculations is no investment. Dynamic indicators include multiple periods, accounting for time preferences that investors can have towards cash flows. The general alternative investment in dynamic calculations is an investment on the capital market with the same risk profile. In general, profitability indicators depict a measure that is built around the profit (understood as difference of revenue and cost).

B.6.5.2 How to calculate profitability indicators

Challenges in profitability calculation for CCU technologies

As profitability is calculated independent of characteristics of certain technologies, no CCU-specific indicators and calculation challenges are necessary. However, the selection of profitability indicators in TEA for CCU remains a challenge: There is currently a lack of standardization, especially in early maturity stages [2]. The use of different indicators makes it difficult to comprehend, reproduce and compare different TEAs for CCU technologies. Practitioners are encouraged to consider the following selection of indicators which are described and sorted by research, development or deployment phases according to the quality of input data needed (the detail of market analysis or the accuracy of cost estimates).

Research phase

The practitioner should normalize the profit to cost in early stages as normalized values simplify displaying and comparing which facilitates selecting concepts and deciding which pathway is favored. The 'relative profit', a dimensionless indicator, is often chosen (*cf.* [25]). Practitioners may choose the specific profit (with the dimension "value per mass") over the normalized form if absolute numbers are important for strategy considerations (*cf.* [86]) or for a rough comparison with established products and deriving cost increments.

Development phase

The 'payback time' is a popular profitability indicator. It is calculated as CapEx divided by the annual profit resulting from plant operation and product selling. The payback time may be calculated in addition to the absolute profit if desired. The date from which on an economic activity generates net profit is also called 'break-even point'. There are multiple definitions of the 'return on investment' (ROI), differing in the items of CapEx or time frame (single period *vs.* project life time or recovery period). Dividing the net returns by the initial CapEx committed, results in the 'static return on investment', which may be given as a useful indicator when comparing the utilization of capital.

From mid-maturity stages onwards, using dynamic indicators becomes versatile. The prediction of future cash flows is very uncertain if the market is not well understood and mistakes in the selection of an adequate discount rate are often made. This leads to substantial errors that often have more impact than neglecting time dependence. Developing an understanding of scenario conditions and predicting future cash flows require an understanding of the market that can usually not be derived until considerable progress in technical development is made. The most prominent dynamic profitability indicator is the 'net present value' (NPV). It is calculated as the sum of all cash flows that are discounted according to the period they occur in with the corresponding assumed discount rate(s). The NPV depicts the amount of money that an investment is worth in period zero. The NPV shall be calculated from (later) development stages and commonly serves as a structural basis for more detailed profitability calculations in deployment stages. The use of NPV in early maturity stages is not recommended. Similar to its static version, the 'dynamic payback time' is the first period in which the sum of all past discounted cash flows is zero or positive. It may be calculated in parallel to a NPV as it can often be read from the same spreadsheet. Similar to the static ROI, a dynamic ROI may be calculated including interest in parallel to an NPV. Including time preference, it is calculated as the ratio of all discounted cash flows to the initial spending. It is popular for comparing the relations of investments' earnings to their initial investments. The 'internal rate of return' (IRR) is the discount rate that leads to a NPV of zero. The IRR is a popular measure when comparing how well different projects perform. However, using the IRR has two disadvantages: 1) Depending on the characteristics of the cash flows, only complex numbers ($\mathbb{C}$) or multiple values can exist. 2) The IRR does not reveal the absolute profit that can be obtained and therefore leads to loss of information. For these reasons, the IRR may be selected but always has to be accompanied with an NPV for the same investment.

Selecting an adequate discount rate in dynamic calculations poses a great challenge. Rather than taking an average capital market interest rate, the practitioner should select an interest rate that represents an investment on the capital market with the same risk profile as the projected technology investment. The capital market is often assumed to be perfect for first calculations and unrestricted in development stages. In later development stages, the practitioner should account for different interest rates for different cost items, for example how CapEx is financed *(e.g. due in period zero and liability financed over several periods, thus increasing the budget in period zero by the cost that is needed for financing it)*. In order to do so, many companies use their weighted average cost of capital (WACC) if the project's risk profile is similar to that of the company. If the project's risk profile is different from that of the company, the WACC shall be adapted to the project's characteristics or other methods *(e.g. capital asset pricing model (CAPM))* can be applied instead. When calculating WACC, the equity interest rate can for example be derived from the shareholders' return expectations [87]. In later development and ultimately deployment phases it should be considered that interest rates are a time-dependent (*cf.* spot rates *vs.* forward rates) since interest rates depend on the life span of the financing instrument.

Deployment phase

Dynamic indicators shall be refined in deployment stages with updated assumptions and prospects of future market developments. Detailed functions and interdependencies of inputs lead to profitability models that are commonly not included in indicator descriptions as given above, although they target the same questions *(e.g. worth of the investment in the present or time after which the investment generates net profit)*. These economic simulations can be based on discrete events (scenarios, see B.6.3 and B.6.4) or analytical functions that describe market, cost and scenario parameter behavior *(e.g. depreciation, taxes, inflation)*. After procurement (and potentially construction and commissioning) is started, cost items shall be updated with actual data of past cash flows in order to reduce uncertainty. It is left to the practitioner's judgement and company-specific frameworks at what point in development or deployment taxes are considered. Tax regulations differ substantially between countries and can be very complex. Including taxes in profitability calculations requires expertise and very precise project (scenario) description. For first calculations, practitioners often choose simplifying assumptions such as one type of tax (income), due date at the same time as income is generated, taxes (or tax rates) proportional to absolute income, tax rates independent of capital origin or company's legal form. These assumptions lead to correction of an NPV's numerator by subtracting tax rate times EBIT (earnings before interest and taxes).

At TRL 9, economic simulations can be conducted for refinements such as plant expansions or minor optimizations that are not considered new technology development. Past economic activities are summarized in accounting for cost checks and profit calculations.

In all phases, the practitioner shall select indicators as requested in goal and scope of the TEA *(e.g. in development and deployment, the practitioner will calculate dynamic indicators unless the TEA's goal and scope specifically states otherwise)*. Indicators not presented here may be selected; if so, it is requested to explain reasons and respective formulas.

B.6.5.3 Further reading

Profitability indicators relevant for CCU in early stages are for example discussed in [2], [25], [26]. A more detailed description of the above indicators and sorting by TRL is given in [20]. Profitability indicators used in the chemical and process industries are covered in standard textbooks for process design (with economic focus), especially [18], [21], [22], also [78], [80], [81], [88] or reports such as [86]. In addition, most aspects of capital budgeting methodology are not technology specific and therefore covered in general economic literature. Single investment appraisal techniques in the context of chemical innovations are discussed in scientific literature, for example in [89], [90].

B.6.5.4 Guidelines

Guideline B. 16 - Calculation of profitability indicators	
Shall	For all phases 1) Present equation and reason for each indicator applied Research 2) Perform qualitative evaluation of profitability prospects if quantitative evaluation is not (yet) possible 3) Calculate quantitative profitability indicators as soon as a mass balance is at hand Development & Deployment 4) Calculate an absolute profit measure as soon as development started (and annual addressable market sales volume is derived from market analysis) 5) Introduce dynamic indicators only with advanced scenario description (usually development phase), prior to deciding about pilot plants 6) Calculate the net present value whenever dynamic indicators are required 7) Consider if a company's WACC is applicable to the project; adapt the WACC to the project's characteristics or obtain a discount rate from other models Deployment 8) Perform detailed economic simulations which consider the project's financial structure in deployment stages 9) Replace cost items with actual cash flows as soon as they are realized
Should	Research 1) Normalize the profit calculated in order to facilitate concept comparison in research phase (report the absolute value) Development & Deployment 2) Select a rate that represents the same risk profile as the present technology for discounting in dynamic indicators 3) Account for different interest rates within one project (in later development)
May	Research 1) Prefer the specific profit over normalized profit if absolute values are needed Development & Deployment 2) Calculate the payback time (static or dynamic) in addition to an absolute profit measure (static profit or NPV respectively) 3) Calculate an ROI (static or dynamic) 4) Calculate an internal rate of return

B.6.6 Normalization and weighting

B.6.6.1 Introduction

Especially for CCU products with diverse technologies and markets, various trade-offs between different indicators and criteria exist *(e.g. OpEx vs. CapEx, market price vs. market volume)*. Normalization and weighting is an optional approach for further processing of previously calculated assessment indicators with the aim of facilitating interpretation and decision-making. Both normalization and weighting can lead to a loss of information however, if only the result is considered. Normalization and weighting metrics and schemes are specific to technologies and projects; they include subjective choices and have to be carried out with great caution.

B.6.6.2 How to conduct normalization and weighting?

Normalization

Normalization is the comparison of different assessment indicators by eliminating the units of measurement of the data, so that relations are depicted instead of absolute values. Common normalization techniques are:[91]

- ***Categorical scaling***: assigning a quantitative or qualitative score to each indicator, which is robust to small changes in data but also entails information loss *(e.g. assigning each indicator based on its value a number of an ordinal scale such as grades between 1 and 10)*.
- ***Rescaling***: deriving values relative to a specified value *(e.g. a scale 0 to 1, where 1 is the highest absolute number measured)*.

Normalization can be used for the comparison of different TEAs. Furthermore, it can be used to show relations within a single TEA or enable combined presentation *(e.g. displaying indicators of multiple criteria on one axis)*. Normalization of results beyond the reference flow is an optional step. If it is applied, results have to be normalized for each assessment indicator separately. Moreover, the reason for normalization and scaling criteria as well as the initial values of the absolute indicators have to be documented.

Weighting

Weighting means assigning quantitative weights to (normalized) indicators. For this guideline weighting also includes aggregating which means adding up weighted indicators. Weights are collected in the goal and scope phase *(e.g. derived from target audience's preferences, expert guesses, company goals or the assessment goal)*. Indicators with different dimensions have to be normalized (preferably to dimensionless indicators) before they are aggregated *(e.g.* $t_{CO2e} / t_{product}$ *and OpEx each have to be normalized before they can be aggregated because they have different denominators)*. Indicators that have the same dimension and that are based on the same assumptions do not require prior normalization. However, normalization is recommended in order to create a common basis and scale. Indicators normalized with categorical scaling cannot be aggregated.

Assigning weights is based on personal decisions and preferences and is thus always subjective. Weighting serves aggregating indicators (usually indicators of different criteria) and includes subjective meanings; aggregated indicators are sometimes demanded by decision makers as they potentially help reducing decision effort. Creating an aggregated indicator leads to reducing visible information, which can facilitate decision-making but at the same time does not necessarily improve the decision.

The weighting approach may be applied

- if interpretation of results and subsequent decision making are based on multiple indicators,
- in order to help make clearer distinctions between results *(e.g. no product scores highest in every indicator)*,
- if comparing an aggregated indicator to a previously defined abort criterion *(e.g. in a stage gate process)*.

The reason for weighting, the weighting scheme and the assigned weights as well as the initial values of the discrete indicators have to be documented.

B.6.6.3 Further reading

Guidance on how normalization and weighting is applied in LCA is explained in more detail in the ILCD Handbook sections 8.3 and 8.4 [4].

B.6.6.4 Guidelines

Guideline B. 17 - Normalization and weighting	
Shall	
Should	
May	1) Apply normalization with great caution. If applied: a) Results have to be normalized for each indicator separately b) Reason for normalization and scaling criteria as well as initial, absolute indicator values have to be documented 2) Apply weighting with great caution. If applied: a) Indicators with different dimensions must be normalized b) Indicators with the same dimension are recommended to be normalized c) Reason for weighting, weighting scheme and weights as well as initial, discrete indicator values have to be documented

B.7 Interpretation

B.7.1 Introduction to interpretation

Interpretation is a review in all stages of the TEA process in order to check consistency, completeness and reliability of model and input parameter assumptions, data quality and associated outputs in relation to goal and scope of the study. This iterative approach is completed if the inventory can address the goal of the assessment sufficiently.

The uncertainty and sensitivity of the assessment output are analyzed to increase the reliability, credibility and robustness of the results and to identify the most influential input variable of the calculated indicators. Interpretation also encompasses the identification of key inventory data that need to be improved and can be useful for the construction of different scenarios. The results of the calculated indicators are interpreted to provide indications for assessment criteria to answer questions posed by the assessment goal. The interpretation can also involve a multi-criteria decision-making step when there is more than one objective defined in the goal of the assessment and trade-offs between different targets need to be made. The outcome of the interpretation phase is a set of conclusions and limitations which serves as a basis for decisions and recommendations for future research, development and deployment.

B.7.2 Uncertainty and sensitivity analysis

B.7.2.1 Introduction

Uncertainty analysis (UA) allows the practitioner to analyze the uncertainty associated with the model output as the result of the propagation of errors in input data as well as uncertainties in the model itself or the context in which the assessment is conducted. The model output refers to any result or indicator of interest that is crucial for the subsequent decision and thus needs to be analyzed in terms of uncertainty and sensitivity. In TEA, this can be the calculated profitability indicator (*e.g. NPV, IRR*). Sensitivity analysis (SA) studies how sensitive the model output is to variations of one or more input variables. UA and SA are complementary as SA reveals how the uncertainty of the output is constructed and discloses key input variables that can contribute most to the uncertainty [92].

The following procedure to analyze uncertainty and sensitivity of calculated indicators is recommended:

1. Characterization of uncertainty
2. Uncertainty analysis
3. Sensitivity analysis
4. Improving data quality by iterative approach

In the case of early technology maturity, complex uncertainty methods can result in substantial noise despite significant effort. For early maturity it is recommended to analyze key input variables by sensitivity analysis or by threshold analysis. A threshold value is the smallest or highest value of an input variable that is sufficient to cause a recognizable change in the model results that would change the decision. Furthermore, uncertainty in early development stages can be analyzed qualitatively when there are only few data for a quantitative computation. As an additional interpretation tool, sanity checks can be applied to quickly evaluate whether the result of the assessment is plausible in terms of physical or economic ration ranges. Initially, in both cases a legitimate indicator shall be selected as output variable, in accordance with the goal of the TEA *(e.g. CO_2 capture cost, revenues, minimum product selling price, profitability indicator)*.

B.7.2.2 How to conduct uncertainty and sensitivity analysis

Characterization of uncertainty

The aim of UA is to quantify the total variation of the output of the model from uncertainties in the inputs of the model or from uncertainties is the model itself [92]. A range of outcomes or confidence intervals rather than one single value leads to more profound and comprehensive decisions. Various methods for UA exist and depend on the source and nature of uncertainty. UA functions as a quality test for the model and its input data by considering all sources of uncertainty simultaneously and validating if the model output supports the underlying decision process.

The classification of sources of uncertainty is divergent in literature and depend on context and scope. They can be classified into four main categories: [4], [93], [94]

- Uncertainties in the quantity of the input variables from errors of measurement or experts' estimations (data accuracy) or stochastic uncertainties due to the probability distributions of variables.
- Uncertainties in model structure and process, meaning how well the model reflects the interrelations of the real system.
- Uncertainties in context and scenarios due to methodological choices of the practitioner in goal and scope phase.

Another source of uncertainty is the 'ignorance of the practitioner' which is not assessable within UA and SA methods but by qualified peer review [95]. Uncertainty decreases with rising maturity levels due to better data or advanced understanding of the technology and conditions its research, development, and deployment is conducted in. This must be considered when comparing results from projects with different maturity levels.

Quantity uncertainty analysis

An uncertainty analysis quantifies the total variation of the outcome due to inherent variations of the inputs of a model [92]. At early maturity stages, a qualitative uncertainty analysis can be alternative or complementary to the quantification of the output variation.

Commonly used methods for the analysis of quantitative uncertainties are intervals (ranges with upper, mid and lower bonds), variance, probability distributions, possibility distributions or fuzzy intervals [92], [94]. If data is available to derive probability distributions, a probability-based method is recommended since it is easy to apply and provides statistical information, such as probability distribution or confidence intervals. Probability distributions are assigned to a set of input variables and are passed through a model (or transfer function) to obtain the distributions of the resulting output. In Figure 6, three input variables (x_1, x_2, x_3) and their respective probability distributions are transferred to the output's probability distribution function [92].

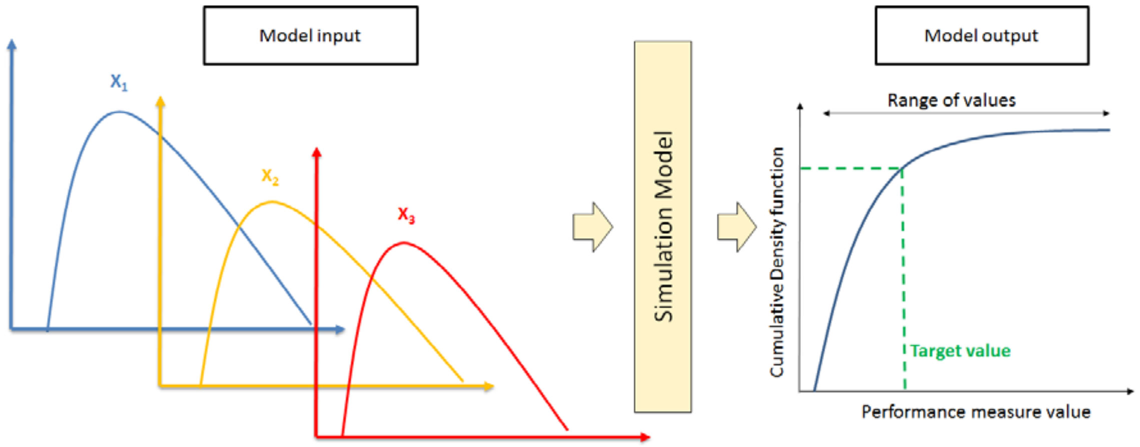

Figure 5. Simulating variable inputs to obtain probability distributions of performance indicator

The output distributions should be used to either describe the range of different potential outputs and their probabilities or estimate the probability that the output will remain in or exceed a specific threshold or performance target value *(e.g. CO_2 price, H_2 price, product price)* [94]. A comprehensive uncertainty propagation method is Monte-Carlo-Analysis; a sampling method where random values from input probability distribution functions are drawn repeatedly to generate the output and its uncertainty. To avoid misinterpretation, the input probability distribution functions should be presented together with the resulting probability distribution function of the output. When using Monte-Carlo-Analysis, the probability distribution functions of the variables must be well known. Especially at early technology maturity, there is often not enough data available for reliable probability distribution functions for the analysis.

Qualitative uncertainty analysis methods can be devised alternatively or complementary when data from different sources is used or when not enough reliable data for stochastic analysis is available. This is especially the case for technologies in early maturity stages, where only some technological and economic data is available. Qualitative methods define uncertainty categories in terms of direction and magnitude and assign them to each input variable and uncertainty source. A very useful approach is to employ simple, relative measures of uncertainty, expressed in terms of 'the degree of confidence'. One example of a qualitative UA of CO_2 polyols is presented in [96], referred as pedigree analysis. A pre-defined pedigree matrix analyses strengths and weaknesses of the knowledge base of each input parameter or model and their respective backgrounds on an ordinal scale *(e.g. scale 1 - 5, low-medium-high, IPCC level of confidence scale)* [97]. Ideally, estimates of confidence should be conducted by experts that are familiar with relevant details of the assumptions, data sources and procedures.

Model uncertainty analysis

The model or context uncertainty can be analyzed by identifying different scenarios and comparing the results or comparing model results with real observations. In order to analyze the model structure uncertainty, the model output needs to be validated with measured data or data from similar systems. To examine these uncertainties reliably, a lot of effort needs to be conducted in order to set up a valid analyzation framework and depends on the involvement of experts [94], [95].

Sensitivity analysis

Sensitivity analysis (SA) examines the sensitivity of the model output by apportioning the variance of the output to one or more input variables. SA also evaluates the contribution of each variable to the output uncertainty and thus reveals key variables that need to be focused on to reduce the uncertainty and to improve inventory data or impact assessment. Identification of key variables can already be executed at early maturity stages whereas for the decomposition of the uncertainty, reliable data is crucial and often not available until medium technology maturity. Sensitivity analysis methods can be broadly classified into local and global methods. While local sensitivity analysis is easier and faster to apply since only one input parameter at a time is varied, global sensitivity methods allow to apportion the output variance to the different input variables and also to calculate interaction effects of two or more input variables *(e.g. CO2 capture cost and CO_2 purity)* [98], [99].

Local sensitivity analysis

Local sensitivity analysis often also called 'one at a time' method, describes a variation of one input variable around a base value keeping all other input variables fixed. The resulting change of the model output in relation to the input variation is quantified as the sensitivity measure. The variation can be chosen individually *(e.g. 20%)* or based on the characterization of the uncertainty such as upper and lower limits of standard deviation or 5th and 95th percentiles of the parameter's distribution or values corresponding to reasonable economic, technical physical constraints *(e.g. material prices, tax rates, inflation rates, equipment configuration)*. A further sensitivity measure is the partial derivative of the model output with respect to each input variable. This method however does not consider uncertainty ranges of the input variables and can lead to misinterpretation if highly sensitive inputs are very certain, vice versa [118]. Calculated results should be presented graphically either as single factor spider (the steeper the slope, the stronger the sensitivity) or tornado graphs (the larger the range, the stronger the sensitivity) as shown in Figure 5. Local sensitivity analysis does not consider any correlations or interactions between different input variables and assumes linearity which leads to a limited informative value of sensitivity results [94].

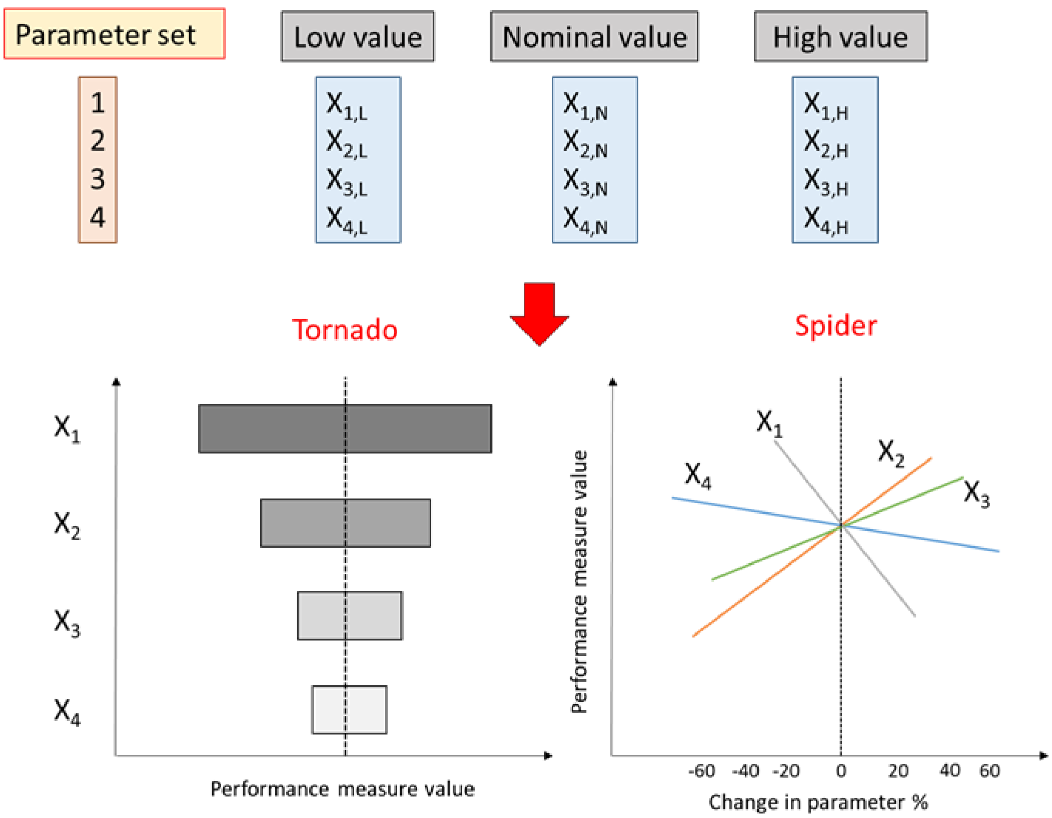

Figure 5. Visual representation of deterministic sensitivity analysis

Global sensitivity analysis

Global sensitivity analysis describes a set of mathematical techniques to investigate how the variation in the output of a numerical model can be attributed to variations of all input variables. Global sensitivity analysis should be applied to analyze the effects on the output of both individual inputs and interactions between the input variables. A common method is the analysis of the correlation between the output and the input space by calculating the regression coefficients of the input variables. The results of the regression analysis, for example regression and correlation coefficients and p-values, can be used to describe the sensitivity of linear as well as non-linear systems. Another econometric approach is the analysis of variance method used to calculate the first order sensitivity index and the total order sensitivity index, calculating the direct contribution to the variance of the individual inputs as well as indirect contributions through interdependencies of input variable [94], [95], [99], [100]. Selection of CCU-specific independent variables for the SA shall incorporate parameters from each system element *(e.g. CO_2 capture, CO_2 conversion plant, H_2 unit, minerals treatment etc.)* in order to obtain a better insight of the individual units and facilitate identification of most influential variables *(e.g. CO_2 price, other input prices, energy consumption and price)*.

Iterative approach for improving key data for inventory

Besides quantifying and allocating the uncertainty of the model output, the combination of uncertainty and sensitivity analyses helps identifying key variables for improving inventory data and calculation of indicators in an iterative way. High priority for improvement of data quality should be placed on data with both a strong sensitivity and a major lack of data quality (see Figure 6; note that the boundaries, axes and square sizes are subjective and derive from the decision maker). If data quality cannot be further improved, the result can be an overall high uncertainty of the results which is to be documented [75]. Complementary, data with a great lack of quality and consequently high uncertainty is recommended not be focused on for improvement if the sensitivity of this data is demonstrated to be very low.

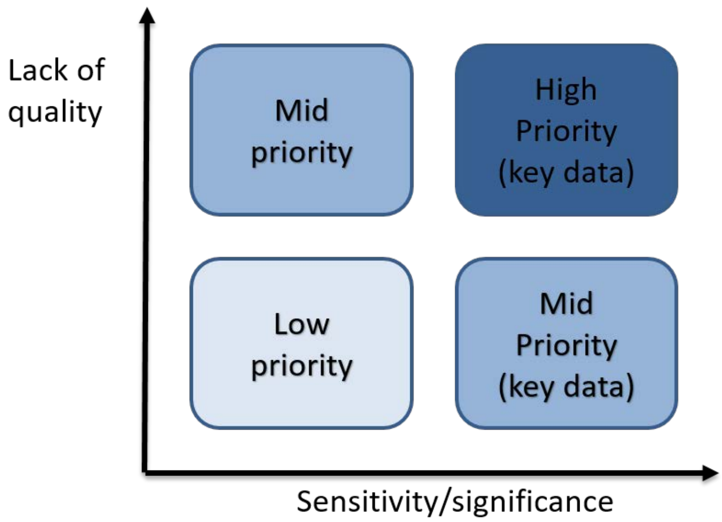

Figure 6. Priority setting for improving key data for inventory, adapted from [4]

The identification of key variables that are most influential to the model output can be useful when constructing different scenarios *(e.g. different energy mixes and their respective prices or different system boundaries and associated costs and prices).* Scenarios are sets of parameters that are derived from choices and assumptions by the practitioner and represent plausible alternative predictions of the future (see B.3.3). A baseline scenario and potentially an optimistic and pessimistic scenario are defined in advance in the goal phase. Developing different scenarios must be justified appropriately with respective assumptions. Scenarios are first defined in the goal phase but might be adapted or further scenarios might be added when reaching the interpretation phase, after identifying key variables that have a great influence on the model output. Other than UA, scenario analysis goes beyond considering the parameters' known uncertainty ranges but rather considers possible future events in a wider scope.

B.7.2.3 Further reading

In quantitative uncertainty methods include Taylor Series Approximation, Monte Carlo Simulations and Bayesian statistical modelling are explained. Qualitative methods of uncertainty analysis tend to be flexible and adaptable to different circumstances as shown in [92], [101]. A large number of local and global sensitivity analysis methods is available ranging from qualitative screening methods to quantitative techniques based on variance decomposition (for reviews see [92], [100]).

B.7.2.4 Guidelines

Guideline B. 18 - Sensitivity and uncertainty analysis		
Shall	1)	Select one or more output variables or indicator that shall be analyzed
	2)	Conduct uncertainty analysis and identify output uncertainty
	3)	Conduct sensitivity analysis and identify key variables
	4)	Provide conclusions, limitations and a basis for recommendations
Should	1)	Conduct local sensitivity analysis for quick screening purposes
	2)	Conduct global sensitivity analysis if the goal is to cover the whole parameter space
	3)	Conduct threshold analysis for identified key variables
	4)	Focus only on improvement of data with strong contribution and sensitivity on the overall result
May	1)	Conduct qualitative uncertainty analysis in research phase (TRL 1-3)
	2)	Derive alternative scenarios from sensitivity analysis

B.7.3 Interpretation of indicators

B.7.3.1 Introduction

The results of the calculated indicators are interpreted to provide indications for assessment criteria to answer questions posed by the assessment goal. Indicators help to compare and choose from multiple alternatives *(e.g. profitability indicators help to choose from investment alternatives)*. The interpretation of assessment indicators gives a positive, indifferent or negative indication - either by depicting a comparison of alternatives *(e.g. profitability indicators)* or are interpreted in comparison to a defined benchmark value *(e.g. technical indicators, CapEx, OpEx)* [20].

B.7.3.2 How to interpret indicators

General remarks

The interpretation of technical, economic or techno-economic indicators shall be done in compliance with the indicator definition, especially with regards to its described limitations. Furthermore, indicators shall be interpreted according to the specifications set in goal and scope; if the goal defines a threshold number for an indicator, the difference of the calculated indicator value to the defined figure can be interpreted. In general, indicator values must always be compared to an alternative value which can be derived from literature, expert guesses or experience from previous projects.

Interpreting profitability indicators

Indications derived from static indicators are recommended to be seen as trends rather than definite statements. Using static indicators poses the risk of underestimation, especially when interest rates are high or the difference between inflation and interest rate is large.[86] Static indicators only deliver limited information and have to be interpreted with caution. The general investment alternative incorporated in static indicators is no investment. Dynamic indicators are particularly sensitive to the used interest rate. The quality of the assumed interest rate has to be considered when forming an opinion about dynamic indicators' values. Outcomes of economic simulations are interpreted like other profitability indicators according to the question they are supposed to answer. The general investment alternative incorporated in dynamic indicators is an investment on the capital market with comparable risk characteristics.

Further remarks on specific profitability indicators:

- For static profit and static ROIs, a positive indication is given if the value is above zero or meets the required target value; when comparing alternatives, the higher value is preferred; in the efficiency form the threshold value is 1.
- For static payback time, a positive indication is given if the payback time is shorter than the expected plant life time; when comparing alternatives, the lower value is the preferred option.
- For NPV and dynamic ROI, a positive indication is given if the value is above zero or meets the required target value; when comparing alternatives, the higher value is preferred.
- For IRR, a positive indication is given if the value is higher than an interest rate for an investment with the same risk characteristics on the capital market or exceeds a target value; IRRs cannot be interpreted independent from a respective absolute value.
- For dynamic payback time, a positive indication is given if the payback time is shorter than the expected plant life time; when comparing alternatives, the lower value is preferred.

Interpreting indicator uncertainty

Uncertainties of different alternatives can be compared by their base cases (for uniform uncertainty distributions) or the expected value of the uncertainty distribution (for non-uniform uncertainty distributions such as normal distribution or skewed distribution). The interpretation of uncertainty ranges of multiple alternatives strongly depends on the practitioners' risk preferences, meaning if the practitioner is risk seeking or risk averse. If the uncertainty range is comparably wide and the practitioner values a chance of a very high outcome better than a higher expected value of an alternative investment, a risk-taking preference is present. Risk preferences may be documented and accounted for as a separate parameter in multicriteria decision analysis. Alternatively, a threshold value within the uncertainty range can be defined under (or above) which the expected values are accounted for with a defined factor. However, risk preferences are already part of the decision-making process and go beyond the assessment process.

B.7.3.3 Further reading

The term "assessment" in implications of its understanding for interpretation are reflected in [20]. In literature, interpretation approaches are usually presented with descriptions of respective indicators. For this reason, the further readings of scope (B.4.5.3) can be consulted.

B.7.3.4 Guideline

Guideline B. 19 - Interpretation of indicators	
Shall	1) Interpretation of indicators shall be in compliance with their definitions as well as with the goal and scope of the study 2) Indicators without an inherent comparison shall be compared to an alternative reference value 3) IRR shall be interpreted only together with absolute profitability indicator 4) Interpretation shall be conducted independently from subsequent decision making step
Should	1) Uncertainty ranges of indicators should be interpreted if different alternatives exist
May	1) Risk preferences of practitioner may be documented for subsequent decision making step

B.7.4 Multicriteria decision analysis

B.7.4.1 Introduction

After evaluating the robustness and reliability of results in previous steps, conclusions and recommendations for decisions can be derived. Multicriteria decision analysis (MCDA) is a method for supporting decisions that involve multiple dimensions or criteria and thus allows to evaluate trade-offs. It allows economic, social and environmental criteria, including competing priorities, to be systematically evaluated [102]. MCDA is typically established in five steps:

1. Identifying objectives
2. Identifying options for achieving the objectives
3. Identifying the criteria to be used to compare the options
4. Analysis of the options
5. Application of a MCDA technique

Two main methodological categories of MCDA exist: Multiple Attribute Decision Making (MADM) and Multiple Objective Decision Making (MODM). While MADM handles problems with a discrete decision space and a predetermined set of alternatives, MODM handles problems that consider a continuous decision space [103]–[105]. These methods are often used for decisions that are based on a combination of quantitative and qualitative information and therefore go beyond quantitative indicators (see B.4.5). MCDA may be used to inform policy makers and other stakeholders of feasible alternatives and aid the decision-making process by presenting complex and interlinked data, impacts and trade-offs clearly and comprehensively.

MADM and MODM may be applied to the interpretation of the TEA as these approaches might help the practitioner subsequent decision-making. If the practitioner examines different process configurations of a specific production process *(e.g. different reactor conditions)*, the investigated criteria could be energy efficiency, processing and investment effort and profitability (see B.4.5). However, preliminary efforts have been made to develop a reliable MCDA framework to interpret technologies at early development stages [106], [107]. MADM and MODM can also be applied to analyze trade-offs between LCA and TEA results (see Wrapping document, A.5).

B.7.4.2 How to conduct multicriteria decision analysis

Multiple Attribute Decision Making (MADM)

MADM methods use normalization and criteria weighting techniques in order to favor a certain aspect of the decision makers' preferences. The problem can be defined as finding the best set of alternatives for the decision maker. Generally, the MCDA problem involves *m* alternatives evaluated on *n* criteria. The grouped decision matrix is depicted in Table 12, where X_{ij} is the rating of alternative *i* with respect to criterion *j* and W_j is the weight of criterion *j*. Several conversion routes and process configurations exist within CCU, even for similar products. MADM may be used to create a common basis for comparisons between different projects. MADM should include a wide range of technical and economic criteria *(e.g. CO_2 capture cost, product market price, employment opportunities)*.

Table 12. Common structure of a MCDA problem

	Criterion 1	Criterion 2	...	Criterion n
Alternative 1	X_{11}	X_{12}		X_{1n}
Alternative 2	X_{21}	X_{22}		X_{2n}
.	.	.		.
.	.	.		.
.	.	.		.
Alternative m	X_{m1}	X_{m2}		X_{mn}
	W_1	W_2	...	W_n

Multiple Objective Decision Making

This concept nearly always provides, not a sole solution, but instead a group of solutions called the 'Pareto optimal set'. The solutions within the Pareto optimal set are termed 'non-dominated'. The graph of the objective functions whose non-dominated vectors are included in the Pareto optimal set is also known as a 'Pareto frontier' (see Figure 7). MODM may be used to identify and display all trade-offs among the investigated indicators. Conflicting concepts should be analyzed which means that achieving the optimum for one objective requires some compromise on one or several other objectives *(e.g. capital cost and operating cost, selectivity and conversion, quality and conversion, and profit and safety cost)*. The mathematical formulation of a MODM problem consists of definition of objective functions and input variables along with equality and inequality constraints. The equality constraints in chemical processes can arise from mass, energy and momentum balances *(e.g. product purity, CO_2 conversion, undesirable side products, reactor temperature)*.

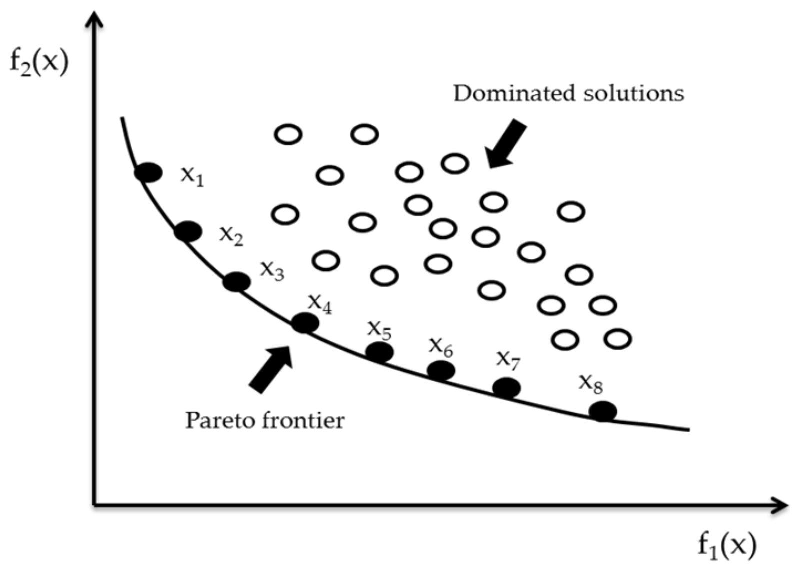

Figure 7. Potential range of solutions for a two-objective optimization problem showing the Pareto frontier

Although there are many choices on the Pareto frontier, in subsequent decision-making one solution will be picked. There are two approaches to find a single solution in MODM, methods with prior preferences (or preference-based procedures) and methods with posterior preferences (or ideal procedures) [108], [109].

B.7.4.3 Further reading

Many MADM methods exist such as Technique for Order Preference by Similarity to Ideal Solution (TOPSIS), Analytic Hierarchy Process (AHP) and its generalization the Analytic Network Process (ANP), Fuzzy Set Theory, Elimination Et Choix Traduisant la Realité (ELECTRE) and Preference Ranking Organization Methods for Enrichment Evaluations (PROMETHEE) [110]. AHP due to its simplicity in procedure has gained popularity although few outranking techniques such as ELECTRE III and PROMETHE are also popular. However, no single MADM model can be ranked as best or worst but every method has its own strength and weakness depending upon the intended application and objective of the assessment [111].

A large number of approaches exists in literature to solve MODM [112]. Among them the most popular are the Non-dominated Sorting Genetic Algorithm and Multi-Objective Simulated Annealing. Classically, a multi-objective optimization model may be scalarized into a single objective optimization problem. Two simple methods in this approach are weighted sum method (WSM) and weighted product method (WPM) [113].

B.7.4.4 Guidelines

Guideline B. 20 - Multicriteria decision analysis	
Shall	
Should	1) Provide holistic information about the whole spectrum of dimensions related to the technology to decision makers
May	1) Conduct Multi criteria decision analysis; if applied shall a) Include a wide range of criteria such as economic, environmental and social b) Investigate conflictive concepts

B.9 Reporting

B.9.1 Introduction

Reporting of the TEA presents the analysis to the audience. Reporting is very specific to the requirements of the audience and can therefore take numerous forms. For example, the requirements for an academic publication will be considerably different to a corporate viability report. Also requirements within an audience type can vary *i.e.* specific reporting requirements for the EU will differ to the US DOE. Therefore, no specific guidelines on the style of the report are given here, instead the guidelines cover aspects that must be covered to ensure transparency and accuracy.

B.9.2 Creating a report for a CCU TEA

B.9.2.1 General reporting principles

TEA results and interpretation should be reported completely, transparently and accurately to the intended audience. The report may take numerous forms *(e.g. academic publication, corporate report)* and should be tailored to the audience's requirements. The reporting should also be aligned to the audience in terms of readability. While readers with R&D expertise *(e.g. researchers, funding agencies)* expect the use of technical terminology, this should be used with care for readers without R&D expertise *(e.g. government agencies, general public).* These audiences require a less technical language to diminish the risk of misunderstanding and misinterpretation [6].

The assessment results shall be clearly reported to the audience in order to avoid ambiguity and misinterpretation. All assumptions, data for calculation, methods, results, respective uncertainties and sensitivities, recommendations and limitations shall be presented transparently and as detailed as possible. The data sources should be explicitly stated. This is also important to guarantee reproducibility and full traceability for the reader [4]. It is recommended that the report includes a clear executive summary and a technical summary table (see Table 16 Annex) to enable the reader to easily access the data used in the assessment. If confidential data is used, this should be clearly stated and then the relevant parts retracted as necessary to avoid confidentiality issues. The report should also include details of who (the practitioner and their background) carried out the analysis and the review process that has been undertaken.

B.9.2.2 Reporting at different technology maturities

For some processes, TEA may be conducted at very early technology maturity stages. In this case, a more qualitative approach should be conducted which is predominantly used to identify hotspots for improvement in process design. The hotspots identified by the qualitative method should be stated clearly and the issues explained. At low maturity, the TEA should not be used as a mechanism to disregard a technology as the uncertainly in the analysis will be high. However, the TEA should be used to inform decision making and next steps in research and development.

At higher levels of technology maturity quantitative approaches can be used alongside qualitative methods. The uncertainty and sensitivity of quantitative analysis should always be included and reflected upon, particularly if generic or average secondary rather than process-specific primary data is used.

B.9.2.3 Reporting of system elements

To enable effective identification of most influential parameters in the process, particularly at low maturity, reporting of indicators for system elements as well as the overall system is encouraged. For example, in the production of methanol, system elements that could be reported would include carbon capture and hydrogen production (if included within the system boundary) and methanol synthesis. By reporting system elements, audiences are easily able to determine the elements that have the highest impacts on the whole system and identify where technology advances would create the greatest benefits.

B.9.2.4 Addressing audiences

Audiences for R&D-perspective TEA

R&D-perspective TEAs are likely to be interesting for R&D experts (academic, industrial or governmental). This audience demands information regarding the technical performance of the product systems and expect the use of technical terminology and detailed reporting of specific technical indicators common for the field *(e.g. turnover frequency or faraday efficiency)*. To describe the big picture, economic or social indicators are typically added at low level of detail. Reporting TEA results to R&D experts can lead to detailed feedback on technical performance or to the adaption of the work in other research groups, which is why confidentiality issues can arise.

Another major audience for R&D-perspective TEAs are funding agencies that require not only information regarding technical performance, but also a description of social and economic benefits. Required indicators are typically at the practitioner's choice, while in certain proposals the calculation of specific indicators *(e.g. CO_2 abatement cost per kg product)* can be necessary. In the latter case and in the case of reporting to governments, cradle to grave assessments are often favored as they can be more transparent when communicating with people not familiar with the topic. Reporting TEA results to funding agencies typically happens in the course of a funding proposal or project report, both crucial to secure R&D funding.

Audiences for corporate-perspective TEA

Corporate-perspective TEAs are likely to be interesting for investors or corporate decision makers *(e.g. management)*. These audiences demand both, the reporting of technical and economic performance, potentially social benefits as well. These audiences typically demand two levels of reporting detail, a summary and a main version (see B.8.2.5). While for the full report economic indicators should be reported at highest level of possible detail *(e.g. NPV, option pricing, liquidity planning)*, technical results either require the introduction of detailed technical terminology or should be reduced to an intermediate level of detail. Reporting is usually very timely, can take place in regular intervals and is connected to important decisions *(e.g. allocation of budget, investment in plant, investment in company shares)*. Reporting to these audiences can lead to feedback especially regarding the economic performance of the product system. There can be a need for both internal and external reporting from a corporate-perspective. If a report is to be released outside of the company, confidentiality issues can occur and dictate that certain data cannot be released. In this case, the report should clearly state if a 'shall' guideline cannot be followed.

Audiences for market-perspective TEA

Market-perspective TEAs are likely to be interesting for policy-related audiences *(e.g. policy makers, regulators, NGOs)*. These audiences demand to understand the larger societal benefits as well as the environmental impacts, which is why for these audiences, indicators integrating TEA, LCA and potential social impact studies are helpful *(e.g. the cost of CO_2 abated, the number of jobs created or maintained, the amounts of fossil imports reduced)*. TEA reports for these audiences should include a summary and a main report (see B.8.2.5). Reporting to these audiences usually takes place in less or fewer regular intervals. Reporting to these audiences can also lead to very important decisions *(e.g. regulation, subsidies)*. Furthermore, it can provide feedback on important concerns that these actors might have on techno-economic aspects of the technology.

Further audiences

Further important audiences are journalists and the wider public. Similar to political audiences, the media and the public demand information about societal benefits and economic impacts, but a much lower level of detail is required. While the indicators can be chosen freely by the practitioner, only a handful of indicators need to be reported and they need to be introduced first. A special challenge when addressing the media and the public is the use of clear and easy to understand language as well as additional image-, audio- and video-based information. Reporting to these audiences is usually irregular and is recommended when there is something new to report. While these audiences do not take immediate decisions on the technology, they can be important multipliers and thus their understanding of the technology's impacts can be crucial for its future success *(e.g. technology acceptance)*.

B.9.2.5 Executive summary

For audiences without R&D expertise, an executive summary of the data, methods, assumptions, limitations, recommendations and results should be included. The executive summary should include clear specific statements which cannot be misinterpreted, for example statements should be phrased such as:

> *This study concluded that the price of methanol produced from CO_2 on a 10 tonne per day plant in Germany using carbon capture and renewable hydrogen from water electrolysis was 4 times higher than the current global market price in 2018 of conventional methanol.*

Rather than:

> *The price of CCU methanol is 4 times the current price.*

The first statement is transparent and clearly shows that the price reported is related to a specific situation, whereas the second statement can easily be misinterpreted to imply that the cost of CCU methanol will be 4 times higher no matter what the inputs, process or location. The later statement could lead to false general conclusions and judgements such as a loss of interest in the technologies or even a rejection of their further development.

B.9.2.6 Reporting of uncertainties and sensitivities

To avoid misinterpretation of results, uncertainty and sensitivity results shall be reported transparently. Following the ILCD Handbook [4], this can be done qualitatively as well as quantitatively. Qualitative reporting should be done concerning the context uncertainty (elements from goal and scope definition) as well as model uncertainty. In early TRLs, quantity uncertainty (lack of knowledge and probabilities) can also be reported qualitatively. All indicators and models selected for the assessment shall be justified. Especially for comparative studies and advanced TRLs, quantitative reporting of quantity uncertainty *(e.g. variance, box plots)* shall be added. The reporting shall include all parameters with high sensitivity (key variables) and their effects to the model result [94].

B.9.2.7 CCU specific reporting

From a techno-economic point of view, the amount of CO_2 utilized in the process needs to be clearly stated in relative or absolute numbers. Moreover, it is essential to state that this amount does not correspond to the amount of CO_2 avoided, which is determined by the LCA. The amount of CO_2 avoided corresponds to the reduction in emissions achieved by the CCU process when compared to the reference scenario. Whereas the amount of CO_2 utilized refers to the amount of CO_2 the process uses to produce the product. It is important to distinguish between used and avoided CO_2 as the values can be very different and so any confusion can lead to misinterpretations.

In addition to reporting results for the complete systems, it may be helpful to report some results for system elements separately. In doing this their effects and impacts on the overall economics can be observed. For example, results and sensitivity of electricity consumption in CCU methanol production, can be reported by each system element (for CO_2 capture, H_2 production, methanol production separately) as well as for the overall system. Reporting sensitivities of system elements separately especially can help in identifying key variables within the system. In all cases, reporting of system elements may be done in addition to reporting for the complete system.

Careful consideration of energy requirements is often an important aspect in CCU processes due to the necessity to use low carbon or renewable energy to avoid additional environmental impacts. When reporting the energy (particularly electricity) requirements, it may be helpful to articulate the real-world implications of that requirement, for example the number of wind turbines needed to produce the required amount or the percentage of a countries current (and future) renewable energy production. A statement on how the intermittency of future energy scenarios has been considered in the modelling should be included.

Where economic incentives are incorporated into the TEA *(e.g. emission certificate prices, emission taxes, gate fees and landfill taxes)*, these should be clearly stated and their impacts clarified. If future scenario modelling is undertaken (see Section 3.3), increases in the incentives can be included based on transparent predictions of growth. As no incentive is permanently guaranteed, it is recommended that the impacts of economic incentives are reported subsequently to the initial analysis without the incentive so that the effect can be fully observed.

B.9.3 Checklists for reporting

Clear reporting enables the reader to follow the methodology and assumptions the practitioner has used. The following checklist provides guidance regarding recommended minimum content for the executive summary and main report and can be used as a quick review process to ensure all essential 'shall' aspects are covered in the report.

Checklist - Executive summary

Goal of the study

- ❑ State goal and study context
- ❑ State the intended application(s) of the results
- ❑ State the reasons for carrying out the study and the decision context

Scope of the study

- ❑ State functional unit
- ❑ State system boundaries
- ❑ State relevant statements on data quality, assumptions

Assessment

- ❑ State main results

Interpretation

- ❑ State any conclusions, recommendation and limitations due to assumptions and methods

Checklist - Main report

Goal of the study

- ❑ State goal – the intended application of the study and the reasons for the study
- ❑ State the target audience for the study
- ❑ State commissioner and authors of the study
- ❑ State limitations in the usability from assumptions or methods
- ❑ State the base case with current conditions

Scope of the study:

- ❑ State product function(s) or product function scenarios
- ❑ State the benchmark process and its scale

- ❑ State the functional unit, including consistency with goal and scope and how performance is measured
- ❑ State elements and boundaries of product system, including a graphical scheme
- ❑ State the technology maturity of system elements and the overall product system
- ❑ State the selected indicators and assessment methods

Inventory

- ❑ State types and sources of the data including the quality
- ❑ State the technical data in SI units and in a technical parameter list
- ❑ State economic data in an economic parameter list
- ❑ State all economic decisions and assumption made

Calculation of indicators

- ❑ State calculation procedures including any assumptions and estimates
- ❑ Explain methodology of financial analysis
- ❑ Include results of technical assessment
- ❑ Include results of economic assessment

Interpretation

- ❑ Include and describe the results
- ❑ Include and describe uncertainty and sensitivity analysis
- ❑ State assumptions and limitation associated with the assumptions, methods and interpretation of results
- ❑ Include conclusions
- ❑ Include recommendations, if any

B.9.3.1 Further Reading

A detailed guidance on LCA reporting principles, elements and targeting at different levels can be found in [4]. The instructions can be for the most part adapted to TEA. For more information on actor-specific issues of stakeholder acceptance of CCU please see [114].

B.9.3.2 Guideline

Guideline B. 21 - Reporting		
Shall	1)	Cover the phases of goal, scope, inventory, assessment and interpretation
	2)	Use clear language to avoid misinterpretations particularly in Executive Summaries
	3)	All assumptions, data for calculation, methods, results, recommendations and limitations shall be presented transparently and as detailed as possible.
	4)	Use the Reporting Checklist to ensure all aspects are covered
Should	1)	Report findings for system elements as well as the whole product systems, to identify key variables
	2)	Take into account the audience and their technical knowledge
	3)	Use a technical summary (Table 16)
	4)	State who carried out the study and how the study has been reviewed
May	1)	Apply the LCA reporting principles (see ILCD handbook), especially when conducting LCA and TEA in parallel

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B.11 Annex

Table 13. Examples of upstream elements for CCU product systems[29], [115], [116]

CO_2 emissions (direct) industry, recent estimates from various years [Mt_{CO2}/year] [29]		CO_2 capture for combustion processes	CO_2 separation for all processes	H_2 production	Electricity production
Coal power plant (PP)	9 031	• Post-process • Oxyfuel • Pre-process • Chemical looping	• Absorption • Adsorption • Chemical looping • Membrane separation • Hydrate-based separation • Cryogenic distillation	• Steam methane reforming • PEM electrolysis cells • Solid oxide electrolysis cells (SOEC)	• Coal-fired PP (fossil coal & bio-based co-firing) • Oil-fired PP • Gas-fired PP (natural gas, biogas) • Nuclear PP • Hydro PP • Wind PP • Photovoltaic PP • Solar-thermal PP
Natural gas PP	2 288				
Cement production	2 000				
Iron and steel production	1 000				
Oil refineries	850				
Oil power plant	765				
Ethylene production	260				
Ammonia production	150				
Bioenergy	73				
H_2 production	54				
Natural gas processing	50				
Waste power plant	60				
Fermentation to biomass	18				

Table 14. Characterizing Technology Readiness Levels for the Chemical Industry [Excerpt from unpublished TUB working paper]

TRL	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Phase	**Research**			**Development**			**Deployment**		
Title	*Idea*	*Concept*	*Proof of concept*	*Preliminary process development*	*Detail process development*	*Pilot trials*	*Demonstration & full-scale engineering*	*Construction and start-up*	*Continuous Operation*
Description	Basic principles observed and reported, opportunities identified, basic research translated into possible applications *(e.g. by brain-storming, literature study)*	Technology concept and application formulated, patent research conducted	Applied laboratory research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)	Concept validated in laboratory environment, scale-up preparation started	Shortcut process models found, simple property data analyzed, simulation of process and pilot plant using bench scale information	Pilot plant constructed and operated with low rate production, products tested in application	Parameter and performance of pilot plant optimized, (optional) demo plant constructed and operating, equipment specification incl. components conferrable to full-scale production	Products and processes integrated in organizational structure (hardware and software), full-scale plant constructed	Full-scale plant audited (site acceptance test), turn-key plant, production operated over the full range of expected conditions in industrial scale and environment, performance guarantee enforceable
Tangible work result	Idea / rough concept / vision / strategy paper	Technology concept formulated, list of solutions, future R&D activities planned	Proof of concept (in laboratory)	Documentation of reproduced and predictable (quantitative) experiment results, first process ideas	Simple parameter and property data, process concept alternatives evaluated	Working pilot plant	Optimized pilot plant, (optional) working demo plant, sample production, finalized and qualified system and building plan	Finalized and qualified system and building plan	Full-scale plant tested and working
Workplace	Sheets of paper (physical or digital), whiteboard or similar	Sheets of paper (physical or digital), whiteboard or similar	Laboratory	Laboratory	Laboratory/mini-plant	Pilot plant, technical centre	Pilot plant, technical centre, (optional) demo plant (potentially incorporated in production site)	Production site	Production site

Table 15. Draft for a technical summary table

System element	Parameter	Unit
A	Flue gas	t/h
(e.g. CO_2 capture)	CO_2 input	t/h
	CO_2 capture	%
	Electricity consumption	MW
	…	
B	Deionised water	t/h
(e.g. Water electrolysis)	…	
C	CO_2 input	t/h
(e.g. CO_2 conversion)	…	
D	Electricity consumption	
(e.g. Purification)	…	

Table 16. Technical Summary Table

GOAL	**CCU product**			
	Intended application and reasons for study			
	Brief description			
	Intended audience			
	Commissioners and Assessors			
	Limitations of study			
SCOPE	**System boundary** (i.e cradle to gate)			
	Benchmark system			
	Plant size			
	Functional Unit			
	System elements and technology maturity	**System elements**	**Efficiency**	**Technology Maturity**
	Assessment indicators	**1**		
		2		
		3		
		4		
		5		
INVENTORY	**Data Sources**			
	Energy sources and scenarios			
			REFERENCE CASE	**CCU TECHNOLOGY**
	Base year			
	Currency			
	Location			
	Plant life time			
	CO_2 source and price (if applicable)			
	Main inputs and prices (if applicable)			
CALCULATION OF INDICATORS	**1.**			
	2.			
	3.			
	4.			
	5			
INTERPRETATION	**Sensitivity Analysis main factors and Hotspots**			
	Uncertainty manipulated variables			
	Main Conclusions	•		
	Recommendations	•		

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PART C
LCA Guidelines

SUPPORTED BY

Contents Part C

C.1 Introduction

C.1.1 General introduction to life cycle assessment

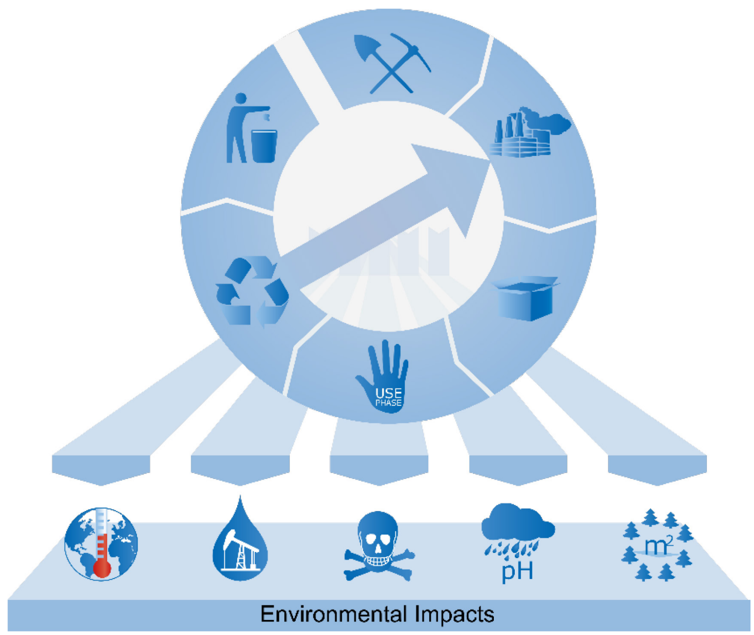

Figure 1: The holistic approach of life cycle assessment accounts for environmental impacts associated with all stages of a product's life cycle (circle in the middle).

Life cycle assessment is a methodology to account for the environmental impacts of a product or service throughout its entire life cycle. The entire life cycle spans from cradle-to-grave, i.e., from raw material extraction through production, packaging, use, end-of-life treatment and recycling to final disposal. Through each stage, the product's life cycle interacts with the environment by consuming natural resources and emitting pollutants. Life cycle assessment is a quantitative method to describe these interactions and their potential environmental impacts[1]. Due to its holistic approach, LCA avoids problem shifting between both environmental impact categories and life cycle stages. Therefore, LCA is a valuable tool in various fields, e.g., product or process design, decision making in industry and policy as well as marketing. The LCA methodology was standardized in the 1990s by the international standardization organization (ISO) in ISO 14040 and 14044 and is still updated and extended regularly.

According to the ISO standard, an LCA study is sub-divided in 4 phases (compare Figure 2):

1. Goal and Scope definition
2. Life cycle inventory analysis
3. Life cycle impact assessment
4. Interpretation

[1] In this guideline, environmental impacts instead of potential environmental impacts is used to improve readability. However, LCA is not able to assess actual environmental impacts.

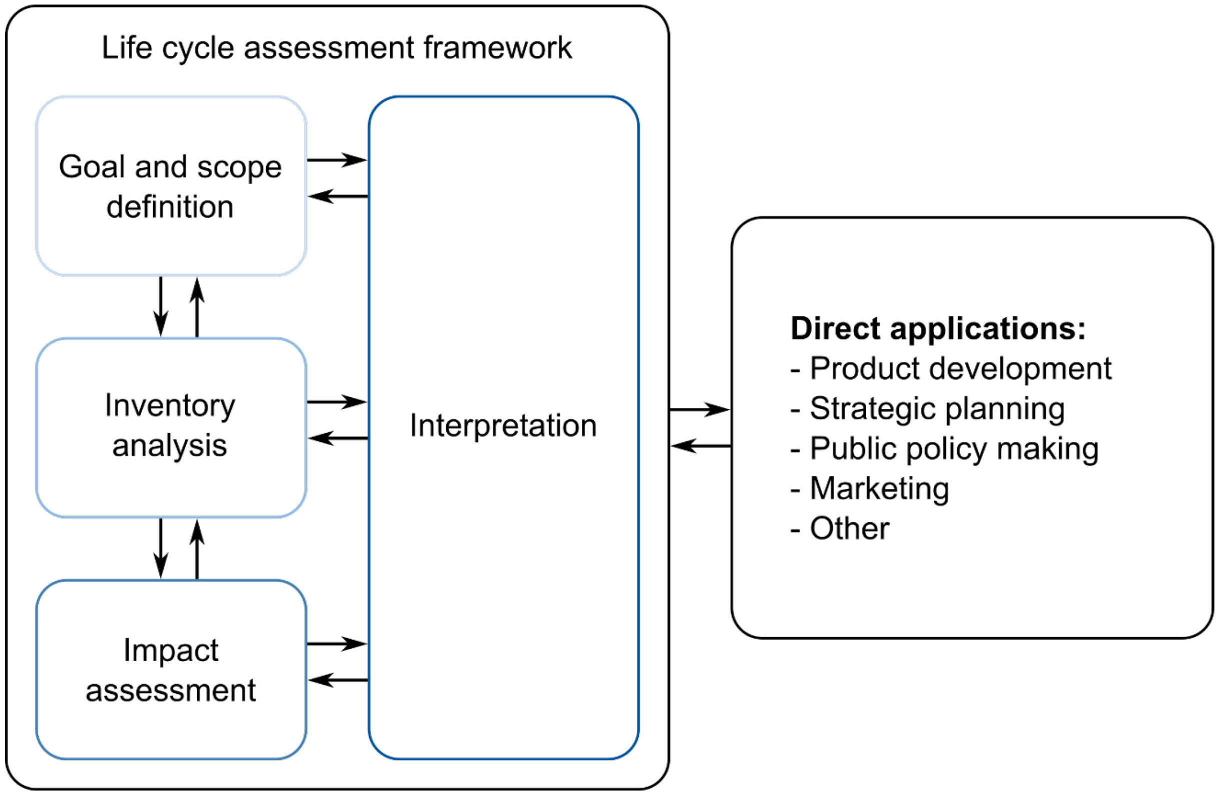

Figure 2: General framework for life cycle assessment [1]

All phases are interdependent, e.g., the gathered life cycle inventories have to suit the initial research question with respect to time and space. In practice, this interdependence renders LCA an iterative approach, as data availability is often not fully known at the beginning of an LCA study. Fig. 2 also shows that the life cycle framework interacts with its supposed direct applications.

The need for standardizing LCA assessment on CCU technologies has been identified by the European Commission [2]. In addition, it was shown that LCA studies on CCU showed a large variation of results even for identical technologies [3]. Therefore, the major goal of this document is standardizing LCA assessments in order to improve transparency and comparability between LCA studies.

C.2 How to read this document

C.2.1 Aim and scope of this document

The application of LCA for CCU technologies is challenging, and substantial methodological choices and pitfalls exist. These difficulties lead to wide differences in current LCA practice in the field of CCU, potentially misleading decision makers. Building upon existing LCA standards and guidelines, this guideline targets CCU-specific challenges for the LCA methodology, and provides recommendations on how to address these challenges in a way that ensures comparability and transparency of the results. This document aims to provide short and concise guidance on CCU-specific LCA challenges and is complementary to existing standards and guidelines. Therefore, general issues of LCA are omitted if these issues are not specific to LCA on CCU. However, since readers might be new to the concept of LCA, we provide a short introduction to each step of an LCA study and further reading is recommended.

This document is based on the life cycle assessment ISO standards 14040 [1] and 14044 [4], the ILCD handbooks [5,6], several textbooks [7–10] and scientific publications [11,12].

C.2.2 Structure of this document

The document is structured according to the LCA workflow and aims to support LCA practitioners while conducting an LCA study (cf. Figure 2). Each chapter provides a short general introduction to the LCA aspect covered. These introductions are provided within boxes and may be skipped by experienced LCA practitioners. Subsequently, CCU-specific challenges are described and recommendations are given. At the end of each chapter, a guideline containing a list of tasks which shall/should/may be performed, is provided.

These guidelines have been developed to enable consistent and comparable LCA studies for CCU. For this purpose, the guidelines are more restrictive than the general ISO-framework. Thus, there may be need to add further tasks to the ones discussed in this guideline since they are important to a specific case study. Such additions are not excluded by the present guideline. However, we believe in the need for a consistent methodological core for LCA of CCU, which these guidelines provide.

C.3 Goal definition

General introduction

Every LCA study starts with the goal definition. According to ISO 14040, the goal definition (4.2.2.) shall unambiguously describe “the intended application of the study, the reasons for carrying out the study, the intended audience of the study and whether the results are to be used in comparative assertions disclosed to public”. All of these items are linked to the goal of the study. Even though the ISO clearly outlines the elements required as part of the goal definition, it is helpful to state the goal as a central research question since such a central question is more often specific than a list of statements [8]. Note that without a precisely defined goal, the result of an LCA study can remain meaningless [8] and not all goal definitions are reasonable. For example, LCA is not able to determine whether or not a product is environmentally sustainable, as this would require an absolute threshold value for sustainability [11]. However, LCA can determine the environmental impacts of products and benchmark the impacts to other products. Therefore, it cannot be emphasized enough how important a precise and reasonable definition of the initial research question is, because the goal definition is the starting point to derive important methodological choices in LCA, such as the definition of the system boundary and co-product allocation.

Further recommended reading:

Baumann and Tillman offer a comprehensible and short description of the goal definition in Chapter 3.1 (Page 74ff.)[8]. A more detailed description of the goal definition is given in the ILCD Handbook in Chapter 5 (Page 29ff.)[5]. The topic also covered in Curran’s handbook in chapter 2.1.1. (Page 17ff.) and in Guinée’s handbook in part 3 chapter 2.2. (Page 456ff.)[7]. Von der Assen et al. (2014) provide a list of exemplary research questions regarding CCU [11].

C.3.1 Defining goals for LCA studies on CCU technologies

Many questions may be answered by LCA. To get an overview, we here start by identifying typical goal definitions for CCU from literature. As stated above, most CCU technologies may be in stages of early development and aim to reduce environmental impacts. Therefore, it is not surprising that most investigated LCA studies on CCU aim at quantifying the potential environmental impact reductions of CCU processes or products in comparison to existing processes [13–31]. Most studies also include a contribution analysis [15–17,20–24,27–29] of environmental impacts to identify hot spots for improvement. One study aims at identifying the CCU technology which makes environmentally most beneficial use of the scarce resource hydrogen produced from renewable energies [32]. Once CO_2-based products are deployed in the markets, LCA can be used for environmental product declaration [33–35].

From this short literature review, the most common research questions are derived:

1. Is a CCU-based product or service environmentally beneficial compared to the same product or service derived from fossil carbon sources?
2. Where are the environmental hot spots for technology improvement to reduce environmental impacts in the life cycle of a CCU product/process?
3. What is the environmentally preferred CCU technology to make best use of a scarce resource, e.g., renewable energy?
4. What are the environmental footprints of products or services used as basis for customer decisions (product declaration)?

All of these research questions imply a comparison between alternatives (explicit or implicit) and thus, intend to support decision making, e.g., which process to use, how to improve the technology or which product to buy (refers to product declaration). In most cases, CCU technologies aim to produce products that are already offered in the market. For this reason, the guideline focusses on comparative assessments, or assessments that are to be used in comparative assertions. Goal definition should use the research questions listed above to derive the specific research question of the study. In addition, the requirements of the ISO 14044 shall be fulfilled as listed in the introduction of this chapter.

For CCU technologies in stages of early development (low technology readiness level, TRL), studies can end up in apple vs oranges comparisons, since most reference technologies are mature and have been optimized over decades. In contrast, low TRL processes usually have higher energy demand or solvent consumption because of not yet established heat integration and/or process optimization. At the same time, low TRL processes lack auxiliary processes such as product purification steps after reaction. Thus, LCA studies on lab-scale processes can under- or over-estimate environmental impacts. These aspects should always be considered in comparative studies if a high TRL technology is compared to a low TRL technology. For low TRL processes, studies are most useful for hot spot analysis. However, a comparison between a low TRL CCU technology and a high TRL reference technology can still reveal valuable insights to guide research. Furthermore, ex-ante assessments may be applied to compare the current low TRL technology at a future industrial scale-up TRL with the future reference process or the technology development [36–42]. Please note that the prediction of future developments introduces another source of uncertainty.

C.3.1.1 Guidelines

Guideline C.1 –Goal definition	
Shall	1) The intended application of the study shall be stated. 2) The reasons for carrying out the study shall be stated. 3) The intended audience of the study shall be stated. 4) It shall be stated whether the results are to be used in comparative assertions disclosed to public.
Should	1) A research question should be chosen from the most common research question (as listed in Chapter C.3.1). 2) The class of the assessed CCU technology should be stated. If the proposed classification is not suitable, it should be justified and reported.
May	

C.4 Scope definition

General introduction

According to ISO 14040, "the scope should be sufficiently well defined to ensure that the breadth, depth and detail of the study are compatible and sufficient to address the stated goal." In other words, it shall be described under which conditions and assumptions the results of the study are valid [11]. Therefore, every aspect of the scope definition is closely related to and has to be in line with the study's goal.

According to ILCD handbook and ISO 14044, the following items need to be unambiguously described or defined in the scope definition:

- The (product) system or process to be studied, its function, functional unit and reference flow (see C.4.1)
- System boundaries, completeness requirements and related cut-offs (see C.4.2)
- The life cycle inventory modelling framework and co-product management (see C.4.3)
- Other life cycle inventory data quality requirements regarding technological, geographical and time – related representativeness and appropriateness (see C.4.4)
- Special requirements for comparative assessments (see C.4.4.1)

Further recommended reading:

The ILCD handbook offers an extensive description of each of the items listed above in Chapter 6 (Page 51ff.) and Baumann and Tillman offer a concise description of the scope definition in Chapter 3.2 (Page 75ff.)[5,8]. Scope definition is also discussed in Curran's handbook (Page 45ff.) and in Guinée's handbook part 2a chapter 2 and part 3 chapter 2.3 (Page 459 ff.) [7,10].

C.4.1 Product system, its function, functional unit and reference flow

General introduction

Life cycle assessment quantifies the environmental impacts of a product or process system on a relative basis with respect to its function, e.g., global warming impact per kg of product. This relative basis is the functional unit, which quantifies the performance of a product system or service. The functional unit then serves as reference system to ensure that comparisons between systems serve equal functions, which is particularly important for comparative studies. 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) to cover a defined area with a defined opacity (functional unit).

A functional unit quantifying the technical performance of a product system or service shall be defined unambiguously.

Note that systems might serve one or more functions, e.g., a combined heat and power system provides both electricity and heat. Therefore, the functional unit might contain more than one reference flow. Furthermore, not all functions might be objectively measurable, e.g., food provides nutrition and sometimes pleasure and thus, LCA studies might exclude additional functions that are out of the scope. Excluded functions shall still be documented and reported.

C.4.1.1 Defining functional units for CCU technologies

Most LCA studies on CCU aim at comparing CCU technologies to a benchmark (cf. Chapter C.3.1). The functional unit ensures sound comparison of the assessed technologies. However, different LCA studies for identical technologies may apply different functional units, which complicates comparisons between studies or even makes them incomparable [3]. To increase comparability among studies, we derive functional units for each class of CCU technologies from current LCA practice.

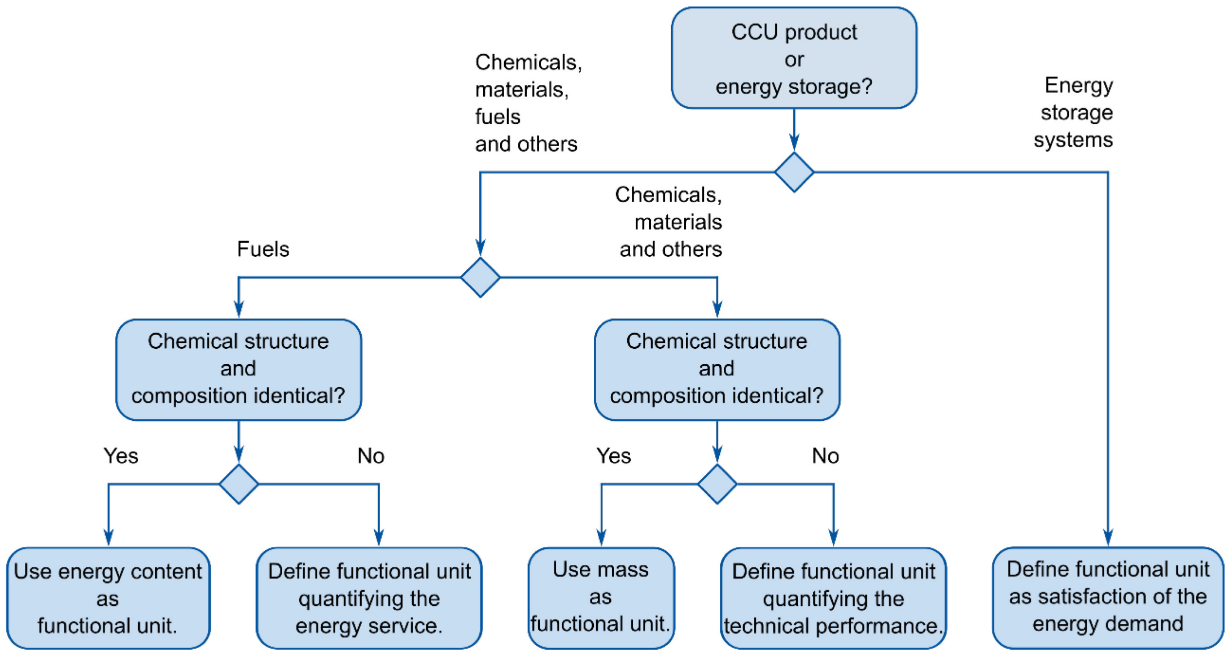

Figure 3: Decision tree for the selection of a suitable functional unit.

For **products with identical chemical structure and composition to their conventional counterparts**, in general, mass shall be used as a basis for comparison since this is the most common trading unit for chemicals, materials and minerals. Other bases for comparison, e.g., amount of species, volume or exergy, could also be applied, since it is ensured that CO_2-derived and conventional products will behave identically in all applications. However, as enhanced comparability is a major goal of this guideline, we recommend using mass for comparisons, since this is the most common measure of trading.

In case of **fuels with identical chemical structure and composition**, energy content (based on the lower heating value, LHV) shall be used, since the value of fuels is measured by their energy content. The lower heating value is recommended since in most energy service the condensation enthalpy of formed water is not accessible due to exhaust temperatures above 100 °C, e.g. power plants, internal combustion engines and most boilers.

For **CO_2-based products with different chemical structure and composition** to their conventional counterparts, a generic functional unit cannot be defined. Instead, the functional unit shall be defined so that the technical performance in the defined application of the products becomes comparable, e.g., compare detergents based on the washing performance and not based on mass.

The functional unit of **CO_2-based fuels with different chemical structure and composition** shall be defined with respect to the purpose of the fuel, i.e., energy services (e.g., supply of electricity or heat) or transportation of persons or goods. The functional unit has to quantify either the precise energy service (e.g., 1 MJ of electricity from a gas turbine of a certain type) or the distance for freight or person transport (e.g., 1 person km driven in a specified vehicle/ship/aircraft), since combustion properties may be different and thus, comparability based on energy content is not guaranteed.

Through decoupling demand and supply, **energy storage systems** offer additional degrees of freedom to operate the energy generation in a more efficient way and thus, can lead to lower environmental impacts. However, potential impact reductions strongly depend on the demand and supply of the energy system in which the energy storage operates and the energy storage characteristics, e.g., charging and discharging rated output, the power ramping capability, i.e. the rate at which the charging or discharging can be dispatched, and the storage duration between charging and discharging. To compare energy storage systems with different storage characteristics, the energy system without any storage system shall be compared to systems with the energy storage alternatives. In a second step, the difference of environmental impacts reductions of the energy storage alternatives can be compared.

C.4.1.2 Guidelines

<table>
<tr><th colspan="2">Guideline C.2 – Functional unit</th></tr>
<tr><td>Shall</td><td>1) A functional unit quantifying the technical performance of a product system or service shall be defined unambiguously.
2) Excluded functions shall still be documented and reported.
3) For products with identical chemical structure and composition to their conventional counterparts, mass shall be used as a functional unit, e.g., 1 kg of substance.
4) For fuels with identical chemical structure and composition to their conventional counterparts, the energy content shall be used, e.g., 1 MJ of substance (LHV).
5) For products with different chemical structure and composition to their conventional counterparts, the function(s) and performance characteristics of the product system shall be stated clearly and an unambiguous measurable functional unit quantifying the technical performance shall be derived.
6) For fuels with different chemical structure and chemical composition to their conventional counterparts, the application shall be stated within the functional unit, e.g., 1 kWh of electricity from combustion in gas turbine (type xy).
7) For energy storage, a functional unit quantifying the storage characteristics shall be defined.</td></tr>
<tr><td>Should</td><td></td></tr>
<tr><td>May</td><td>1) LCA studies may exclude additional functions that are out of the scope. Excluded functions shall still be documented and reported.</td></tr>
</table>

C.4.2 System boundaries, completeness requirements and related cut-offs

General introduction

The system boundary defines which processes and life cycle stages are needed to fulfil the function as defined by the functional unit and thus, are part of the analyzed product system. For this purpose, the product system is separated by the system boundary from the technosphere and the ecosphere. The technosphere contains all other technical systems transformed by humans and the ecosphere refers to the environment containing all other systems. For comparative studies, each product system has its own system boundary but system boundaries should be comparable.

Flows that are exchanged between processes are called technical flows and flows exchanged between processes and the environment are called elementary flows. Technical and elementary flows are gathered in the life cycle inventory (see Chapter C.5). Elementary flows are characterized according to their environmental impact in the life cycle impact assessment.

Product systems exchange countless technical flows with other product systems and thus, complex networks of products systems are formed. As a result, the system boundaries for an LCA study of a simple product would need to cover processes from the entire world. However, accurate results can still be achieved by assessing a limited number of processes and flows. For this purpose, only significant flows and processes are accounted for and other processes and flows are neglected (cut-off). Cut-off criteria are used to separate significant flows from negligible flows and can be based on the share of mass and energy balance or environmental contribution. The latter is the most accurate cut-off criterion. E.g., highly toxic substances might not have a significant contribution to mass and energy balances, but may have major contribution in toxicity impact categories.

Applying cut-off reduces completeness of study. Thus, the desired level of completeness and applied cut-off criteria shall be clearly described in the scope definition and the resulting process system shall be described, e.g., by drawing a flow sheet of the studied system.

C.4.2.1 Life cycle phase coverage for CCU technologies

Figure 4: The cradle-to-grave approach accounts for the entire life cycle of a product system. A cradle-to-gate study ends at the factory gate and does not account for any downstream environmental impacts

LCA is a holistic methodology covering the entire life cycle from cradle-to-grave. However, in situations where technical performance and, thus, downstream emissions are identical, a cradle-to-gate approach is sufficient. In a cradle-to-gate approach, the system boundaries cover the product system from extraction of raw materials to the factory gate and thus, not the entire life cycle is covered in these analyses (compare Figure 4). In fact, in some situations, it is practically unfeasible to cover the entire life cycle, e.g., if a product has numerous potential, but unknown, applications. In the following, we derive archetypical system boundaries for CCU technologies in agreement with the CCU classes derived in Part A 3.2.

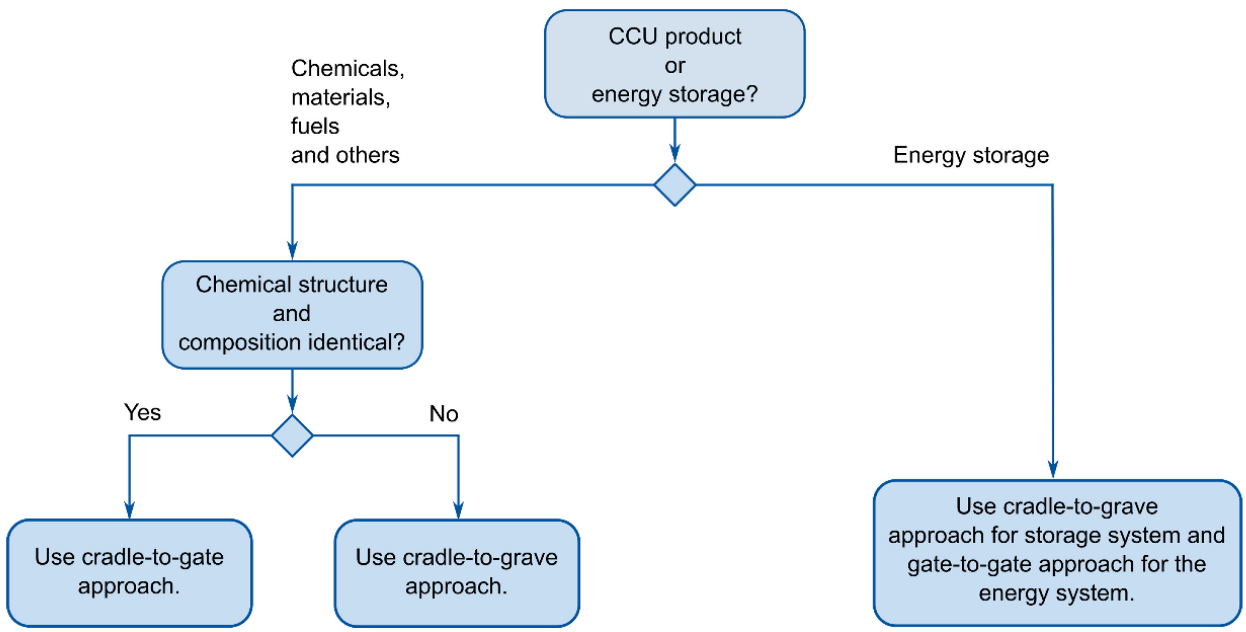

Figure 5: Decision tree for the selection of system boundaries

For **products and fuels with identical chemical structure and composition to their conventional counterparts,** a cradle-to-gate approach is sufficient since the products cannot be differentiated and thus, downstream life cycle phases are identical (compare Figure 6).

System boundaries for **products with different chemical structure and composition to their conventional counterparts,** such as *CO_2-based materials* (e.g., consumer products) shall cover the entire life cycle from cradle-to-grave. A cradle-to-gate approach is only applicable if differences in technical performance and end-of-life treatment do not differ significantly. In all other cases, materials perform differently and environmental impacts from downstream processes will not be identical. Therefore, LCA studies shall cover the entire life cycle to avoid problem shifting from one life cycle phase to the other (compare Figure 5).

For ***fuels* with different chemical structure and composition to their conventional counterparts,** a cradle-to-grave approach shall cover the raw material acquisition, production, and transport as well as use and end-of-life which often occur simultaneously during combustion. Omitting combustion can lead to qualitatively incorrect results, if fuels change engine efficiencies and tailpipe emissions [43].

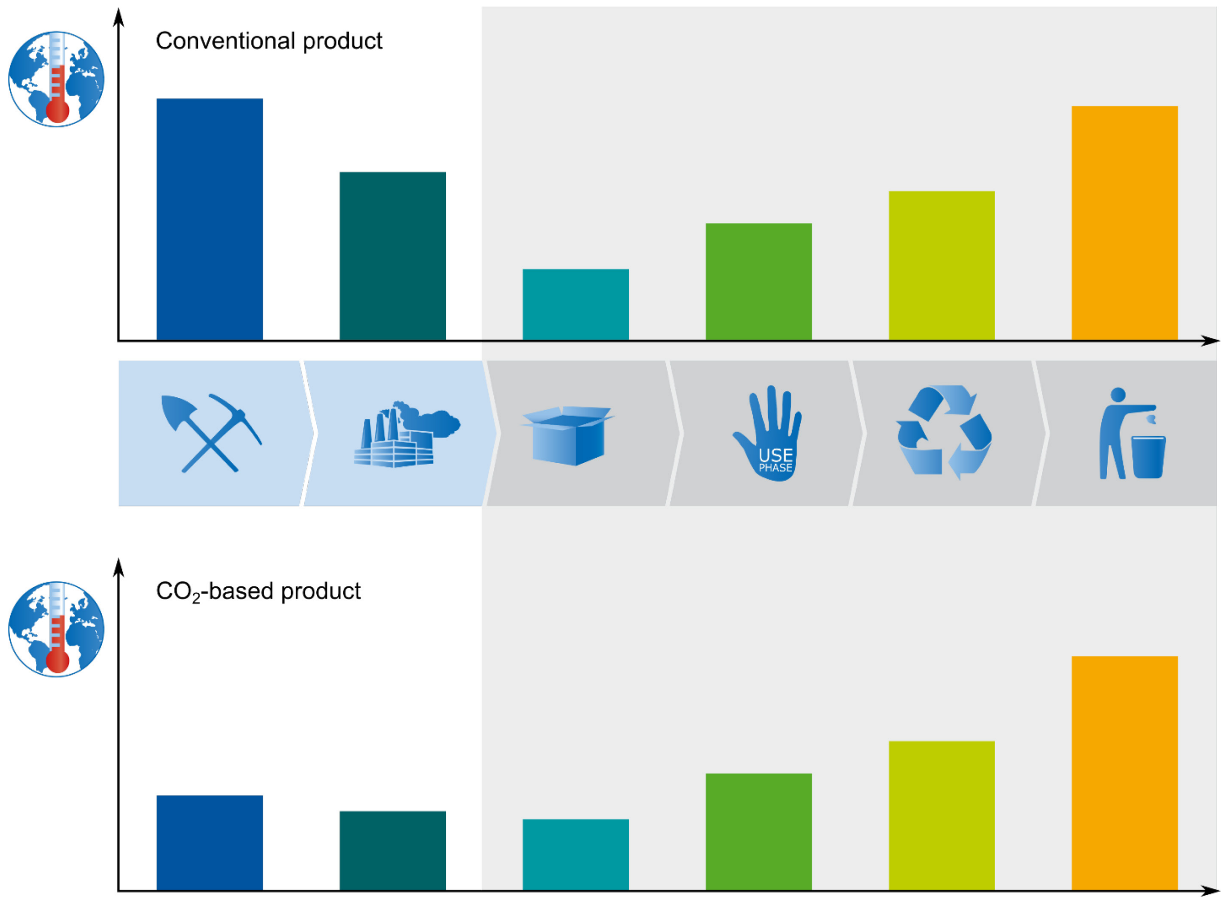

Figure 6: Comparison of environmental impacts for products with identical chemical structure and composition over the entire life cycle. Impacts only differ during raw material acquisition and production phases and thus, comparative studies only have to consider these phases.

However, if the study aims to compare **fuels with identical chemical structure and composition to their conventional counterparts** it is ensured that both fuels will behave identically in all potential applications and thus, a cradle-to-gate approach is justified.

In other cases, omitting the combustion might still be necessary if the potential application is unknown, e.g., in early stages of development.

For the comparison of **energy storage system**, the system boundaries shall cover the entire energy system and the entire life cycle of the energy storage.

Table 1: Selection of functional units and system boundaries for CO_2-based technologies

CCU classification	**Fuels**		**Chemicals, materials, and others**		**Energy storage systems**
	with identical chemical structure and composition	with different chemical structure and composition	with identical chemical structure and composition	with different chemical structure and composition	with identical storage characteristics
Basis for comparison	Energy content	Energy service provided	Mass	Technical performance	Energy system with and without energy storage
System boundaries	Cradle-to-gate	Cradle-to-grave	Cradle-to-gate	Cradle-to-grave	Cradle-to-grave for storage system and gate-to-gate for energy system in which the storage system operates
System boundaries		For preliminary studies only: cradle-to-gate		For preliminary studies only: cradle-to-gate	

C.4.2.2 Upstream environmental impact from CO_2 capture

CO_2 emitted to the environment is an elementary flow. Thus, captured CO_2 is often treated intuitively as a consumed emission $\left(GW_{CO_2} = -1\frac{kg_{CO2e}}{kg_{CO2}}\right)$. However, captured CO_2 is a product of human transformation and in consequence, CO_2 is a technical flow, i.e., a chemical feedstock. Thus, treating CO_2 as negative emission is usually incorrect and captured CO_2 has to be treated like any other feedstock [44]. CO_2 sources shall be included in system boundaries as environmental impacts occur due to the CO_2 supply. Assessments shall comprise all process steps leading to environmental impacts including CO_2 source, CO_2-purification and transport as shown in Figure 7.

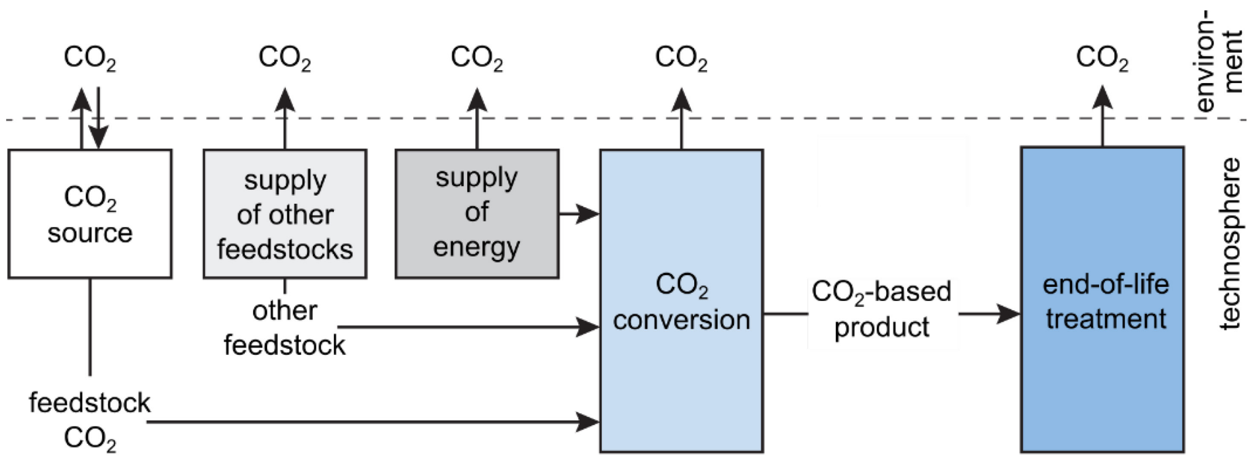

Figure 7: Schematic life cycle of CCU technologies span from the CO_2 source, supply other feedstocks and energy to the end of life treatment. In all life cycle stages, environmental impacts should be considered. Adopted from [12].

C.4.2.3 Guidelines

Guideline C.3 - System boundaries	
Shall	1) System boundaries shall be clearly defined and unambiguously described according to Table 1. 2) System boundaries of all product systems to be compared shall be described. 3) CO_2 sources shall be included in system boundaries as environmental impacts occur due to the CO_2 supply.
Should	
May	1) System boundaries other than stated in Table 1 may be applied if differences in downstream processes are not significant or a preliminary study shall be conducted. 2) In early stage of development, a cradle-to-gate approach may be applied for a preliminary LCA. In these cases, results have limited validity and shall be interpreted with caution.

C.4.3 Life cycle inventory modelling framework and solving multi-functionality

General introduction

The life cycle inventory modelling framework defines how data is gathered and processed during life cycle inventory. The framework defines how interactions with other product systems are handled, in particular, how to solve multi-functionality problems. Product systems can show multi-functionality in three ways:

- multiple outputs (co-production of several valuable products),
- multiple inputs (treatment of several wastes) and
- in- and output systems (treatment of a waste(s) and production of valuable product(s)).

Multi-functionality needs to be resolved, if environmental impacts of a single function are needed or if functions of compared systems are not equal.

Several methodological choices exist in LCA methodology regarding multi-functionality. The following methods are given by standards [45–48] and guidelines [5,49,50]:

- Sub-division
- System expansion
- Substitution
- Allocation using underlying physical relationship
- Allocation using underlying other relationship

The methodological choices are described in Chapter C.4.3.1.

C.4.3.1 Data inventory for CCU processes

The system boundaries for LCA studies on CCU technologies start with acquisition of raw materials and either end at the factory gate or at the end of the products life cycle (cf. Chapter C.4.2).

Sooner or later during an LCA study, process data will not be available from direct measurements. A company can usually only measure data within its factory gates. The missing upstream and downstream data in the life cycle inventories can be supplied by other companies or LCA databases. If the specific supplier of up-/downstream services is known or the production process of an input can be identified, inventory data specific to the process should be used. In other cases, this information might be not available, because products are purchased from a market, e.g. electricity traded at the stock market. In these cases, a specific technology is not available and a market mix shall be used instead.

The use of market mixes can be assumed until the additional demand or supply of the CCU technology triggers large-structural changes[2]. An example for a large-scale structural change could be the installation of additional electrical power capacities in response to an excessive electricity demand by a CCU technology, which could also affect production and consumption patterns in wide parts of the economy through changes in electricity prices. Such large-scale structural effects, however, may occur for a large-scale market introduction of CCU products. Nevertheless, accessing large-scale structural changes is typically beyond the scope of conventional LCA studies. The development of methods for this purpose by integration of complex market models is topic of current research. In this guideline, we focus on the scope of conventional LCA studies.

Therefore, first process specific inventory data shall be used, if this information is available. Then averaged market mixes for the regarding input shall be used.

C.4.3.2 Solving multi-functionality

Most CCU systems are multi-functional, because CO_2 sources often provide a main product and CO_2 and/or the conversion process itself produces multiple products (Figure 8) [11]. For example, ammonia is produced by reacting hydrogen with nitrogen. Hydrogen can be co-produced with CO_2 in the steam-methane-reforming process. As poison to the catalyst for ammonia production, CO_2 has to be separated prior to the formation of ammonia and subsequently, a pure CO_2 stream is released. If CO_2 is now captured from ammonia synthesis, the main-product ammonia and the co-product CO_2 are produced simultaneously (Figure 8). If the environmental impacts for the produced CO_2 stream are required, the total emissions of the system need to be split between the main and the co-product.

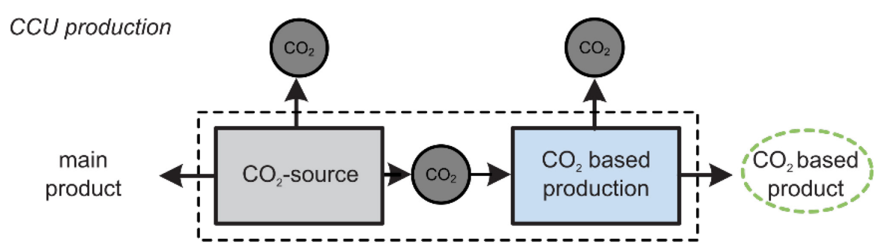

Figure 8: Stand-alone system analysis: Carbon capture from point source leads to the joint production of the CO_2-based product (functional unit, green dashed line) and the main product of the point source

This problem is called multi-functionality. Other co-products or functions may occur throughout the life cycle of CCU products. In general, the problem of multi-functionality is not a CCU-specific problem. The problem can be addressed using established LCA methodologies. However, a number of methodological choices have to be made. Therefore, we first present the hierarchy of methods to solve multi-functionality which is generally valid

[2] Following the ILCD handbook, this shall be assumed as long as the additional supply or demand of the production system under study does not exceed a threshold value of 5 % of the annual market size of a supplied or demanded product. The threshold value of 5 % refers to an estimated share of production capacity which is annually decommissioned, i.e., production plants in the end of their life time [5]. If the additional supply or demand of the production under study exceeds 5 % production capacity, plants are decommissioned that would otherwise still produce and thus, large structural changes apply. This might be the case if CCU technologies are deployed on a global scale and thus, CCU technologies trigger large-scale changes. The ILCD handbook refers to this as the distinction between goal situation A and B.

according to ISO 14044 and other guidelines. Subsequently, we demonstrate how the methods can be applied to a CO_2 source since the multi-functionality problem at the CO_2 source is at the core of most CCU processes.

Hierarchy of methods for solving cases of multi-functionality

Existing *s*tandards [45–48] and guidelines [5,49,50] rank methods for solving multi-functionality in a hierarchy which should be consistent with the stated goal definition.

1. First, check if multi-functionality can be solved by gathering individual process data and apply sub-division.
2. If subdivision cannot solve the multi-functionality problem, apply system expansion.

Note that results obtained via system expansion are joint impacts due to the production of more than one product and thus, are not specific to a single product of the CCU technology. This might be in conflict with the initial research question and a modification of the question might be needed. If product-specific assessments are needed to answer the initial research question the following hierarchy of allocation method shall be applied. Please note that results obtained via system expansion shall always be computed.

3. First, substitution shall be applied.
4. If substitution is not possible, e.g., because there is no process available to be substituted, apply allocation: First using an underlying physical relationship and then an underlying other relationship, e.g., economic value.

In the following, the alternative methods to solve multi-functionality are described and applied to account for the supply of CO_2.

Sub-division:

Sub-division solves the problem of multi-functionality by separating an aggregated (black box) unit process with multiple functions into smaller unit processes and gathering input and output data of these smaller unit processes, e.g., a factory with multiple products that are produced in independent processes can be sub-divided into individual production lines.

Cases where sub-division is applicable are not a problem of multi-functionality in a strict sense, but a problem of missing data. If this missing data can be gathered, multi-functionality can be fully resolved and thus, sub-division shall always be applied first. Sub-division shall even be applied if multi-functional unit processes remain, as this leads to smaller and simpler product systems.

Application to the CO_2-source: Sub-division is not applicable to the CO_2-source since CO_2 is always produced jointly with the main product.

System expansion

System expansion expands the functional unit to include other functions of the product systems than were originally stated in the goal and scope definition. If this expanded function is still meaningful, the multi-functionality problem is resolved.

Application to CO_2-source: CCU processes are often multi-functional, e.g., when the CO_2 source co-produces another product such as electricity. As discussed above, CCU processes are often compared to conventional processes. To compare both product systems, each product system needs to fulfil the same functional unit and therefore, the system boundaries and the functional unit are changed for the product systems. For the comparison of the CCU process with two products (product of CO_2 source and product of CO_2-process) to a conventional system (Figure 9), the main product of the CO_2 source is added to the functional unit and the conventional system is expanded with the CO_2 source without capture (Figure 10).

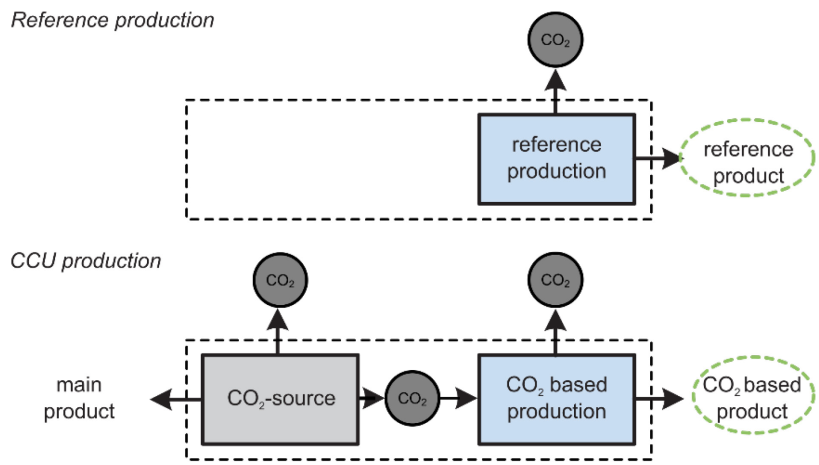

Figure 9: Comparison of a CCU production and a reference production: CCU system produces a main product besides CO_2-based product, i.e., the CCU system has additional functions not included in the functional unit (dashed green line). Thus, the conventional and CCU system are not comparable due to different functions.

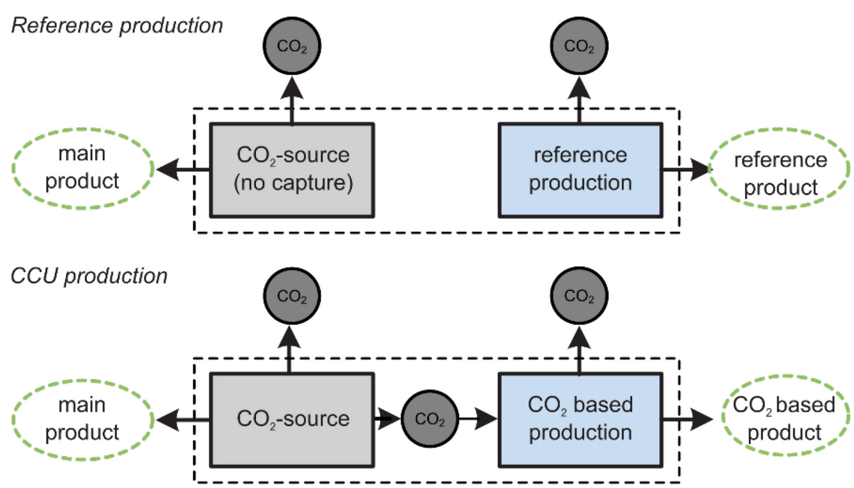

Figure 10: System expansion approach to compare a CCU production with a conventional production: the main product of CO_2-source is included in functional unit and the status-quo production system is expanded with the conventional production of the main product without carbon capture

Note that a process used for system expansion (not in the case of CO_2-sources) can be multi-functional as well and subsequent system expansion may be needed. In theory, one could end up modelling the entire global technosphere. However, this endless chain of system expansion is usually interrupted by the defined cut-off criteria (compare Chapter C.4.2).

Substitution:

Substitution does not include additional functions in the functional unit. Instead, a credit is given for the production of the co-product to represent the environmental burdens avoided by the substitution of the conventional production system which would have been used otherwise. The functional unit remains as stated in the goal and scope definition, but the system boundary is altered for the product system where substitution is applied. In comparative assessments, the system boundary and functional unit of the conventional product system(s) remains unchanged.

Similar to the approach presented in Chapter C.4.3.1 “Data inventory for CCU processes”, first a specific process to be substituted shall be identified and used. In all other cases, a market averaged process mix shall be assumed [5].

Application to CO_2-source: For CO_2 sources, the substituted process is usually the same source but without capture (Figure 11). This assumption is valid as long as not all CO_2 from this source is already fully utilized.

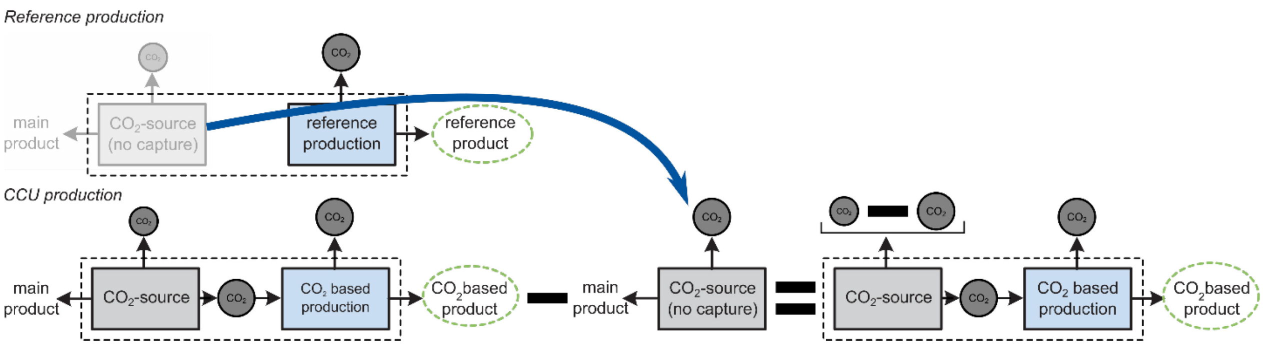

Figure 11: Substitution: The production of the main product without carbon capture is avoided and thus, the CCU system is credited for the otherwise emitted CO_2, but has to carry the burdens of purification, compression and transport

Both approaches, system expansion and system expansion via substitution, are mathematically equivalent; however, results, meaning and interpretation of results are not, because system boundaries and functional unit are altered. System expansion via substitution can lead to negative results (e.g. negative CO_2 emissions). This might be misinterpreted to mean that the system is beneficial to the environment by taking up emissions (e.g., that the amount of CO_2 in the atmosphere is reduced), however the negative numbers usually only mean that the system produces less emissions than the conventional system. Thus, the unlimited production of the analyzed system will not lead to an infinite benefit, but the net benefit is valid until the market of the substituted product system is fully satisfied. As a conceptual advantage, substitution conserves the causal interaction between processes by accounting for impacts in other life cycles.

Allocation:
Allocation sub-divides the multi-functional process into processes with exactly one function. Subsequently, the emissions of the multi-functional process are distributed among the functions reflecting an underlying physical causal or other relationship.

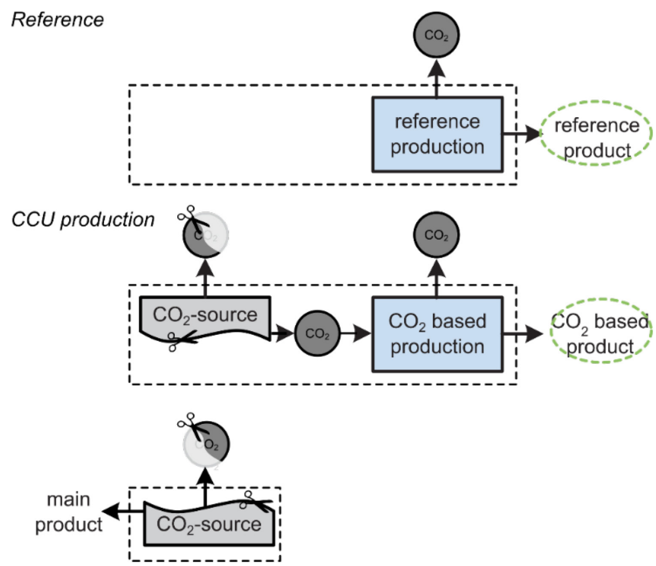

Figure 12: Allocation sub-divides the CO_2-sources into two processes and distributes the environmental burdens of the CO_2 source between the main product and the feedstock CO_2 production using underlying physical relationship or other relationship. The CCU production system becomes a mono-functional system and can be compared to the conventional production since functional units agree.

Allocation following an underlying physical causal relationship:

According to ISO 14044, an underlying physical causal relationship shall be applied first, by quantifying how input and outputs physically relate to a function of the system. For example, the chlorination of benzene delivers mono-chlorobenzene, ortho- and para-dichlorobenzene and hydrochloric acid. The amount of chlorine consumed by the process is directly physically related to the amount of the chlorine incorporated in the products. Therefore, the amount of chlorine in each product is the physical criterion to distribute the chlorine flow between the products of benzene chlorination. Another way to establish a physical causality is to quantitatively change the functions and observe how the inputs and outputs are affected. The distribution of the inputs and outputs should than reflect this quantitative change of inputs and outputs[3]. Note that more than one relationship can be applicable within one process.

Application to CO_2-source: A physical causality can be found by quantitatively changing the amount of main product and the product CO_2 produced and observing how the inputs and outputs are affected. Setting the amount of main product to zero, leads to a process without inputs, outputs and product CO_2. Therefore, the amount of main product affects the inputs and outputs of the process. Varying the amount of product CO_2 changes the amount of CO_2 emitted, since captured CO_2 is no longer emitted, but inputs and outputs related to the capture process, e.g. electricity for compression, are also changed. In consequence, 1 kg of CO_2 provided by the CO_2-source leads to an emission reduction of 1 kg CO_2-eq. and an increase of emissions related to the capture process. The result is identical to the substitution approach.

Allocation following another underlying relationship:

If a physical causal relationship cannot be applied, another underlying relationship shall be used. For this purpose, the multi-functional process is sub-divided into mono-functional processes and the environmental burdens of the multi-functional process are distributed among the mono-functional processes according to attributes of the product or functions. The most commonly applied attribute is economic value of products or

[3] The ILCD handbook refers to this as "virtual sub-division".

functions. Since the multi-functional process is artificially sub-divided, the physical causality between processes is lost, i.e. the independent production of former jointly produced products. In addition, the selection of the attribute is to some extent arbitrary.

Application to CO_2-source: The selection of a suitable product attribute to distribute the emissions of the CO_2-source among the main product and the CO_2 -source can be difficult. Mass can be applied to all processes except power plants, since electricity has no mass and thus, all emissions would be distributed to CO_2. Energy is not a suitable attribute since CO_2 does not contain any energy, i.e., the lower heating value is zero. The economic value of CO_2 is uncertain, since the capture process has costs, the price of CO_2 might be positive and thus, economic allocation would attribute the product CO_2 with emissions of the CO_2 source. However, it can also be argued that CO_2 has a negative economic value since it is a waste stream, which needs to be treated. In this case, the main product would also carry some burdens of the utilization process, which would serve as a treatment process.

As each applied criterion would significantly alter the environmental impact attributed to CO_2 and an objective selection of one allocation criterion is not possible, a sensitivity analysis is always needed.

C.4.3.3 Guidelines

Guideline C.4 - Life cycle inventory modeling framework and solving multi-functionality	
Shall	1) If multi-functionality occurs within the defined system boundaries: I. Sub-division shall be applied. If not possible: II. System expansion shall be applied. If product-specific assessments are needed to answer the initial research question the following hierarchy of allocation method shall be applied. Note that system expansion shall always be applied and product-specific assessment may be applied additionally if needed. III. System expansion via substitution shall be applied. This step should be only in addition to system expansion. If not possible: IV. Allocation using first underlying physical causalities shall be applied. This step should be only in addition to system expansion. A sensitivity analysis is needed if more than one criterion seems applicable. If not possible: V. Other underlying relationship(s) shall be applied. A Sensitivity analysis with regard to applicable criteria shall be conducted.
Should	
May	

C.4.4 Data quality

General introduction

Data gathered for the life cycle inventory shall have sufficient quality to answer the initial research question. Since data gathering is time consuming, it is beneficial to keep in mind what level of data quality should be achieved to produce reliable results. Thus, the goal and scope definition shall state which data will be used and what level of data quality will be sufficient.

Data can be qualified through the following items: Representativeness, completeness, uncertainty as well as methodological appropriateness and consistency.

Representativeness means how the collected inventory data represents the true inventory of the process for which data is collected regarding technology, geography and time. Completeness of inputs and outputs refers to how well the inventory enables the impact assessment to produce reliable results, e.g., mass as cut-off criteria might neglect highly toxic substances. Data measurements or process simulation have finite accurateness, and thus, data uncertainty is introduced with each collected data set. Methodological appropriateness and consistency refers to the selected modelling approach, e.g., attributional or consequential. Modelling approaches should not be mixed to ensure consistency. Note that this guideline describes an attributional approach.

C.4.4.1 Guidelines

Guideline C.5 – Data quality	
Shall	1) It shall be stated which data is used and what level of data quality is sufficient
Should	
May	

C.4.5 Special Requirements for comparative studies

Any study intended for external communication shall be reviewed. For comparative studies or studies to be used in comparative assertions disclosed to public, a critical review shall be conducted by an independent and qualified review panel. More information about the review process can be found in the ILCD handbook, the ISO standard and the PEF guideline [1,4,5,50]. Note that external review also allows studies to leave out confidential information in the public report and thus, can protect intellectual property.

C.4.5.1 Guidelines

Guideline C.6 – Special requirements for comparative studies	
Shall	1) Any study intended for external communication shall be reviewed. 2) For comparative studies or studies to be used in comparative assertions disclosed to public, a critical review shall be conducted by an independent and qualified review panel. More information about the review process can be found in the ILCD handbook [5], the ISO 14071 [51] and GHG protocol [49].
Should	
May	

C.5 Life cycle inventory (LCI)

General introduction

In the life cycle inventory phase, the actual data is gathered and the product system is modelled according to the goal and scope definition. The modelling usually starts by drawing a flow chart of the product system with the system boundaries as defined during scope definition. All relevant unit processes with their relevant elementary and technical flows should be represented in the flow chart. Then, incomplete mass and energy balances for each unit process are collected (see also cut-off criteria in Chapter C.4.4) and documented. From the collected data, usually a linear, non-dynamic flow model is built and elementary flows are calculated for the product system on the basis of the functional unit.

Further recommended reading:

The ILCD handbook presents a detailed description in Chapter 7 (page 153ff.) on life cycle inventory [5]. See Baumann and Tillman for a practical introduction to the construction of the flowchart, data collection and the calculation of environmental loads in Chapter 4 (page 97ff.) [8]. Also see Curran's handbook for an introduction to life cycle inventory Chapter 3 (page 43ff.) and Chapter 5 for sourcing life cycle inventory (page 105ff.) [7]. Guinée's handbook provides very detailed rules for the collection of process data, data management, calculation methods and methods to avoid cut-off by estimation methods in part 2a chapter 3 (page 41 ff.) [10].

C.5.1.1 Guidelines

Guideline C.7 – Life cycle inventory (LCI)	
Shall	1) System boundaries shall be described and represented in a flow chart. 2) Inventories shall be documented and reported, at least to external reviewers
Should	1) All relevant unit processes with their relevant elementary and technical flows should be represented in the flow chart.
May	

C.5.2 Estimation methods to bridge data gaps

During LCA studies, practitioners are often confronted with limited data availability and thus, estimation methods to bridge data gaps have been developed. In the following, commonly applied estimation methods are presented and further readings are provided. These methods may be used to bridge data gaps but the generated data should be replaced by measured values as soon as possible.

C.5.2.1 Second-law analysis

With thermodynamic analysis, a second-law analysis can be conducted based on stoichiometric reaction schemes, mass-, energy-, exergy- and entropy balances. By assuming second-law efficiency of 100%, an absolute best-case scenario is obtained. If this best-case scenario does not offer environmental benefits, the considered process will never offer any environmental benefits. In particular, for low TRL technologies, the second-law analysis is a useful tool to sort out technologies. Therefore, the second-law analysis shall be used to establish a best-case scenario.

C.5.2.2 Gate-to-Gate inventory estimation

In cases where specific information of chemical processes is missing, e.g. for feedstocks, the database Ecoinvent uses a yield of 95% based on a stoichiometric mass balance and a product averaged energy demand and other auxiliaries can be assumed as a rough estimation [52–54].

Jiménez-Gonzáles *et al*. (and Kim *et al*.) provide a design-based method to estimate gate-to-gate inventory information when direct data is not available [55,56]. The provided method defines transparent rules for data collection and provides several rules of thumb, e.g., for the estimation of mass balance, energy requirements and energy recovery rates. Based on this method, Kim *et al*. show for 86 chemicals that the gate-to-gate process energy ranges for half of the organic chemicals from 0 to 4 MJ per kg and for half of the inorganic chemicals from -1 to 3 MJ per kg.

A method to estimate gate-to-gate process energy consumption when no process engineering is available, is provided by Bumann *et al*. [57] which correlates the process energy demand with the energy index provided by Sugiyama *et al*. [58]. The proposed method is based on a simplified process model consisting of a reactor and separation unit and information of the chemical reaction, e.g., educts, products, co-products and by-products, reaction conditions and thermodynamic data. From this data, an energy index is computed and used for the estimation of gate-to-gate energy consumption. The average deviation of this method is around 30%.

C.5.2.3 Artificial neural networks

Finechem is a software tool to estimate the environmental impacts of processes from the molecular descriptors of the desired product using neural networks [59,60] and can be helpful if no process information is available. The neural network was trained with industrial data and thus, the method might be limited to predict molecules comparable to those in the training set. In addition, the molecular descriptors limit the range of application, as isomeric compounds and polymers cannot be differentiated. Furthermore, as this method uses solely the molecular descriptors of the product as an input, alternative production pathways cannot be assessed by this method. This is in particular a shortcoming for CCU technologies which aim to substitute identical products, fuels or materials.

C.5.2.4 Guidelines

Guideline C.8 – Estimation methods		
Shall	1)	If no other data is available, a best-case scenario based on stoichiometric schemes and thermodynamics shall be used to calculate potential environmental impact reductions.
Should		
May	1)	Estimation methods may be applied to bridge data-gaps. If applied, methods and assumptions shall be reported.
	2)	Techniques to forecast future technology development may be applied. If applied, the forecast shall cover both the CCU and the reference technology and shall not exceed physical limitations.

C.5.3 Selection of reference processes

The selection of a reference process has significant impact on the reduction potential of the assessed CCU technology. Therefore, the reference process has to be carefully selected. In general, reference processes shall be those processes the CCU process compete with in the market, i.e. the marginal process. However, the identification of the marginal process may introduce complex market interactions, in particular if the process has more than one function. Therefore, the reference process shall be modelled as the average market mix if further information is missing and if no large-scale structural changes occur (compare Chapter C.4.3.1).

However, CCU technologies in particular in stages of early development, do not compete with current technologies, since their market launch lies in the future. Instead, these CCU processes compete with the technologies established in the future. Thus, comparing CCU technologies in stages of early development to currently used processes does not reflect reality. Therefore, the time dimension is crucial for assessing ecological benefits of CCU. For this purpose, future development techniques, e.g. learning curves, may be applied to both the CCU technology and the reference process, as both processes underlie development [38]. Methods to apply learning curves are described by Gavankar *et al*. [39] and Cespi *et al*. [61]. Note that forecasting techniques shall not exceed physical limitations, e.g., the second law of thermodynamics. In addition, changes in the background system shall be accounted for, e.g. the changes in the energy supply due to higher shares from renewables.

However, predicting future technologies is potentially beyond the scope and experience of many LCA practitioner and thus, if no reliable predictions on future developments are available, the current best available technology should be used as the reference technology.

C.5.3.1 Guidelines

Guideline C.9 - Selection of reference process		
Shall	1)	The reference process shall be the marginal process. If no marginal process can be identified, the market mix shall be assumed.
Should	1)	For processes in stages of early development, the current best available technology should be selected as the reference process.
May	1)	For processes in stages of early development, techniques to forecast future technology development may be applied. If applied, forecasts shall cover the CCU technology, the reference technology and the background system. Physical limitations shall not be exceeded.

C.6 Life cycle impact assessment

General introduction

Life cycle impact assessment (LCIA) is the phase of an LCA study where the elementary flows computed in the life cycle inventory phase are translated into their potential environmental impacts. LCIA enhances the readability and comparability of results, since the number of environmental impacts is usually significantly lower than the number of elementary flows. Environmental impacts are caused due to complex cause-effect chains in the natural environment and can be reported at different points within the cause-effect chain. In LCA, the main distinction is made between mid- and endpoint. At midpoint level, substances are aggregated that have the same primary effects, e.g., infrared absorption as primary effect leading to climate change. In contrast to midpoint indicators, endpoint indicators aim to quantify how the areas of protection human health, natural environmental and natural resources are affected by the product system, e.g., how coral reefs die due to temperature rise caused by enhanced radiated forcing of emitted greenhouse gases from the product system. Endpoint indicators aim to make midpoint results more comprehensible, however, endpoints introduce more uncertainty in that they account for complex cause-effect chains that are sometimes barely understood and in addition, rely on the comparability of different damages done to the areas of protection, e.g., mal-nutrition caused by droughts compared to heat stress. Therefore, the uncertainty of impact assessment methods increases with the level of aggregation.

For life cycle impact assessment at midpoint level, elementary flows are multiplied with their characterization factor for a specific impact category, e.g., climate change. The characterization factor quantifies the environmental impact within an impact category relative to a reference substance, e.g., CO_2 for climate change. All substances are normalized to the reference substance according to common mechanisms.

Further recommended reading:

For more details on impact assessment, please see "ILCD handbook. Framework and requirements for life cycle impact assessment models and indicators" by the Joint Research Center [62] or "Life cycle impact assessment" by Hauschild [9]. In depth information about life cycle impact assessment and the CML method can be found in Guinée's handbook[10].

C.6.1 Life cycle impact assessment methods

Key driver for CCU is to lower GHG emissions and our dependence on fossil resources. Not surprisingly, global warming and fossil resource depletion (or fossil-based cumulative energy demand) are usually selected as impact categories in LCA studies on CCU. The introduction of CCU technologies may further affect a variety of environmental impacts and the holistic LCA approach aims to avoid problem shifting from one impact category to another. Therefore, impact categories shall not be omitted from LCA studies to avoid misleading decision-making if impact categories are:

- Relevant, i.e., accounted elementary flows contribute in these categories and
- Assessable, i.e., impact assessment methods exist and these methods are reliable.

However, the selection of impact categories and methods is not straightforward: Numerous impact categories exist and sometimes even multiple methods for one impact category exist. Furthermore, the uncertainty of impact assessment models varies as more or less complex cause-effect chains are involved and methods are more or less advanced. In consequence, different impact assessment models are used in practice leading to differences in LCA results.

The CML impact assessment methodology in its most recent version should be used for impact assessment as the "International Environmental Product Declaration (EPD) System" uses CML as a default for product category rules. To the best of the authors knowledge (July 2018) the most recent version of CML is 2016. Additionally, a second set of methodology should be applied if this methodology is geographically more appropriate than CML [63,64]. In this way, comparability and geographical representativeness are guaranteed at the same time.

For Europe, the Joint Research Center provides a selection of impact categories and methods which were defined in a stakeholder's dialogue involving LCIA model developers and LCA practitioners and thus, the JRC recommendation should be followed for Europe [6]. For the United States the EPA developed TRACI 2.0 as impact assessment methodology and thus, TRACI 2.0 should be used for studies in the U.S. [65].

Note that life cycle impact assessment should be limited to midpoint indicators, because the level of uncertainty increases with endpoint indicators or single point indicators. Also note that a detailed knowledge of impact assessment method is necessary to interpret and report results properly, e.g., human toxicity assessments have high uncertainty and thus, results differing by 2-3 orders of magnitude might still be interpreted correctly as "identically toxic" [9].

C.6.1.1 Guidelines

Guideline C.10 - Life cycle impact assessment methods		
Shall	1) 2)	CML impact assessment methodology shall be used as a default LCA studies for CCU technologies shall analyze midpoints indicator categories
Should	1)	In addition to CML, a second, geographically more appropriate method should be applied. For Europe, JRC recommended methods should be used and for the U.S., TRACI 2.0
May	1)	Other categories or methods may be applied, but shall be justified, documented and reported.

C.6.2 Temporary storage of CO_2

CCU products offer temporary carbon storage. Due to temporary carbon storage, CO_2 emissions can be delayed and thus, do not contribute to climate change during the time of storage. Therefore, temporary storage is not an independent or additional benefit.

The relevance of temporary storage depends on the class of CO_2-based product or fuel considered:

For **CO_2-based products and fuels with identical chemical structure and composition to their conventional counterparts,** carbon storage does not offer any additional benefits since the product life is identical after leaving the factory gate for both products and the amount of carbon chemically bonded is identical. Therefore, the time between production and end-of-life treatment and the amount of CO_2 released during end-of-life treatment is identical. Thus, the emission time profile is identical after factory gate (blue and green line in Figure 13) and there is no additional effect storing CO_2.

For **CO_2-based products different in chemical structure and composition to their conventional counterparts,** emission time profiles are not identical (red line in Figure 13) and thus, temporary storage may be significant (Figure 14). However, note that temporary storage offers a benefit only once. Once all counterparts have been substituted, the composition remains constant and thus, emission time profiles are identical again.

For **CO_2-based fuels different in chemical structure and composition to their conventional counterparts**, temporary storage is usually not significant, since the storage duration is short compared to climate change dynamics.

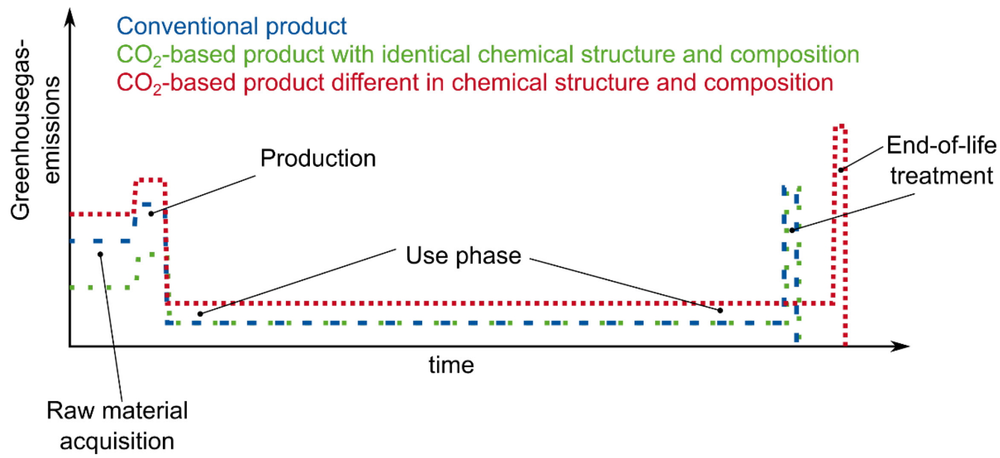

Figure 13: Emissions time profiles for different products. CO_2-based products with identical chemical structure and composition to their conventional counterparts have identical emissions timing profiles after production. CO_2-based products different in chemical structure and composition can have different emissions during use-phase and end-of-life treatment and different life spans and thus, the emissions timing profile can be different.

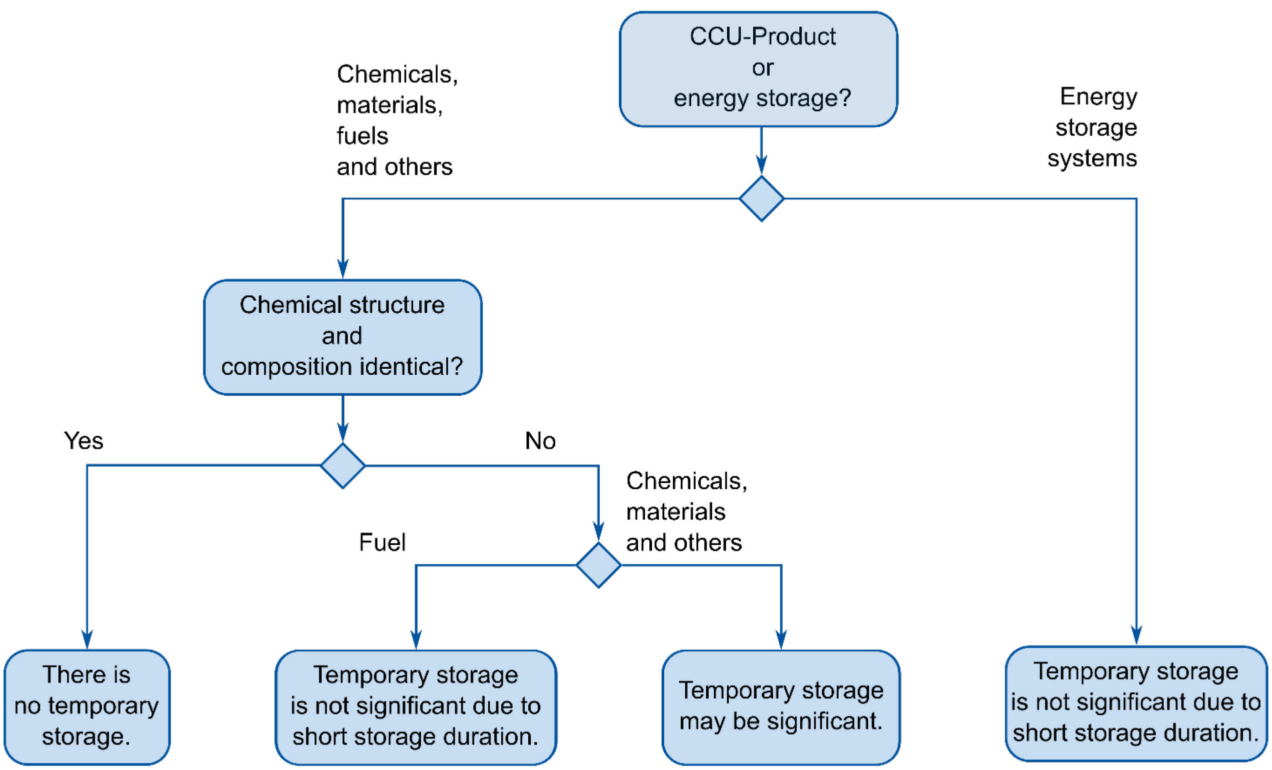

Figure 14: Decision tree for determining if temporary storage is significant for LCA study.

The effect of temporary CO_2 storage is known from bio-based products and methods to account for temporary storage exist [66–68]. However, classic LCA does not account for temporary storage or emission timings, "as LCA per se is not discounting emissions over time" (ILCD handbook p. 226). LCA models are usually static and do not account for dynamic effects such as discounting emissions over time [69]. To follow the established LCA principles, delayed emission shall not be discounted over time. Instead, emission time profiles, the amount and duration of carbon stored may be reported as a separate item. Note that for permanent storage[4] a discounting method is not needed because end-of-life emission never occur and thus, are zero. If end-of-life emissions are zero, the effect of storage is thus already considered.

C.6.2.1 Guidelines

Guideline C.11 - Guideline Temporary storage of CO_2		
Shall	1)	Delayed emission shall not be discounted over time as a default.
Should		
May	1)	If delayed emissions occur, an emission time profile of the conventional product and the CO_2-based products different in chemical structure and composition shall be reported. The amount and duration of carbon stored shall be reported.

[4] Permanent storage can be assumed if CO_2 is sequestered for 100.000 years.

C.7 Life cycle interpretation

General introduction

The phase of life cycle interpretation has two purposes:

1) Closing the feedback loop during the iterative steps of LCA studies, e.g., through evaluating the gathered life cycle inventory in the light of the goal definition and
2) Evaluating results to derive robust conclusions and potential recommendations at the end of an LCA study.

During iterative steps, significant issues such as relevant life cycle stages and unit processes are identified through contribution analysis, sensitivity analysis etc. In cases, where these issues have significant influence on the results and/or gathered data quality is not sufficient, either the model shall be refined or the goal and scope shall be adapted.

The iteration ends if the question posed in the goal definition can be sufficiently answered. For this purpose, the completeness and consistency of the study is evaluated with qualitative methods, e.g., expert's opinion or quantitative methods such as uncertainty and sensitivity analysis.

Finally, conclusions are drawn. The conclusions answer the initial research question explicitly, honestly, in an unbiased way and entirely based upon the results of the study. Therefore, conclusions drawn shall be based solely on the data quality, system boundaries, methodologies and results.

Recommendations are a subjective interpretation of the conclusions and thus, shall exclusively be based on the conclusion.

Further recommended reading:

Please see Chapter 4.5. of ISO 14044 [4] or Chapter 9 of the ILCD handbook for more information on interpretation [5]. See Baumann and Tillman for practical introduction and guidance for presentation of results [8].

C.7.1 Carbon neutral products and negative emissions

CCU technologies consume CO_2 to produce value-added products. Thus, intuitively CCU technologies may be thought of as technologies with potentially zero emissions or net-negative emissions.
CO_2 is usually considered to be captured from fossil or biogenic point sources or directly from the atmosphere via direct air capture. Fossil point sources release carbon previously stored in underground compartments, while biogenic point sources releases carbon previously consumed from the atmosphere.

CCU technologies can theoretically be carbon neutral over the entire life cycle:

- if CO_2 is captured from the atmosphere (via biogenic point sources or direct air capture) and the CO_2 is released at the end-of-life (Figure 15 a)
- <u>or</u> if CO_2 is captured from fossil point sources and CO_2 is sequestered or permanently stored in the product (Figure 15 b)
- and if all other GHG emissions are zero over the life cycle.

CCU technologies have potentially negative emissions (Figure 15 c):

- if CO_2 is captured from the atmosphere (via biogenic point sources or direct air capture)
- and if CO_2 is sequestered or permanently stored in the product
- and if overall life cycle GHG emissions are lower than the amount of CO_2 fixed.

If the amount of atmospheric CO_2 capture and fixation is equal to other fossil emissions over the life cycle, the process is carbon neutral.

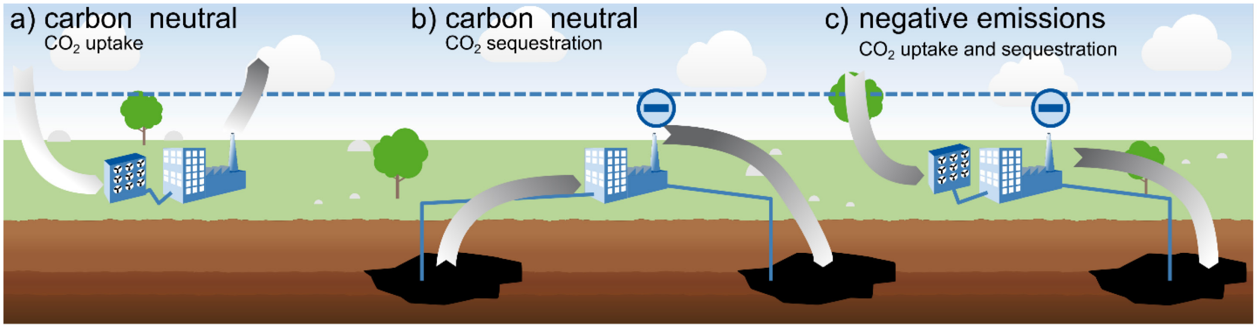

Figure 15: Case a) Carbon neutral CO_2-uptake: CO_2 is taken from the atmosphere and is re-emitted after the product life cycle. Case b) Carbon-neutral CO_2 sequestration: Fossil carbon is taken from underground reservoirs and CO_2 is sequestered after product life cycle. Cases a) and b) are only carbon neutral if no emissions occur during the product life cycle. c) Negative emissions: CO_2 is taken from the atmosphere and sequestered after the product life cycle. Case c) will only have negative emissions if emissions over the entire lifecycle are less than 1 kg CO_2-eq. per kg CO_2 up taken.

In all other cases, CCU technologies have positive CO_2 emissions over the life cycle. Still, emissions can be lower than for competing conventional processes (compare case d) in Figure 16). In this case, the CCU process also contributes to climate change mitigation through substitution, and hence is carbon reducing. Even though such processes lead to lower CO_2 emissions compared to the status quo, they are not carbon negative. In particular, this also holds for carbon-reducing processes with negative CO_2 emissions obtained from substitution. Through applying substitution (compare Chapter C.4.3.1 "Solving multi-functionality") or cradle-to-gate analysis, negative LCA results can be computed. However, such negative LCA results only reflect a comparison. In particular, negative LCA results do not necessarily imply that the CCU product is carbon neutral or even has negative emissions over its life cycle. Therefore, negative CO_2 emissions obtained from substitution shall be clearly stated as environmental benefit compared to the benchmark technology and not as negative CO_2 emissions over the life cycle. In addition, avoided CO_2 emissions and other environmental impact from substitution shall be reported separately.

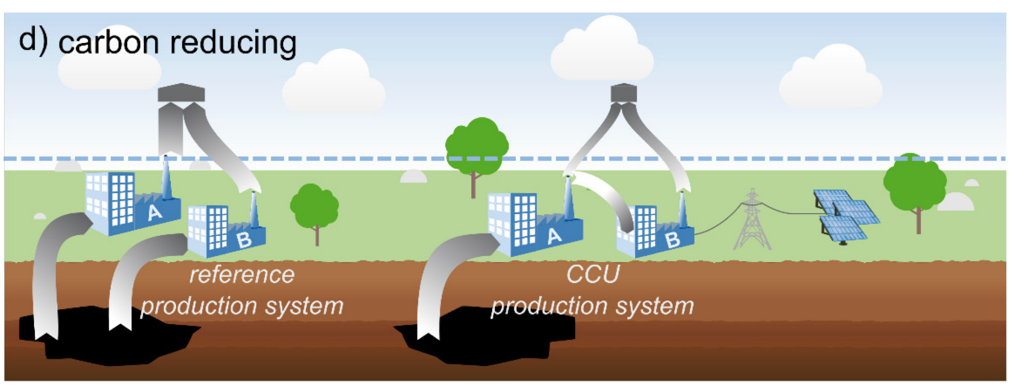

Figure 16: Case d) carbon reducing: CCU technologies can offer lower CO_2 emissions than the status quo and thus, may be considered as carbon reducing technologies.

C.7.1.1 Guidelines

Guideline C.12 - Interpretation	
Shall	1) In cases, where issues such as life cycle stages, unit processes, transportation or energy consumption have a significant influence on the results and/or gathered data quality is not sufficient, either the model shall be refined or the goal and scope shall be adapted. 2) Conclusions drawn shall solely be based on the data quality, system boundaries, methodologies and results. 3) Recommendations are a subjective interpretation of the conclusions and thus, shall exclusively be based on the conclusions. 4) Negative emission in cradle-to gate studies shall not be interpreted as CO_2 sinks if life does not end with permanent carbon fixation. 5) Emission reductions due to substitution effects shall be interpreted as environmental benefits and not as negative emissions. 6) Emissions reductions due to substitution effects shall be reported separately.
Should	
May	

C.7.2 Uncertainty and Sensitivity analysis

General introduction

Uncertainty and sensitivity analyses enable the LCA practitioner to understand the robustness of the results and help to draw conclusions. There are three major sources of uncertainty: parameter uncertainty, model uncertainty and uncertainty due to choices [70].

Parameters derived from imprecise measurements or estimations of experts introduce parameter uncertainty. The definition of system boundaries, selection of processes and impact assessment methods introduces model uncertainty. Uncertainty due to choices results, for example, from the determination of the functional unit or allocation criteria [70].

According to ISO 14040 and ISO 14044, data quality requirements for LCA studies should address all sources of uncertainty mentioned above. Therefore, LCA practitioners shall include an assessment of these uncertainties in order to understand the uncertainty of the overall model results. In addition, the uncertainty of the overall model results shall be documented and interpreted according to the goal and scope of the study.

In the following, methods to quantify the impact of these uncertainties are described and two levels of recommendation are provided. This section is adapted from Igos *et al*. [71]: First, a basic approach is described using sensitivity analysis and scenario analysis and second, an intermediate approach using uncertainty analysis. The basic approach shall be applied and the intermediate approach should be applied if possible.

Please note that uncertainty assessment in general is already covered sufficiently by standards and guidelines. However, the following section describes how methods can be applied to CCU technologies.

Basic approach

In the basic approach, input variables shall be identified that have uncertainties with high impacts on the uncertainty of the model output. For this purpose, a sensitivity analysis shall be carried out. Sensitivity analysis is a systematic procedure to estimate the effects that alternative choices for methods and data have on the outcome of a study [4]. The most basic approach to carry out a sensitivity analysis is the one-at-a-time approach. For the one-at-a-time approach, input variables shall be varied separately one after the other to quantify the sensitivity of the model results towards the considered input variable. For this purpose, the input variables shall be varied within realistic ranges. The results of the sensitivity analysis may be sorted to identify key variables with the highest influence to the overall output uncertainty. If the variation of the input variables reveals weak points of the study that are not in line with the LCA study's goal and scope, the goal and scope definition shall either be refined or data quality and modelling approach shall be reviewed until significance of results according to goal definition is achieved.

Once the key variables are identified, either a scenario analysis, i.e., the evaluation of alternative choices, or the calculation of threshold values for key variables shall be carried out.

For a scenario analysis, a number of sets of key variables shall be defined. These sets, i.e., the scenarios, shall be analyzed in relation to the model results of the baseline scenario. Typically, best and worst case scenarios should be defined to quantify the range of the model results.

CCU technologies often make use of energy or high energetic reactants, e.g., hydrogen to activate CO_2. The production of those high energetic reactants or the supply of energy can lead to high environmental impacts. In consequence, assumptions on environmental impacts of these inputs have been identified as the major source of varying results in LCA studies on CCU technologies. Thus, the environmental impacts related to the high energetic reactants are often the key variables in studies on CCU technologies [3]. Furthermore, CCU technologies are emerging technologies and thus, the derived scenarios shall consider the transition of the background system. For this purpose, the practitioner shall define a scenario representing the status-quo, a fully decarbonized future and a transition scenario. An example for electricity generation is presented in Table 2. The status-quo is taken from the Energy Technology Perspectives report published by the International Energy Agency [72]. In fully decarbonized industry the greenhouse gas emissions of the energy supply will be fairly close to zero, while in a transition scenario the emissions will lie somewhere in between the status-quo and a fully decarbonized industry (e.g. 50% of the current emissions). Even though these scenarios are derived in a very simply way and the scenarios will perform badly at forecasting, valuable insights from a scenario analysis like this can be gained, e.g. the dependence on clean energy supply can be shown. Since the generation of scenarios can be time and resource demanding, scenarios for the supply of electricity, hydrogen, CO_2, heat and natural gas (as methane) for the European context are provided in the annex of this document (see C.9.1.).

Table 2: Exemplary scenarios

Input	Unit	Status-quo	Transition	Full decarbonized
Electricity	kg CO_2-eq /MJ	0.091[5]	0.046	0

However, note that scenario analysis can suffer from ambiguity because the definition of scenarios relies on the LCA practitioner and can hardly become an automated part of LCA calculations [73].

[5] Calculated from [72]

As an alternative to scenario analysis, threshold values for key variables can be calculated. A threshold value is the smallest (or highest) value of an input variable that is sufficient to achieve environmental benefits compared to the benchmark process. For example, a hydrogen electrolysis process that consumes 50 kWh electricity per kilogram hydrogen is only ecologically beneficial compared to steam reforming of methane (with a global warming impact of 10.7 $kgCO_2$-eq per kilogram hydrogen) if the global warming impact of electricity supply falls below a value of 0.214 $kgCO_2$-eq per kWh electricity [74]. In this case, the threshold value of electricity would be 0.214 $kgCO_2$-eq per kWh. For a sound interpretation the calculated threshold values should lie within physical and thermodynamic limits.

Intermediate approach

Based on the basic approach, the LCA practitioner should carry out an intermediate approach to quantify the uncertainty of the model output using uncertainty analysis. According to the ISO 14044, uncertainty analysis is a "systematic procedure to quantify the uncertainty introduced in the results of a life cycle inventory analysis due to the cumulative effects of model imprecision, input uncertainty and data variability" [4]. Therefore, uncertainty analysis is a measurement of the reliability of the model output towards the underlying decision process. Uncertainty analysis is usually carried out using stochastic methods, e.g., Monte Carlo simulation [75–78], or perturbation theory, e.g., analytical uncertainty propagation [73,79–83].

In the intermediate approach, the Monte Carlo simulation is recommended since it is the most common method to carry out an uncertainty analysis and it is integrated in current LCA software, e.g., SimaPro, OpenLCA and GaBi. In a Monte Carlo method, all input variables are varied randomly within their defined ranges for a fixed number of model simulations. In consequence, the range of the model results is a value for the probability distribution and thus, a value for the overall model uncertainty. The Monte Carlo method requires a high number of simulations in order to obtain representative results and therefore, high computational power or high calculation time. Usually, 10,000 Monte Carlo sets are generated, but Wei Wei *et al*. showed that 1 million might be necessary to achieve sufficient accuracy of results [84]. In general, convergence cannot be guaranteed [71]. Therefore, the number of Monte Carlo sets should be as high as possible, but at least 1,000 [71].

In comparative studies, Monte Carlo analysis shall not be carried out independently for each alternative, since the comparison of probability distribution can lead to wrong interpretations, i.e., a large overlap of two probability distributions might be misinterpreted as an indistinct decision, where an integrated Monte Carlo analysis of the difference of the alternative reveals a clear advantage of alternative A (compare Figure 17).

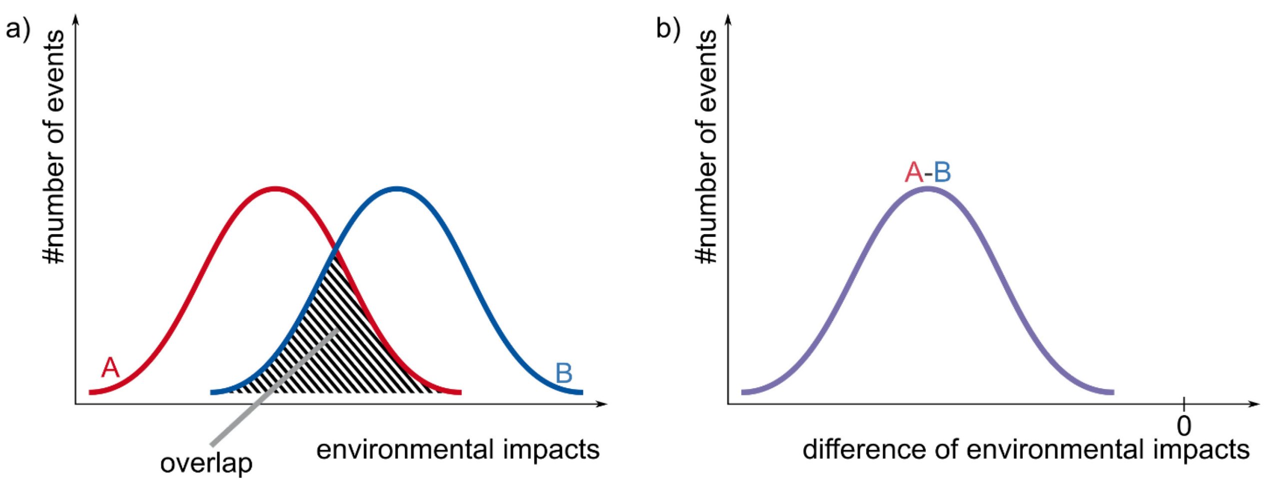

Figure 17: a) Results of an independent Monte Carlo analysis for alternatives A and B. b) Results of Monte Carlo analysis for the difference of technologies.

Therefore, a comparison of different technologies shall be carried out in a joint Monte Carlo simulation. Furthermore, a comparison between different technologies in a joint Monte Carlo simulation step shall always be related to the same background system to ensure consistent results. For instance, the conventional synthesis of methanol requires high amounts of carbon monoxide and hydrogen whereas the CO_2-based production pathway requires high amounts of carbon dioxide and hydrogen. To ensure a fair comparison between both technologies and thus, a consistent result of the uncertainty analysis, the background production system of hydrogen has to be the same for each individual Monte Carlo simulation step. For this reason, using aggregated processes in Monte Carlo analysis can be misleading and thus should be avoided.

Uncertainty and sensitivity analysis are important for comparative studies to identify whether calculated differences of environmental impacts are significant or not. Note that significant difference may not be revealed by sensitivity analysis. This does not mean that no difference exists, but that the study could not prove any. Furthermore, note that ignorance, as an additional source of uncertainty, can neither be assessed by uncertainty nor by sensitivity analysis “but may be revealed by qualified peer review” [5].

Communication of uncertainty assessment results

The communication of uncertainty assessment results is important to avoid misleading interpretations and to ensure the credibility of the assessment [85]. Therefore, the communication of the results of the basic approach shall include parameters with high sensitivity and their effects to the overall model results. The results of the scenario analysis and calculated threshold values shall be reported separately to the results of the sensitivity analysis. The intermediate uncertainty assessment approach should furthermore include the results of the uncertainty analysis. The results of the uncertainty analysis should be interpreted with regard to their effect on the reliability of the LCA results.

C.7.2.1 Guidelines

Guideline C.13 - Uncertainty and Sensitivity analysis	
Shall	1) As minimum requirement for uncertainty assessment, a basic uncertainty approach covering sensitivity analysis and scenario analysis shall be applied to identify key variables and to reflect how potential background system changes effect the technologies under study. 2) If variation of the input variables reveals weak points of the study that are not in line with the LCA study’s goal and scope, the goal and scope definition shall either be refined or the data quality and modelling approach shall be reviewed until the significance of the results according to the goal definition is achieved. 3) If Monte Carlo analysis is applied for comparative studies, the analysis shall consider the alternatives in one joint Monte Carlo analysis.
Should	1) The intermediate approach should be applied to quantify the uncertainty of the results. 2) Aggregated processes should not be used for Monte Carlo analysis, since important variables in the foreground system cannot be varied in the background system. 3) For the scenario analysis the standard scenarios provided in the Annex C.9.1 should be used.
May	

C.8 Reporting

General introduction

The ISO standard 14044 recommends "The results and conclusions of the LCA shall be completely and accurately reported without bias to the intended audience." Assumptions made on data and methods should be transparently reported and enable the reader to understand the limitations of the results. Presented results should enable readers to understand the complexity and trade-offs of the LCA study. The results and interpretation presented should be in line with the goals of the study. The reports may be limited if sensitive or confidential information and data may not be published (please see Chapter 10 of the ILCD handbook for further information).

The ILCD handbook describes three elements of a report: executive summary, technical summary and main report.

The executive summary should address a non-technical audience, typically decision makers. Therefore, the executive report focuses on the results, limitations, conclusion and recommendations. The technical summary addresses a technical audience and focusses on the main findings, while still being as transparent and consistent as the main report. The main report provides all details of the study.

Further readings:

More details can be found in Chapter 5 of ISO 14044 [4] or in Chapter 10 of the ILCD handbook[5].

C.8.1 CCU specific reporting

In the following, a checklist for an executive summary and main report is provided. This checklist is derived from the ISO 14044 and the ILCD handbook and additionally includes CCU-specific items. The assessment results shall be clearly reported to the audience in order to avoid ambiguity and misinterpretation.

The report shall include an executive summary and a technical summary table (see Annex 10.4) to provide easy access to the data used in the assessment. The main report shall report all assumptions, data for calculation, methods, results and limitations as transparently and in as much detail as possible. This is also important to help assure reproducibility and full traceability.

Confidential information may be left out in the main report to avoid confidentiality issues and should be reported in a separate, confidential part available to the reviewing process. If confidential data is not disclosed to the public, this should be clearly stated and then the relevant parts retracted as necessary to avoid confidentiality issues.

Checklist - Executive summary

Goal of the study

- ❑ State the intended application of the study
- ❑ State the reasons for carrying out the study
- ❑ State the intended audience of the study
- ❑ State whether the results are to be used in comparative assertions disclosed to public
- ❑ State unambiguously the research question(s)
- ❑ State the classification of the assessed CCU technology

Scope of the study

- ❑ State functional unit clearly and unambiguously according to guideline and report changes due to solving of multi-functionality
- ❑ State system boundaries according to guideline
- ❑ State relevant issues with data quality and assumptions
- ❑ State technology readiness level (TRL) of processes and sub-processes
- ❑ Report production or storage capacity
- ❑ Report geographical scope
- ❑ State software system (and version) and data library (and version) used
- ❑ State type of review and provide additional information about reviewers

Life cycle inventory and life cycle impact assessment

- ❑ State main results of life cycle inventory and life cycle impact assessment
- ❑ If results are reported on a relative basis, report basis
- ❑ Describe uncertainty and sensitivity analysis and report results separately

Interpretation

- ❑ State any conclusions, recommendation and limitations

Checklist – Main report

Goal of the study

- ❑ State the intended application of the study
- ❑ State the reasons for carrying out the study
- ❑ State the intended audience of the study
- ❑ State whether the results are to be used in comparative assertions disclosed to public
- ❑ State unambiguous research question(s)
- ❑ State the classification of the assessed CCU technology
- ❑ State limitations due to the assumptions and methods, e.g., if study is preliminary
- ❑ State commissioner of the study and other influential actors
- ❑ State technology readiness level (TRL) of processes and sub-processes
- ❑ Report production or storage capacity
- ❑ State review process and review experts, if any

Scope of the study:

- ❑ State functional unit clearly and unambiguously according to guideline, report changes due to solving of multi-functionality
- ❑ State performance characteristics, any omission of additional function in comparison and how performance is measured (might apply for products different in chemical structure and composition to their conventional counterparts)
- ❑ State system boundaries according to guideline and cut-off criteria including a system boundaries flow chart
- ❑ State omitted life cycle stages and processes (might apply for products different in chemical structure and composition to their conventional counterparts)
- ❑ State relevant issues with data quality and assumptions
- ❑ State method(s) to solve multi-functionality
- ❑ State impact assessment methods

- ❑ State data quality needs and how energy and material inputs and outputs are quantified
- ❑ State software system (and version) and data library (and version) used
- ❑ State type of review and provide additional information about reviewers

Life cycle inventory

- ❑ Include flow diagram of assessed process system(s)
- ❑ State types and sources of required data and information
- ❑ State calculation procedures
- ❑ State all assumptions made
- ❑ Describe sensitivity analysis for refining system boundaries
- ❑ Include calculated full LCI results (if this not contradicts with confidentiality)
- ❑ State data representativeness and appropriateness of LCI data
- ❑ If results are reported on a relative basis, report basis
- ❑ State results obtained from scenario analysis (including scenarios) and threshold values, if any

Life cycle impact assessment

- ❑ Include results of life cycle impact assessment
- ❑ State if impact categories coverage is reduced, e.g., in case of carbon footprinting
- ❑ If results are reported on a relative basis, report basis
- ❑ State if delayed emissions occur and include emission time profile if needed
- ❑ If applied, state discounting method and discounted results

Life cycle interpretation

- ❑ Include and describe the results
- ❑ Negative emission in cradle-to-gate studies shall not be interpreted as CO_2 sinks if life does not end with permanent carbon fixation
- ❑ Emission reductions due to substitution effects shall be interpreted as environmental benefits but not as negative emissions.
- ❑ Describe uncertainty and sensitivity analysis and report results separately
- ❑ Include completeness check
- ❑ Include consistency check
- ❑ State assumptions and limitation associated with the interpretation of results
- ❑ Include conclusions
- ❑ Include recommendations, if any

C.9 Annex

C.9.1 Description of modeling of standardized scenarios

The provided inventories have been modelled with the LCA Software GaBi and some of the inventories[6] could only be provided due to the courtesy of Thinkstep [74]. In the following, a description of the modelling is provided. Please note that the provided data sets do not aim to represent the status-quo or the future in an accurate way. Instead, the scenarios provided should help to avoid scenario generation for each LCA study and in addition, the scenarios allow a comparison between technologies as they serve as a harmonized input.

Four inventory data sets are provided:

1. Status-quo
2. Low decarbonized
3. High decarbonized
4. Full decarbonized

The scenarios have been generated by applying a simple rule: first the greenhouse gas emissions of the electricity grid mix are computed and then the other technologies are selected such that the lowest greenhouse gas emissions are always achieved for each input. The only exception is the CO_2 supply, in highly or fully decarbonized scenarios, as fossil power plants will no longer be available as a CO_2 source. Instead, it is assumed that a direct air capture process supplies the CO_2. In Table 3 the selected technologies are listed.

Table 3: Selected Technologies for scenarios

	Status quo	**Low decarbonized**	**High decarbonized**	**Full decarbonized**
Hydrogen	Steam methane reforming	PEM electrolysis	PEM electrolysis	PEM electrolysis
CO_2	Coal power plant	Coal power plant	Direct air capture	Direct air capture
Heat	Natural gas vessel	Electrode vessel	Electrode vessel	Electrode vessel
Natural gas (methane)	Natural gas	Natural gas	Methanation	Methanation

C.9.1.1 Electricity:

For the current electricity generation, the mix of electricity production for the EU is used from the GaBi database (EU-28: Electricity grid mix ts). For low and high decarbonized scenarios, the mix of electricity production for the EU is modelled according to the 2°C scenario of the Energy Technology Perspectives report for the years 2030 and 2050 respectively. The inventories for the electricity technologies are taken from the GaBi database [74]. As inventories for European technology mixes are not available, inventories representing Germany are used as a proxy. In the Energy Technology Perspectives report carbon capture and storage (CCS) technologies are used, but no inventories for the used CCS technologies are available. Therefore, electricity technologies with CCS are modelled the same as conventional electricity technology, but with zero CO_2 emissions. This can be assumed, if the capture rate is 100%, the energy demand for capture, compression and storage of CO_2 is

[6] LCIA results of the following processes are published with permission of Thinkstep: EU-28: Electricity grid mix ts, DE: Electricity from wind power ts EU-28: Heat ts, DE: Hydrogen ts

zero and CO_2 is stored permanently. In the full decarbonized scenario electricity comes 100% from renewables and thus, wind energy is used as a proxy process (DE: Electricity from wind power ts) [74].

C.9.1.2 Hydrogen

Currently, hydrogen is mainly produced by steam reforming of hydrocarbons. Therefore, for the status quo production of hydrogen, a steam methane reforming inventory has been used (DE: Hydrogen ts). For the hydrogen generation via electrolysis an alkaline water electrolysis has been modelled according to Koj *et al*. [86]. The impact of the electricity demand of the electrolysis is then calculated according to the energy scenario.

C.9.1.3 CO_2

For CO_2 supply two sources are considered: capture from exhaust gases of a coal-fired power plant [87] and direct air capture [12].

C.9.1.4 Heat

Heat is either supplied by a natural gas boiler (EU-28: Heat ts) or by an electrode boiler. The electrode boiler is assumed to simply convert electricity to steam with an efficiency of 95%. No other inventory was considered.

C.9.1.5 Natural gas

Natural gas is either supplied by the natural gas network of Europe from the extraction of fossil natural gas or by methanation from CO_2 and hydrogen.

The natural gas network of Europe is modelled by weighting the national natural gas supply processes from the GaBi database according to their relative market volume in Europe. The market volume of the national gas markets are based on data from Eurostat and are assumed to remain constant over time. The following assumptions are made in the modelling of the natural gas network:

- For the national markets of Malta and Cyprus no data is available, thus they are not considered in the EU natural gas mix.
- For the countries of Bulgaria, Croatia, Denmark, Estonia, and the Czech Republic no national process are available in the GaBi database [74]. The national market of these countries combined contribute less than 4% to the total European market and are neglected.
- The market share of the other countries has been adjusted accordingly to reach 100%.

The methanation is modelled according Müller *et al*. [88].

C.9.1.6 Life cycle impact assessment results for standardized scenarios

CML 2016 January	Scenario			
Supply of 1 MJ electricity	**Status-quo**	**Low decarbonized**	**High decarbonized**	**Full decarbonized**
Abiotic Depletion (ADP elements) [kg Sb eq.]	4,90E-08	1,20E-07	1,50E-07	1,50E-07
Abiotic Depletion (ADP fossil) [MJ]	1,3	0,47	0,18	0,036
Acidification Potential (AP) [kg SO2 eq.]	0,00035	8,90E-05	9,20E-05	8,50E-06
Eutrophication Potential (EP) [kg Phosphate eq.]	3,20E-05	1,30E-05	1,10E-05	9,50E-07
Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.) [kg DCB eq.]	0,00025	0,00018	0,00018	2,00E-05
Global Warming Potential (GWP 100 years) [kg CO2 eq.]	0,12	0,042	0,011	0,003
Global Warming Potential (GWP 100 years), excl biogenic carbon [kg CO2 eq.]	0,12	0,042	0,017	0,003
Human Toxicity Potential (HTP inf.) [kg DCB eq.]	0,0056	0,0037	0,0038	0,0013
Marine Aquatic Ecotoxicity Pot. (MAETP inf.) [kg DCB eq.]	14	18	20	0,61
Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]	5,50E-12	3,30E-13	3,40E-13	2,50E-14
Photochem. Ozone Creation Potential (POCP) [kg Ethene eq.]	2,20E-05	6,80E-06	4,70E-06	3,40E-07
Terrestric Ecotoxicity Potential (TETP inf.) [kg DCB eq.]	8,70E-05	8,80E-05	9,00E-05	2,10E-05

CML 2016 January	Scenario			
Supply of 1 kg H_2	**Status-quo**	**Low decarbonized**	**High decarbonized**	**Full decarbonized**
Abiotic Depletion (ADP elements) [kg Sb eq.]	8,60E-07	2,20E-05	2,80E-05	2,90E-05
Abiotic Depletion (ADP fossil) [MJ]	190	85	34	8,1
Acidification Potential (AP) [kg SO2 eq.]	0,0055	0,017	0,018	0,0028
Eutrophication Potential (EP) [kg Phosphate eq.]	5,60E-04	0,0025	0,002	0,00022
Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.) [kg DCB eq.]	0,0026	0,036	0,035	0,0068

Global Warming Potential (GWP 100 years) [kg CO2 eq.]	11	7,6	2,1	0,67
Global Warming Potential (GWP 100 years), excl biogenic carbon [kg CO2 eq.]	11	7,7	3,1	0,66
Human Toxicity Potential (HTP inf.) [kg DCB eq.]	0,015	0,71	0,75	0,3
Marine Aquatic Ecotoxicity Pot. (MAETP inf.) [kg DCB eq.]	15	3,20E+03	3,50E+03	1,30E+02
Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]	6,10E-13	6,10E-10	6,10E-10	5,50E-10
Photochem. Ozone Creation Potential (POCP) [kg Ethene eq.]	1,20E-03	0,0013	0,00091	0,00013
Terrestric Ecotoxicity Potential (TETP inf.) [kg DCB eq.]	0,00018	0,016	0,017	0,0044

CML 2016 January	**Scenario**			
Supply of 1 kg H_2	**Status-quo**	**Low decarbonized**	**High decarbonized**	**Full decarbonized**
Abiotic Depletion (ADP elements) [kg Sb eq.]	6,00E-08	1,40E-07	8,50E-07	8,70E-07
Abiotic Depletion (ADP fossil) [MJ]	1,6	0,57	1	0,21
Acidification Potential (AP) [kg SO2 eq.]	0,00043	0,00011	0,00052	4,80E-05
Eutrophication Potential (EP) [kg Phosphate eq.]	3,90E-05	1,60E-05	6,20E-05	5,40E-06
Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.) [kg DCB eq.]	0,0003	0,00022	0,001	0,00011
Global Warming Potential (GWP 100 years) [kg CO2 eq.]	-0,85	-0,95	-0,94	-0,98
Global Warming Potential (GWP 100 years), excl biogenic carbon [kg CO2 eq.]	0,15	0,051	0,095	0,017
Human Toxicity Potential (HTP inf.) [kg DCB eq.]	0,0069	0,0045	0,022	0,0076
Marine Aquatic Ecotoxicity Pot. (MAETP inf.) [kg DCB eq.]	17	22	1,10E+02	3,4
Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]	6,70E-12	4,00E-13	1,90E-12	1,40E-13
Photochem. Ozone Creation Potential (POCP) [kg Ethene eq.]	2,70E-05	8,30E-06	2,70E-05	1,90E-06
Terrestric Ecotoxicity Potential (TETP inf.) [kg DCB eq.]	0,00011	0,00011	0,00051	0,00012
Abiotic Depletion (ADP elements) [kg Sb eq.]	6,00E-08	1,40E-07	8,50E-07	8,70E-07

CML 2016 January	Scenario			
Supply of 1 MJ Heat	**Status-quo**	**Low decarbonized**	**High decarbonized**	**Full decarbonized**
Abiotic Depletion (ADP elements) [kg Sb eq.]	0,00	1,20E-07	1,60E-07	1,60E-07
Abiotic Depletion (ADP fossil) [MJ]	1,10	0,49	0,19	0,038
Acidification Potential (AP) [kg SO2 eq.]	0,00	9,40E-05	9,60E-05	8,90E-06
Eutrophication Potential (EP) [kg Phosphate eq.]	0,00	1,40E-05	1,20E-05	1,00E-06
Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.) [kg DCB eq.]	0,00	0,00019	0,00019	2,10E-05
Global Warming Potential (GWP 100 years) [kg CO2 eq.]	0,07	0,044	0,012	0,0032
Global Warming Potential (GWP 100 years), excl biogenic carbon [kg CO2 eq.]	0,07	0,044	0,018	0,0032
Human Toxicity Potential (HTP inf.) [kg DCB eq.]	0,00	0,0038	0,004	0,0014
Marine Aquatic Ecotoxicity Pot. (MAETP inf.) [kg DCB eq.]	0,48	19	21	0,64
Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]	0,00	3,50E-13	3,50E-13	2,60E-14
Photochem. Ozone Creation Potential (POCP) [kg Ethene eq.]	0,00	7,10E-06	4,90E-06	3,50E-07
Terrestric Ecotoxicity Potential (TETP inf.) [kg DCB eq.]	0,00	9,20E-05	9,50E-05	2,20E-05

CML 2016 January	Scenario			
Supply of 1 kg natural gas (methane)	**Status-quo**	**Low decarbonized**	**High decarbonized**	**Full decarbonized**
Abiotic Depletion (ADP elements) [kg Sb eq.]	0,000	0,00	0,00	0,00
Abiotic Depletion (ADP fossil) [MJ]	49,000	52,00	20,00	4,80
Acidification Potential (AP) [kg SO2 eq.]	0,001	0,01	0,01	0,00
Eutrophication Potential (EP) [kg Phosphate eq.]	0,000	0,00	0,00	0,00
Freshwater Aquatic Ecotoxicity Pot. (FAETP inf.) [kg DCB eq.]	0,001	0,02	0,02	0,00
Global Warming Potential (GWP 100 years) [kg CO2 eq.]	0,480	0,480	-1,40	-2,30
Global Warming Potential (GWP 100 years), excl biogenic carbon [kg CO2 eq.]	0,480	0,480	2,10	0,59

Human Toxicity Potential (HTP inf.) [kg DCB eq.]	0,004	0,43	0,45	0,18
Marine Aquatic Ecotoxicity Pot. (MAETP inf.) [kg DCB eq.]	3,700	1900,00	2200,00	77,00
Ozone Layer Depletion Potential (ODP, steady state) [kg R11 eq.]	0,000	0,00	0,00	0,00
Photochem. Ozone Creation Potential (POCP) [kg Ethene eq.]	0,000	0,00	0,00	0,00
Terrestric Ecotoxicity Potential (TETP inf.) [kg DCB eq.]	0,000	0,01	0,01	0,00

C.9.2 Technical Summary Table

GOAL	CCU product		
	Goal		
	Brief description		
	Intended audience		
	Functional unit		
	Limitations & assumptions		
SCOPE	Boundary (i.e., cradle-to-gate)		
	Location		
	Time frames		
	Multi-functional approach	☐Sub-division ☐System expansion ☐System expansion via substitution ☐Virtual sub-division ☐Mass allocation	☐Energy allocation ☐Economic allocation ☐ Closed loop scenarios ☐Other (please specify)…………………
INVENTORY	Data source	☐Primary sources ☐Secondary sources ☐Stoichiometric data	☐Process modelling based data ☐Mixes sources ☐Other (please specify)……………………
	Energy sources (select all that apply)	☐Grid mix ☐Power station with Carbon Capture ☐Wind ☐Solar	☐Nuclear ☐Hydro ☐Future (see timeframes) ☐Other (please specify)………………….
	Main sub-processes and TRLS	**SUB-PROCESS**	**TRL** TRL TRL TRL
	Database & software used		
ASSESSMENT	LCIA method	☐ CML ☐ ILCD recommendation: v.____ ☐ TRACI 2.0 OTHER IMPACT METHODS ☐……………………………………….	SINGLE CATEGORIES: ☐ Climate change ☐ CED ☐ use TOX

	Highlighted results (graphical, text or tabular format)	
INTERPRETATION	**Main conclusions**	
	Sensitivity analysis	☐No ☐ Yes (please specify below)

C.10 References

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