

# Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO<sub>2</sub> Utilization (Version 1.1)

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# PART A General Assessment Principles



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## Foreword from the Global CO<sub>2</sub> Initiative

Since the publication of Version 1.0 of these Guidelines in 2018, the urgency to counter the causes of climate change and the associated catastrophic effects on human well-being has become ever more apparent. Climate change is one of the greatest challenges of our time. A major cause of anthropogenic climate change is the excessive release of carbon dioxide into the atmosphere. Left unaddressed, ecosystems will fundamentally change, and with that, 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 maintain global temperature increase during this century to well below two degrees Celsius relative to pre-industrial levels. This will require a variety of strategies, including increased use of renewable power generation and broad-scale electrification, increased energy efficiency, and carbon-negative technologies.

The Global CO<sub>2</sub> Initiative, launched in 2016 during the meeting of the World Economic Forum with the goal of catalyzing innovative research in CO<sub>2</sub> utilization, seeks to get CO<sub>2</sub> capture and use recognized and implemented as a mainstream climate solution.

The Global CO<sub>2</sub> Initiative's [roadmap](#) to a global market for CO<sub>2</sub>-based products identified a trillion-dollar opportunity by 2030 for CO<sub>2</sub> capture and utilization across a wide array of industry sectors. Key to the successful launch of a new carbon economy will be comprehensive assessments of the environmental and economic benefits of new technologies and products.

Life cycle assessment (LCA) is necessary to demonstrate that a technology could contribute to mitigating environmental impacts, whereas techno-economic assessment (TEA) will show how the technology could be competitively delivered in the market. Together they provide a valuable toolkit for promoting the development of carbon capture and utilization (CCU) technologies. While neither LCA nor TEA are new tools, their application to carbon capture and utilization was not comprehensively defined and described. The ensuing confusion concerning the comparability of different studies, and the validation of underlying data and methods motivated the development and publication of “Techno-Economic Assessment and Life Cycle Assessment for CO<sub>2</sub> Utilization, Version 1.0.”

Over the past two years, these Guidelines have been widely distributed and used, and have inspired an international collaboration to further harmonize LCA and TEA for CO<sub>2</sub> utilization, coordinated by the Global CO<sub>2</sub> Initiative and supported by EIT Climate-KIC.

This revised version 1.1 of the Guidelines has been developed by a team of researchers at TU Berlin, RWTH Aachen, the University of Sheffield, the Institute for Advanced Sustainability Studies Potsdam, and the University of Michigan. Several workshops, and feedback from practitioners and users of LCA and TEA studies, have contributed to this updated version.

We hope that this document will be useful to you and we [invite feedback](#) to help us produce version 2.0.

**Global CO<sub>2</sub> Initiative, September 2020**

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## List of Abbreviations

<b>AACE</b>	Association for the advancement of cost engineering
<b>AHP</b>	Analytic hierarchy process
<b>ANP</b>	Analytic network process
<b>BFD</b>	Block flow diagram
<b>CapEx</b>	Capital expenditure
<b>CAPM</b>	Capital asset pricing model
<b>CCS</b>	Carbon capture and storage
<b>CCU</b>	Carbon capture and utilization
<b>CEPCI</b>	Chemical Engineering Plant Cost Index
<b>CML</b>	Institute of Environmental Sciences of the University of Leiden
<b>CO<sub>2</sub></b>	Carbon dioxide
<b>COGM</b>	Cost of goods manufactured
<b>COGS</b>	Cost of goods sold
<b>DIN</b>	Deutsches Institut für Normung
<b>EBIT</b>	Earnings before interest and taxes
<b>EIA</b>	Energy Information Administration
<b>ELECTRE</b>	Elimination Et Choix Traduisant la Réalité
<b>ETS</b>	Emission trading system
<b>EU</b>	European Union
<b>FCI</b>	Fixed capital investment
<b>FOAK</b>	First of a kind
<b>GHG</b>	Greenhouse gas
<b>GWP</b>	Global warming potential
<b>H<sub>2</sub></b>	Hydrogen
<b>IEA</b>	International Energy Agency
<b>IEAGHG</b>	International energy agency greenhouse gas program
<b>ILCD</b>	International reference life cycle data
<b>IPCC</b>	Intergovernmental Panel on Climate Change
<b>IRR</b>	Internal rate of return
<b>ISBL</b>	Inside battery limits
<b>ISO</b>	International Organization for Standardization
<b>JRC</b>	European Commission's Joint Research Centre
<b>LCA</b>	Life cycle assessment
<b>LCC</b>	Life cycle costing
<b>LCI</b>	Life cycle inventory
<b>LCOE</b>	Levelized cost of electricity
<b>LHV</b>	Lower heating value
<b>MADM</b>	Multiple attribute decision making
<b>MCDA</b>	Multicriteria decision analysis
<b>MODM</b>	Multiple objective decision making
<b>NGO</b>	Non-governmental organization
<b>NOAK</b>	Nth of a kind
<b>NOX</b>	Nitrous oxides
<b>NPV</b>	Net present value
<b>OAT</b>	One at a time
<b>OME</b>	Oxymethylene ether
<b>OpEx</b>	Operating expenditure
<b>OSBL</b>	Outside/off-site battery limits
<b>P&amp;ID</b>	Piping and instrumentation diagram

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<b>PEM</b>	Proton-exchange membrane
<b>PFD</b>	Process flow diagram
<b>PROMETHEE</b>	Preference Ranking Organization Methods for Enrichment Evaluations
<b>R&amp;D</b>	Research and development
<b>RED</b>	Renewable energy directive
<b>ROI</b>	Return on investment
<b>SA</b>	Sensitivity analysis
<b>SI UNITS</b>	International System of Units
<b>SMR</b>	Steam methane reforming
<b>TEA</b>	Techno-economic assessment
<b>TOPSIS</b>	Technique for order preference by similarity to ideal solution
<b>TRL</b>	Technology readiness level
<b>UA</b>	Uncertainty analysis
<b>UN</b>	United Nation
<b>US DOE</b>	United States Department of Energy
<b>US EPA</b>	United States Environmental Protection Agency
<b>USD</b>	United States Dollars
<b>VDI</b>	Verein Deutscher Ingenieure
<b>WACC</b>	Weighted average cost of capital
<b>WPM</b>	Weighted product method
<b>WSM</b>	Weighted sum method

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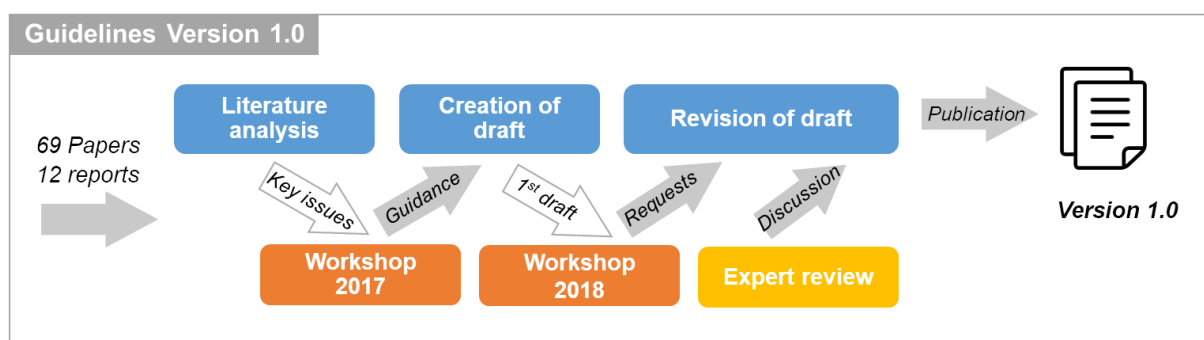


## A.1 Introduction

In times of climate change, research on CO<sub>2</sub> utilization is gaining momentum in industry, academia, and policy spheres, leading to a vast number of promising technologies, for example in the fields of CO<sub>2</sub>-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 for analyzing 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.

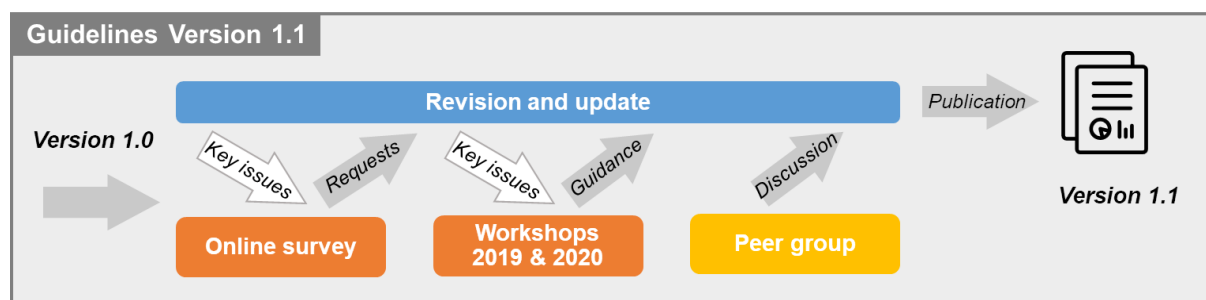
The methods applied in TEA and LCA, especially at differing stages of technology maturity and for selected indicators, currently lack standardization in academia and industry across most fields of CO<sub>2</sub> utilization (e.g., there is no CCU protocol for LCA yet derived from the ISO approach). Hence, ‘apples-to-apples’ comparisons of different technologies remain difficult [3]. Most CO<sub>2</sub> utilization technologies are currently in early stages of development; to date, only some have entered the demonstration plant stage but many more are anticipated. Entering the demonstration phase requires increased investment, and such funding needs 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 standardized guidelines for TEA and LCA of CO<sub>2</sub> utilization.

The present TEA and LCA Guidelines for CCU are intended to substantially reduce ambiguity in methodological choices and to 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 development of version 1.0 [4] of the Guidelines involved several stages, including an extensive literature study, guidance and requests from several stakeholder workshops, and multiple discussion rounds of peer-review, allowing for close participation of the CCU community and ensuring high scientific quality (see Figure 1).



**Figure 1.** The process of creating the Guidelines document (version 1.0), involving literature analysis, draft creation and revision, involving stakeholder workshops and expert review

Version 1.0 of the Guidelines has been revised with the continued participation of the CCU community. This updated version 1.1 of the Guidelines is based on comments received from prior stakeholder workshops, requests from an online survey of guideline users, guidance from two further stakeholder workshops, and discussion by an expert peer group (see Figure 2).



**Figure 2.** The process of creating the Guidelines document (version 1.1), involving revised drafts and updates based on an online survey, stakeholder workshops, and peer group discussion

Several reports and articles present the Global CO<sub>2</sub> Initiative's and Climate-KIC's efforts to produce TEA and LCA guidelines for CCU. Besides version 1.0 [4] and the revised version 1.1 presented here, three peer-reviewed articles were published to date regarding TEA guidelines for CCU [5], LCA guidelines for CCU [6], and the harmonization of guidelines for CCU across organizations [7] (see Table 1).

**Table 1.** List of guideline documents and articles

Guideline documents and articles	Guideline documents
	<ul style="list-style-type: none"> <li>▪ Techno-Economic Assessment &amp; Life Cycle Assessment Guidelines for CO<sub>2</sub> Utilization, Version 1.0 (2018)</li> <li>▪ Techno-Economic Assessment &amp; Life Cycle Assessment Guidelines for CO<sub>2</sub> Utilization, Version 1.1 (2020) [THIS PUBLICATION]</li> </ul> <p>Peer-reviewed guideline articles</p> <ul style="list-style-type: none"> <li>▪ Sick <i>et al.</i> (2019). The Need for and Path to Harmonized Life Cycle Assessment and Techno-Economic Assessment for Carbon Dioxide Capture and Utilization</li> <li>▪ Zimmermann <i>et al.</i> (2020). Techno-Economic Assessment Guidelines for CO<sub>2</sub> Utilization</li> <li>▪ Müller <i>et al.</i> (2020). A Guideline for Life Cycle Assessment of Carbon Capture and Utilization</li> </ul>

In addition, a range of connected reports have been produced that provide further orientation, examples, and discussion summaries. These include an orientation report for commissioners and decision-makers,[8] as well as worked examples on methanol and OME production[9], [10], mineralization [11], setting goals in TEA [12], creation of LCA inventories [13], and interpretation of LCA results [14]. Summaries of discussions at stakeholder workshops held in Ann Arbor 2019 and Brussels 2019 were also published (see Table 2) [15], [16]. All documents are available online at [www.globalco2initiative.org](http://www.globalco2initiative.org).

Table 2. List of publications closely connected to the Guidelines

<b>Connected publications</b>	<p><b>Publication for study commissioners and decision makers</b></p> <ul style="list-style-type: none"> <li>▪ Making Sense of Techno-Economic Assessment &amp; Life Cycle Assessment Studies for CO<sub>2</sub> Utilization: A guide on How to Commission, Understand, and Derive Decisions from TEA and LCA studies, Version 1.0 (2020)</li> </ul> <p><b>Worked examples for practitioners</b></p> <ul style="list-style-type: none"> <li>▪ Methanol Worked Examples for the TEA and LCA Guidelines for CO<sub>2</sub> Utilization (2018)</li> <li>▪ Mineralization Worked Examples for the TEA and LCA Guidelines for CO<sub>2</sub> Utilization (2018)</li> <li>▪ OME Worked Example for the TEA Guidelines for CO<sub>2</sub> Utilization (2019)</li> <li>▪ A Guide to Goal Setting in TEA: A Worked Example Considering CO<sub>2</sub> Use in the Domestic Heating Sector (2020)</li> <li>▪ Building an LCA Inventory: A Worked Example on a CO<sub>2</sub> to Fertilizer Process (2020)</li> <li>▪ Interpretation of LCA results: A Worked Example on a CO<sub>2</sub> to Fertilizer Process (2020)</li> </ul> <p><b>Workshop reports</b></p> <ul style="list-style-type: none"> <li>▪ Workshop on LCA/TEA for CO<sub>2</sub>-based Products (2019)</li> <li>▪ Towards a Common Understanding of LCA and TEA for CO<sub>2</sub> Utilization technologies: An Exchange Among Policymakers, Industry and Practitioners (2020)</li> </ul>
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Version 1.0 of the Guidelines was updated by four partners, IASS Potsdam, RWTH Aachen, The University of Sheffield, and TU Berlin, supported by the Global CO<sub>2</sub> Initiative and EIT Climate-KIC. The fruitful discussions with all contributors, reviewers, and with colleagues are gratefully acknowledged. The outstanding peer group contributions from colleagues at The University of Michigan, the US National Energy Technologies Laboratory (NETL), the US National Renewable Energies Laboratory (NREL), the National Research Council of Canada, and Argonne Labs are highly appreciated.

## 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**' introduces both TEA and LCA; Part B, the **TEA Guidelines**; and Part C, the **LCA Guidelines** (see Figure 3). As these Guidelines follow a commercial and product-oriented approach, the section on TEA is presented first. This order can, however, be reversed by practitioners depending on individual needs. The document parts are marked and color-coded at the top of each page.

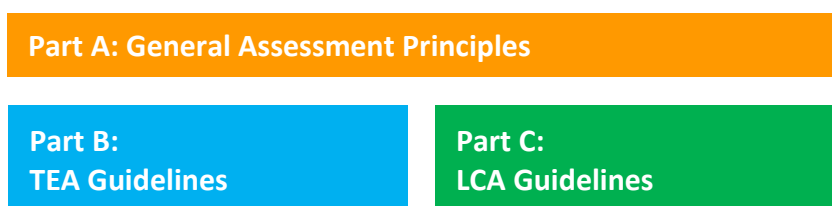


Figure 3. Structure of the TEA & LCA Guidelines document

### A.2.2 Scope of this Document

A thorough review of published TEAs and LCAs for CCU technologies 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<sub>2</sub> prices, calculating OpEx and CapEx, integrating LCA and TEA*). These difficulties lead to wide differences in current TEA and LCA practices in the field of CCU that may potentially misinform decision makers.

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

For LCA, general concepts are omitted if these issues are not specific to CCU. Instead, we provide short and concise guidance on CCU-specific assessment challenges to complement existing ISO standards and guidance. However, since readers might be new to the concept of LCA, a short introduction to each step of LCA is provided together with further reading. For TEA, general concepts are introduced in all chapters.

TEA and LCA remain two separate approaches in this document, as is currently common practice for assessments conducted in industry and in the academic literature. There is strong demand for an integrated approach to TEA and LCA, and discussion has begun on integration methods and best practices. However, commonly accepted methods and best practices remain to be developed and therefore cannot be included at present.

### A.2.3 Intended Audience

This document is aimed at practitioners seeking to create comprehensible and consistent TEAs and LCAs in the CCU field. Practitioners come from academia, industry, or government, and work in the areas of technology assessment, research and development, or funding. 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 can use this document to understand the challenges and pitfalls of 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. Instead they aim to help practitioners to conduct sound assessments efficiently, avoid common mistakes, and to derive meaningful results that can be compared to other studies. The Guidelines provide a consistent methodological core for conducting all LCA and TEA CCU studies. This document serves as an addition to conventional existing standards (in particular for LCA) and literature, and does not replace any chemical engineering, economic, or project planning principles. However, since the aim is 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 a need to add further tasks to those discussed in these Guidelines, if they are important to a specific study. This document provides a detailed set of provisions on separate TEA and LCA studies for CCU. Furthermore, some initial guidance is provided on integrated TEA and LCA studies.

### A.2.5 The Provisions

Each chapter concludes by recommending provisions for conducting TEA or LCA for CCU. These recommendations follow three categories, termed: *shall*, *should*, and *may*:

- **Shall:** these are the minimum requirements for achieving a standardized TEA/LCA for CCU. Every TEA/LCA produced using these Guidelines must meet these basic requirements. All provisions in this category must be addressed.
- **Should:** these provisions cover a recommended level of analysis and should be applied to produce a TEA/LCA of greater depth.
- **May:** these provisions produce the most detailed TEA/LCA. They will not be applicable in all studies, and may be applied as determined by the practitioner.

If specific provisions from this work are referenced in the TEA or LCA report, they can be addressed by provision topic or number, as for example “[Provision Topic] Shall: Provision 2” or “A.X Should: Provision 3.”

Table 3. Template for provisions

Provisions A.X - [Topic]	
<b>Shall</b>	1) Provision 1 2) Provision 2
<b>Should</b>	1) Provision 1 2) Provision 2
<b>May</b>	1) Provision 1 2) Provision 2

## A.3 Carbon Capture and Utilization

### A.3.1 Introduction

Carbon capture and utilization (CCU) is the capture of carbon dioxide (CO<sub>2</sub>) from industrial flue gas or the atmosphere and its subsequent conversion into value-added products (see Figure 4). CCU has already shown its potential to reduce environmental impacts such as greenhouse gas (GHG) emissions and fossil fuel depletion in comparison to conventional technologies. However, CCU alone cannot mitigate climate change since the amount of CO<sub>2</sub> that is potentially convertible to chemicals, fuels, and materials is much less than that currently emitted [1]. Furthermore, many CO<sub>2</sub>-based products lie thermodynamically uphill; in other words, a large amount of energy is generally required to chemically reduce the CO<sub>2</sub>. For other CCU technologies such as mineralization, no energy is required to convert the CO<sub>2</sub>, but those processes often have slow kinetics and require energy-intensive preparation of reactants (*e.g.*, grinding of olivine and other minerals). Therefore, the environmental benefits and economic viability of CCU technologies often depend on the context and boundary conditions of each case (*e.g.*, availability of electricity with a low carbon footprint and low prices).

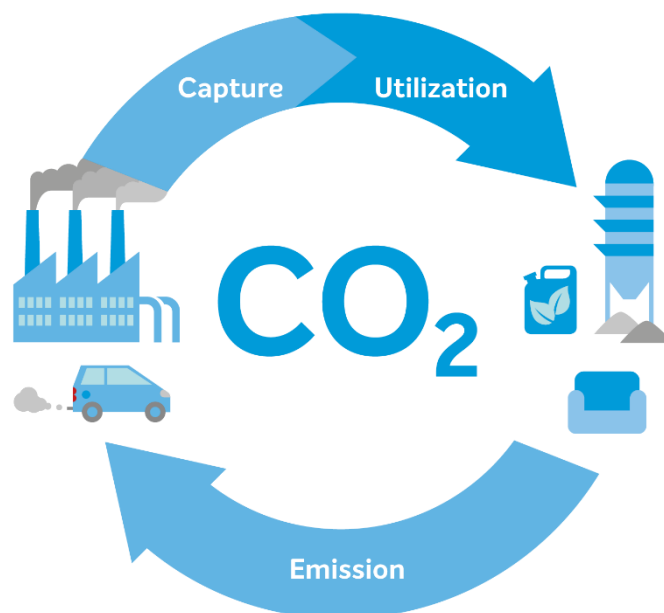


Figure 4. The CO<sub>2</sub> utilization cycle; Source: [1]

Interest in CCU has increased in the last decade, with a sharp increase in the number of 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 products have already entered the market (*e.g.*, CRI's Vulcanol, Covestro's Cardyon, and Carbon8's C8Agg). A 2016 market study for CCU products projected an annual revenue of up to 800 billion USD through 2030, relating to an annual uptake of up to 7 billion tonnes of CO<sub>2</sub> [17]. CCU markets can be categorized into two groups: niche markets (small volumes but high margins) such as plastics, chemicals, and carbon fibers; and bulk markets (large volume but low margins) such as concrete, asphalt, and fuels; through their large volumes, bulk markets can also provide substantial potential for emissions mitigation.

The strong 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 feedstocks.
- CCU can offer new pathways for synthesizing existing or new products, and thereby open new markets (see [18]).
- CCU can address challenges associated with chemicals, fuels, materials, waste treatment, and the mitigation of industrial CO<sub>2</sub> emissions, for integrating renewable electricity into the chemical and transportation sectors, and overall for industrial symbiosis and a circular economy.
- CCU can reduce the complexity of chemical reaction pathways (see [18]–[20]).
- CCU can increase process efficiency and reduce input price volatility.
- CCU can potentially reduce environmental impacts beyond climate change, as demonstrated for CO<sub>2</sub>-based fuels that reduce nitrous oxide (NO<sub>x</sub>) and soot emissions (see [19]).
- CCU technologies can even be carbon-negative if combined or integrated with CO<sub>2</sub> sequestration (*e.g., through mineralization*).

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

- The vast majority of CCU processes have high energy demand or require 'high-energy' co-reactants, which can increase operating costs and environmental impacts.
- CCU processes often require new plants, and many include high-pressure processes, both of which increase capital expenditure.
- CCU mostly focusses on low-margin, large-volume industrial markets requiring substantial investment.
- CCU addresses the chemical, fuel, and materials industries that face high costs in adapting existing processes and display very slow product adaption rates (slow market uptake).
- Reduction of environmental impacts is one important criterion for commercialization of CCU. If a CCU technology does not reduce overall environmental impacts it is unlikely to be successfully commercialized as a measure for mitigating emissions.

Since both the economic and environmental benefits of CCU technologies are important criteria for guiding future research and deployment, comprehensive assessments are required. Commonly accepted methods include LCA for comprehensive environmental assessment and TEA for assessing technical feasibility and economic viability.

### A.3.2 Classification of CCU Technologies

In these Guidelines, CCU technologies are classified according to their differences from compared products or services and by their intended application. Classification is not mandatory for LCA or TEA studies. However, it can help inform methodological choices (*e.g., the definition of the functional unit*). Since products or services are classified by their intended application, each might fall into different classes (*e.g., methanol can serve as both a chemical intermediate and fuel*).



The following CCU classes are defined:

- CO<sub>2</sub>-based products
  - Having identical chemical structure and composition to their reference/benchmark counterparts (e.g., chemicals or intermediates such as syngas, ethylene, methanol, oxalic acid, formic acid, and dimethyl carbonate).
  - Having different chemical structure and composition to their conventional reference/benchmark counterparts (e.g., materials such as thermosets, foams, elastomers, mineral aggregates, bricks, and carbon nanotubes).
- CO<sub>2</sub>-based fuels
  - Having identical chemical structure and composition to their reference/benchmark counterparts (e.g., methane).
  - Having different chemical structure and composition to their reference/benchmark counterparts (e.g., CO<sub>2</sub>-based methanol vs. reference/benchmark gasoline for use as a drop-in fuel).
- Energy storage systems (e.g., CO<sub>2</sub>-based methane that is stored and subsequently used for dispatchable electricity production).

The provisions and best practices presented in this document can also be applied to technologies not belonging to the CCU classes presented above, but should be applied with caution.

### A.3.3 Further Reading

For a general introduction to carbon capture and utilization we recommend the brochure “CO<sub>2</sub> Utilization Today” by TU Berlin (2017) [1], the report “Putting CO<sub>2</sub> to Use” by the International Energy Agency (2019) [21], and the overview article “The Technological and Economic prospects for CO<sub>2</sub> Utilization and Removal” by Hepburn *et al.* (2019) [22]. The books “Carbon Dioxide Utilization Fundamentals” [23] and “Carbon Dioxide Utilization Transformations” [24] provide a good starting point for research on any CCU-related topic. A comprehensive review of LCA for CCU is presented in the article “Sustainable Conversion of Carbon Dioxide: An Integrated Review of Catalysis and Life Cycle Assessment” by Artz *et al.* (2018) [18].

Detailed information on the future potential and developments of CCU can be accessed in the reports “Accelerating Breakthrough Innovation in Carbon Capture, Utilization and Storage” by Mission Innovation (2018) [2], “Global Roadmap for Implementing CO<sub>2</sub> Utilization” by the Global CO<sub>2</sub> Initiative (2016) [17], “Low Carbon Energy and Feedstock for the European Chemical Industry” by the German Society for Chemical Engineering and Biotechnology (Dechema) (2017) [25], and the article “Climate Change Mitigation Potential of Carbon Capture and Utilization in the Chemical Industry” by Kätelhon *et al.* (2019) [26].

## A.4 Technology Maturity

### A.4.1 Introduction

The term ‘technology maturity’ describes the stage of development of individual system elements / unit process or the overall product system. The selection of assessment methods and indicators depends on 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 within a TEA or LCA.

Technology maturity can be subdivided into the three major phases of applied research, development, and deployment. For a more detailed analysis, the concept of technology readiness level (TRL) can be used. The major maturity phases can be associated with distinct TRLs. Commonly used general TRL concepts relevant to CCU include those from the US Department of Energy [27] and the European Commission Horizon 2020 program [28]. However, specific TRL descriptions for the chemical and process industries are lacking at present. This has proven to make assigning TRLs difficult and subjective for TEA practitioners [29], especially in the case of CCU. Table 4 combines the general TRL concepts from the US DoE and EU Horizon 2020 and adapts them for the chemical and process industries (further details can be found in Table 12, chapter B.10).

**Table 4. Characterizing technology readiness levels for the chemical industry (excerpt from [30])**

TRL	Phase	Title	Description
1	<b>Research</b>	<i>Idea</i>	Basic principles observed and reported, opportunities identified, basic research translated into possible applications
2		<i>Concept</i>	Technology concept and application formulated, patent research conducted
3		<i>Proof of concept</i>	Applied laboratory research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)
4	<b>Development</b>	<i>Preliminary process development</i>	Concept validated in laboratory environment, scale-up preparation started
5		<i>Detailed process development</i>	Shortcut process models identified, simple analysis of property data, simulation of process and pilot plant using bench-scale information
6		<i>Pilot trials</i>	Pilot plant constructed and operated at low production rate, products tested in application
7	<b>Deployment</b>	<i>Demonstration &amp; full-scale engineering</i>	Parameters and performance of pilot plant optimized, (optional) demo plant constructed and operating, equipment specification incl. components conferrable to full-scale production

TRL	Phase	Title	Description
8	Deployment	<i>Construction and start-up</i>	Products and processes integrated in organizational structure (hardware and software), full-scale plant constructed
9		<i>Continuous operation</i>	Full-scale plant audited (site acceptance test), turn-key plant, production operated over the full range of conditions expected in industrial scale and environment, performance guarantee enforceable

Applied research is conducted mainly in TRLs 1–3 but often expands into later TRLs; 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, in TRL 1. Systematic development is started in TRL 4 and is mainly conducted until TRL 6, but can last until plant commissioning in TRL 8. Deployment begins with detailed planning of a full-scale plant in TRL 7 and is completed with running production in TRL 9.

Once a TRL is assigned to a system element (TEA) or unit process (LCA) and product system, the technological maturity also clarifies what data can theoretically be available to the TEA practitioner. If these data do not exist, are unavailable, or lack sufficient 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 indications of data availability and study limitations. Therefore, technology maturity **shall** be defined in each assessment.

Technology maturity is specific to each product system and each system element (TEA) / unit process (LCA). The technology maturity **shall** therefore be defined first for each individual system element / unit process, and second for the overall product system. The overall maturity of the product system **shall** equal that of the least mature system element / unit process (*e.g., when the systems elements H<sub>2</sub> generation and CO<sub>2</sub> capture are at deployment stage, CO<sub>2</sub> separation is at development stage, and the CO<sub>2</sub> utilizing reaction is at the research stage, the overall CCU product system is defined as being at the research stage*). While any maturity concept can be used, the concept and its criteria **shall** be clearly documented. For greater transparency and comparability, it is recommended that the TRL concept **should** be used to identify technology maturity. Furthermore, the chosen 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 a high level of technology maturity. However, the maturity of a system

element / unit process cannot be simply derived from other product systems unless their data are available for the assessment study. Furthermore, the system elements / unit processes of the similar product system may differ and not necessarily match the product system in focus. It is therefore necessary to rate technology maturity for all system elements / unit processes based on the data available for the actual process that is currently in research, development, or deployment. System elements / unit processes that are not the focus of the research, development, or deployment and therefore not implemented in earlier stages can be excluded from maturity rating.

#### A.4.2.3 Further Reading

Relevant sources discussing TRL include: “Technology Readiness Assessment Guide” by the US Department of Energy (2011) [27], “The TRL Scale as a Research and Innovation Policy Tool, EARTO Recommendations” by the European Association of Research Technology Organisations, EARTO (2014) [29], and the “General Annex G., Technology Readiness Levels (TRL)” by the HORIZON 2020 program [28].

#### A.4.2.4 Provisions

<b>Provisions A.1 - Technology Maturity</b>	
<b>Shall</b>	1) Technology maturity shall be defined in each assessment: first for each system element / unit process 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 / unit processes
	3) The maturity concept and its criteria shall be clearly documented
<b>Should</b>	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
<b>May</b>	

## A.5 Integration of TEA and LCA

### A.5.1 Introduction

When implementing new CO<sub>2</sub> utilization technologies, technological, economic, and environmental criteria can be taken into consideration. Both TEA and LCA can support this decision making. TEA compares technological feasibility and economic opportunity, whereas LCA compares environmental impact reductions. By integrating TEA and LCA, the relationships between technological, economic, and environmental criteria and indicators can be systematically analyzed [31]–[33]. Integration of TEA and LCA enables the joint interpretation of identified hotspots (for further details see A.5.2.1) and a balancing of trade-offs between technological, economic, and environmental aspects when searching for outcomes (*e.g., selecting an alternative feedstock might improve economic performance but worsen environmental impacts*).

The integration of TEA and LCA can be approached either by ex-ante integration, conducting a single study that covers the criteria of both TEA and LCA; or by ex-post integration after the individual TEA and LCA studies have been conducted separately, linking the results from both assessments. Three main types of integration can be characterized based on the approach taken:

- Qualitative, discussion-based integration
- Combined indicator-based integration
- Preference-based integration

In order to integrate studies, the data selected from the TEA and LCA must match the level of alignment required by the integration goal. The key aspects of each type, and key aspects of alignment are presented in the following paragraphs.

As this is an evolving area of study, many aspects of the methodology are yet to be defined. As such, we do not seek to provide provisions here for undertaking such studies, but instead present the types of integration, means of selecting between these types, and highlight further key issues (alignment of system elements, data, and multifunctionality) that could help practitioners avoid pitfalls.

### A.5.2 Types of TEA / LCA Integration

#### A.5.2.1 Qualitative, discussion-based integration

Qualitative, discussion-based integration, aims to compare economic and environmental results through detailed discussion. The qualitative discussion can include the whole process, hotspots in sub-processes, and/or trade-offs, as required, to achieve the integration goal. In this type of integration, the overall system boundaries of the TEA and LCA parts can differ, but those system elements selected for integration need to be sufficiently aligned in scope for the discussion to be meaningful.

Identifying hotspots can benefit the analysis. Here, a hotspot is a process or input that has a significant influence on the technical, economic, or environmental performance of the plant or process. Common hotspots 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. Hotspots can be identified in either the TEA or LCA, followed by a qualitative analysis of whether there are similar effects in the respective technical, economic, or environmental indicators.

### A.5.2.2 Combined indicator-based Integration

In combined indicator-based integration, TEA and LCA results are related by calculating a combined indicator (e.g., *greenhouse gas (GHG) abatement cost*). This type of integration is generally conducted for the whole process rather than for single system elements. As a quantitative result is produced, the scope of the two studies must be highly aligned in order to limit additional errors resulting from integration. Indicators which combine results from TEA and LCA, such as abatement costs, are commonly used to analyze economic and environmental efficiency and to rank alternatives, and are therefore of particular interest for CCU options. However, combined indicator results are, in general, limited to a specific point in time and do not reflect potential changes over time; this must be accounted for in the interpretation phase.

The following example utilizes a combined indicator: GHG abatement cost ( $c_{abated}$ ). Similar methodology can be applied to calculate other combined enviro-economic indicators. Although combined indicators for CCU are often based on greenhouse gas emissions, other environmental indicators need to be included in the combined analysis in order to broaden the scope from carbon footprinting to encompass multiple LCA indicators. GHG abatement cost can only be calculated if the CCU process has lower GHG emissions than the benchmark, otherwise no emissions are abated and the indicator is meaningless. GHG abatement cost ( $c_{abated}$ ) 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 boundaries and are set with respect to a single functional unit that is used consistently in both the techno-economic and environmental parts of the analysis.

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

The lower the GHG abatement cost, the higher will be 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 might need market incentives or that the CO<sub>2</sub>-based product needs to achieve a premium price over the conventional counterpart to be economically viable. Note that negative values of GHG abatement cost do not serve as an indicator of environmental viability, as other impact categories, such as human toxicity or eco-toxicity, must be taken into account to avoid ‘burden shifting’ of environmental impacts from one impact category to another. Comparing the GHG abatement cost of various technology options (e.g., *via marginal abatement cost curves*) can be conducted in a ranked list, for example in the form of an environmental-merit-order [34], [35].

While abatement costs are specific to the functional unit, the abatement of an overall CCU 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 approximated by the plant capacity and a load factor; this does not apply for multiple products), and the difference in specific GHG 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 total global market penetration. Subsequently, the comparison of this abatement potential to Socolow's stabilization wedges (reduction of one Gt CO<sub>2</sub>-eq. per year) can reveal whether the technology can significantly contribute to climate change protection [36]. However, this comparison is only of a qualitative, informative nature, as unforeseen changes might occur during scale-up.

### A.5.2.3 Preference-based Integration

Preference-based integration aims to include the decision maker's preferences by following a multi-criteria approach that can consider technical, economic, and environmental factors simultaneously. Based on the concepts of multi-criteria decision analysis (MCDA): TEA and LCA criteria (and, ultimately, preferences for these criteria) are selected and their respective indicator results are used as the basis for a concrete decision. This approach can include normalization and weighting of each criterion, to enable summing up the separate results. MCDA can be applied to the whole process or individual system elements (*e.g., elements identified as hotspots*). Multi-criteria decision analysis (MCDA) can be conducted to evaluate the interdependencies of the most influential technology barriers, cost drivers, and environmental impacts in order to determine the most beneficial outcome based on the goals of the study. Both multiple-objective decision making and multiple-attribute decision making can be applied. MCDA can also include the use of combined indicators. Note that LCA standards and guidelines do not recommend the application of weighing and aggregation, as these steps can lead to a decreasing understanding of underlying trade-offs. It is beyond the scope of these Guidelines to recommend specific MCDA methods, as the method chosen needs to be based on the goal and scope of the integrated study. Further details on MCDA can be found in chapter B.7.4.

### A.5.2.4 Three-step Approach to Select a Suitable Form of Integration

The integration type will be selected during the goal and scope phase of an integrated assessment, as the practitioner first needs to define what kinds of information need to be provided to the target audience. Three steps can be followed to select a suitable integration type: 1) defining the integration purpose; 2) identifying restrictions imposed by technology maturity; 3) identifying resource limitations for the assessment.

In the first step it is recommended to define the purpose of the integrated assessment in order to understand how TEA and LCA results need to be linked and interpreted. If the purpose is to analyze hotspots within the process concept from an economic and environmental perspective, then qualitative discussion-based integration is recommended. In this case, single system elements are often of interest and there is a need to prevent any loss of information due to aggregating and normalizing TEA and LCA results. If the purpose is to benchmark a technology against a variety of alternatives based on a single comparable indicator (*e.g., GHG abatement cost*), then combined indicator-based integration is recommended. In this case, the target audience is presented with a relative measure, which overcomes complex assessment results as it can easily be interpreted. If the purpose is to support the selection of an alternative technology by already including the decision makers' preferences within the integrated assessment, then preference-based integration applying multi-criteria decision analysis (MCDA) is recommended. In this case, the underlying criteria can be weighted to allow the aggregation of multiple indicator results into a single value and enable a quick decision process.

The second step identifies potential limitations arising from the level of data availability corresponding to the maturity of the assessed technology. At low technology readiness levels (TRLs 1–3) qualitative discussion-based integration is recommended, as the uncertainty in the data is usually greater due to estimated procedures. If possible, any additional loss of information due to normalizing or aggregating results via combined indicators or MCDA needs to be avoided. For higher levels (TRLs 4–9) all forms of integration are equally appropriate.

The third step identifies potential limitations imposed by the resources available to the practitioner, typically including limited time, budget, or expertise for conducting the assessment. Generally, when resources are limited, qualitative discussion-based integration is recommended, as no additional effort is required to mathematically link the indicator results. With increasing resource availability, combined indicator-based and preference-based integration can also be performed.

### A.5.3 Alignment of TEA and LCA

#### A.5.3.1 Alignment of System Elements

These 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 hotspots and areas for improvement; 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 raised to improve yields, 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 straightforward and clearer in reporting.

#### A.5.3.2 Alignment of Data

By aligning the underlying data of the two assessments – for example by choosing the same goal, functional unit, and system boundaries for the studies – uncertainty in the interpretation of the integrated LCA and TEA results is decreased. However, attempts to integrate an LCA and TEA that have only a low degree of alignment will introduce additional uncertainty and possibly lead to unreliable conclusions. For this reason, practitioners need to state the required level of alignment in the goal and scope phase.

To achieve a high level of data alignment between TEA and LCA, the system boundaries can be redrawn if necessary, scopes aligned, and aspects of the analysis repeated to reduce the uncertainty of integration. However, this approach is time consuming, as aspects of the analysis might have to be repeated. For high levels of data alignment, the following items must 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 multifunctionality (sub-division, system expansion, substitution or allocation using underlying physical or other relationship)
  - Temporal and geographical representation of the study
- Inventory: in particular, processes and data used, including electricity supply
- Scenarios applied (necessary if combined indicators are also 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 a single, all-encompassing integration goal. For example:

- TEA goal: What is the technical viability and economic performance of methanol production via CO<sub>2</sub> 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<sub>2</sub> 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 located in Germany, which uses wind energy for CO<sub>2</sub> hydrogenation, be optimized to maximize technological, economic, and environmental performance?

### A.5.3.3 Aligning and Solving Multifunctionality

TEA aims to assess the technical feasibility and economic viability of production and sales, mostly from the perspective of a producer (as described in this Guideline document). LCA aims to calculate the environmental impacts of a production system with all its functions (as defined in the goal and scope). TEA does not usually deal with upstream multifunctionality in the same way as LCA. It is not common practice within TEA to apply system expansion, including upstream and downstream processes or functions in the functional unit. For example, if the study analyzes a CCU plant for which a cement plant is the CO<sub>2</sub> source and system expansion is applied in LCA, then upstream processes such as cement production would be included within the system boundaries, leading to the inclusion of multiple functions (so-called ‘basket of functions’) such as cement and the CCU product(s) within one single functional unit. In practice, in a common TEA the system boundaries would not include the production of cement but only the CO<sub>2</sub> input flow (e.g., by calculating the costs of CO<sub>2</sub> capture from the CO<sub>2</sub> source or by assuming CO<sub>2</sub> costs via a market price for CO<sub>2</sub>). While system expansion can be applied when conducting TEA, it can cause complications involving detailed modelling and data collection for the CO<sub>2</sub>-providing process, which might not be known in detail. If product-specific indicators are required, then system expansion is not appropriate. Instead, the hierarchy described in the LCA Guidelines, chapter C.4.3.2, is recommended to resolve the multifunctionality.

## A.6 Screening

In CCU, as in most rapidly developing fields, many research and development projects are competing for resources to reach mass deployment. Each of these project candidates undergo various evaluations, for example to receive government-funded research grants or to pass a company's internal stage-gates. TEA and LCA provide robust tools to evaluate mature technologies; however, to evaluate R&D projects, TEA and LCA need to be conducted at a lower level of detail, referred to as 'screening.' For the purpose of this document, we define screening as a quick form of assessment with a low degree of detail, intended to pre-select promising alternatives. The goal and scope of a study define what degree of detail is sufficient for the pre-selection process.

The aim of screening is to reliably differentiate promising from unpromising candidates. Two methods are commonly used for screening: group-ranking and threshold-ranking. In group-ranking, a group number is defined for assessment criteria and candidates are selected according to their ranking until the group is full (*e.g., the top 5 candidates to reduce environmental impacts and maximize profits*). In threshold-ranking, inclusion thresholds are defined for assessment criteria and all candidates that meet the inclusion criteria are selected (*e.g., all candidates that reduce environmental impacts compared to a fossil benchmark while also showing financial profit*). Often, these screening assessments are carried out for the first, rough pre-selection of a group that will then be analyzed in more detail in a second step. As innovative projects contain confidential information, most screening assessments are not reviewed or published.

The TEA and LCA Guidelines presented here can, in principle, also be applied to screening. It is recommended to carry out an integrated assessment approach (TEA + LCA) for screening. Using the screening approach affects all phases of the assessment. Crucial points and questions include:

- Practitioners need to clearly state the purpose of the screening
- Relevant screening criteria and indicators need to be selected, and relevant functional units and system boundaries need to be defined
- Practitioners need to identify appropriate amounts and quality of data and select relevant estimation methods
- The limitations of the selected screening approach and potential burden-shifting needs to be discussed
- Practitioners need to ensure that the results and limitations are communicated clearly and in the language of the intended audience, and also embrace (internal) reviewing

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# PART B TEA Guidelines

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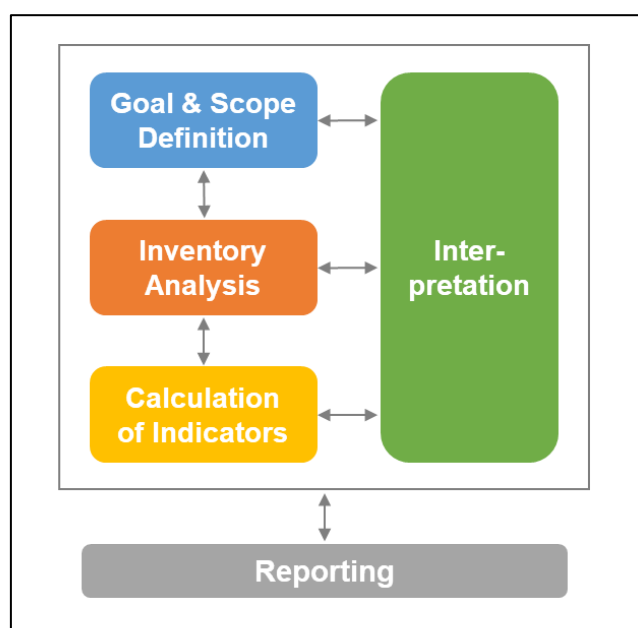
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## B.1 Introduction to Techno-Economic Assessment

Techno-economic assessment (TEA) is a methodology framework for analyzing 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. TEAs typically focus on the production phase, reflecting the perspectives of a producer. The inclusion of further upstream and downstream life cycle stages is possible, for example to analyze the technical or economic performance of products during the use or disposal phases.

For these Guidelines, TEA has been subdivided into the following phases: Goal and Scope Definition, Inventory Analysis, 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 the results. While conducting each phase, 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 need to revisit a previous phase to modify the assessment, if recommended by the interpretation phase. After completing all phases of the TEA, the goal, scope, and inventory 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 help identify the next steps in technology development or in 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 a single product as well as a combination of products. In this document, 'services' will also be referred to as a '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 in order to reduce development effort and time to market.

Note that specific TEA results require specific assumptions, thereby making the study context-specific with respect to factors such as location, time horizon, or access to information. Furthermore, TEA provides results relating to questions of technology and economics, while leaving aside environmental impacts and social aspects. TEA can support project-specific decision making in both technological and economic contexts, such as R&D support or investment decisions. Reliably applying TEA results in a generalized context, such as for global policy making, can be quite challenging and therefore requires considerable caution.

## B.2 How to Read this Document

### B.2.1 Scope of this Document

A thorough review of published TEAs for carbon capture and utilization (CCU) technologies has identified a number of methodological challenges and pitfalls (*e.g.*, *setting system boundaries for multifunctionality, selecting comparable indicators, identifying Technology Readiness Level, selecting CO<sub>2</sub> prices, calculating Operational Expenditure (OpEx) and Capital Expenditure CapEx, and integrating LCA and TEA*). This leads to differences in current TEA practice, which can be confusing and misleading for readers and decision makers. This document and its attachments summarize and extend commonly applied assessment concepts, present 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 Guidelines aim to provide an overview of standard TEA practice together with specific guidance on the challenges of conducting TEA for CCU. In general, each chapter or sub-chapter consists of an introduction, a 'how to....' section, some CCU examples, suggested further reading, and recommended Guidelines for that topic.

### B.2.2 Linking TEA and LCA

The link between techno-economic (TEA) and life cycle (LCA) assessments is strong in many industries, especially for CCU. All CCU processes aim to synthesize products in an economically viable way, and most seek to reduce environmental impacts; therefore, both LCA and TEA are needed to assess the viability of a process. Subsequently, the structure proposed here follows in part the methodological structure of a LCA as presented in ISO standards 14040 and 14044 and the ILCD Handbook. By applying good TEA practice concepts as well as introducing concepts used in LCA, these Guidelines aim to enable systematic and transparent assessment together with better integration of TEA and LCA 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 more reliable comparisons of results between different studies. Consequently, each chapter covers specific techno-economic aspects and, if applicable, how these are linked to LCA principles.

## B.3 Goal Definition

### B.3.1 Introduction to Goal Definition

The first step in 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 in combination then frame all subsequent 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 are not available.

It is important to note that the assessment goal is specific to the individual study and the practitioner's perspective. Even when focusing on the same product system, the assessment goal can vary between studies depending on factors such as the scope and size of the project, technological maturity, the region, and time horizon. For example, when assessing laboratory-scale technologies, the goal for an early research project at a university or company might be to identify general technical viability and overall economic potential. In comparison, 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, 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 while also remaining meaningful, or else the study needs to be discontinued.

### B.3.2 Perspectives and Principles of Assessment Goals

#### B.3.2.1 Introduction

Analysis of the CCU literature shows that comparisons between studies are challenging [2], especially when comparing technologies of varying disciplines, markets, and technological maturity (*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 manner proposed below can appear uncommon for TEAs today; however, this approach is useful as it facilitates comparisons between differing technologies, products, and markets that are necessary for CCU.

#### B.3.2.2 How to Define TEA Goals for CCU

##### B.3.2.2.1 Plausible Process Concepts

First and foremost, all assessments need to be based on process concepts that are technologically plausible. Prior to the assessment, a 'plausibility check' needs to be conducted by the TEA practitioner (*e.g., checking that proposed concepts do not violate the first or second laws of thermodynamics; checking mass and energy balances*). When the plausibility check indicates that process concepts are implausible, the process concept needs to be corrected or the assessment terminated altogether. The latter is sometimes referred to as a 'show stopper.'

#### B.3.2.2.2 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 1). Practitioners **should** state the intended TEA perspective.

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 must first be conducted for each application individually before a comparison can be carried out.

#### B.3.2.2.3 Principles of Goal Definition

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

- The study context, especially comparison to 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 organization, university, company, individual*)
- limitations in usability resulting from assumptions or methods (*e.g., time, location, or specific use cases of the products*)



Table 1. Common TEA perspectives, questions, and goal examples

Common perspectives	Description	Common goal-related questions	Goal examples
<b>R&amp;D-perspective</b>	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	<ul style="list-style-type: none"> <li>▪ What are major cost and value drivers?</li> <li>▪ What product performance characteristics have to be met?</li> <li>▪ What aspects need to be worked on (next)?</li> <li>▪ How does the current development state rank amongst alternatives?</li> <li>▪ Do we fund CCU research and development of project X?</li> </ul>	<ul style="list-style-type: none"> <li>▪ <i>(Scientific) assessment of economic potential of product or technology</i></li> <li>▪ <i>Planning of next R&amp;D steps or priorities</i></li> <li>▪ <i>Decisions on funding program</i></li> </ul>
<b>Corporation-perspective</b>	Analysis of projects in development and deployment; assessment of investment alternatives and comparison to existing processes; use of detailed process data is common	<ul style="list-style-type: none"> <li>▪ How does the CCU product perform against current and upcoming benchmarks?</li> <li>▪ Is the CCU product in a future scenario economically viable?</li> <li>▪ How does the investment in a CCU product deployment / demonstration project / full-scale plant compare to alternatives?</li> </ul>	<ul style="list-style-type: none"> <li>▪ <i>Business case for new CCU plant</i></li> <li>▪ <i>Economic due diligence for investment in CCU start-up</i></li> </ul>
<b>Market-perspective</b>	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	<ul style="list-style-type: none"> <li>▪ What are current states, favorable conditions, best practices, and necessary actions for regional CCU value chains?</li> <li>▪ What regulatory clarification and support (type, timing, and budgets) is required for specific CCU products or services?</li> </ul>	<ul style="list-style-type: none"> <li>▪ <i>Local CO<sub>2</sub> supply chains</i></li> <li>▪ <i>National CO<sub>2</sub> regulations</i></li> <li>▪ <i>Comparing multiple product applications, comparing best resource use of CO<sub>2</sub>, H<sub>2</sub>, electricity</i></li> </ul>

### B.3.2.3 Further Reading

Goal concepts and definitions of LCA are described briefly in the standard ISO 14044:2006 (Environmental management — Life cycle assessment — Principles and framework) [3] and in more detail in the ILCD Handbook [4].

### B.3.2.4 Provisions

Provisions B.1 - Goal Definition	
<b>Shall</b>	1) The study context (especially comparison to what, location, time horizon, scale, and involved partners) shall be stated
	2) The intended application and reasons for the study shall be stated
	3) The target audience for the study shall be stated
	4) The commissioners and authors of the study shall be stated
	5) The limitations in usability resulting from assumptions or methods shall be stated
<b>Should</b>	1) The intended TEA perspectives (R&D, corporation, market) should be stated
<b>May</b>	

## 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 – although not equally likely – states of the world, which represent plausible conditions under different assumptions; whether or not the scenario is plausible depends on the study context. Scenarios and scenario analysis provide a creative and flexible approach to support coordinated decision making that has long-term consequences. The practitioner can design the scenario according to their needs. 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 utilizing scenario analysis, it is important that practitioners analyze and clearly communicate to stakeholders the nature and magnitude of all inherent uncertainties [5], [6].

The starting point of an analysis is often a “base case” scenario, in which current trends are extended into the future (*e.g., absence of carbon pricing*). Additional scenarios to the base case need to test the limits of an unknown future and question the base case scenario (*e.g., the presence of a carbon tax, low-carbon technology subsidies or tax benefits, or a cap and trade scheme with low versus high prices*); the most surprising scenarios can provide insightful information. Various processes for creating scenarios are described in the literature, some of which are presented in the further reading sections (see chapter B.3.3.3). The combination of qualitative and quantitative techniques and close involvement with stakeholders helps to create more robust, diverse, and relevant scenarios. As each new scenario can provide additional insight but also requires additional effort, the literature generally recommends creating three to five scenarios; the final number is subject to the practitioner's judgement. To make more efficient use of

available research time and budgets, practitioners are encouraged to openly report, discuss, and share scenario data [5], [6].

### B.3.3.2 How to Define Scenarios for CCU Assessments

Scenario analysis is a useful approach, since TEA studies support decisions that have long-term implications, especially for CCU products that often require substantial investment. TEA scenarios can either be defined during the initial goal phase or when reaching the interpretation phase at which key data for improvement are identified and the study goal can be refined through further iteration (also see the iterative approach in chapters B.5.2 and B.7.2).

If scenario analysis is applied, all scenarios used for analysis **shall** be distinct and both physically and economically plausible (also see plausible process concepts in B.3.2.2). The scenarios used **should** alter various factors as necessary to account for potential temporal changes (*e.g., analysis of various competing technological developments, consequences of large-scale technological adoptions, different potential states in future markets, regulatory frameworks, and 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. Current, mature technologies shall be included in the base case scenario; however future technologies currently under development can also be included in the base case scenario if documentation is provided on their process design at the current development stage. Scenarios **shall** be developed in consultation with the stakeholders of the study, to ensure they remain relevant to the target audience. Scenario assumptions and data should be made openly accessible in order to facilitate future work. Moreover, scenarios featuring future, clean technologies **should** be considered. The analysis and reporting of uncertainties for each scenario is important and is further described in the interpretation and reporting chapters (see chapters B.7.2 and B.8.2.6).

If TEA and LCA are integrated with high level of data alignment, the same set of scenarios **shall** be used (see chapter A.5). 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 C.9).

### B.3.3.3 Further Reading

Guidance on scenario development and planning can be found in the literature [5]–[7].

## B.3.3.4 Provisions

<b>Provisions B.2 - Assessment Scenarios</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Scenarios used shall be distinct and both physically and economically plausible</li> <li>2) The base case scenario shall serve as a baseline for analysis, extending current trends</li> <li>3) Current, mature technologies shall be included in the base case scenario; however future technologies can be included in the base case scenario if documentation on process design in the current development stage is provided</li> <li>4) Scenarios used shall be developed in interaction with the stakeholders of the study</li> <li>5) If TEA and LCA are integrated with high level of data alignment, the same set of scenarios shall be used</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Scenarios used should factors as necessary to account for potential temporal changes</li> <li>2) Scenario assumptions and data should be provided via 'open access'</li> <li>3) Scenarios featuring future, clean technologies should be considered</li> </ol>
<b>May</b>	

## B.4 Scope Definition

### B.4.1 Introduction to Scope Definition

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. Furthermore, the TEA Guidelines introduce a concept for maturity-based selection of indicators and methods.

The first step of the TEA scope phase is to identify and describe the analyzed product system; the central elements are precise and quantitative description of the function(s) and selection of the comparison metrics in the form of functional units and reference flows. The next step is to specify the analyzed system elements and define system boundaries. This is followed by selecting benchmark systems for comparison. Finally, the technological maturity of the product system will be used to select suitable assessment indicators.

From the assessment scope, the requirements are derived for the inventory phase (for example for data quality) and the reporting phase [3], [4].

CCU-specific challenges with the scope phase are that many CCU products provide similar but non-identical performance to benchmark products (*e.g., in the case of materials, a different molecular structure can lead to different behavior compared to conventional solutions, providing acceptable or possibly even improved performance in certain applications*). This is why, in many cases, CCU researchers and developers try to match the CCU product's performance to existing standards, aiming to achieve 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 fuels, or as electricity storage, thereby requiring cross-sector analysis.

To enable the future integration of TEA and LCA, key terminology will be adopted from ISO 14040 and the ILCD Handbook and further defined in the next chapter.

### B.4.2 Product Application and Functional Units

#### B.4.2.1 Introduction

For the purpose of this document, the term 'product' describes goods, services, events, or combinations thereof. 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 a coating product for exterior walls*). The product system can have one or multiple output flows, also called co-products or by-products.

The term 'function' means to qualitatively and quantitatively specify the analyzed product system (*e.g., production of coating for exterior walls*). To derive the function of the product system, an understanding of the analyzed product is crucial. Therefore, according to the assessment goal, TEA practitioners are required to further define and select one or multiple relevant market applications of the product, meaning the purpose or value proposition (*e.g., the purposes of an external wall coating might be weather protection and long lifespan*). Applications can be specified by market segments (*e.g., products intended for street art versus home renovation*). Hence, the selection of a relevant application forms the basis for defining the function of the analyzed system. Therefore, the TEA Guidelines focus on the concepts used in selecting

relevant applications, which is relatively uncommon in the field of LCA. A detailed description of the concepts common in LCA can be found in the further reading recommendations (see chapter B.4.2.3).

The ‘functional unit’ describes the qualitative and quantitative aspects of the function, to enable valid comparisons between different alternatives, thereby covering information relating to “what,” “how much,” “how well,” and “for how long” (e.g., *decorative coating for home renovation of 1 m<sup>2</sup> outdoor wall, providing 90% opacity over 10 years*). The ‘reference flow’ describes the flow needed to meet the functional unit of the analyzed product system (e.g., *a 25-liter bucket of the analyzed paint product*). It is the flow to which all other input and output flows are set into relation with. Note that for a product system with multiple functions, the functional unit can also have multiple reference flows.

## B.4.2.2 How to Define CCU Product Applications, Functional Units, and Reference Flows

### B.4.2.2.1 CCU Product Applications

In general, to derive a suitable function for the analyzed system the product application **shall** be defined according to the study goal and clearly documented in the assessment report. If one application has been identified, it is important to keep in mind that CCU products can provide additional applications (e.g., *carbonation of mineral slags serves the purpose of waste treatment but also creates aggregates for cement*). Cross-sectoral analysis facilitates 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 a chemical versus a fuel*), following the provisions for each application individually.

For products with a small number of applications, one typical application or a relevant ‘application-mix’ **should** be defined. For example, in the case of CO<sub>2</sub>-based ethanol, either fuel for transportation can be defined as typical application, or the shares of transport modes (light passenger, commercial, and heavy duty) can be defined as the application-mix. If only one of the multiple applications can be carried out at a time (alternative functions), then the inclusion of only one typical application in the assessment is sufficient (e.g., *polyols for flexible or rigid foams; seasonal, grid-scale electricity storage*).

For base chemicals, materials, or other products with a large or even practically indefinite number of applications, or where the application is non-specific (meaning that there are broad uses for a product), 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 the transparency and comparability of the study.

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 specialties*). As corporate-perspective TEAs focus on the needs of customers and users, 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 as essential, desirable, or 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 2.

Table 2. Examples of CCU product applications and market segments (not exhaustive)

CCU class	Chemical products	Material products	Fuels	Energy storage systems
<b>Product application</b>	Methanol for chemical production	Polyols for flexible foams Waste treatment for industrial ash	Fuels for efficient and clean transportation	Delaying energy use and thus decoupling energy supply from demand
<b>Market segment</b>	Chemicals with low carbon footprint	High-quality flexible foams for mattresses Low-quality aggregates for low-cost concrete	Fuels with low NOx/soot emissions for heavy duty vehicles	Seasonal, grid-scale electricity storage

#### B.4.2.2.2 Functional Units and Reference Flows

Similarly to the application, the functional unit **shall** be defined according to the study goal and clearly documented in the assessment report. The functional unit **shall** be defined based on 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 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 that of existing materials; compare performance of new power storage device with different characteristics to that of 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 3.

Table 3. Examples of CCU substitutes, basis for comparison, functional units, and reference flows (not exhaustive)

<b>Properties</b>	<b>Substitutes</b>				<b>Non-substitutes</b>
<b>CCU class</b>	Chemical products	Material products	Fuels	Energy storage systems	All
<b>Basis for comparison</b>	Mass	Material performance	Energy	Storage performance	Service or performance provided
<b>Functional unit</b>	<i>e.g., mass, plant output</i>	<i>e.g., mass, plant output</i>	<i>e.g., energy, mass, plant output</i>	<i>e.g., energy, plant output</i>	Compare performance of new versus existing solutions
<b>Reference flow</b>	<i>e.g., 1 t methanol, 1.6 Mt/a plant output</i>	<i>e.g., 1 t concrete, 50 kt/a plant output</i>	<i>e.g., 1 MJ of H<sub>2</sub>, 2.5 Mt/a diesel output</i>	<i>e.g., storing 1 MJ of electricity, 80 MWh battery</i>	<i>e.g., 1 t, 1 MJ, output of a plant</i>

#### B.4.2.3 Further Reading

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



#### B.4.2.4 Provisions

<b>Provisions B.3 - Definition of Product Systems and Functional Units</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) The product application(s), functional unit, and reference flow shall be defined according to the study goal and shall be stated in the assessment report</li> <li>2) The functional unit shall be defined based on the good judgement of the practitioner following these principles:               <ol style="list-style-type: none"> <li>a. For products with the same structure, composition, or characteristics as benchmark products (substitutes), the functional unit shall be defined on a mass or energy basis</li> <li>b. For products with a structure or characteristics different to benchmark products (non-substitutes), the functional unit shall be derived from the product performance</li> </ol> </li> <li>3) If the TEA study is conducted together with an LCA, the functional unit shall be consistent for both studies</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) The definition of the product application should follow these principles:               <ol style="list-style-type: none"> <li>a. For products with a small number of applications, one typical application or a relevant application-mix should be defined</li> <li>b. For products with a large number of applications, the products itself should serve as the 'application.' In this case, a detailed technical description of the product should also be provided</li> <li>c. The product application should be defined specific to market segments</li> </ol> </li> <li>2) Corporate-perspective TEAs should include a description of at least one customer group and their needs</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Multiple product applications may be assessed and compared against each other, following the provisions for each application individually</li> <li>2) For products with a large number or unspecified applications, the functional unit may describe the output of a plant</li> </ol>

### 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, which can be a process unit, a unit operation, or an item of 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, and various inputs for waste treatment*), the latter are often referred to as multifunctional product systems or as having '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 is 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.

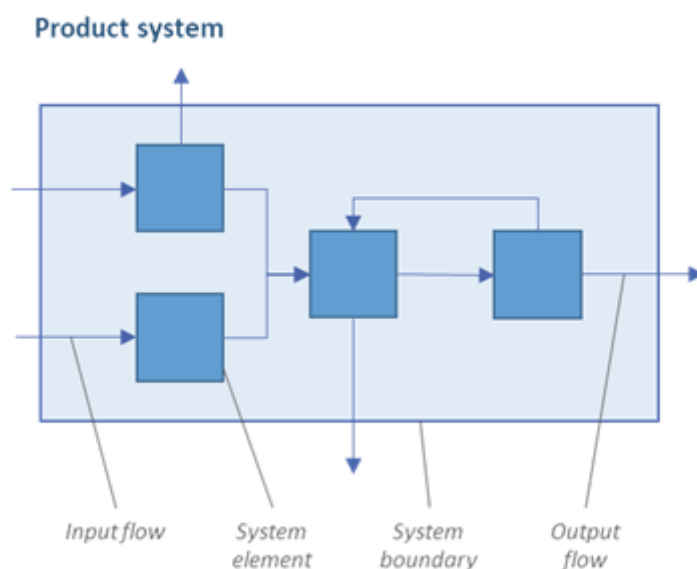


Figure 2. Example product system, showing elements, boundaries, and input & output flows

### B.4.3.2 How to Define Elements and Boundaries for CCU Product Systems

#### B.4.3.2.1 Deriving CCU System Elements

When defining system elements, it is essential to choose an appropriate level of detail. Process units **shall** be used as basis for system elements (*e.g., electrolysis, CO<sub>2</sub> 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*).

Assessments need to be conducted not only for the overall product system as a whole, but also for each system element individually, meaning that each system element **should** serve as the accounting unit for inventory, calculation, interpretation, and reporting. For example, if the product system contains an electrolyzer (system element), the relevant energy and mass flows and cost would be collected, calculated, interpreted, and reported for the individual electrolyzer unit and a break-even cost and operating hours could be calculated.

#### B.4.3.2.2 Deriving CCU System Boundaries

Overall, the system boundaries **shall** be derived from the assessment goal and **shall** be consistent throughout the study. The TEA system boundaries can be derived from two points of view: from the perspective of the study, or 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 system boundaries around the activities of a real or

hypothetical 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 C.4.2.1); in the case of TEA, one could argue that the resource extraction impacts are represented by 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 analyzing the full cost for society, but also the benefits and losses as well as the market power of each player in the value chain. For example, 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 those of benchmark products (non-substitutes), any TEA assessment with gate-to-gate boundaries **should** include price–performance correlations with benchmark products that need to be available in sufficient quality. If these correlations are not available, the boundaries **should** be extended to cradle-to-grave in order to include the impacts from the whole life cycle, which necessitates properly accounting for the technological and economic implications of further processing steps, use, or disposal phases (also see LCA Guideline, chapter C.4.2.1).

While the use of cradle-to-grave boundaries is not currently common practice for TEA, they **may** be used to align a TEA study with an LCA study in case of an integrated assessment. Cradle-to-grave boundaries can also be used if required by a TEA audience or goal. If the practitioner intends to integrate TEA and LCA with a very high degree of data alignment, then identical system boundaries **shall** be defined for both TEA and LCA. This means that if the LCA is set to include CO<sub>2</sub> capture, separation, and transportation (see LCA Guidelines chapter C.4.2), then identical system boundaries are required. Also, in the case of independent TEAs that do not require a high level of data alignment with LCA, practitioners **should** include key CCU processes, such as CO<sub>2</sub> capture, separation, and transport, in the assessment.

With respect to extending the boundaries to cradle-to-grave, another commonly applied tool is life cycle costing (LCC) [9]–[12]. Generally, the significant freedom of methodological approaches in both TEA and LCC makes it impossible to define clear differences among the tools. Depending on the goal and scope of the study, TEA and LCC can be similar in choice of criteria, indicators, methods, and boundaries. For example, both TEA and LCC can adopt a customer, producer, investor, or governmental perspective and can focus on the life cycle of a project or product. Nevertheless, their inherent perspectives found in the literature tend to be different. TEA studies are typically limited to cradle-to-gate boundaries and have an investor focus. This limitation is often required for technologies in research and development stages, as is common for the field of CO<sub>2</sub> utilization. In contrast, LCC is typically intended to cover the full life cycle, thereby showing a strong cost focus, leaving aside not only technical feasibility but also revenue- and profit-related indicators or criteria – the major factors in all business and investment decisions. Recent discussions have examined the question of integrating LCC and LCA, which could be helpful when addressing an integrated techno-economic-environmental assessment study with cradle-to-grave boundaries (see [11], [13]–[15]).

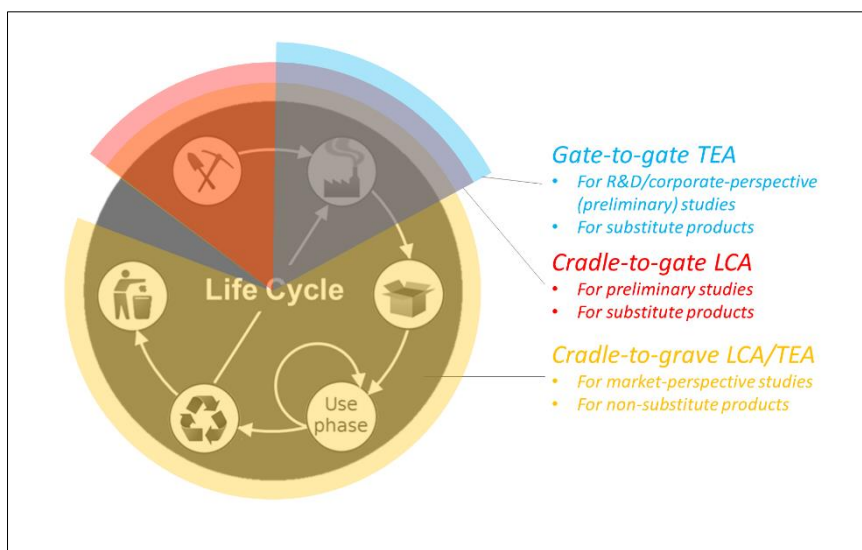


Figure 3. The scope of TEA and LCA in the product life cycle, adapted from [16]

### B.4.3.3 Including or Excluding CCU Upstream Processes in System Boundaries

A common question for CCU product systems is whether to include or exclude CO<sub>2</sub> capture, separation, and transport processes. Other common important upstream processes include H<sub>2</sub> production, electricity production, and many more. For examples, see Table 11 in the Annex (list is not exhaustive).

The decision on whether to include or exclude an upstream or downstream process **shall** be made for each process individually and **shall** not be taken to improve results, but instead based on the assessment goal, material and energy flows, as well as on data requirements, and potentially the audience or stakeholder perspective.

Following the iterative approach utilized in the data collection phase (see chapter B.5.2), it might be that an upstream process is excluded at first, but then added to the process design and techno-economic assessment later, when its 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 are 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<sub>2</sub>, H<sub>2</sub>, or electricity are provided without charge. For example, if CO<sub>2</sub> can be used economically, the gain in value for the CO<sub>2</sub> consumer and the emitter will demand compensation; if CO<sub>2</sub> emissions are fiscally penalized, they create an additional burden for the emitter, and the CO<sub>2</sub> consumer will demand compensation for consumption.

#### B.4.3.3.1 Multifunctional Product Systems

For product systems with multiple functions, the 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. Selecting a suitable approach for solving multifunctionality challenges 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 Guidelines chapter B.5.3.2). A general overview of different approaches for solving data and system boundary issues in case of multifunctionality is presented in the LCA section of these Guidelines (see chapter C.4.3).

#### B.4.3.3.2 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.4.3.4 Further Reading

Principles of Life Cycle Costing in combination with LCA are described by the Society of Environmental Toxicology and Chemistry (SETAC) [14]. Furthermore, a larger number of life cycle costing standards for a range of specific industries have been defined by ISO, DIN, and VDI among others.

### B.4.3.5 Provisions

<b>Provisions B.4 - Definition of System Elements and System Boundaries</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Process units shall be used as the basis for system elements</li> <li>2) The system boundaries shall be derived from the assessment goal and shall be consistent throughout the study</li> <li>3) If TEA and LCA are intended to be integrated with a very high degree of data alignment, then identical system boundaries shall be defined for both TEA and LCA</li> <li>4) The decision on whether to include or exclude a key upstream or downstream process shall be made for each process individually, and key processes shall not be included or excluded to improve results</li> <li>5) If an upstream process is excluded from the final system boundaries the reasoning shall be explained</li> <li>6) Product systems, elements, and boundaries shall be presented in a graphical scheme and specifications for all input flows shall be described</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) System elements should serve as the unit for accounting and recommendations</li> <li>2) For non-substitute products, any gate-to-gate assessment should either include price–performance correlations or the boundaries should be extended to cradle-to-grave to include the impacts from the whole life cycle</li> <li>3) Key CCU processes, such as CO<sub>2</sub> capture, separation, and transport, should be included in the assessment</li> <li>4) For product systems with multiple functions, function dependencies should be taken into account</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) The system elements may be further refined as unit operations or even unit equipment</li> <li>2) In case of an integrated assessment, cradle-to-grave boundaries may be used to align a TEA study with an LCA study</li> </ol>

## B.4.4 Benchmark Product Systems

### B.4.4.1 Introduction

The term ‘benchmark product’ describes products other than the one in focus, which provide 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 to describe a characteristic – preferably a quantitative variable of a benchmark product (here referred to as ‘benchmark value’).

The term ‘substitute’ describes a product that not only fulfills the same application as the benchmark product, but also provides the same performance: substitution therefore requires identical chemical structure and composition for chemical or fuel products, and identical characteristics across different energy storage systems. The term ‘non-substitute’ is used for products that potentially provide the same application but that differ in 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 via thermochemical, electrochemical, biochemical, or photochemical pathways*) and belong either to existing technology regimes (*e.g., CO<sub>2</sub>-based methanol compared to conventionally produced methanol*) or to new ones (*e.g., transport by CCU fuel vehicles compared to transport by battery electric vehicles*). Comprehensive understanding of the product application is essential for identifying and selecting relevant benchmark products (see chapter B.4.2).

Benchmark products (and services) and their benchmark systems **shall** be selected according to application and assessment goal (*e.g., an average-size benchmark system*). 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 to include two promising future material concepts*). Note that if the time horizon of the assessment goal is in the future, then learning curves and improvements have to be included for both the product and the benchmark systems (see chapter B.5.3.2 and B.6.3.2).

### B.4.4.3 Further Reading

Principles and concepts for chemical product design are described in the work of Cussler and Moggridge (2011) [8]. Approaches for segmentation of applications or identification of benchmarks can be found in Saavedra (2016) [17].

### B.4.4.4 Provisions

Provisions B.5 - Definition of Benchmark Systems	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Benchmark products and benchmark systems shall be selected and stated according to the product application and assessment goal</li> <li>2) The currently most common or best-in-class products shall be selected as benchmark products; multiple benchmark products can be included</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Customer needs should be used to identify utility and competitive advantage</li> <li>2) Benchmark products that are likely to become relevant in the future should be included</li> </ol>
<b>May</b>	

## B.4.5 Assessment Indicators

### B.4.5.1 Introduction

In the following, ‘criterion’ refers to a parameter in decision making (*e.g., profitability*), ‘indicator’ refers to a representative measure for a criterion (*e.g., net present value*), and ‘method’ refers to 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 derives 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 per kWh of energy stored, cost per tonne of CO<sub>2</sub> used*). 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 chapter A.5.2.2.

Both internal company and external market views 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 4), 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

#### B.4.5.2.1 Common Indicators for TEAs in CCU

TEA results are difficult to compare as practitioners use indicators of their particular interest, with the result that studies do not have a common indicator basis. This lack of indicator standardization is evident in 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 to evaluating and comparing CCU technologies [2]. Example criteria and indicators are shown in Table 4.



Table 4. Example criteria and indicators

Area	Criterion	Indicator examples
<b>Technical</b>	Energy demand	<i>Heat demand, cooling demand, electricity demand, primary energy demand</i>
	Energy efficiency	<i>Lower heating value efficiency, higher heating value efficiency, energy/exergy efficiency, CO<sub>2</sub> capture penalty</i>
	Mass demand	<i>Mass demand of individual inputs, mass of CO<sub>2</sub> converted</i>
	Mass efficiency	<i>Atom economy, yield, percentage of CO<sub>2</sub> converted</i>
<b>Economic</b>	Processing effort	<i>Operational expenditure (OpEx)</i>
	Investment effort	<i>Capital expenditure (CapEx)</i>
	Product margin	<i>Market-derived margin for product, company-internal margin</i>
	Product volume	<i>Market volume for product, company-internal demand</i>
	Resource availability	<i>Market volume for feedstocks, company-internal availability of resources, number of suppliers</i>
	Profitability	<i>Profit, net present value, internal rate of return</i>
	Profit/cost per functional unit	<i>Cost per kg benchmark product equivalent, cost per km, cost per MJ stored</i>
<b>Techno-economic</b>	Technology maturity	<i>Technology Readiness Level (TRL) regarding market introduction (Horizon 2020 definition), company internal maturity rating</i>

As many TEAs apply TRL, OpEx, and CapEx, using varying definitions and equations for calculation, these three indicators and their methodological approaches are covered in this document (for TRL see section A, chapter A.4, for CapEx and OpEx see chapters 0 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 the experience of the TEA practitioner. An overview of calculation methods can be found in the recommended literature listed in the further reading. Indicators and methods can be selected from the list presented above, or from the pool of indicators used in similar TEA studies.

#### B.4.5.2.2 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. Note that aggregated indicators must be used with caution if they require

normalization and weighting. Weightings reflect subjective choices based on quantitative or qualitative criteria (see chapter B.6.6).

#### *B.4.5.2.3 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 of whether data are 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 and development to deployment phases, various processes and economic data all become 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 increasingly 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 12) in the TEA Guidelines Annex. The use of economic indicators according to the TRL scale from Table 12 is further discussed here. Indicators can either exclude or include changes over time, further called static and dynamic indicators (for example, see chapter B.6.5.2). 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 early research stage, the use of quantitative indicators is not meaningful; instead, qualitative evaluation can be conducted, for example multi-criteria rankings [8], [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 materials and other cost items. In the development phase, the market view is completed with the projected sales volume in order to calculate an absolute profit. Furthermore, the product definition is sufficiently accurate to predict future revenues; dynamic economic indicators can be used. Plant optimizations or changes in capacity planning can be evaluated. 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 through 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 (*e.g.*, *accounting for inflation*). 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 chapters 0 and B.6.4). In the deployment phase, dynamic indicators can be used at an even greater level of detail. Assessments can be refined to provide complex simulations of future economic activities prior to constructing a full-scale plant. At TRL 9, cost and profitability checks are carried out in conventional accounting.

### B.4.5.3 Further Reading

General cost estimates and profitability analysis in the chemical industry are described in the process design literature [18], [21], [22]. The selection of economic indicators in research and development is described in the following papers [20], [23]–[25]. The use of indicators in CCU TEAs is described in the following paper and report [2], [26].

### B.4.5.4 Provisions

<b>Provisions B.6 - Assessment Indicators and Methods</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Selected indicators shall be compliant with the assessment goal</li> <li>2) Selected indicators and calculation methods shall be compliant with data availability, which is associated with technology maturity</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Indicators from both technical and economic fields should be included in the assessment</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Aggregated indicators may be selected but must be used with caution</li> </ol>

## 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], as summarized with minor adaptations in Provisions B.7. These criteria must be met during the scope, inventory, and calculation phases.

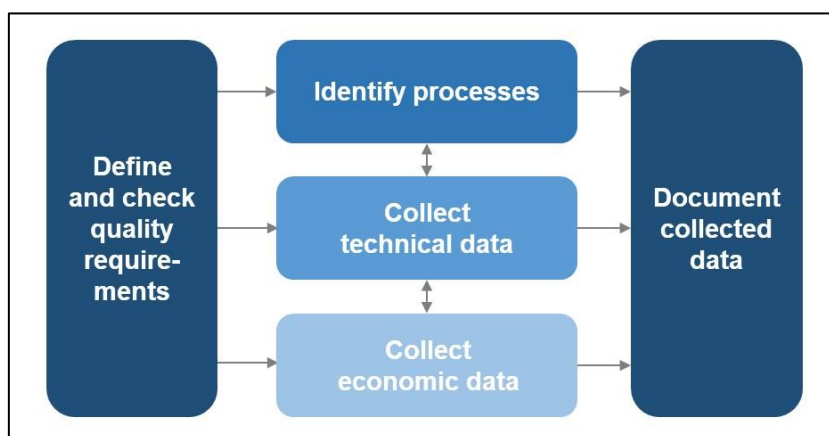
### B.4.6.1 Provisions

Provisions B.7 - Consistency and Reproducibility	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Methods and assumptions shall be applied in a sufficiently consistent way to all processes, parameters, and flows of the analyzed systems, including benchmark systems</li> <li>2) Sufficiently consistent data regarding accuracy, precision, and completeness shall be applied</li> <li>3) Inconsistencies shall be documented. If significant, the inconsistencies shall lead to the adaptation of the goal or shall be taken into account for interpretation and reporting</li> <li>4) All selected methods for calculating indicators shall be described clearly, including why they were chosen</li> <li>5) Methods and method selection shall be documented               <ol style="list-style-type: none"> <li>a) <i>For public reports:</i> in an appropriate and transparent way that would enable another TEA practitioner to sufficiently reproduce the assessment and results</li> <li>b) <i>For confidential reports:</i> in a separate, confidential file that shall be made available to the critical reviewers in confidentiality</li> </ol> </li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) System boundaries, methods, and assumptions should be applied in a sufficiently consistent way so that the results can be related to other studies by another TEA practitioner</li> <li>2) The documentation should begin from the project start; documentation should be guided by reporting needs</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) The assessment may include suggested ways or techniques to avoid pitfalls in assessment procedures</li> </ol>

## B.5 Inventory Analysis

### B.5.1 Introduction to Inventory Analysis

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 are collected, economic data are collected, and data are 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 data quality and detail required for each system element might vary between LCA and TEA as determined by differing goals 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 involved, as will be described in the following chapter B.5.2.3. Deriving economic data for input CO<sub>2</sub> 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 is collected and documented transparently to describe specific conditions of the market, value chain, and their limitations. The description of the specific context is highly important to ensure meaningful comparisons among studies.

## B.5.2 Interim Quality Control and Types of Data

### B.5.2.1 Introduction

Interim quality control helps to ensure consistency and reproducibility in the TEA study (see chapter 0). It is conducted in parallel with data collection and saves time and effort by already verifying during data collection whether the required data quality is achieved. Data quality requirements and principles of data documentation have to be clear before collecting data. Consideration of technology maturity is important for understanding which data are available for TEA or else need to be estimated, depending on 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.

### B.5.2.2 Types of Data and Sources

Different types and sources of data exist that are relevant for TEA, as indicated by the 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 averages (*e.g., published energy use of a real process, material prices from one's own supplier quotes, measured input flows or energy efficiencies, and other technical process data as documented in patents, etc.*)
- **Average data:** data reflecting industry averages on the basis of reported measured data comprising several processes (*e.g., average CO<sub>2</sub> 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 have not been measured from an existing process but are 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 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 are not based on measurements of the respective process (*e.g., via similar patents, process engineering models, data bases, etc.*)

### B.5.2.3 How to Control Data Quality?

#### B.5.2.3.1 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., system elements assessed in high detail at the unit equipment level generally require higher-quality data than when only describing the inputs and outputs of a process unit*).

#### B.5.2.3.2 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 chapter B.7.2). Conducting sensitivity analysis early and in parallel with inventory collection helps ensure that data are collected at sufficiently high quality where needed. Data quality itself can also be evaluated in parallel by conducting uncertainty analysis (see detailed description in chapter B.7.2). The requirements for data quality are defined by goal and scope and are strongly connected to the results of the sensitivity analysis, with high sensitivity generally necessitating high data quality. Therefore, both analyses are helpful for characterizing each parameter along the inventory collection, as is required for the iterative approach explained in the next chapter.

#### B.5.2.3.3 Iterative Approach for Choosing Relevant Data Types and Sources

The practitioner **should** aim to collect all relevant available data, the extent of which generally increases with technology maturity. Multiple iterations of data collection **should** be conducted in order to reduce the overall effort by helping to identify and increase the quality of significant data points (*e.g., focusing on data that make a large quantitative contribution to the TEA results as identified by sensitivity analysis, also see B.7.2.2 and Figure 9*).

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, initially allowing the inclusion of low-quality data with the goal of subsequently identifying those data points that make a high quantitative contribution. In the second and following iterations, the quality requirements and collection effort for these data points are increased (*e.g., to check the sensitivity of a CCU polymer TEA to propylene oxide as an input, a price obtained from open Internet platforms could provide an appropriate indication; in the case of high sensitivity, a second price could be obtained from a commercial price data base; thirdly, 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 be unable to answer the questions posed in the goal. Thus, the 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 these data increasingly represent 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 readily available secondary sources might be sufficiently representative in the first iteration of data collection to identify significant data points (*e.g., CO<sub>2</sub> capture cost or H<sub>2</sub> production cost derived from published studies on similar processes, methanol cost from data bases reflecting industry averages, experience-based estimates, etc.*).
- Average or generic data from secondary sources might be sufficiently specific for system elements that are not core elements of the process development (*e.g., processes 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 periods of 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 of high quality regarding a specific, novel production process; however these technology-specific price data might not be representative for your scenario if an average across multiple suppliers or mature technologies has to be accounted for*)

#### B.5.2.4 Data Availability as a Challenge in Data Collection

The technology maturity of a product system gives an indication of whether certain data points can be collected directly at high quality or else need to be estimated. Incomplete data sets need to be sufficiently completed by means of estimation before they 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., during the research and development phases, specific data on process design and related costs are unlikely to be available; cost estimation methods enable the practitioner to fill data gaps in order to estimate the cost for a full-scale plant, which can further be distinguished between first of a kind, not including learning curves versus nth of a kind, including learning curves*). Applying suitable cost estimation methods at early technology maturity poses a major challenge. A general overview of cost estimation methods and harmonization approaches required for calculation of TEA indicators is presented in chapter B.6. Furthermore, estimation methods to bridge technical data gaps can be found in the LCA section of the Guidelines (see chapter C.5.2).

#### B.5.2.5 Confidentiality as a Challenge in Data Collection

Particularly in academic TEAs, practitioners face the problem of acquiring cost and market price data that are confidential to the technology providers or users, thus often resulting in incomplete data sets. Additionally, even when industrial performance data and cost data are published, the underlying assumptions are often not clearly stated. This causes problems of transparency and credibility for TEA practitioners, especially for more mature technologies. Practitioners **shall** clearly state any problems encountered in acquiring confidential data.

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 to ensure anonymity
- Providing relative relationships between data points rather than absolute data values in the TEA report
- Collection, anonymization, and provision of data by a trustworthy third party
- Selected exchange or publication of basic results for industrial process design and simulations

#### B.5.2.6 Further Reading

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



## B.5.2.7 Provisions

<b>Provisions B.8 - Interim Quality Control and Approximations</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Quality requirements shall be defined for each collected data set according to the assessment goal</li> <li>2) Data quality shall be checked and documented during data collection</li> <li>3) Problems encountered in acquiring confidential data shall be clearly stated</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Data available at the corresponding technology maturity should be collected</li> <li>2) Multiple iterations of data collection should be conducted in order to reduce the overall effort by helping to identify and increase the quality of significant data points; In each iteration, data types and sources should be chosen according to quality requirements</li> <li>3) If data quality cannot be improved to a satisfactory level, either the goal and scope should be adjusted or the study should be discontinued</li> <li>4) Process-specific and primary data should be used with increasing maturity of the assessed process</li> <li>5) Readily available generic or average data should be used from secondary sources where sufficiently representative</li> </ol>
<b>May</b>	

## B.5.3 Collecting Data

## B.5.3.1 Introduction

The collection of technical and economic data can be done in parallel or in consecutive steps. Economic information in the form of costs and prices is 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 as well as individual system elements. This means that by conducting a thorough TEA including sensitivity analysis, the potential for improvement of individual system elements can be identified, which is then fed back into the process design for further development. A scenario analysis can serve to evaluate the potential overall economic impact of identified future technological improvements.

### B.5.3.2 How to Collect Data in CCU Projects

Practitioners **shall** plan and prepare data collection according to the data requirements, selected methods and indicators, and overall assessment goal. Technical data are obtained from the process design; the level of detail **shall** follow the identified system elements (*e.g., material, energy, and 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 their technical parameters are essential parts of technical data collection (see chapter 0).

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., suppliers' price quotes for a reactor vessel, country-specific salaries from public or proprietary data bases, sales platforms, cost of high-pressure steam based on expert estimates, literature values from similar published processes, etc.*). The acquisition of input prices and especially equipment prices can involve non-standardized names, requiring the practitioner to thoroughly understand the process design in order to identify the correct prices (*e.g., different names for the same items or the same name for different items*). Other economic parameters relevant to the cost estimation of a projected plant are highly dependent on the specific scenario (*e.g., considering how cost data might differ between the original location and that of the studied scenario*). An example list of such parameters can be found in chapter B.5.6.2. A more detailed explanation of the use and application of important economic parameters can be found in chapter B.6 on the calculation of indicators. 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 greater certainty of particular parameters is required. Note, that prices for material and energy flows can vary substantially depending on where these are sourced from. In the case of highly integrated plant infrastructure, company internal prices might be relevant; in other cases, average market prices serve as a good estimate. However, in general, there are no free feedstocks, and therefore costs of some kind must be accounted for.

When collecting technical and economic data from different sources, practitioners **should** carry out harmonization, which means maintaining uniformity and aligning assumptions. For technical data this may entail, for example, persisting with the choice of higher or lower heating value; In the case of economic data, this may entail averaging price fluctuations including inflation, or adapting data to the same year for comparative purposes.

### B.5.3.3 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 in production plant equipment, engineering costs, 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 the potential cost data for a planned plant, where real data are not yet available. The choice of the cost estimation method depends on data availability and the requirements of the analysis. 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 0 and B.6.4.

#### *B.5.3.3.1 Adapting Data Quality and Data Sources to Technology Maturity*

Practitioners **should** adapt the quality of price data and the number of data sources to technology maturity. In the early research and development stage, market-average price data **should** be used (*e.g., from a commercial market study based on multiple sources or even multiple studies*); typically, the inclusion of a few secondary data sources will meet the data requirements at this stage of the analysis. In the development stage, experts **should** include market-average price data that are date- and location-specific; typically, secondary sources are still sufficient, but multiple sources need to be included. In the deployment stage, practitioners **should** use process-specific data and primary sources.

#### *B.5.3.3.2 Sales Prices and Market*

Besides collecting cost data from a process plant perspective, the estimation of sales prices and market volumes are essential for understanding profitability. Market analysis can become necessary not only for main products, but also for other inputs and outputs of product systems (*e.g., if their small market volume becomes limiting to large-scale implementation*). Sales prices and market volumes are derived from market analyses 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 are rarely static but instead subject to certain dynamics that must be analyzed to understand the profitability of new processes. Hence, a statement is required on whether an average price or specific prices are selected. The sales price of substitutes can be derived from price 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 those of benchmark products. However, estimating the market volume for non-substitutes can be challenging. The market volumes of any known benchmark product can be used to derive those of non-substitutes. Further limitations, such as target market locations (*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 included to refine the estimation of market volumes.

#### *B.5.3.3.3 Potential Sources of Secondary Cost-Data*

Table 5 lists some public and restricted sources for statistical and industrial cost data. Commonly, information from a variety of sources must be combined in order to achieve the desired data point.

Table 5. Selected sources of primary and secondary cost-data

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

#### B.5.3.4 Description of Technical and Economic Context

A purely generic TEA, not focusing on specific market conditions, might produce unrepresentative results. Therefore, practitioners **shall** describe the temporal and regional context of the study (*e.g., value chain characteristics*) as well as their related limitations and risks. Furthermore, practitioners **shall** justify context-specific assumptions and parameters (*e.g., regional requirements and restrictions; supply chain mechanisms and availability; time frame, scale, and production capacity; availability of required investment, etc.*). This description is crucial for the collection of meaningful economic inventory with respect to the predefined scope of the study (see chapter B.4).

An assessment **should** be conducted of whether sufficient access to the local value chain for both input material and 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 in order to prevent underestimates of given limitations. Besides project-specific risks regarding feedstock, regulatory frameworks can also differ markedly between locations, thereby impacting the feasibility of the TEA project (*e.g., subsidies on feedstock, taxes, site regulations, etc.*).

##### B.5.3.4.1 Multifunctionality

Product systems can have multiple inputs or outputs, leading to a case of “multifunctionality,” which is especially challenging when comparing product systems with different outputs. How to address multifunctionality in TEA depends on the goal and perspective of the study. A general overview of the different concepts for solving multifunctionality is presented in the LCA Guidelines (see chapter C.4.3) as well as in Part A (see chapter A.5).

Even in the case of a multifunctional product system it is common practice in TEA to calculate indicators for the whole product system without explicitly presenting indicators for individual products (*e.g., the overall economic feasibility of the project is assessed rather than attempting to present each function's individual*

*contribution to the final result*). However, for some TEA studies, especially with a corporate perspective, the allocation of costs to each product function might be a key question. A common allocation approach for TEA is economic allocation. This means that the full cost of the studied product system can be allocated to each function after deriving each product value, based either on external sales prices from markets 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 gas sales prices*). However, economic allocation is challenging in cases of highly uncertain prices and therefore requires careful consideration (*e.g., for intermediates without specific market value, for non-substitute products, or for novel future products and processes*).

If a TEA study is conducted together with an LCA study and integration of both studies is aimed for, the required level of data alignment between the two studies needs to be defined. If the required level of data alignment is very high, then the multifunctionality approach **shall** be identical for TEA and LCA. If the integrated assessment only requires a low level of data alignment, then the multifunctionality approach for TEA can be selected independently from LCA, meaning that, for example, allocation in TEA can follow any principle that ensures meaningful results for the particular product system.

#### *B.5.3.4.2 Deriving Flow Prices*

For economic data in the inventory model, prices play a crucial role. It is necessary to derive prices for all input flows, meaning any material and energy flows that enter the system boundaries. Furthermore, to compare the results with other existing studies, it might be of interest to derive a price of a flow between system elements (*e.g., internal cost of CO<sub>2</sub> capture, internal cost of hydrogen electrolysis*).

Deriving flow prices, in general, depends on three, consecutive factors: technical specifications, assessment boundaries, and location (see Figure 5). First, practitioners **shall** match the technical specifications of the input flow to the requirements of the product system, such as in quantity, quality, and development over time. If the flow does not meet these requirements, practitioners need to revise the flow source or production technology, modify the system boundary, or change the system elements. For example, if an input flow does not reach the purity required by the product system, a purification step could be added to the product system. Second, practitioners **shall** then derive flow prices according to whether the source, production, or additional handling steps – such as purification, compression, or heating – of a flow are included or excluded by the system boundaries. In the example given above, experts need to account for the added purification step in the assessment. Note that if practitioners decide to include source, production, and handling in the assessment, the discussed flow does not cross the system boundaries and is not an input to the product system but instead flows between system elements; nevertheless, deriving a price for such a flow might be of interest. Third, practitioners **shall** further derive flow prices according to whether specific locations are defined for the input source, transportation, and storage. In the example above, production might occur within the same industrial park, and experts could therefore include a simple cost of transportation by pipeline. When the prices for input flows cannot be derived, practitioners could redefine the goal via an iterative approach. This approach was first presented in [28].

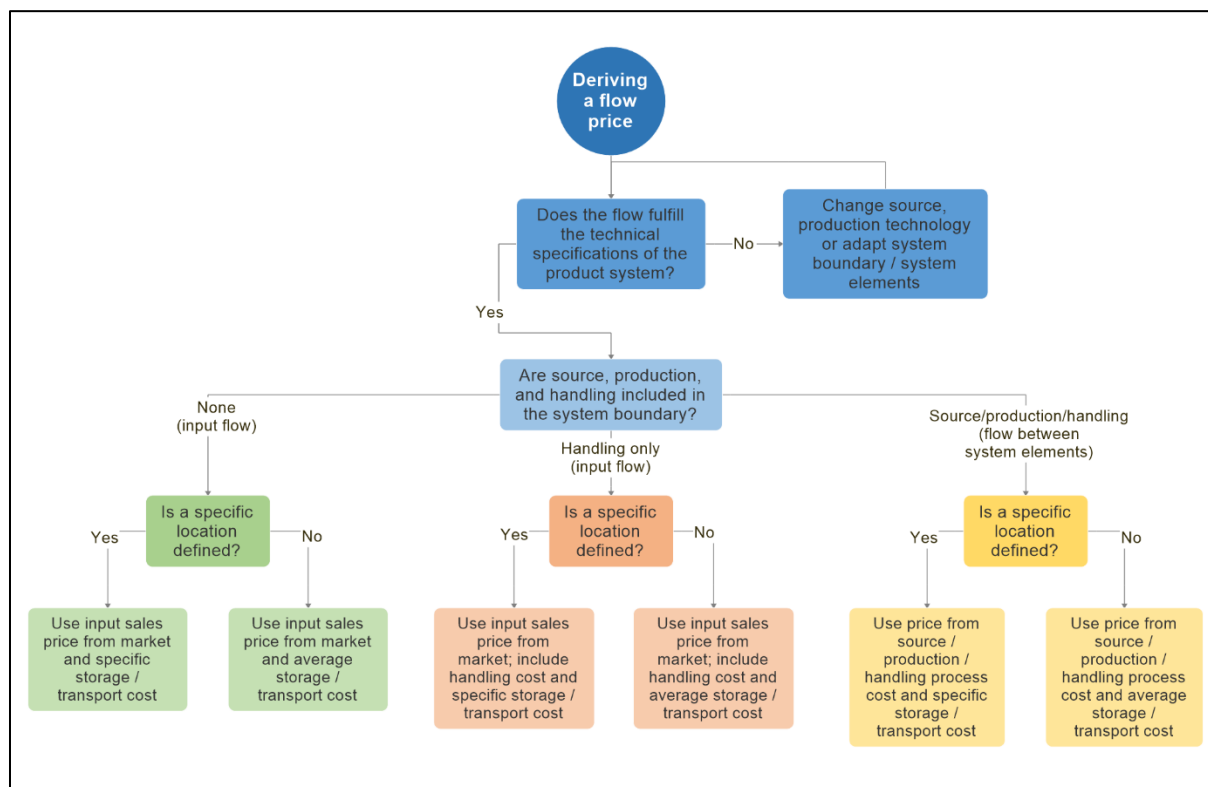


Figure 5. Deriving a flow price (as published in [28])

### B.5.3.5 Further Reading

Additional information on types and acquisition of technical data from process design as well as widely accepted methods for acquiring economic data can be found in the literature on process design [18], [21], [22], [27].

## B.5.3.6 Provisions

<b>Provisions B.9 - Collecting Data</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Data collection shall be planned and prepared according to data requirements, selected methods and indicators, and overall assessment goal</li> <li>2) The level of detail of the technical data shall follow the identified processes along the system elements</li> <li>3) The temporal and geographic context as well as their related limitations and risks shall be described, and context-specific assumptions and parameters shall be justified</li> <li>4) If both LCA and TEA studies are integrated and the goal of the integrated assessment requires a very high level of data alignment between TEA and LCA, then the same method for solving multifunctionality shall be applied, else the method can be selected independently from LCA</li> <li>5) Three consecutive factors shall be considered when deriving flow prices: <ol style="list-style-type: none"> <li>a. Technical specifications: the technical specifications of the input flows shall match the requirements of the product system</li> <li>b. System boundaries: the flow price shall then be derived according to whether the source, production, or additional handling steps of a flow are included or excluded by the system boundaries</li> <li>c. Location: flow prices shall be further derived according to whether specific locations are defined for input source, transportation, and storage</li> </ol> </li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) When collecting technical and economic data from different sources, harmonization should be carried out, which means maintaining uniformity and aligning assumptions</li> <li>2) The quality of price data and the number of data sources should be adapted to technology maturity: <ol style="list-style-type: none"> <li>a. In the early research and development stage, market-average price data should be used</li> <li>b. In the development stage, market-average price data that are date- and location-specific should be included</li> <li>c. In the deployment stage, process-specific data and primary sources should be used</li> </ol> </li> <li>3) Accessibility to the local value chain for both input material and product sales should be assessed</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Regions or addressable market segments or market growth rates may be included to refine the estimation of market volumes</li> </ol>

## B.5.4 Deriving a CO<sub>2</sub> Price

### B.5.4.1 Introduction

For many CCU-TEA studies, the price of CO<sub>2</sub> is a decisive factor for profitability, which is why calculation or estimation of CO<sub>2</sub> prices needs to be planned and executed carefully. Different approaches for deriving CO<sub>2</sub> price are reported in the literature, calling for clear documentation regarding CO<sub>2</sub> sources and purity, cost type, and any dependencies on location and regulation.

Typical pitfalls that TEA practitioners need to avoid when selecting CO<sub>2</sub> prices in TEA of CCU include:

- Assuming zero cost for CO<sub>2</sub>
- Assuming emission trading price or emissions tax as CO<sub>2</sub> price
- Assuming greenhouse gas abatement cost instead of CO<sub>2</sub> capture cost (see following paragraph)

### B.5.4.2 CO<sub>2</sub> Capture Cost and Greenhouse Gas Abatement Cost

In the following, the terms CO<sub>2</sub> capture cost and greenhouse gas (GHG) abatement cost are discussed in more detail. The amount of CO<sub>2</sub> captured states the amount of CO<sub>2</sub> emissions that is separated and available for further processing in a plant equipped with CO<sub>2</sub> capture technology. CO<sub>2</sub> capture cost (or cost of CO<sub>2</sub> captured) relates all resulting costs of the process to the amount of CO<sub>2</sub> captured (*e.g., cost/tCO<sub>2</sub> captured*). The costs include all operational and capital expenditures of capturing CO<sub>2</sub> from flue gas or air over the whole lifetime of the unit.

In contrast, the amount of GHG abated states the difference in overall greenhouse gas emissions, measured in CO<sub>2</sub> equivalents, between a system with CO<sub>2</sub> capture and the benchmark system without CO<sub>2</sub> capture, including the additional GHG emissions caused by the capture process, transportation, and potentially storage or production processes. 'Greenhouse gas abatement cost' relates all resulting costs of the capture, transport, and storage or production processes to the greenhouse gas emissions abated in CO<sub>2</sub> equivalents (*e.g., cost/tCO<sub>2e</sub> abated*). GHG abatement cost is a widely used measure from the field of CO<sub>2</sub> capture and storage (CCS). Note that the capture and benchmark plant both provide the same functional unit, for example the amount of product. In the literature, the emission impacts of transport and storage are often excluded [29]. However, the IPCC recommends the calculation for the full system, including capture, transport, and storage. In the case of CCU systems this full approach increases assessment complexity, as both the CCU system and the benchmark system would have to include the corresponding production processes for the desired product within the system boundaries. As defined by LCA (see chapter C.4.3), system expansion would therefore be required, adding the benchmark process of the CO<sub>2</sub> utilization process to the overall benchmark system. The two ways of reporting GHG abatement cost (capture only or full system) usually result in different values. Hence, the practitioner is required to carefully analyze any information found on GHG abatement cost.

Generally, GHG abatement cost tends to be higher than CO<sub>2</sub> capture cost because capture requires additional plants and energy, leading to increased emissions and thereby decreasing the potential reduction in emissions [30]. To obtain results for overall GHG emissions, a life cycle assessment approach is required, thereby underlining the strong linkage between LCA and TEA. The use of GHG abatement cost as a combined enviro-economic indicator is further explained in the Wrapping Document, part A.



### B.5.4.3 How to Derive a CO<sub>2</sub> Price

The CO<sub>2</sub> price and its calculation or estimation strongly depend on the system elements in the product system, meaning whether CO<sub>2</sub> source, capture process, purification, compression, or transport are included or excluded from the assessment boundaries. If the CO<sub>2</sub> capture process is included in the system boundaries, the CO<sub>2</sub> capture cost needs to be calculated by estimating the required capital and operational expenditures of the system elements associated with capture, purification, compression, and transport. Otherwise, a suitable market price for CO<sub>2</sub> must to be assumed (see Figure 5 and chapter B.5.3.2). In order to find a suitable market price, it is recommended to consider nearby plants that have adequate CO<sub>2</sub> emission streams and to consider average costs for capturing and compressing CO<sub>2</sub> at these plants as well as transporting the CO<sub>2</sub>. In the case of high-purity CO<sub>2</sub> streams ready for use, capture is not relevant and instead compression and transport are the cost drivers. Note that commercial price quotes for CO<sub>2</sub> from industrial gas businesses can be used as conservative indications of the upper price limit only where no information on capture cost is available. Practitioners **shall** report the CO<sub>2</sub> capture cost; if such information is unavailable, an explanatory statement **shall** be included.

### B.5.4.4 Deriving CO<sub>2</sub> Costs from the Literature

Generally, when considering published data on CO<sub>2</sub> costs, careful consideration of all underlying technological constraints and assumptions made in the original publication is required, documenting non-transparent or missing information (*e.g., original assumptions regarding type and source of energy, statements on whether costs of capture are for a single system element or the full process, etc.*). Valuable information on CO<sub>2</sub> cost can be obtained from studies in the academic literature as well as industrial and public sources. Depending on the scope of the TEA, reports on specific emission sources and capture technologies or aggregated reviews across multiple studies can be useful to estimate average costs. Information from renowned (inter-)governmental or industrial organizations dealing with climate issues is relevant for filling data gaps and validating any estimated data. Furthermore, such literature is more likely to be updated at regular intervals, thus providing information on how technology classes have matured in terms of cost performance. Information on current and future political instruments relevant for CCU technologies is also discussed in the abovementioned sources as well as in governmental media such as reports provided by political bodies.

When investigating the literature on CO<sub>2</sub> cost data, it would help practitioners to review the research on both carbon capture and utilization (CCU) and carbon capture and storage (CCS). Note that in the literature both CO<sub>2</sub> capture cost and greenhouse gas abatement cost could be reported. Recommendations on how to deal with each cost type are provided in a dedicated paragraph further below. The following sources are recommended for obtaining cost data:

- Academic literature studies on CCU and CCS:
  - Specific technology studies: Increasingly providing detailed data on CO<sub>2</sub> costs specific to CO<sub>2</sub> emission source, capture technology, time frame, and location
  - Literature reviews: Listing, analyzing, and comparing reported data on CO<sub>2</sub> costs from specific technology studies and studies on policy aspects effecting cost
  - Scientific conference and workshop contributions: Recent or previously unpublished data are potentially introduced at scientific conferences or in reports on 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*)
  - EU Zero Emissions Platform (*e.g., The Costs of CO<sub>2</sub> Capture report*)
  - US National Energy Technology Laboratory (*e.g., carbon storage publications*)
  - United Nations Industrial Development Organization (*e.g., CCS – Roadmap*)
  - Other CCU-based research projects and platforms

#### B.5.4.5 CO<sub>2</sub> Emission Sources and Costs

CO<sub>2</sub> cost generally differs depending on the selected CO<sub>2</sub> source, due to differing CO<sub>2</sub> purity and the 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<sub>2</sub> streams as an input, others can utilize less pure CO<sub>2</sub> streams. Since purification requires additional efforts and has important impacts on costs, practitioners **should** select a CO<sub>2</sub> source by considering the lowest purity and level of compression that is technically required by process, and by considering the associated transportation requirements.

Many industrial CO<sub>2</sub>-emitting sources exist, such as power stations and plants producing cement, steel, or ammonia (see Table 6). Depending on sector and time, as well as capture technology and final stream purity, reported CO<sub>2</sub> capture costs range between 5 USD and 180 USD per tonne of CO<sub>2</sub>, or even higher for some sectors [29]–[32]. The open access EU Eurostats Prodcom database reports an average EU-28 market value for CO<sub>2</sub> of 0.078 Euros per kg of CO<sub>2</sub> 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) [33]. Any technology-specific cost data presented in this document would rapidly become outdated due to technological advances. However, technology-specific literature and review studies provide information on cost ranges for orientation. Practitioners **should** check and harmonize selected cost data or cost ranges from the literature to ensure the use of appropriate units, base years, scales, etc. A selection of the most common CO<sub>2</sub> sources is presented in Table 6.

Table 6. The range of CO<sub>2</sub> emitters in various sectors potentially providing CO<sub>2</sub> streams of differing purity

CO <sub>2</sub> emission 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
Aluminum production
Pulp and paper

If the goal and scope of the study define a certain location then a location-specific CO<sub>2</sub> price needs to be derived, otherwise a location-average CO<sub>2</sub> price is sufficient (see Figure 5 and B.5.3.2). Location-specific CO<sub>2</sub> prices are usually relevant for product systems including the source type, capture, and transport of CO<sub>2</sub> within the system boundaries, thus requiring data on locally available CO<sub>2</sub> emission sources. Location-average CO<sub>2</sub> prices are usually relevant for product systems excluding the specific source, capture process, and transport of CO<sub>2</sub> from system boundaries, thus requiring data on averaged CO<sub>2</sub> cost from regionally relevant sources with average assumptions about transport costs.

Practitioners **should** investigate the local proximity of the CO<sub>2</sub> source to the investigated utilization plant in relation to transport costs. In most cases the transportation of CO<sub>2</sub> is relatively costly, especially if there is no dedicated infrastructure, such as a pipeline system, in place. CO<sub>2</sub> transport cost will most likely decrease with closer proximity of the capture location to the utilization plant.

#### B.5.4.6 Regulation and CO<sub>2</sub> Price

As introduced in chapter B.5.4.1, the price for CO<sub>2</sub> flow cannot be derived based on prices of CO<sub>2</sub> emission certificates or taxes. Nevertheless, it is recommended that practitioners investigate the influences of regulations for CO<sub>2</sub> emission, as the regulatory framework can affect the overall revenues of analyzed CCU projects. In other words, they can play a crucial role in determining the economic feasibility of a given project.

As far as current regulations on CO<sub>2</sub> emissions are concerned (*e.g., emission-trading-systems (ETS), renewable energy directive RED II, 45Q, Low-Carbon Fuel Standard, etc.*), they are all region-specific and employ differing policy mechanisms from each other. Moreover, the regulations are subject to various factors and likely to change over time. Hence, for TEA studies, regulations need to be considered in accordance with specific scenarios and therefore no general guidelines can be given here. Also, it is recommended to exclude regulations on CO<sub>2</sub> emissions from base case scenarios, thereby maintaining the

comparability of different TEA studies on CCU. Instead, practitioners are encouraged to check the impacts of relevant regulations in additional scenarios and by means of sensitivity and uncertainty analyses.

Before practitioners decide to include any CO<sub>2</sub> emission regulations in TEA studies for CCU projects, great attention needs to be paid to the focuses of current regulations. Many regulations focus on CCS and thus often see CO<sub>2</sub> storage as an integral part in financing incentives (*e.g.*, ETS). Consequently, it is unclear to what extent CO<sub>2</sub> emissions transferred to CCU installations are deductible, thereby making these regulations inapplicable to some CCU projects. Nonetheless, as CCU schemes attract increasing attention in recent years, calls have emerged to develop criteria that can expand the applicability and improve the integrity of CO<sub>2</sub> emission regulations. For instance, in an unprecedented ruling the European Court of Justice determined that calcination emissions can be deducted for their use in precipitated calcium carbonate production, making it essentially eligible for ETS. In response, revisions to ETS have been under review. In summary: the inclusion of CO<sub>2</sub> emission regulations in TEA requires practitioners to have detailed insights into the various current policy mechanisms and even their potential future changes.

#### B.5.4.7 Steps for Documenting the CO<sub>2</sub> Price

As described above, the boundaries defined during the goal and scope phases indicate whether data need to be derived from process development or from literature reports on emission sources and resulting CO<sub>2</sub> capture costs. In the case of literature values, it is not recommended to base the choice of emission source on the lowest CO<sub>2</sub> price available without critically reviewing the underlying sources and capture processes, as these might cause higher environmental burdens compared to alternatives. In the case of reported CO<sub>2</sub> cost ranges for a specific source or capture technology, analysis is required regarding the harmonization of underlying values and development state of reported technologies. For scenarios other than the base case the CO<sub>2</sub> price **may** be approximated by greenhouse gas abatement cost or else **may** be adjusted by regulatory mechanisms such as emissions trading, emissions taxes, or other CO<sub>2</sub>-related subsidies or penalties.

The following underlying technological and economic assumptions **shall** be documented:

- Technologies: capture, compression, transport, and storage concepts; CO<sub>2</sub> concentrations, flow rates, flow conditions
- Prices: process-specific or average cost of CO<sub>2</sub> capture
- Limitations: regional restrictions, reference year, and applied transformation factors

#### B.5.4.8 Further Reading

An overview of CO<sub>2</sub> emission sources and reported CO<sub>2</sub> capture and GHG abatement costs is provided in [30]–[32]. There is an extensive published literature on carbon capture technologies. Overviews of available and emerging capture technologies are provided in [34]–[37].

### B.5.4.9 Provisions

Provisions B.10 - Deriving a CO <sub>2</sub> Price	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) CO<sub>2</sub> capture cost shall be reported; if such information is unavailable, an explanatory statement shall be included</li> <li>2) Technological and economic assumptions shall be documented</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) The CO<sub>2</sub> source should be selected by considering CO<sub>2</sub> at the lowest purity and level of compression that is technically required by the process, and by the associated transportation requirements</li> <li>2) Selected cost data or cost ranges from the literature should be checked and harmonized to ensure the use of appropriate units, base years, scales, etc.</li> <li>3) Local proximity of the CO<sub>2</sub> source to the utilization plant should be investigated in relation to transport costs</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Regulatory adjustments (e.g., ETS) or cost-lowering mechanisms may be applied in additional scenarios except in the base case</li> </ol>

## 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<sub>2</sub>, which will partly be introduced in the following chapters. Some typical CCU key inputs are electricity, hydrogen, mineral sources, fly ash, catalysts, fossil hydrocarbons, together with microorganisms and culture media for bioconversion. There is no ranking of importance among the described inputs, as the practitioner compiles the inventory according to the underlying process design and required data quality. Deriving prices for these flows depends on the three factors mentioned in chapter B.5.3.2: technical specifications, assessment boundaries, and location.

### 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<sub>2</sub> is a decisive factor for profitability, which is why calculation or estimation of H<sub>2</sub> prices needs to be planned and executed carefully. Being strongly connected to energy input, H<sub>2</sub> generation can have both substantial economic and environmental impacts.

Typical pitfalls the TEA practitioner needs to avoid when deriving H<sub>2</sub> prices in TEA of CCU include:

- Unintentionally selecting an inexpensive hydrogen source that, in practice, has severe impacts in the life cycle assessment, resulting in increased overall CO<sub>2</sub> emissions in the CCU process
- Assuming free or negative electricity prices in the base case scenario
- Assuming H<sub>2</sub> from intermittent (dynamic) electricity sources without considering the impacts on technological feasibility or economic potential (*e.g., OpEx versus CapEx trade-off at different loads*)

- Assuming H<sub>2</sub> production scales for particular technologies that are economically or technologically unfeasible
- Assuming an optimistic future scenario of H<sub>2</sub> generation as the base case

#### B.5.5.2.1 Present and Future H<sub>2</sub> Generation Routes

Hydrogen is an essential input for the chemical and petrochemical sectors, and can be produced by various processes, currently mainly from fossil raw materials. Production costs and therefore also H<sub>2</sub> price differ significantly between production processes. Depending on the regional concentration of industrial sites, hydrogen production can either be located on-site or off-site. The user can produce hydrogen on-site for direct application, either in dedicated plants as captive H<sub>2</sub> or as a byproduct of other processes. So-called ‘merchant’ H<sub>2</sub> is produced off-site by a commercial H<sub>2</sub> supplier. An overview of current and future H<sub>2</sub> production technologies and estimated production costs can be found in technology roadmaps such as those provided by the International Energy Agency (IEA) [38]–[40]. The current predominant H<sub>2</sub> generation processes are listed in Table 7.

**Table 7. Present hydrogen generation routes and global market shares (2014)**

H <sub>2</sub> generation route	Global market share 2014 [38]	Market
Large-scale steam-methane reforming (SMR)	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 [39]–[41]:

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

The energy required for producing H<sub>2</sub> (calculated from the heat of formation) from fossil sources, biomass, or water differs considerably, being much lower for hydrocarbons than that for water electrolysis [42]. This makes energy requirements 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. This does not take into account the level of environmental pollution caused by these technologies, making it crucial to consider environmentally friendly alternatives as H<sub>2</sub> sources.

Besides local feedstock and electricity prices, the 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<sub>2</sub> source and given the infrastructure at CCU plant, additional transport and storage costs also need to be considered.

#### B.5.5.2.2 Steps for Deriving the H<sub>2</sub> Price

In this document, no specific prices for hydrogen will be stated, as such data rapidly become outdated due to technological advances and dependence on fluctuating input prices. Chapter B.5.5.6 provides references to publications providing cost information for H<sub>2</sub> production technologies.

Similar to the CO<sub>2</sub> price, the H<sub>2</sub> price needs to represent cost of production or a market price. It is of considerable importance to consider transportation and storage of H<sub>2</sub>, as the energy required for compression and the safety requirements for storage need to be reflected in the attributed costs. H<sub>2</sub> production and related processes (e.g., separation, transport, and storage) can be included in system boundaries if economically significant (e.g., in case of large demand for merchant hydrogen from off-site production). An analysis of local conditions is necessary to adequately provide information about prices, especially in relation to the regulatory framework and the availability of the feedstocks required for the multiple potential production technologies.

- If H<sub>2</sub> production is included within system boundaries, the H<sub>2</sub> price need to be calculated based on the full location-specific process
- If H<sub>2</sub> production is excluded from system boundaries, the H<sub>2</sub> price need to be collected either from a supplier quote or a location-average estimate specific to the production route
- H<sub>2</sub> transport and storage need to be represented in the H<sub>2</sub> price, independent of their inclusion within system boundaries

In accordance with Guideline B.2, for the base case scenario, a current, mature H<sub>2</sub> generation process needs to be selected. In additional scenarios, future, low-carbon-footprint H<sub>2</sub> generation processes can also be considered for cost estimation. The scale and maturity of the selected H<sub>2</sub> generation process **shall** be discussed regarding current and future technological and economic viability. Technological parameters (e.g., process type, efficiency, and operating time) and those fore energy sources and electricity prices (e.g., cost type, time, and location) affecting hydrogen production cost **shall** be clearly documented.

The price of H<sub>2</sub> derived from water electrolysis is strongly dependent on both the cost and selected type of electricity. If a grid electricity mix is selected, the cost calculation needs to be based on an electricity spot price and H<sub>2</sub> 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), the cost calculation needs to be based on intermittent energy supply or levelized cost of electricity (LCOE) according to assessment goal and scope. In other words, a dynamic costing based on intermittent energy supply must be conducted when a detailed analysis is required, otherwise estimation based on LCOE is adequate. Also, practitioners have to take into account data availability and quality (see chapter B.5.2.3) when selecting the approach for estimating H<sub>2</sub> cost. If satisfactory data cannot be obtained to estimate the cost of producing H<sub>2</sub> from intermittent energy supply, then estimation based on LCOE by assuming reasonable full-load hours can be conducted. The price of H<sub>2</sub> from steam-methane reforming is dependent on methane price, therefore cost calculation can be based either on methane spot or contract prices.



### B.5.5.3 Consumption of Electricity

Depending on technology type, electricity consumption can contribute significantly to the economic performance of a process. Some technologies include energy-intensive mechanical processing steps, whereas 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, and subsidies. The importance of electricity for hydrogen production via electrolysis is discussed in chapter B.5.5.2.

Since CCU technologies have potential to reduce CO<sub>2</sub> emissions, the choice of electricity source also becomes vital in many CCU studies. Electricity from renewable resources is of particular interest, as carbon-neutral energy production can be achieved. However, present limitations include insufficient local availability and considerable production costs. If practitioners select electricity from renewable sources, then availability **shall** be discussed and temporal and regional contexts **shall** be documented. For reasons of comparability, the locally available electricity grid mix **should** be considered in the TEA, in either the base case or an additional scenario. Clear documentation needs to be provided on the chosen energy sources, including both fossil energy carriers and renewable sources.

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

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

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

### B.5.5.4 Inputs for Mineralization

Mineralization technologies use the carbonation of mineral oxide to produce various materials and aggregates; there are generally two types of feedstock: mined minerals (*e.g., olivine, serpentine*) and mineral wastes (*e.g., fly ash and steel slags*). Additionally, there are a number of carbon curing technologies, which introduce CO<sub>2</sub> during the hardening process of concrete structures.

Typical cost drivers are extraction of the mineral, transportation to the CCU plant, as well as mechanical preprocessing to prepare the mineral feedstock by energy-intensive grinding and milling of the raw material to obtain the required particle size. Preprocessing scenarios and their resulting energy demand as well as transportation scenarios **should** be assessed. The required purity of the CO<sub>2</sub> input stream can be low, as the presence of impurities such as NO<sub>x</sub> has no effect on the carbonation reaction. Costs for additional inputs



such as acids and bases as well as the disposal of resulting waste after carbonate formation need to be accounted for. The value and market volume of the resulting carbonate products must be carefully investigated within the temporal and regional context.

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, certain national policies or mechanisms, such as tax relief or other tailored subsidies, might provide economic incentives to choose CCU as an alternative treatment for industrial waste. Therefore, practitioners **should** investigate the local regulatory context for compensation of industrial mineral waste treatment. Financial incentives of this kind can have a major effect on the overall cost performance of a particular process, potentially making it economically viable.

### B.5.5.5 Further Inputs

#### *B.5.5.5.1 Fossil-Based Organic Compounds*

If additional inputs in the form of fossil-based organic compounds are required for CCU technologies involving chemical conversion (*e.g., synthesis of polycarbonates via reaction of CO<sub>2</sub> and propylene oxide*), then the following considerations form part of the inventory collection. The prices of fossil-based organic compounds are strongly dependent on the markets for fossil resources, as reflected by global crude oil and natural gas prices. Generally, there is a trend in which the closer the chemical is to the crude oil resource within the value chain, the closer will also be the market price. However, supply–demand relationships might result in deviating prices and always need to be considered as well. Furthermore, the future availability of such fossil-based organic compounds is dependent on the regional availability of their fossil resources, which can be subject to physical scarcity and political restriction. Hence, when compiling the economic inventory, price volatilities and risks concerning the availability of input sources **should** be accounted for. Especially when looking at long-term strategies for the assessed CCU process, potential resource scarcity can have a major impact on profitability. Sources and methods for estimating the prices of raw materials are further discussed in chapter B.6.4. Any assumptions and justifications regarding fossil-based feedstocks **should** be carefully documented.

#### *B.5.5.5.2 Catalysts for Chemical Conversions*

Metal-based catalysts (heterogeneous or homogeneous) are of major importance for many CCU technologies involving 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 economically feasible conversion. The design of suitable catalysts and the technical development of processes for the catalytic conversion are crucial research activities. The production of catalyst materials can be highly cost-intensive, especially if it requires rare metals, expensive ligands, or advanced carrier materials. When compiling the inventory, the required catalyst inputs need 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 for entire new production facilities that would need to be constructed based on specific supply contracts. For cost estimation approaches see also chapter B.6.4. Depending on the recycling rate of the catalyst material, the make-up cost for replacement of the catalyst after a predefined period of time **should** also be investigated. Any risks arising from limited options to procure rare metals on regional and global markets **should** be evaluated in line with the time frame defined in the scope phase.

#### B.5.5.5.3 Algae Production for CCU

The use of algae to convert CO<sub>2</sub> from atmospheric 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<sub>2</sub>, water, nutrients, and light. The management of the culture medium and the subsequent harvesting process to efficiently separate biomass from the culture medium are currently among the main cost drivers. Water inputs need to be evaluated for composition (purified water or waste water) as well as temporal and regional availability. Other important parameters include light (sunlight or artificial) for biological conversion, energy required 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** - H<sub>2</sub> price estimation for different production routes can be found in various reports [38], [40], [41]. A general overview of H<sub>2</sub> production technologies can be found in Ullmann's Encyclopedia of Industrial Chemistry (2011) [42]. Information regarding conversion efficiency, life time, maturity, and future predictions can be found in the IHS Markit - Hydrogen Handbook (2015) [43].

**Mineralization inputs** - Information about current developments is provided, for example, by Pan *et al.* (2015) [44].

**Algae production for CCU** - Reviews of technology development and future predictions can be found in literature sources [45]–[47]

## B.5.5.7 Provisions

<b>Provisions B.11 - Other Key Inputs for CCU Technologies</b>	
<b>Shall</b>	<p><b><u>Hydrogen as Input</u></b></p> <ol style="list-style-type: none"> <li>1) The scale and maturity of selected H<sub>2</sub> generation process shall be discussed regarding current and future technological and economic viability</li> <li>2) Technological parameters and those for energy sources and electricity prices affecting hydrogen production costs shall be clearly documented</li> </ol>
	<p><b><u>Electricity as Input</u></b></p> <ol style="list-style-type: none"> <li>3) If electricity from renewable sources is selected, then availability shall be discussed and temporal and regional contexts shall be documented</li> </ol>
	<p><b><u>Electricity as Input</u></b></p> <ol style="list-style-type: none"> <li>1) Electricity from grid mix should be considered either in the base case or additional scenarios</li> <li>2) Any electricity price in the base case should not be set at zero cost</li> </ol>
<b>Should</b>	<p><b><u>Mineralization</u></b></p> <ol style="list-style-type: none"> <li>3) Preprocessing scenarios and their resulting energy demand as well as transportation scenarios should be assessed</li> <li>4) The local regulatory context for compensation of industrial mineral waste treatment should be investigated</li> </ol>
	<p><b><u>Further Inputs</u></b></p> <ol style="list-style-type: none"> <li>5) For fossil-based compounds, price volatilities and risks concerning the availability of input sources should be investigated and any assumptions and justifications regarding fossil-based feedstocks should be carefully documented</li> <li>6) For metal catalysts, make-up costs for replacement of catalysts should be investigated and any risks concerning future supply of rare metals should be evaluated</li> </ol>
<b>May</b>	

## 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 need to be ensured to enable quick and transparent comparisons of important parameters. A description of the technical and economic context of the study and of the collected data are vital parts of the assessment documentation. The documentation needs to be in a suitable format depending on the needs of the practitioners, for example in tables and flow sheets, and in units that are easy to compare.

### B.5.6.2 How to Ensure Documentation

#### B.5.6.2.1 Documenting Data and Assumptions

To prepare for the reporting phase it is helpful to document relevant technical conditions and assumptions (e.g., temperature; pressure; purities and compositions; assumed conversion efficiencies; equipment dimensions, durability, and lifetime) as well as relevant economic conditions and assumption parameters (e.g., location, currency exchange rates, depreciation periods, interest rates, operating hours, lifetimes, base years, time or location transformation by CEPCI Index or inflation indices) throughout the data collection.

Practitioners **shall** document relevant data, such as parameters, decisions, and assumptions, for all scenarios, preferably throughout the collection process. Data **shall** be documented based on the functional unit and reference flow, and **may** additionally be documented in absolute values. Practitioners **should** document data for each system element independently to enable subsequent analysis, supporting further process development and improvement, which is one major goal of TEA. Characteristics and limitations **shall** be documented – preferably at the beginning of the study – such as regional and temporal context including limitations of market, value chain, scale and production capacity, base year, or underlying thermodynamic limits of chemical conversions. This is particularly important if novel technologies are assessed, which have not yet been optimized to the level of mature benchmarks. The overestimation of efficiencies needs to be avoided, thereby necessitating transparent documentation of all technical assumptions. Furthermore, practitioners **should** document any data quality issues throughout the data collection phase.

#### B.5.6.2.2 Documentation Formats

All collected data need to be documented in a suitable format. The required content differs according to the assessed process as well as the practitioner's demands. Any chosen documentation format needs to list all technical parameters and underlying assumptions in such a way that ensures an overview and facilitates comparison. An example of a tabulated list of technical parameters is provided in Table 13 of the report annex. In particular, economic data **should** be collectively displayed in a separate list that is easily accessible, located either at the beginning or within the annex of each report. The specific needs of different practitioners vary, and not all economic parameters are relevant for each study. For illustration, examples of the main economic parameters are listed in Table 14.

A conventional flow diagram, consisting of system elements together with mass and energy flows, **may** be extended by relevant TEA data, to visualize technical and economic parameters efficiently (“TEA flow sheet”). The TEA flow sheet can differ from technical flow sheets, depicting the process design, as it only includes information relevant for TEA. The various system elements can be represented at different levels of detail (e.g., electrolysis as a black box, methanol synthesis as a PFD). In addition, relevant economic data can be included to describe energy and material flows along the depicted system elements. The TEA flow sheet is a useful tool for enabling TEA practitioner to focus on the system elements that are relevant within

the system boundaries and to enable visualization of the main technical and economic parameters required for assessment. Optionally, the TEA flow sheet could be limited to a graphical representation of only the most significant parameters as defined through the iterative approach. This approach can visualize potential hot spots along the process steps.

#### B.5.6.2.3 Uniformity of Scientific Units

The transparency and comparability of different TEA results are strongly dependent on the consistent use of scientific units. Practitioners **shall** document parameters in SI units (International System of Units/Système international d'unités), due to their broad acceptance and clear definitions; If practitioners choose not to use SI units, clear documentation and unit definitions **shall** be provided.

#### B.5.6.3 Provisions

<b>Provisions B.12 - Documentation in Data Collection</b>	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Relevant data, such as parameters, decisions, and assumptions, shall be documented for all scenarios, preferably throughout the collection process</li> <li>2) Data shall be documented based on the functional unit and reference flow</li> <li>3) Characteristics and limitations shall be documented – preferably at the beginning of the study</li> <li>4) Parameters shall be documented in SI units, or else clear documentation and definitions shall be provided for all non-SI units utilized</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Data should be documented for each system element independently</li> <li>2) Data quality should be documented throughout the data collection process</li> <li>3) Economic data should be collectively displayed in a separate list that is easily accessible, located either at the beginning or in the annex of each report</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Data may be documented in absolute values</li> <li>2) A conventional flow diagram, consisting of system elements together with mass and energy flows, may be extended by relevant TEA data</li> </ol>

## B.6 Calculation of Indicators

### B.6.1 Introduction to Calculation of Indicators

Suitable assessment indicators are selected in the goal and scope phases and then collected and documented in the inventory phase data for calculation. The calculation of assessment indicators itself forms a separate phase and is covered in this chapter. Calculation 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.

As CCU technologies cover a wide range of specialisms within the field of chemistry (*e.g., thermochemical, biochemical, electrochemical, photochemical, etc.*) and include projects at varying technology maturity, a large variety of technical indicators exists. While this multitude cannot be discussed in detail in this guideline, general best practices in the calculation of assessment indicators are presented at the beginning of this chapter. Subsequently, the economic indicators for capital expenditure (CapEx) and operational expenditure (OpEx) as well as a selection of profitability indicators are presented, and the chapter concludes by discussing normalization and weighting of the results.

CapEx and OpEx are intermediate indicators that are either directly interpreted compared to benchmark values of the same indicator or else aggregated in further calculations, especially in all profitability indicators (*e.g., net present value*) or in enviro-economic indicators (*e.g., CapEx /  $t_{CO_2e}$* ). The importance of CapEx and OpEx in CCU is acknowledged in separate sections of this chapter by proposing methodological approaches. CapEx and OpEx feed the calculation of profitability indicators, which are outlined in a separate section as they are especially important for decision making in business-driven contexts. In particular, CapEx and OpEx generate the cost of goods manufactured (COGM), which then gives cost of goods sold (COGS) with general expenses considered. Ultimately, profitability indicators can be calculated from cost of goods sold, revenues, and risk (see Figure 6).

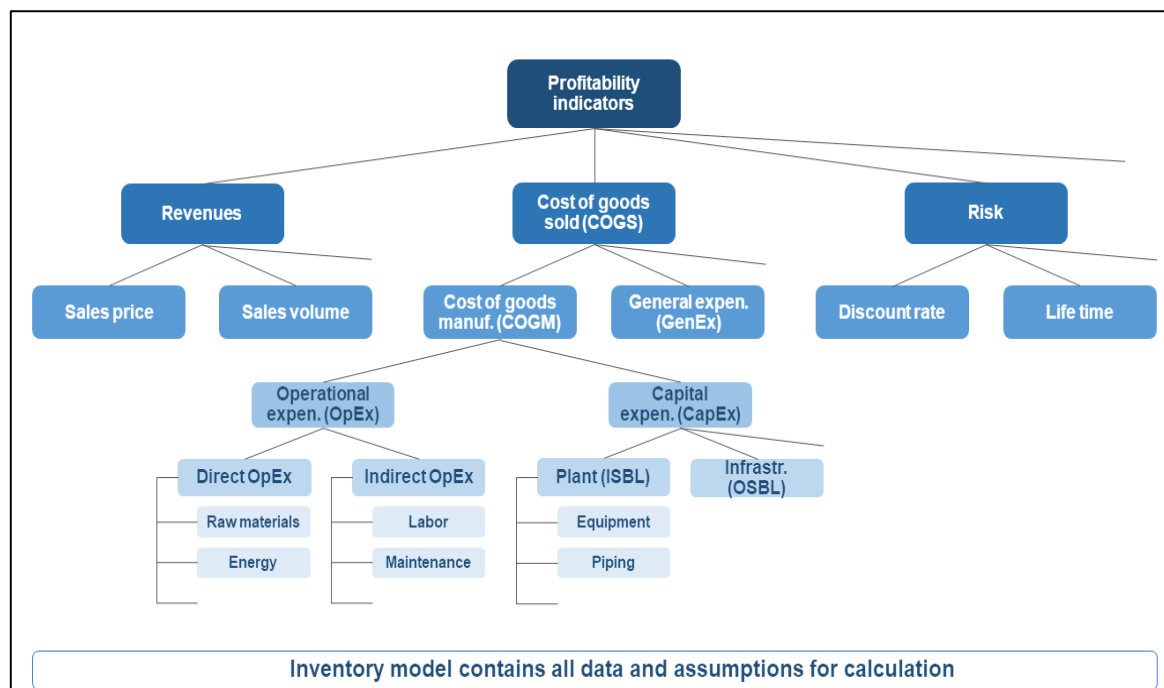


Figure 6. Calculation hierarchy for economic indicators, adapted from Buchner et al. [20]

## 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 for non-specialist readers to comprehend. 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

First and foremost, practitioners **shall** select methods of indicator calculation that comply with the goal and scope of TEA (*e.g., with the audience's demands for accuracy*). While practitioners conduct calculation of indicators according to their needs, some general principles need to be kept in mind. We recommend that practitioners choose quantitative assessment over qualitative assessment. However, in very early maturity stages such as TRL 1, some quantitative data might not be available, and a qualitative assessment might be useful to derive first recommendations. Seamless reiteration (*e.g., allowing indicators to update following changes of the inventory*), transparency, and reproducibility are major challenges in the calculation phase. To avoid possible inconsistencies in data and to enable seamless reiteration, practitioners **shall** link inventory data to calculation of indicators (*e.g., linking data points to equations in a separate calculation spreadsheet*). To ensure transparency, calculation of indicators **shall** be conducted separately from inventory. Furthermore, practitioners **should** store results in a separate file from the calculation of indicators (*e.g., spreadsheet*). For better reproducibility, practitioners **should** select methods that are commonly used in the literature. Further, practitioners **should** select methods that are as accurate as the available data permit following an iterative approach. Nevertheless, uncommon methods can also be used when necessary, but note that the motivation and explanation for such decisions **shall** be stated. To avoid potential ambiguity in producing and/or utilizing the calculations, all assumptions, requirements, and adjacent estimates **shall** be stated (*e.g., company internal estimation and budget authorization frameworks*). In addition, the equation employed and the reasons for choosing each indicator **shall** be presented.

Calculations **shall** be conducted for the overall product system as well as for each system element individually, thereby allowing better comparability and analysis of system element alternatives (*e.g., inclusion or exclusion of CO<sub>2</sub> capture, H<sub>2</sub> products*). The level of calculation detail can vary between system elements according to data requirements (*e.g., black box or detailed process*). While the assessment can be conducted for each system element individually, data describing flows between system elements, for example market data, can prove difficult to obtain and might therefore impede the calculation of aggregated indicators, such as profitability indicators, for the respective system element. If the data required for a selected calculation or estimation are found to be unobtainable, the required data need to be collected in the following iteration of the assessment (see iterative approach in chapters B.5.2 and B.7.2).

### B.6.2.3 Further Reading

Many best practices can be found in textbooks for process engineering [18], [21], [22]. Specific cost estimation frameworks and groups of methods are presented by several authors [48]–[52].

### B.6.2.4 Provisions

Provisions B.13 - Best Practices in Indicator Calculation	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Methods that comply with the goal and scope of TEA shall be selected</li> <li>2) Inventory data shall be linked to calculation of indicators</li> <li>3) Calculation of indicators shall be conducted separately from inventory</li> <li>4) If uncommon methods are used, motivation and explanation shall be stated</li> <li>5) All assumptions, requirements, and adjacent estimates shall be stated</li> <li>6) The equation employed and the reasons for choosing each indicator shall be presented</li> <li>7) Calculations shall be conducted for the overall system as well as for each system element individually</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Results should be stored in a separate file from the calculation of indicators</li> <li>2) Methods commonly used in the literature should be used</li> <li>3) Methods that are as accurate as the available data permit should be selected, following the iterative approach</li> </ol>
<b>May</b>	

## 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 CapEx is an important economic indicator (see scope, chapter 0) 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 detailed data.
- CCU projects belong to different fields of technology. A variety of methods for CapEx estimation is available; however, from the literature it is not always evident which methods are best applied for a given detail and quality of input data.

For these reasons, a brief general methodology overview is presented in this chapter. The next chapter provides guidance, applicable to CCU projects, on how to estimate CapEx (see chapter 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, 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*), see Figure 6.



In general, methods for the estimation of CapEx vary regarding their use of data. Frameworks for CapEx estimation methodology are widely adopted in chemical engineering and are referred to in this document as they facilitate choice of methods. The AACE International Cost Estimate Classification System [53] presents the most common framework. The following clusters of methods estimating FCI or ISBL cost were identified:

- ‘Short methods’ calculate costs from one or few characteristic parameters and often include cost-capacity curves or scales of operation factors (see [54], [55]).
- ‘Parametric techniques’ derive cost from process characteristics and related parameters; most are based on the number of significant process steps and other characteristic process parameters (see [56], [57] for low-detail methods, and [58], [59] for high-detail methods).
- ‘Factored methods’ apply factors to equipment cost to calculate other direct or indirect cost items. Some authors apply one, global factor to cumulative equipment cost to calculate ISBL (see [60], [61]), while others estimate single cost items via detailed factors that are individually adapted to single components (see [62]–[64]).
- ‘Unit cost line items’ derive costs from rigorous design and offer 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 adaptations of detailed factors for single equipment.
- ‘Cost transformation’ describes the adoption or transfer of similar plants’ CapEx to a projected plant, usually based on capacity or other significant plant parameters (*e.g., by using the popular six-tenths power rule* [65], [66] *or adaptations* [48]). 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

#### B.6.3.2.1 General CapEx Estimation Framework

Table 8 provides an overview of a cost estimation methodology and serves as an orientation to the selection of adequate methods; the table is based on the AACE International Recommended Practice 18R-97 [67] and includes types of methods as described above.

**Table 8. Typical methods for capital expenditure estimation in different technology maturity phases of a project**

<i>Technology maturity phases</i>	Research	Development	Deployment
AACE Estimate Classes	5 and 4	4 and 3	2 and 1
Typical methods adapted from AACE	<ul style="list-style-type: none"> <li>▪ Short methods</li> <li>▪ Parametric techniques (low detail)</li> <li>▪ Factored methods</li> <li>▪ Cost transformation</li> </ul>	<ul style="list-style-type: none"> <li>▪ Component factored methods</li> <li>▪ Parametric techniques (high detail)</li> <li>▪ Inclusion of unit cost line items</li> <li>▪ Cost transformation</li> </ul>	<ul style="list-style-type: none"> <li>▪ Unit cost line items (high detail or based on design quantities)</li> <li>▪ Still undefined items: detail component factored methods (or "forced detail")</li> </ul>

#### B.6.3.2.2 Method Selection

In this context, method selection means the use of rough estimation in the first iteration, especially with short methods. Subsequent iterations identify the parameters to which CapEx is most sensitive (see chapter B.7.2.2) and then select more accurate methods. While the most accurate estimates possible are preferred in general, a simpler methodology can be applied. As system elements with different maturity can be present within a single product system, a combination of different methods might be necessary for the calculation of a complete CapEx.

As mentioned in chapter B.6.2, calculation methods need to be as precise as possible (exploiting best available data) but can only be as precise as available data permit (indicated by technology maturity) to lead to the most accurate overall cost possible and subsequently the best decision basis.

For estimating ISBL CapEx, in cases where the similarity and quality of available data of similar plants are considered sufficient, cost transformation **should** be applied. For estimating ISBL CapEx in deployment phases, in which cash flows can be sufficiently forecasted, the highest level of accuracy for estimations is needed. Two exceptions apply:

- If practitioners require equipment specifications for a complete estimate but cannot derived them from technical development at the point of assessment, they **may** assume them 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 the assessment into a certain pathway for future development.
- If practitioners judge CapEx to be of minor importance compared to OpEx, they **may** lower the accuracy demands of CapEx estimation.

Especially for larger plants, OSBL cost can contribute a major share to the overall CapEx estimate. In early- to mid-maturity stages, OSBL cost **should** be 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 this section 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. In stages of high technology maturity, all CapEx items **should** be estimated independently: In particular, OSBL **should** be estimated independently of ISBL.

#### *B.6.3.2.3 Challenges in CapEx Estimation for CCU Technologies*

For CCU plants, the distinction between inside (ISBL) and outside (OSBL) facilities is often unclear. For example, energy and utility provision can either be seen as core plant functions or as connections to the outside world (grid). Thus, practitioners **should** provide a clear assignment of components to either ISBL or OSBL. In addition, practitioners need to pay attention to the scaling factors of ISBL and OSBL as these might deviate. Usually, the ratio of ISBL to OSBL decreases with increasing plant size.

Cost estimation methods, especially parametric techniques, are typically based on company experience of processes that utilize fossil resources. In addition, various 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 understand the economic composition of a plant and identify key cost drivers. Practitioners should keep in mind that CapEx estimates at early technology maturity involve large uncertainties, which need to be reflected in the interpretation (see chapter B.7).

Moreover, at mid to high technology maturity, the cost scaling of the main component **should** be analyzed. While the 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 that might not follow such scaling effects. In this case, short methods and some parametric techniques tend to underestimate CapEx.

#### *B.6.3.2.4 Contingency*

Depending on project management decisions, practitioners **may** include costs for unforeseeable events and circumstances as contingency costs when estimating CapEx. Contingency can mean the following: [18], [21], [22], [68]–[70]

- Allowance for ‘known unknowns’: specific, known but unquantified items (*e.g.*, currency exchange rate fluctuations, estimation errors, metal price changes)
- General contingency for ‘unknown unknowns’: 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, construction date)

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

Contingency can be calculated using 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 heuristics [71], [72]. Probabilistic techniques use either expected values of cost impacts of a range of potential events [73] 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 level of certainty that the budget will not be overrun [74], and this 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 in which a plant will be situated, which usually accompanies increasing technology maturity. External threats (force majeure) that determine general contingency are not directly affected by technology maturation. An overall contingency value less than 10% of FCI is not recommended [18], [21], [22].

#### B.6.3.2.5 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 costs. The first plant of a particular kind is likely to require significantly higher CapEx than subsequent examples. 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
- 'N<sup>th</sup> of a kind' (NOAK): several plants exist that employ the same or similar technologies and learning rates can be estimated

If required by the goal and scope, practitioners may convert the CapEx of a FOAK plant to the CapEx of a NOAK plant by including learning curve effects, as described in the literature [75]–[78]. When applying CapEx learning curve effects, great caution is required to ensure 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 the near future*). In addition, the expectation that the market volume will support multiple plants needs to be justified. Furthermore, it must be considered that learning curve effects can also apply to benchmark systems, which is especially important when directly comparing CapEx to other systems or when calculating profitability.

#### B.6.3.3 Further Reading

The most prominent methods for CapEx estimation are described in the process design literature, for example in [18], [21], [22], [79], [80]. Detailed information on contingency estimation is available from various sources, including the AACE International recommended practices: 41R-08, 42R-08, 43R-08, and 44R-08 [71]–[74].

## B.6.3.4 Provisions

Provisions B.14 - Estimation of Capital Expenditure	
<b>Shall</b>	
<b>Should</b>	<ol style="list-style-type: none"> <li>1) At early to mid technology maturity               <ol style="list-style-type: none"> <li>a. For estimating ISBL, in cases where the similarity and quality of available data of similar plants are considered sufficient, cost transformation should be applied</li> <li>b. OSBL cost should be estimated in total as a factor applied to ISBL cost</li> </ol> </li> <li>2) At mid to high technology maturity, the cost scaling of the main components should be analyzed</li> <li>3) At high technology maturity               <ol style="list-style-type: none"> <li>a. all CapEx items should be estimated independently</li> <li>b. OSBL should be estimated independently of ISBL</li> </ol> </li> <li>4) Components should be clearly assigned to either ISBL or OSBL</li> <li>5) CapEx estimation should be conducted critically using multiple methods in parallel</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) If equipment specifications are required but cannot be derived, they may be assumed for economic calculations ('forced detail')</li> <li>2) If CapEx is found to be of minor overall importance, the accuracy demands for CapEx estimation may be lowered</li> <li>3) Contingency may be included in a CapEx estimate</li> <li>4) Learning curve effects may be included to estimate NOAK plant CapEx</li> </ol>

## 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 other hand, 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].

Operational expenditure is an important economic indicator (see chapter 0). Especially for high-volume products that compete in 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 reactants (*e.g., H<sub>2</sub>, epoxides*), thereby making reliable data for these inputs a crucial factor.

Two key terms in OpEx estimation are ‘cost increment’ and ‘factored estimation’. A cost increment means the 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

### B.6.4.2.1 General OpEx Estimation Framework

Similar to the estimation of CapEx, the most accurate estimates possible for OpEx are preferred; however, a less accurate methodology might be applied in order to reduce estimation effort if the goal and scope definitions allow it. Table 9 shows proposed OpEx estimation methodology as well as required data and sources along the technology maturation phases of research, development, and deployment.

**Table 9. Proposed methodology for operational expenditure estimation**

Phase	Research	Development	Deployment
Material	<ul style="list-style-type: none"> <li>Based on stoichiometry, measured mass flows, or design/simulation</li> </ul>	<ul style="list-style-type: none"> <li>Based on measured mass flows or design/simulation</li> </ul>	<ul style="list-style-type: none"> <li>Based on measured mass flows or design/simulation</li> </ul>
Energy, utilities & other variable OpEx	<ul style="list-style-type: none"> <li>Based on measured energy flows or design/simulation</li> <li>Factored estimation (based on material cost)</li> <li>Cost increments from similar plants</li> </ul>	<ul style="list-style-type: none"> <li>Based on measured energy flows or design/simulation</li> <li>Cost increments from similar plants</li> </ul>	<ul style="list-style-type: none"> <li>Based on measured energy flows or design/simulation</li> </ul>
Fixed OpEx	<ul style="list-style-type: none"> <li>Simple factored estimation</li> <li>Cost increments from similar plants</li> </ul>	<ul style="list-style-type: none"> <li>Detailed factored estimation</li> <li>Cost increments from similar plants</li> </ul>	<ul style="list-style-type: none"> <li>Detailed factored estimation</li> <li>Separate calculation of fixed OpEx items</li> </ul>
General expenses & freight	<ul style="list-style-type: none"> <li>Factored approach</li> </ul>	<ul style="list-style-type: none"> <li>Factored approach or company-specific</li> </ul>	<ul style="list-style-type: none"> <li>Company-specific</li> </ul>
Main price data and sources	<ul style="list-style-type: none"> <li>Price data: market-average</li> <li>Sources: few, secondary</li> </ul>	<ul style="list-style-type: none"> <li>Price data: market-average</li> <li>Sources: multiple, secondary</li> </ul>	<ul style="list-style-type: none"> <li>Price data: process-specific</li> <li>Sources: few, primary (supplier quotes)</li> </ul>

OpEx estimation is largely dependent on cost increments and factor estimation, as well as on similarity of plants. No general provisions for increments or factor estimation can be given here, since they are technology-specific and can vary considerably. Furthermore, no quantitative approach is available for judging degrees of similarity among plants. These issues are left to the practitioner's careful consideration and judgement of the company-specific and technology-specific characteristics. In the research and development phase, and if data from similar plants are available at a substantial degree of similarity and quality, practitioners need to consider cost increments for calculating OpEx.

#### B.6.4.2.2 Variable OpEx: Raw Material Cost

The costs of 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 subsequent stages, the mass balance for the OpEx estimate is based on actual mass flows from the conducted process (*e.g., laboratory experiments, pilot trials, plant operation*). Mass balances for system elements that are not yet built are determined following process design (*e.g., through process simulation*).

Raw material prices can be obtained from primary or secondary sources (see chapter B.5.2). Using specific raw material prices from suppliers is preferable but often challenging, especially for development projects that lack trustworthy relationships with suppliers or those in the early stages with unknown trade conditions.

#### B.6.4.2.3 Variable OpEx: Energy, Utilities, and Other Costs

The costs of 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 for system elements that are not yet built are determined following process design (*e.g., through process simulation*). In both the research and development phases, practitioners can simplify variable OpEx estimations, subject to proper justification:

- If practitioners judge energy cost to be of minor importance, it **may** be estimated as a share of the total raw material cost.
- If practitioners judge utilities or other variable costs to be of minor importance, these costs **may** be estimated as a share of the total energy cost.

Practitioners can obtain energy prices from data bases similar to those for raw material prices. For plant integration into existing sites where utility supply already exists, 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 must be approached in the same way.

#### B.6.4.2.4 Fixed OpEx

As mentioned above, practitioners can adapt fixed OpEx from the data for similar plants, estimate it via factors or specific correlations, or also project it in detail. In the late research phase, once the FCI estimate is available, practitioners are recommended to use a factored approach for estimating fixed OpEx. Factors for fixed OpEx estimation are either directly applied to CapEx or major OpEx items. A variety of estimation factors and typical OpEx items are available from the literature [18], [20]–[22], [81], [82]. Practitioners need to carefully adapt the factored estimation of fixed OpEx to the projected scenario (*e.g., increased maintenance factor for plants with higher operating pressure or greater safety demands*). No quantitative approach is available for judging degrees of similarity between plants in order to deduce appropriate cost increments. In the deployment stage, all major fixed OpEx items need to be calculated in detail.

#### B.6.4.2.5 General Expenses & Freight

The relevant market costs 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. For the estimation of general expenses, a factored approach is often chosen during research phases, whereas in more advanced phases of development and deployment company-specific values can be added. Freight can account 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 to each product and its related sales activity.

#### B.6.4.3 Further Reading

Methods for estimation of operating labor demand, as a basis in factored estimation, are available in the literature [18], [22], [79]. Cost items and values for factored estimation as well as correlations for single cost items of fixed OpEx are available from textbooks [18], [21], [22], [81], encyclopedias [83], and research articles [20], [84].

#### B.6.4.4 Provisions

<b>Provisions B.15 - Estimation of Operational Expenditure</b>	
<b>Shall</b>	
<b>Should</b>	
<b>May</b>	<ol style="list-style-type: none"> <li>1) If of minor importance, energy cost may be estimated as a share of the total raw material cost</li> <li>2) If of minor importance, utilities or other variable costs may be estimated as a share of the total energy cost</li> </ol>

### B.6.5 Calculation of Profitability Indicators

#### B.6.5.1 Introduction

For interpretation and decision making for profit-oriented stakeholders in business-driven contexts (*e.g., manager, shareholders, or creditors*), profitability indicators present the most important basis, adding a market view to the internal cost. Profitability indicators are “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 [85].



## B.6.5.2 How to Calculate Profitability Indicators

### B.6.5.2.1 Static and Dynamic Profitability Indicators in General

Two types of profitability indicators can be distinguished: static and dynamic [86], which are presented in the following. Static indicators consider only one period or an average of multiple periods. The general alternative action in static calculations is ‘no investment.’ Popular static profitability indicators are relative profit, payback time, and return on investment. The ‘relative profit,’ a dimensionless indicator, is often chosen (see [25]); if absolute numbers are important for strategic considerations, practitioners can choose the absolute profit over relative profit (see [87]) or a rough comparison with established products and deriving cost increments. ‘Payback time’ and break-even points are popular profitability indicators. The Payback time is calculated as CapEx divided by the profit of the period, measuring the number of periods required to recoup initial costs and reach the break-even point. The ‘break-even point’ is the point in time at which the total cost and profits are equal, after which subsequent economic activity generates net profit for the future. A third popular profitability indicator is the ‘return on investment’ (ROI), which is calculated by dividing profit by CapEx. Note that ROI equations presented in the literature differ in the items of CapEx or time frames (single period vs. project life time or recovery period).

Dynamic indicators include multiple periods, accounting for investors' preferences for the timing of cash flows. The general alternative investment in dynamic calculations is an investment in the capital market with the same risk profile. The most prominent indicator of dynamic profitability is ‘net present value’ (NPV), which is calculated as the sum of all cash flows that are discounted according to the period they occur in, with corresponding assumed discount rate(s). NPV depicts the amount of money that an investment is worth in period zero. The use of NPV in early maturity stages is not recommended. Similarly to its static version, the ‘dynamic payback time’ is the duration until the first period in which the sum of all past discounted cash flows is zero or positive. Dynamic payback time can be calculated in parallel to NPV as it requires the same data. The dynamic ROI can include interest and time preference; it is calculated as the ratio of all discounted cash flows relative to initial spending. Another popular dynamic profitability indicator is the ‘internal rate of return’ (IRR), comparing relative earnings to initial investments, measuring the discount rate that leads to a NPV of zero. IRR is a popular measure when comparing how well different projects perform. However, using IRR has disadvantages [88]: For example, depending on cash flow characteristics, practitioners might end up with multiple solutions, or else solutions in the domain of complex numbers ( $\mathbb{C}$ ). Another example is that the IRR does not reveal the absolute profit that can be obtained, and thereby leads to loss of information. For these reasons, IRR can be selected but must always be accompanied by NPV for the same investment. In addition to the presented quantitative profitability indicators, there might be additional economic factors of interest that are difficult to translate into monetary measures and are therefore left to qualitative evaluation (*e.g., availability of qualified personnel, see [79]*).

### B.6.5.2.2 Profitability Indicators at Different Technology Maturity Stages

At the research stage, using static indicators is sufficient. Practitioners **should** use one indicator that normalizes profit to cost because normalized values simplify the comparison of alternatives, thereby assisting in deriving recommendations. From the development phase onwards, using dynamic indicators becomes versatile. When the addressable market volume is derived, practitioners **should** calculate an absolute profit measure. From (later) development stages onwards, practitioners **should** calculate NPV. NPV commonly serves as a structural basis for more detailed profitability calculations during the deployment stages.

In the deployment stages, dynamic indicators need to be refined 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.*, the present worth of the investment, or the worth of the investment after it generates net profit). These economic simulations can be based on discrete events (scenarios, see chapters 0 and B.6.4) or analytical functions that describe the behaviors of markets, costs, and scenario parameters (*e.g.*, depreciation, taxes, inflation). After procurement (and potentially construction and commissioning) has started, cost items need to 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 to determine at what point during development or deployment to consider issues of taxation. 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 initial calculations, practitioners often choose simplified assumptions, such as applying a single 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 technological developments. Past economic activities are summarized in accounting for cost checks and profit calculations.

#### *B.6.5.2.3 Challenges in the Calculation of Profitability Indicators for CCU Technologies*

The selection of profitability indicators in TEA for CCU remains a key challenge: There is currently a lack of standardization, especially at early maturity stages [2]. The use of different indicators makes it difficult to comprehend, reproduce, and compare 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.

When calculating dynamic profitability indicators, a second key challenge is the selection of an adequate discount rate. 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 when discounting for dynamic indicators. 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 overall company. If the project's risk profile differs from that of the company, the WACC needs to 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 [89]. The capital market is often assumed to be perfect for first calculations and unrestricted in research and early development stages. In later development stages, the practitioner can adapt interest rates to cost items, for example how CapEx is financed. In later development and in deployment, the time dependency of interest rate needs to be considered (*cf.* spot rates vs. forward rates), since interest rates depend on the life span of the financing instrument; practitioners **should** adapt interest rates to different financing instruments.

When calculating dynamic profitability indicators, a third key challenge is the prediction of future cash flows. Future cash flows are very uncertain if the market is not well understood, leading to errors that have large impacts on the results. Developing an understanding of scenario conditions and predicting future cash flows require an understanding of the market, which can usually not be derived until considerable progress in technical development is made. When applying dynamic indicators, practitioners **should** describe scenarios in great detail.

### B.6.5.3 Further Reading

Profitability indicators used in the chemical and process industries are covered in textbooks for process design, especially [18], [21], [22] or reports such as [87]. Capital budgeting methods are covered in the general economic literature; single investment appraisal techniques in the context of chemical innovations are discussed, for example, in [90], [91]. Profitability indicators relevant for CCU in early stages are discussed, for example, in [26], [92]–[94].

### B.6.5.4 Provisions

Provisions B.16 - Calculation of Profitability Indicators	
<b>Shall</b>	
	<ol style="list-style-type: none"> <li>1) One indicator that normalizes profit to cost should be used</li> <li>2) When the addressable market volume is derived, an absolute profit measure should be calculated</li> <li>3) From later development stages onwards, NPV should be calculated</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>4) When applying dynamic indicators, an interest rate should be selected that represents the same risk profile as the projected technology</li> <li>5) In later development and deployment, interest rates should be adapted to different financing instruments</li> <li>6) When applying dynamic indicators, scenarios should be described in great detail</li> </ol>
<b>May</b>	

## B.6.6 Normalization and Weighting

### B.6.6.1 Introduction

Especially for CCU products involving diverse technologies and markets, various trade-offs are required between different indicators and criteria (*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 involve subjective choices and must be conducted with great caution.

### B.6.6.2 How to Conduct Normalization and Weighting?

#### B.6.6.2.1 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 [95]:

- **Categorical scaling:** assigning a quantitative or qualitative score to each indicator, which is robust to small changes in data but also entails some information loss (*e.g., assigning each indicator, based on its value, a number on 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 **may** be applied as an optional step; if it is applied, results have to be normalized for each assessment indicator separately, and the reasons for selecting normalization and scaling criteria as well as the initial values of the absolute indicators must be documented.

#### B.6.6.2.2 Weighting

Weighting means assigning quantitative weights to (normalized) indicators. For these TEA Guidelines weighting also includes aggregating, which means adding up weighted indicators. Weights are collected during the goal and scope phase (*e.g., derived from target audience's preferences, expert opinions, company goals, or the assessment goal*). Indicators with different dimensions have to be normalized (preferably to dimensionless indicators) before they are aggregated (*e.g.,  $t_{CO_2e} / t_{product}$  and OpEx must each 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 by categorical scaling cannot be aggregated.

Assigning weightings is based on personal decisions and preferences and is thus always subjective. Weighting serves the aggregating of indicators (usually indicators of different criteria) and includes subjective meanings; aggregated indicators are sometimes demanded by decision makers as they potentially help to reduce 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 compared to decisions based on non-aggregated information.

Weighting can be applied if the interpretation of results and subsequent decision making are based on multiple indicators, in order to help make clearer distinctions between results (*e.g., no single product scores highest in every indicator*), or if comparing an aggregated indicator to a previously defined criterion for canceling the assessment (*e.g., in a stage gate process*). Weighting **may** be applied as an optional step; if applied, practitioners must normalize indicators with different dimensions. Practitioners are recommended to normalize indicators with the same dimension and must also document the reasons for weighting, the weighting scheme, and the assigned weights as well as the initial discrete indicator values.

#### B.6.6.3 Further Reading

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

## B.6.6.4 Provisions

<b>Provisions B.17 - Normalization and Weighting</b>	
<b>Shall</b>	
<b>Should</b>	<ol style="list-style-type: none"> <li>1) Normalization of results beyond the reference flow may be applied as an optional step, but only with great caution. If applied:               <ol style="list-style-type: none"> <li>a) Results have to be normalized for each indicator separately</li> <li>b) Reasons for selecting normalization and scaling criteria as well as initial, absolute indicator values must be documented</li> </ol> </li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>2) Weighting may be applied as an optional step, but only with great caution. If applied:               <ol style="list-style-type: none"> <li>a) Indicators with different dimensions must be normalized</li> <li>b) Indicators with the same dimension are recommended to be normalized</li> <li>c) Reason for weighting, weighting scheme, and the assigned weights, as well as initial, discrete indicator values have to be documented</li> </ol> </li> </ol>

## B.7 Interpretation

### B.7.1 Introduction to Interpretation

The interpretation stage comprises a review of all stages of the TEA process in order to check the consistency, completeness, and reliability of the model and input parameter assumptions, data quality, and associated outputs in relation to the 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 identifies key inventory data that need to be improved, and can be useful for constructing different scenarios. A key challenge in the interpretation stage is assessing the information provided by indicators and corresponding criteria, in order to satisfactorily answer the questions posed by the assessment goal. The interpretation can also involve a multi-criteria decision analysis step when the assessment goal includes multiple objectives that potentially require trade-offs between different targets. The outcome of the interpretation phase is a set of conclusions and limitations that serve 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. UA deals with 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 for the base case, and any additional scenarios that are crucial for the subsequent decision and thus need 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 in one or more input variables. UA and SA are complementary, as SA reveals how any uncertainty within the output is constructed, and discloses key input variables that can contribute most to the uncertainty [96].

In the case of low technology maturity, complex uncertainty methods can result in substantial noise. Therefore, it is recommended to focus efforts on key input variables that are identified by sensitivity analysis. Furthermore, uncertainty during early development stages can be analyzed qualitatively when there too few data for reliable quantitative assessment. As an additional interpretation tool, plausibility checks can quickly evaluate whether the assessment result produces plausible physical or economic ratio ranges. Such plausibility checks can already be performed as part of the goal definition (see chapter B.3.2.2). Based on the plausibility checks, practitioners can decide whether to move forward with the assessment, revise the process designs, or terminate the assessment.

### B.7.2.2 How to Conduct Uncertainty and Sensitivity Analysis

In the interpretation phase, practitioners **shall** provide conclusions, limitations, and a basis for recommendations with respect to the calculated results. Interpretation of an indicator result is based on information gained from UA and SA of its key input variables (*e.g., CO<sub>2</sub> capture cost, revenues, minimum product selling price, profitability indicator*). The following procedure is recommended to analyze the uncertainty and sensitivity of calculated indicators:

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

### B.7.2.3 Characterization of Uncertainty

Practitioners **shall** conduct uncertainty analysis to identify the total variation of the model output caused by uncertainties in the inputs or in the model itself [96]. The use of a range of outcomes or a confidence interval (such as that produced by uncertainty analysis) leads to more profound and comprehensive decisions than those based on a single value. Various methods are available for UA, which are selected according to the source and nature of uncertainty (also see B.7.2.6 Further Reading). UA serves as a quality test for the model and its input data by considering all sources of uncertainty. This enables verification of whether the model output properly supports the underlying decision process.

The literature includes differing classifications for sources of uncertainty, which depend on context and scope. Sources of uncertainty fall within three main categories [4], [97], [98]:

- Quantitative uncertainties in the input variables resulting from measurement errors 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 the practitioner's methodological choices in the goal and scope phases

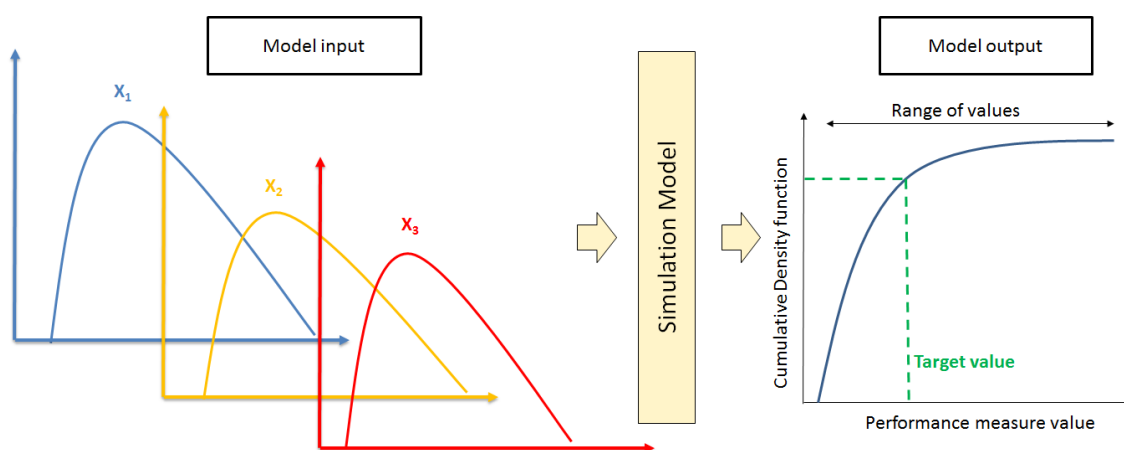
Another source of uncertainty is the 'ignorance of the practitioner,' which is not assessable within UA and SA methods but by qualified peer review [99]. Uncertainty decreases with increasing maturity levels, as a result of improved data or better understanding of the technology and the conditions under which its research, development, and deployment are conducted. These disparities in data quality and levels of understanding must be considered when comparing results from projects involving different maturity levels.

## B.7.2.4 Uncertainty Analysis

### B.7.2.4.1 Quantitative Uncertainty Analysis

An uncertainty analysis quantifies the total variation in the outcome due to inherent variations in the inputs to a model [96]. At early maturity stages, a qualitative uncertainty analysis can be an alternative or complementary to the quantification of output variations.

Commonly used methods for analyzing quantitative uncertainties include intervals (ranges with upper, mid, and lower bounds), variance, probability distributions, possibility distributions, and fuzzy intervals [96], [98]. If relevant data are available, a probability-based method is recommended since these are easily applied and provide statistical information such as probability distributions and 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 7, three input variables ( $x_1$ ,  $x_2$ ,  $x_3$ ) and their respective probability distributions are transferred to the probability distribution function of the output [96].



**Figure 7. Simulating variable inputs to obtain probability distributions of a performance indicator**

The output distributions can be used to either describe the range of different potential outputs and their probabilities or to estimate the probability that the output will remain within or exceed a specific threshold or performance target value (*e.g.*,  $CO_2$  price,  $H_2$  price, product price) [98]. One comprehensive uncertainty propagation method is Monte Carlo analysis, a sampling method in which 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 need to 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 during early technology maturity, there is often insufficient data available to produce reliable probability distribution functions for the analysis.

In the research phase, qualitative uncertainty analysis methods **may** be devised as alternative or complementary methods when data from different sources are used; when insufficient reliable data are available for stochastic analysis; or where only some technological and economic data are 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 [100], termed pedigree analysis. A pre-defined pedigree matrix analyzes the 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) [101]. Ideally, confidence estimates can be conducted by experts that are familiar with relevant details of the assumptions, data sources, and procedures.

#### B.7.2.4.2 Model and Context Uncertainty Analysis

The model or context uncertainty can be analyzed by identifying different scenarios and comparing the results, or by comparing and validating model results with real observations or with alternative models. In order to analyze the structure of the model uncertainty, the model output needs to be validated with measured data or with data from similar systems. To examine these uncertainties reliably much effort is required to set up a valid analysis framework. Context uncertainty can be further analyzed and reduced by peer review in which experts who are independent of the assessment check its applicability and resulting limitations [98], [99].

### B.7.2.5 Sensitivity Analysis

Practitioners **shall** conduct sensitivity analysis to reveal key variables that need to be focused on to reduce the uncertainty and to improve inventory data or impact assessment. Sensitivity analysis (SA) examines the sensitivity of the model output by apportioning the variance in the output to one or more input variables. Identification of key variables can already be executed at early maturity stages, whereas more detailed deconstruction of uncertainty requires reliable data that are often unavailable until medium technology maturity. Sensitivity analysis can be broadly classified into local and global methods. Local sensitivity analysis is easier and faster to apply, since only one input parameter at a time is varied, whereas global sensitivity methods allow the output variance to be apportioned to the different input variables and to calculate the interaction effects among two or more input variables (e.g., *CO<sub>2</sub> capture cost and CO<sub>2</sub> purity*) [102], [103].

#### B.7.2.5.1 Local Sensitivity Analysis

For the first assessment iteration, practitioners **should** carry out local sensitivity analysis. For all sensitivity analysis methods, the resulting change in the model output in relation to the input variation is quantified as the sensitivity measure. The 'one at a time' (OAT) local sensitivity analysis describes the variation of one input variable (e.g., *material prices, tax rates, inflation rates, or equipment configuration*). The variation in OAT takes a minimum and maximum value around a base value (e.g.,  $\pm 10\%$ ) with all other input variables fixed within reasonable technical, physical, or economic constraints. In 'one-way' local sensitivity analysis this variation of the input variable is extended to cover its entire predetermined range, showing the variation in the output variable between its extremes and making non-linear correlations visible. The 'n-way' sensitivity analysis extends the analysis from one input variable to multiple (n) input variables, showing the dependencies between the input variables [104], [105].

A further sensitivity measure is the partial derivative of the model output with respect to each input variable. However, this method does not consider the uncertainty ranges of the input variables and can lead to misinterpretation if highly sensitive inputs are very uncertain. The results can be presented graphically, either as single-factor spider (the steeper the slope, the stronger the sensitivity) or tornado (the larger the range, the stronger the sensitivity) graphs, as shown in Figure 8. Local sensitivity analysis does not consider any correlations or interactions between different input variables, and assumes linearity, which leads to limited informational value of the sensitivity results [98].

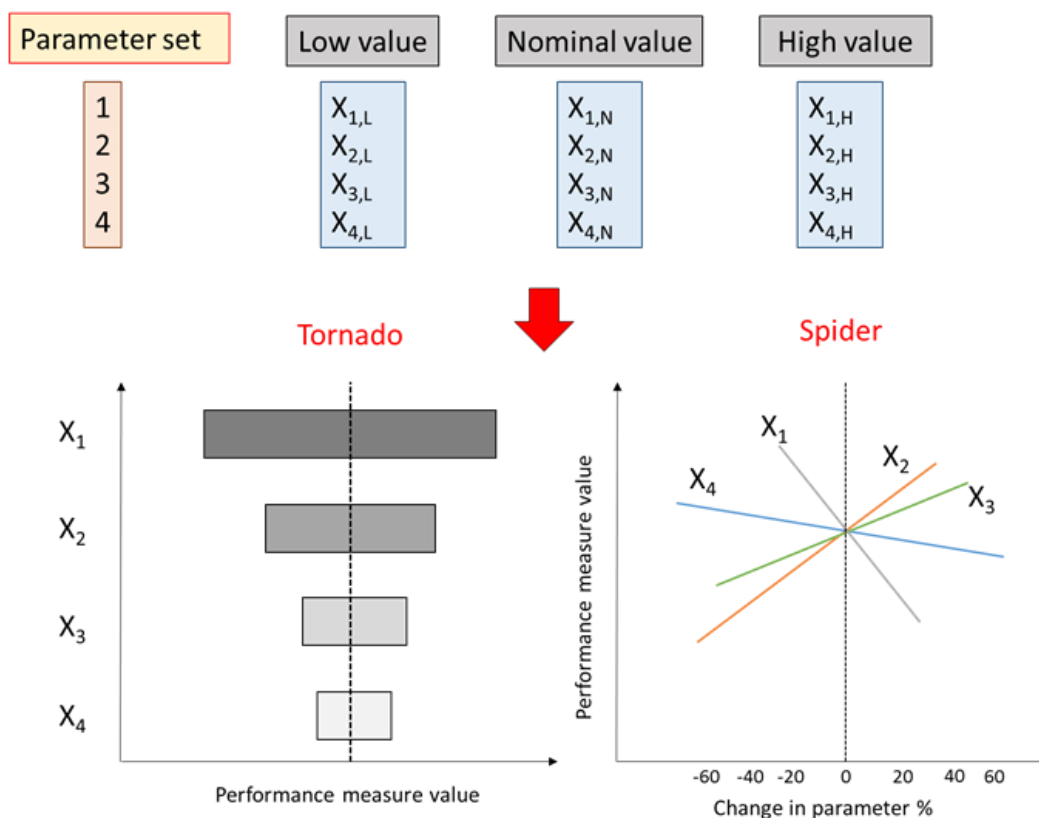


Figure 8. Visual representation of deterministic sensitivity analysis

#### B.7.2.5.2 Global Sensitivity Analysis

To cover the whole parameter space, global sensitivity analysis **should** be applied to analyze the effects on the output of both individual inputs and interactions between the input variables. 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. A common method is to analyze 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, a method used to calculate the first-order and total-order sensitivity indices. This calculates the direct contributions to the variance of the individual inputs as well as indirect contributions through interdependencies among input variables [98], [99], [103], [106]. The selection of CCU-specific independent variables for SA needs to incorporate parameters from each system element (e.g., *CO<sub>2</sub> capture, CO<sub>2</sub> conversion plant, H<sub>2</sub> unit, minerals treatment, etc.*) in order to obtain better insight into the individual units and facilitate identification of the most influential variables (e.g., *CO<sub>2</sub> price, other input prices, energy consumption, and price*).

#### B.7.2.5.3 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 identify key variables for improving the inventory data and calculation of indicators in an iterative way. Practitioners **should** focus the improvement of data quality to those data items that have insufficient quality yet strongly influence the sensitivity of the overall result (see Figure 9); note that the boundaries, axes, and square sizes are subjective and derive from the decision maker).

If data quality cannot be further improved the results can lack overall certainty, which needs to be documented [50]. Conversely, practitioners do not need to focus on improving data items that are already of high quality or have demonstrated very low sensitivity.

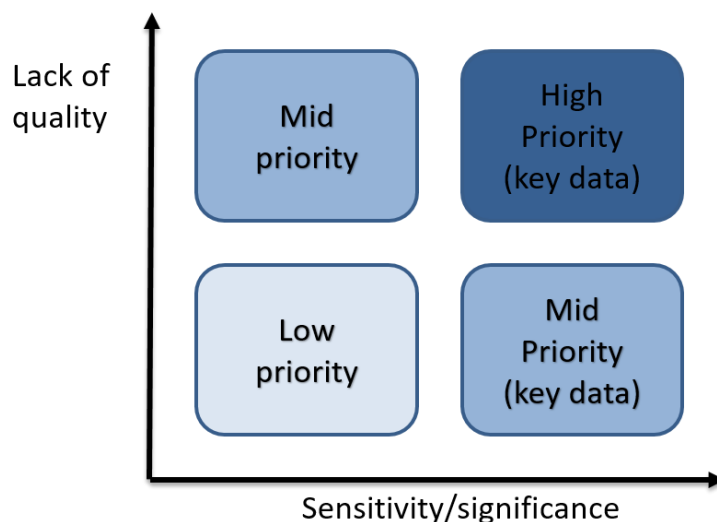


Figure 9. Priority setting for improving key data for inventory, adapted from [4]

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 chapter B.3.3). A baseline scenario and potentially an optimistic and pessimistic scenario are pre-defined during the goal phase. The development of different scenarios must be justified appropriately with respective assumptions. Scenarios are first defined during the goal phase but might be adapted, or further scenarios might be added, when reaching the interpretation phase, after identifying key variables that greatly influence the model output. Other than UA, scenario analysis goes beyond considering the parameters' known uncertainty ranges and instead considers a broader scope of possible future events.

#### B.7.2.6 Further Reading

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 [96], [106]). Qualitative methods of uncertainty analysis tend to be flexible and adaptable to different circumstances, as shown in [96], [107]. Quantitative uncertainty methods such as Taylor Series Approximation, Monte Carlo simulations, and Bayesian statistical modelling are described in standard textbooks [108]–[110].

### B.7.2.7 Provisions

Provisions B.18 - Sensitivity and Uncertainty Analysis	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Conclusions, limitations, and a basis for recommendations with respect to the calculated results shall be provided</li> <li>2) Uncertainty analysis shall be conducted and output uncertainty identified</li> <li>3) Sensitivity analysis shall be conducted and key variables identified</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) For the first assessment iteration, local sensitivity analysis should be conducted</li> <li>2) To cover the whole parameter space, global sensitivity analysis should be conducted</li> <li>3) Efforts to improve data quality should focus on data items that are of insufficient quality yet strongly influence the sensitivity of the overall result</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Qualitative uncertainty analysis may be conducted in the research phase</li> </ol>

## B.7.3 Interpretation of Indicators

### B.7.3.1 Introduction

The information and trends revealed by the indicators are interpreted in order to answer the original questions posed by the assessment goal. Indicators help to compare and choose between multiple alternatives (*e.g., profitability indicators help to choose between investment alternatives; cost-based indicators allow comparison between different CO<sub>2</sub> emission reduction technologies with respect to the marginal abatement cost curve*). The interpretation of assessment indicators gives a positive, neutral, or negative signal about the opportunities of a given technology or product. This can either derive from comparison of alternatives (*e.g., profitability indicators*) or from comparison with a defined benchmark value (*e.g., technical indicators, CapEx, OpEx*) [20].

### B.7.3.2 How to Interpret Indicators

#### B.7.3.2.1 General Remarks

The interpretation of technical, economic, or techno-economic indicators **shall** be conducted in compliance with the indicator definition, especially according to its described limitations. This also requires that interpretation of indicators is in accordance with the specifications set in the goal and scope. In general, indicator values **shall** be compared to an alternative value (*e.g., based on selected benchmark systems*). Key indicators and key indicator values can be derived from the results and discussion sections of similar studies or by iteratively applying uncertainty and sensitivity analyses (see Figure 9).

#### B.7.3.2.2 Threshold analysis for key input variables

After defining thresholds for indicators (*e.g., minimum selling price lower than benchmark price*), practitioners can employ a type of local sensitivity analysis, termed threshold analysis, to identify the threshold values of input variables at which the indicator results lead to a change in the main conclusion.

Threshold analysis **should** be conducted for identified key input variables (*e.g., CO<sub>2</sub> input price, H<sub>2</sub> input price, etc.*).

A break-even point is the threshold at which a project becomes profitable. For example, a break-even analysis could be applied to determine the maximum price for electricity that allows the project to be profitable with an NPV greater than zero.

#### *B.7.3.2.3 Interpreting Profitability Indicators*

Indications derived from static indicators are recommended to be regarded 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 [87]. Static indicators only deliver limited information and must be interpreted with caution. The general investment alternative incorporated in static indicators is 'no investment.' Dynamic indicators are particularly sensitive to the interest rate utilized. The quality of the assumed interest rate must be considered when forming opinions on the values of dynamic indicators. The outcomes of economic simulations are interpreted as per other profitability indicators according to the question they are intended 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 lifespan of the plant; when comparing alternatives, shorter payback time 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 the interest rate for an investment with the same risk characteristics on the capital market, or exceeds a target value; Practitioners **shall** interpret IRR together with respective indicators of absolute profitability
- For dynamic payback time, a positive indication is given if the payback time is shorter than the expected plant lifespan; when comparing alternatives, the shorter payback time is preferred

#### *B.7.3.2.4 Interpreting Indicator Uncertainty*

Indicator uncertainty determines whether the result can be used for deriving conclusions and recommendations according to the goal and scope. If the indicator shows unacceptably high uncertainty, improvement of the data quality, adaption of the TEA goal, or cancellation of the assessment is required. If the indicator uncertainty is acceptable, practitioners can compare the indicator results and their uncertainties to benchmark values. The interpretation **should** involve absolute indicator results as well as the uncertainty ranges.

Uncertainty ranges can take the form of uniform distributions or non-uniform distributions, such as normal distributions or skewed distributions. The interpretation of uncertainty ranges of multiple alternatives strongly depends on the decision-makers' risk preferences, meaning whether the decision maker is risk-seeking or risk-averse. Risk preferences **may** be documented for subsequent decision-making steps, for

example in multi-criteria decision analysis. Alternatively, a threshold value within the uncertainty range can be defined, above (or below) which the expected values are accounted for with a defined factor.

### B.7.3.3 Further Reading

In the literature, interpretation approaches are usually presented with descriptions of respective indicators. Therefore, the further reading (chapter B.4.5.3) provides additional information on this issue.

### B.7.3.4 Provisions

Provisions B.19 - Interpretation of Indicators	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) The interpretation of any indicators shall be conducted in compliance with their definition, especially according to its described limitations</li> <li>2) Indicator values shall be compared to an alternative value</li> <li>3) IRR shall be interpreted only together with respective indicators of absolute profitability</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) The interpretation of indicators should involve absolute indicator results as well as the uncertainty ranges</li> <li>2) Threshold analysis should be conducted for identified key variables</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Risk preferences of practitioners may be documented for subsequent decision-making steps</li> </ol>

## B.7.4 Multi-Criteria Decision Analysis

### B.7.4.1 Introduction

Multi-criteria decision analysis (MCDA) is a method for supporting decisions that involve multiple dimensions or criteria and thus allows evaluation of trade-offs. It allows economic, social, and environmental criteria, including competing priorities, to be systematically evaluated [111]. For example, 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 chapter 0). MCDA is typically established in five steps:

1. Identifying objectives
2. Identifying options for achieving the objectives
3. Identifying the criteria to be used in comparing 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 [112]–[114]. 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 chapter 0). MCDA can 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 (see Wrapping document, A.5).

### B.7.4.2 How to Conduct Multi-Criteria Decision Analysis

MCDA **may** be applied to the interpretation of the TEA as it might help in subsequent decision making. The whole spectrum of criteria relevant for decision making **should** be presented to decision makers. Preliminary efforts have been made to develop a reliable MCDA framework to interpret technologies at early development stages [115], [116]. The principles of MADM and MODM are explained in the following paragraphs.

#### B.7.4.2.1 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 task 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 10, where  $X_{ij}$  is the rating of alternative  $i$  with respect to criterion  $j$  and  $W_j$  is the weight of criterion  $j$ . The criteria rankings are multiplied by their corresponding weights and then summed for each alternative to provide a final score. Several conversion routes and process configurations exist within CCU, even for similar products. MADM can be used to create a common basis for comparisons between different projects, including benchmark systems. The goal and scope define the required range of technical and economic criteria as expressed by their indicators (*e.g.*,  $CO_2$  capture rate, GHG abatement cost, product market price, employment opportunities).

**Table 10. Common structure of a MCDA problem**

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

Many MADM methods have been developed, including: 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 Réalité (ELECTRE), and Preference Ranking Organization Methods for Enrichment Evaluations (PROMETHEE) [117]. AHP has gained popularity due to its procedural simplicity, although a few other techniques, such as ELECTRE III and PROMETHEE, are also popular. However, no single MADM model can be ranked as best or worst; instead, each method has its own strength and weakness depending upon the intended application and objective of the assessment [118].

#### B.7.4.2.2 Multiple-Objective Decision Making (MODM)

This concept nearly always provides not a single 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 10). MODM may be used to identify and display all trade-offs among the investigated indicators. This means that achieving the optimum for one objective requires some compromise in one or several other objectives (e.g., *capital cost versus operating cost, selectivity versus conversion, quality versus conversion, or profit versus safety cost*). The mathematical formulation of a MODM problem consists of defining 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<sub>2</sub> conversion, undesirable side products, reactor temperature*).

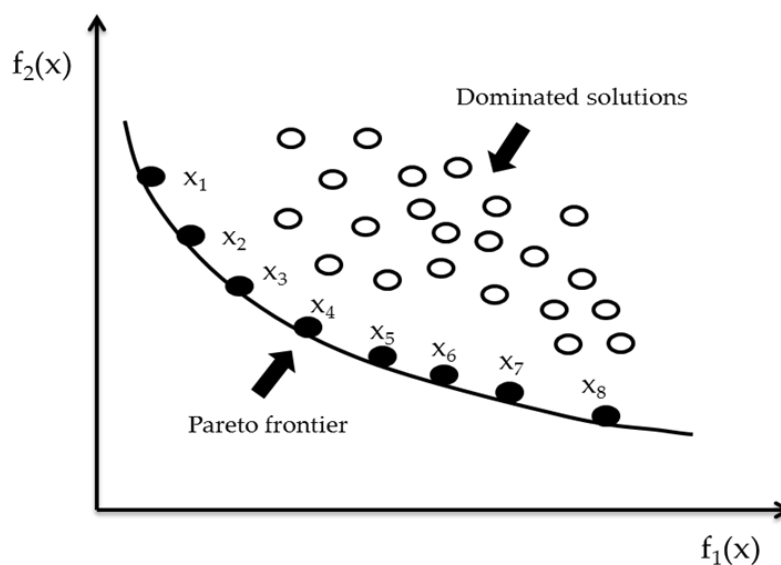


Figure 10. Potential range of solutions for a two-objective optimization problem showing the Pareto frontier

Although there are many choices on the Pareto frontier, in subsequent decision making one solution will be picked. There are two approaches to finding a single solution in MODM: methods with prior preferences (or preference-based procedures) and methods with posterior preferences (or ideal procedures) [119], [120].

The literature includes many approaches to solving MODM [121]. Among 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 for this are the weighted sum method (WSM) and weighted product method (WPM) [122].

#### B.7.4.3 Further Reading

Additional information about the selection and application of MCDA approaches can be found in research articles from various fields [123]–[128].



## B.7.4.4 Provisions

<b>Provisions B.20 – Multi-criteria Decision Analysis</b>	
<b>Shall</b>	
<b>Should</b>	1) The whole spectrum of criteria relevant for decision making should be presented to decision makers
<b>May</b>	2) Multi-criteria decision analysis may be applied to the interpretation of the TEA

## B.8 Reporting

### B.8.1 Introduction

The reporting phase 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. Furthermore, requirements within an audience type can vary (*e.g., specific reporting requirements for the EU will differ from those for the US DOE*). Therefore, no specific provisions on the style of the report are given here; instead, the provisions cover aspects that must be included to ensure transparency and accuracy.

### B.8.2 How to Create a Report for a CCU TEA

#### B.8.2.1 General Reporting Principles

Regarding the content of the TEA report, practitioners **shall** cover all phases of the study in the TEA report, meaning the contents of the goal, scope, inventory, indicator calculation, and interpretation phases. If the provisions of this Guidelines document are applied, conformity **should** be declared and explanations **should** be provided for any deviations. The report **should** list the names and backgrounds of the practitioners that conducted the study and include a description of whether and how a review was conducted. Practitioners **may** apply LCA reporting principles in addition to TEA reporting, especially when conducting LCA and TEA in parallel.

The report **shall** present in a transparent manner all important assumptions, relevant inventory data and their sources, calculation methods and results, as well as respective uncertainties and sensitivities, recommendations and limitations. In the main report, practitioners **shall** set indicator results in relation to uncertainties and sensitivities in the main report to avoid misinterpretation. Furthermore, practitioners **may** provide the calculation model used in the analysis to allow readers to test different assumptions and adapt the calculation to their needs.

The format and language of the TEA are decisions for the practitioner, but need to reflect the requirements of the audience. Practitioners **shall** present findings using clear language to avoid misinterpretation, particularly in Executive Summaries. The reporting **should** be aligned to the requirements of the audience in terms of commonly accepted terminology, presented content, as well as selected presentation format. Reports **should** include a summary in written form (such as an Executive Summary) and a technical summary in table form (see Table 15 Annex), to enable the reader to easily access the data used in the assessment. Practitioners need to state data sources clearly, which is important to ensure reproducibility and full traceability for the reader [4]. If confidential data were used and details are redacted in the report, practitioners need to include a statement about what information has been omitted.

#### B.8.2.2 Addressing Audiences

While readers with R&D expertise (*e.g., researchers, funding agencies*) expect the use of technical terminology, the report must also be accessible to readers who lack specialist expertise (*e.g., government agencies, general public*), to reduce the risk of misunderstanding and misinterpretation. The report can take numerous forms (*e.g., academic publication, corporate report*) and needs to be tailored to the audience's requirements. The readability of the report also needs to be aligned to the target audience(s).

#### B.8.2.2.1 Audiences for R&D-perspective TEA

R&D-perspective TEAs are likely to be of interest to R&D experts (academic, industrial, or governmental). This audience demands information regarding the technical performance of the product systems, and expects the use of technical terminology and detailed reporting of specific technical indicators common to 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. To illustrate and measure the social effects (*e.g., job creation, injury rate, workers' rights*) for a product system or project, social LCA assessments approaches can be used [129]. Reporting TEA results to R&D experts can lead to detailed feedback on technical performance or to the adaptation of the work in other research groups, which is why confidentiality issues can arise.

Another major audience for R&D-perspective TEAs is funding agencies, which require not only information on technical performance, but also a description of social and economic benefits (*e.g., creation of jobs, local value chains, and new industries*). Required indicators are typically at the practitioner's choice, while in certain proposals the calculation of specific indicators (*e.g., GHG abatement cost per kg product*) might 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 audiences who are unfamiliar with the topic. Reporting TEA results to funding agencies typically occurs in the course of a funding proposal or project report, both of which are crucial to securing R&D funding.

#### B.8.2.2.2 Audiences for Corporate-perspective TEA

Corporate-perspective TEAs are likely to be of interest to investors or corporate decision makers (*e.g., management*). These audiences demand the reporting of both technical and economic performance, and potentially social benefits as well. These audiences typically demand two levels of reporting detail, comprising a summary and a main version (see chapter B.8.2.5). While for the full report economic indicators need to be reported at the highest level of possible detail (*e.g., NPV, option pricing, liquidity planning*), technical results either require the introduction of detailed technical terminology or need to be reduced to an intermediate level of detail. Reporting is usually very timely, can take place at regular intervals, and is connected to important decisions (*e.g., budget allocation, 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 arise and might dictate that certain data cannot be released.

#### B.8.2.2.3 Audiences for Market-perspective TEA

Market-perspective TEAs are likely to be of interest to 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 they find indicators that integrate TEA, LCA, and potential social impact studies to be helpful (*e.g., the cost of greenhouse gas abated, the number of jobs created or maintained, reductions in fossil fuel imports*). Reporting to these audiences usually takes place at fewer or less 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 concerning the techno-economic aspects of the technology.

#### B.8.2.2.4 Further Audiences

Additional important audiences include journalists and the wider public. Similarly 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 prior to detailed discussion. A special

challenge when addressing the media and the public is the use of clear and easily understood 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.8.2.3 Reporting at Different Technology Maturities

Throughout all technology maturity stages a major task of the reporting phase is to present information for further decision making. At low technology maturity, decision making focusses on technology development. This is why practitioners need to inform audiences about the identified hotspots as well as underlying assumptions and limitations. Furthermore, the main sources and levels for qualitative – and, if available, quantitative – uncertainty are reported.

At higher levels of technology maturity the amount of reported information tends to increase. As uncertainties decrease, reporting focusses mainly on the results. Inventories consist of higher levels of process-specific primary data rather than generic or averaged secondary data, due to more knowledge about the process design. As the calculation models become more complex, transparent reporting of the data used for the calculation is required. This includes the reporting of main issues identified in quantitative uncertainty and sensitivity analyses, both to place any resulting conclusions into perspective and to ensure comparability of results.

### B.8.2.4 Reporting of System Elements

To facilitate comparisons with other studies and to enable effective identification of the most influential parameters in the process, particularly at low maturity, practitioners **should** report findings for system elements as well as the whole product system. 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 largest impacts on the whole system and identify where technological advances would create the greatest benefits.

### B.8.2.5 Executive Summary

For audiences without R&D expertise, an executive summary of the data, methods, assumptions, limitations, recommendations, and results needs to be included. It is recommended that the executive summary includes clear specific statements that cannot be misinterpreted. For example, statements can be phrased as:

*This study concluded that the price of methanol produced from CO<sub>2</sub> at 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 four times higher no matter what the inputs, process, or location. The latter statement could lead to incorrect general conclusions and judgements, such as loss of interest in a technology or even rejection of

its further development. Practitioners can add their personal recommendation on the technology, for example regarding its feasibility, but only following a transparent summary of the results, so that the audience can relate the results and recommendation and derive their own view.

### B.8.2.6 CCU-specific Reporting

From a techno-economic point of view, the amount of CO<sub>2</sub> 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 greenhouse gas abated, which is determined by the LCA. The amount of greenhouse gas abated corresponds to the reduction in greenhouse gas emissions achieved by the CCU process when compared to the reference scenario. In contrast, the amount of CO<sub>2</sub> utilized refers to the amount of CO<sub>2</sub> that the process uses to produce the product. It is important to distinguish between CO<sub>2</sub> used and greenhouse gas abated as the values can be very different and so any ambiguity can lead to misinterpretations (see chapter C. 4.2.2, Part C).

In addition to reporting the results for complete systems, it can be helpful to report some results for system elements separately. In doing so, their effects and impacts on the overall economics can be observed. For example, the results and sensitivity of electricity consumption in CCU methanol production, can be reported by each system element (for CO<sub>2</sub> capture, H<sub>2</sub> production, and methanol production separately) as well as for the overall system. Reporting the sensitivities of system elements separately can be especially helpful for identifying key variables within the 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 in order to avoid additional environmental impacts. When reporting the energy requirements (particularly electricity), it can be helpful to articulate the real-world implications of that requirement, for example the number of wind turbines needed to produce the required energy or the percentage of a country's present (and future) renewable energy production.

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 chapter B.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.8.3 Checklists for Reporting

Clear reporting enables the reader to follow the methodology and assumptions employed by the practitioner. The following checklist provides guidance regarding recommended minimum content for the executive summary and main report, and can be used as a quick reference guide to ensure that all essential 'shall' aspects are covered in the report. Practitioners **may** use the Reporting Checklist to ensure all aspects are covered.

### Checklist – Executive Summary

#### Goal Definition

- State goal and context of the study
- State intended application(s)

#### Scope Definition

- State product application and functional unit
- State system boundaries
- State benchmark products and systems
- State assessment indicators and methods

#### Inventory Analysis

- State key assumptions, relevant parameters, and their data quality

#### Calculation of Indicators

- State main results

#### Interpretation

- State conclusions, limitations, and recommendations, if any

### Checklist – Main report

#### Goal Definition

- State goal, study context, and the reasons for the study
- State the intended application and target audience of the study
- State commissioners and authors of the study
- State limitations in the applicability of the study
- State the analyzed scenarios and their conditions

#### Scope Definition

- State product application(s), functional units, and reference flows
- For corporate-perspective TEAs, state at least one customer group and their needs
- State elements and boundaries of product system in a graphical scheme, potentially state reasons for excluding upstream processes
- State benchmark products and systems
- State technology maturity for system elements and the overall product system
- State the selected indicators and assessment methods, including data availability associated with technology maturity
- Document remaining inconsistencies, if any

### Inventory Analysis

- Document technological and economic parameters, decisions and assumptions, where possible based on functional unit and reference flow
- Justify context-specific assumptions and parameters, discuss scale and maturity, as well as temporal, geographic, and regulatory context and related limitations and risks, especially for key inputs such as CO<sub>2</sub>, hydrogen, electricity, minerals, fossil feedstocks, or catalysts
- State types and sources of data, including quality and confidentiality
- Report CO<sub>2</sub> capture cost; otherwise, if not available, include statement
- Document characteristics and limitations of data utilized
- Document data in SI units or provide unit definitions
- Document data for each system element independently
- Display economic data collectively

### Calculation of Indicators

- State calculation procedures, including potential additional assumptions and estimates utilized
- Present equations for each indicator applied; for uncommon methods, describe motivation
- State all relevant results for the overall system as well as for each system element individually

### Interpretation

- Describe uncertainty and sensitivity of the results
- Provide conclusions, presenting the whole spectrum of criteria relevant for decision making
- Discuss limitations
- State recommendations, if any

## B.8.4 Further Reading

A detailed guidance on LCA reporting principles, elements and targeting at different levels can be found in the ILCD Handbook [4]; for the most part these instructions can be adapted to TEA. For more information on actor-specific issues of stakeholder acceptance of CCU, see Jones *et al.* (2017) [130].

## B.8.5 Provisions

Provisions B.21 – Reporting	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) All phases of the study shall be covered in the TEA report</li> <li>2) Important assumptions, relevant inventory data and their sources, calculation methods, and results, as well as respective uncertainties and sensitivities, recommendations and limitations, shall be presented in a transparent manner</li> <li>3) Indicator results shall be set in relation to uncertainties and sensitivities in the main report</li> <li>4) Clear language shall be used in the TEA report</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>5) If the provisions of this Guideline document were applied, conformity should be declared and for deviations an explanation provided</li> <li>6) The report should list the names and backgrounds of the practitioners that conducted the study and include a description of whether and how a review was conducted</li> <li>7) The reporting should be aligned to the requirements of the audience in terms of commonly accepted terminology, presented content, as well as selected presentation format</li> <li>8) Reports should include a summary in written form (such as an Executive Summary) and a technical summary in table form</li> <li>9) Findings for system elements as well as the whole product system should be reported to facilitate comparison with other studies</li> <li>10) If economic incentives are included in the calculation, these <b>should</b> be clearly stated and their impacts clarified</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) LCA reporting principles may be applied in addition to TEA reporting, especially when conducting LCA and TEA in parallel</li> <li>2) The calculation model used in the analysis may be provided to allow readers to test different assumptions and adapt the calculation to their needs</li> <li>3) The Reporting Checklist may be used to ensure all aspects are covered</li> </ol>



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## B.10 Annex

Table 11. Examples of upstream elements for CCU product systems [30], [131], [132]

CO <sub>2</sub> emissions (direct) industry, recent estimates from various years [Mt <sub>CO2</sub> /year] [30]	CO <sub>2</sub> capture for combustion processes	CO <sub>2</sub> separation for all processes	H <sub>2</sub> production	Electricity production	
Coal power plant (PP)	9 031	▪ Post-process	▪ Absorption	▪ Steam-methane reforming	• Coal-fired PP (fossil coal & bio-based co-firing)
Natural gas PP	2 288	▪ Oxyfuel	▪ Adsorption	▪ PEM electrolysis cells	• Oil-fired PP
Cement production	2 000	▪ Pre-process	▪ Chemical looping	▪ Solid oxide electrolysis cells (SOEC)	• Gas-fired PP (natural gas, biogas)
Iron and steel production	1 000	▪ Chemical looping	▪ Membrane separation		• Nuclear PP
Oil refineries	850		▪ Hydrate-based separation		• Hydro PP
Oil power plant	765		▪ Cryogenic distillation		• Wind PP
Ethylene production	260				• Photovoltaic PP
Ammonia production	150				• Solar-thermal PP
Bioenergy	73				
H <sub>2</sub> production	54				
Natural gas processing	50				
Waste power plant	60				
Fermentation to biomass	18				

Table 12. Characterizing technology readiness levels for the chemical industry [52]

TRL	1	2	3	4	5	6	7	8	9
Phase	Research			Development			Deployment		
Title	Idea	Concept	Proof of concept	Preliminary process development	Detailed process development	Pilot trials	Demonstration & full-scale engineering	<i>Construction &amp; start-up</i>	<i>Continuous Operation</i>
Description	Basic principles observed and reported, Opportunities identified, Basic research translated into possible applications <i>(e.g., by brainstorming, literature study)</i>	Technology concept and application formulated, Patent research conducted	Applied laboratory research begun, 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 conditions expected at 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) experimental results, First process ideas	Simple parameter and property data, Alternative process concepts 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 center	Pilot plant, technical center, (optional) demo plant (potentially incorporated in production site)	Production site	Production site



Table 13. Draft for a technical summary table

System element	Parameter	Unit
<b>A</b> (e.g., CO <sub>2</sub> capture)	Flue gas	t/h
	CO <sub>2</sub> input	t/h
	CO <sub>2</sub> capture	%
	Electricity consumption	MW
<b>B</b> (e.g., Water electrolysis)	...	
	Deionized water	t/h
	...	
<b>C</b> (e.g., CO <sub>2</sub> conversion)	CO <sub>2</sub> input	t/h
	...	
<b>D</b> (e.g., Purification)	Electricity consumption	
	...	

Table 14. Examples of economic parameters and assumptions to be documented (adaptation to each specific TEA study is necessary)

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

Table 15. Technical summary table

<b>GOAL</b>	<b>CCU product</b>			
	<b>Intended application and reasons for study</b>			
	<b>Brief description</b>			
	<b>Intended audience</b>			
	<b>Commissioners and assessors</b>			
	<b>Limitations of study</b>			
<b>SCOPE</b>	<b>System boundary (i.e., cradle to gate)</b>			
	<b>Benchmark system</b>			
	<b>Plant size</b>			
	<b>Functional unit</b>			
	<b>System elements and technology maturity</b>	<b>System elements</b>	<b>Efficiency</b>	<b>Technology maturity</b>
	<b>Assessment indicators</b>	<b>1</b>		
		<b>2</b>		
	<b>3</b>			
	<b>4</b>			
	<b>5</b>			
<b>INVENTORY</b>	<b>Data sources</b>			
	<b>Energy sources and scenarios</b>			
		<b>REFERENCE CASE</b>	<b>CCU TECHNOLOGY</b>	
	<b>Base year</b>			
	<b>Currency</b>			
	<b>Location</b>			
	<b>Plant life time</b>			
	<b>CO<sub>2</sub> source and price (if applicable)</b>			
<b>Main inputs and prices (if applicable)</b>				
<b>CALCULATION OF INDICATORS</b>	<b>1.</b>			
	<b>2.</b>			
	<b>3.</b>			
	<b>4.</b>			
	<b>5</b>			
<b>INTERPRETATION</b>	<b>Sensitivity analysis: main factors and hotspots</b>			
	<b>Uncertainty analysis: main factors</b>			
	<b>Main conclusions</b>	•		
	<b>Recommendations</b>	•		

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# PART C LCA Guidelines

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## Contents Part C

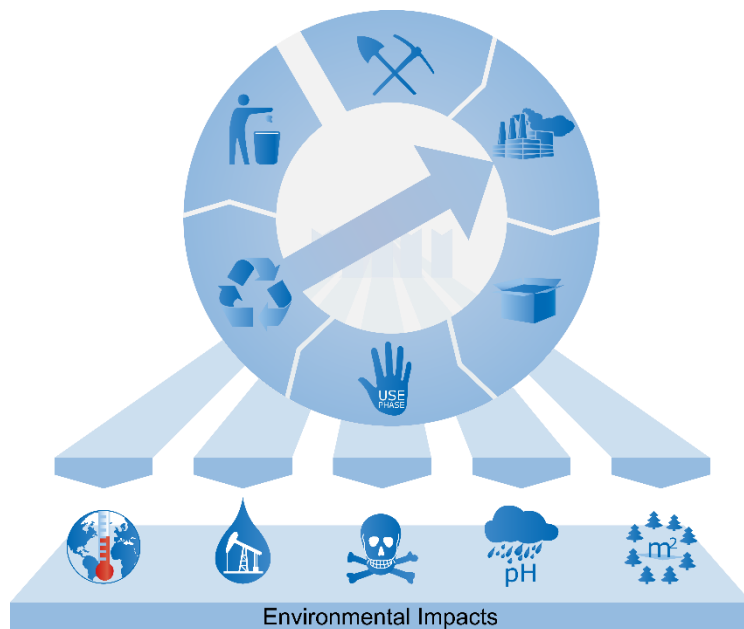
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## C.1 Introduction

### 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 (central circle)

Life cycle assessment (LCA) is a methodology to account for the environmental impacts of a product or service throughout its entire life cycle. The 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<sup>1</sup>. Due to its holistic approach, LCA avoids shifting problems 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 Organization for Standardization (ISO) in ISO 14040 and 14044 and is still updated and extended regularly.

According to the ISO standards, an LCA study is sub-divided into four phases (Figure 2):

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

<sup>1</sup> To aid readability, these Guidelines use the term “environmental impacts” instead of “potential environmental impacts.” However, in practice, LCA is only able to assess potential rather than actual environmental impacts.

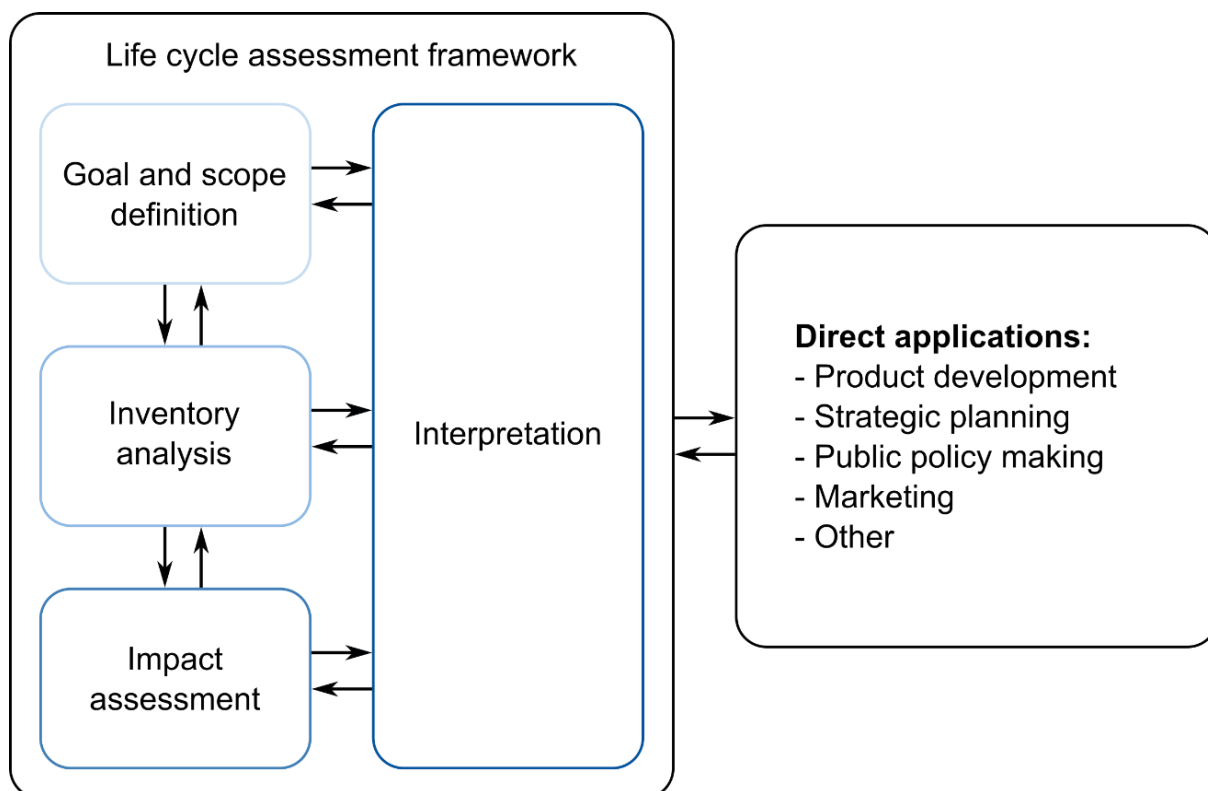


Figure 2. General framework for life cycle assessment [1]

All phases are interdependent, e.g., the gathered life cycle inventories must fit the goal and scope with respect to time and space. In practice, this interdependence renders LCA an iterative approach, as data availability is often uncertain at the beginning of an LCA study. Furthermore, the entire life cycle assessment framework is influenced by its supposed direct applications and vice versa (Figure 2).

The need for standardizing LCA assessment of CCU technologies has been identified by the European Commission [2]. In addition, it was shown that LCA studies of CCU showed large variation in results even for identical technologies [3]. Therefore, the major objective of this document is to standardize 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, involving substantial methodological choices and various pitfalls. These difficulties lead to wide differences in current LCA practice in the field of CCU, which may be misleading for decision makers. Building upon existing LCA standards and guidelines, the present Guidelines document 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 provides short and concise guidance on CCU-specific challenges for LCA and is complementary to existing standards and guidelines. Therefore, general issues of LCA are omitted if they are not specific to 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 recommend sources of further reading.

This document is based on the life cycle assessment standards ISO 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 (Figure 2). Each chapter provides a short general introduction to the LCA aspect to be discussed. These introductions are provided within boxes and may be skipped by experienced LCA practitioners. Subsequently, CCU-specific challenges are described and recommendations are given. Each chapter concludes by providing a list of provisions that shall/should/may be performed.

These provisions have been developed to enable consistent and comparable LCA studies for CCU, and are therefore more restrictive than the general ISO framework. Thus, there may be a need to add further tasks to those discussed in this document if they are important for a specific case study. Such additions are not excluded by the present provisions. However, there is a need for a consistent methodological core for LCA of CCU, which these provisions provide.



## C.3 Goal Definition

### General Introduction

Every LCA study starts with the goal definition. According to ISO 14044, 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 the 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]; furthermore, 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 these impacts relative to other products. Therefore, the importance of establishing a precise and reasonable definition of the initial research question cannot be over-emphasized, because the goal definition is the starting point for deriving important methodological choices in LCA, such as defining the system boundary and co-product allocation.

*Further recommended reading:*

*Baumann and Tillman offer a short and comprehensible description of the goal definition in Chapter 3.1 (p. 74ff.) [8]. A more detailed description of the goal definition is given in Chapter 5 of the ILCD Handbook (p. 29ff.) [5]. The topic is also covered in Chapter 2.1.1 of Curran's handbook (p. 17ff.) and in part 3 Chapter 2.2. (p. 456ff.) of Guinée's handbook [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 of CCU Technologies

LCA can answer many different kinds of questions. To get an overview, we start by identifying typical goal definitions for CCU from the literature. As stated above, most CCU technologies are in early stages of development and aim to reduce environmental impacts. Therefore, it is not surprising that most LCA studies of CCU aim to quantify the potential reduction of environmental impacts that can be achieved by CCU processes or products relative to existing processes [13–31]. Most studies also include a contribution analysis [15–17, 20–24, 27–29] of environmental impacts to identify opportunities for improvement. LCA can also evaluate which CCU technology makes the most environmentally beneficial use of scarce resources, such as hydrogen produced from renewable energies [32]. Once CO<sub>2</sub>-based products are deployed in markets, LCA can be used for environmental product declaration [33–35].

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

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 the 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 – for product declaration – which product to buy*).

In most cases, CCU technologies aim to provide less environmentally harmful alternatives to products that are already offered in the market. For this reason, these Guidelines focus 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 for each study. Furthermore, the class of the assessed CCU technology **should** be stated, as classification can help to resolve methodological issues (A.3.2). If a classification is deemed to be unsuitable, this **should** be reported and the reasons explained. In addition, the requirements of ISO 14044 **shall** be fulfilled as listed in the introduction to this chapter. Following the ILCD recommendation, each assessment **shall** state its potential limitations and **shall** identify the commissioner of the assessment and all other influential actors. For CCU technologies in stages of early development (low technology readiness level, TRL), studies can result in comparisons of ‘apple vs. oranges’, since most conventional reference technologies are mature and have been optimized over decades. In contrast, low-TRL processes usually have higher energy demand or solvent consumption, for example, because heat integration and/or processes are not yet known or optimized. At the same time, low-TRL processes lack auxiliary processes such as product purification steps after reaction. Thus, LCA studies of lab-scale processes can either under- or over-estimate environmental impacts. These aspects **should** always be considered in studies comparing a high-TRL technology to a low-TRL technology (see Provisions A.1). For low-TRL processes, studies are most useful to identify opportunities for environmental improvement via contribution analysis followed by sensitivity analysis. However, a comparison between a low-TRL CCU technology and a high-TRL reference technology can still provide 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 a future reference process or a technological development [36–42]. Note that the prediction of future developments introduces another source of uncertainty.

### C.3.1.1 Provisions

Provisions C.1 - Goal Definition	
<b>Shall</b>	1) The intended application of the study shall be stated
	2) The reasons for conducting 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 the public
	5) Potential limitations shall be identified and clearly reported
	6) The study commissioner and all other influential actors shall be stated
<b>Should</b>	1) A research question should be chosen from the most common research questions (as listed in C.3.1)
	2) The class of the assessed CCU technology should be stated. If a classification is deemed to be unsuitable, this <b>should</b> be reported and the reasons explained.
<b>May</b>	

## 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** describe the conditions and assumptions under which the results of the study are valid. Therefore, every aspect of the scope definition is closely related to and must be aligned with the study's goal.

According to the 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 (C.4.1)
- System boundaries, completeness requirements, and related cut-offs (C.4.2)
- The life cycle inventory modeling framework and co-product management (C.4.3)
- Other life cycle inventory data-quality requirements regarding technological, geographical, and time-related representativeness and appropriateness (C.4.4)
- Special requirements for comparative assessments (0)

*Further recommended reading:*

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

### C.4.1 Product System, its Function, Functional Unit, and Reference Flow

#### General Introduction

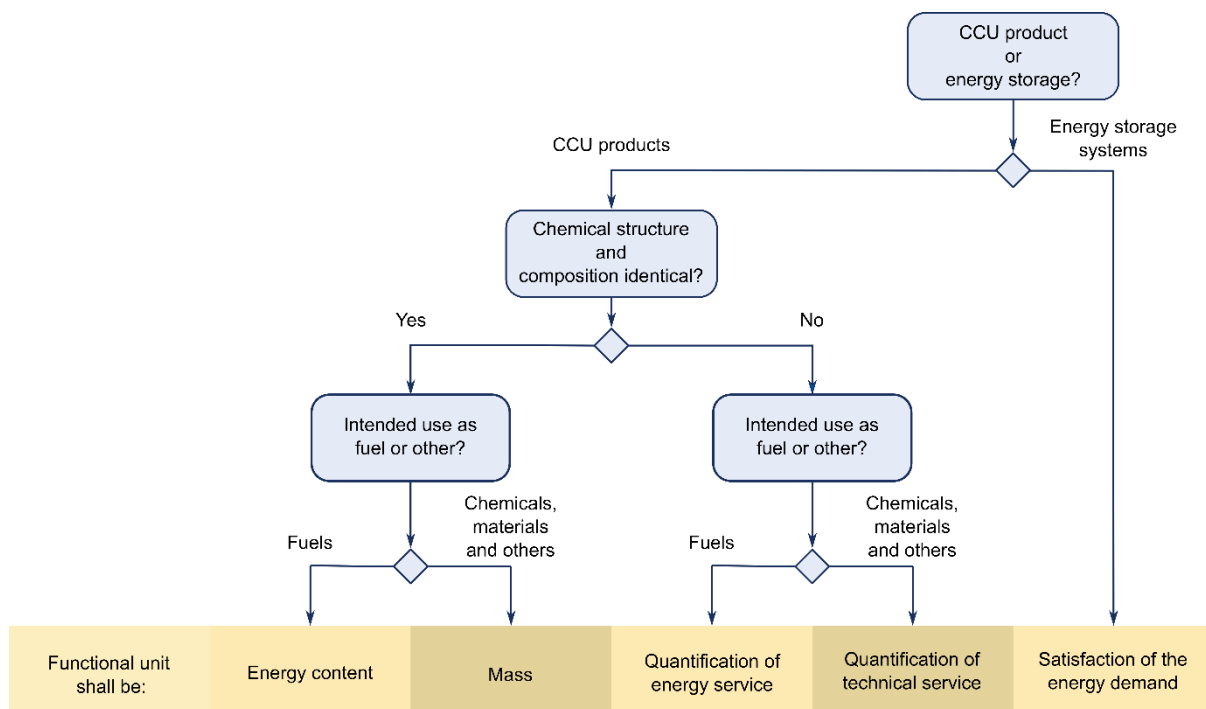
Life cycle assessment quantifies the environmental impacts of a product or process system on a relative basis with respect to its function (*e.g., global warming impact per kg of product*). This relative basis is the functional unit, which quantifies the performance of a product system or service. The 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 from 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 at 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 beyond this scope. Excluded functions **shall** still be documented and included in the final report.

### C.4.1.1 Defining Functional Units for CCU Technologies

Most LCA studies of CCU aim to compare CCU technologies against a benchmark (C.3.1). The functional unit ensures reliable comparison of the assessed technologies. However, different LCA studies for identical technologies might apply different functional units, thereby complicating comparisons between studies or even making them incomparable [3]. To increase comparability among studies, we derive functional units for each class of CCU technologies from current LCA practice and provide a decision tree to define a suitable functional unit (Figure 3).



**Figure 3. Decision tree for LCA of CCU: a) suitable functional unit.** For calculation of the energy content, the lower heating value is recommended. If the respective chemical structures or compositions are not identical, define the functional unit in such a way that the performance is comparable for the defined application of the products. Note that combustion characteristics might differ between chemically dissimilar fuels, and thus the energy service of a specific application must be compared rather than the energy content. Assessments of energy storage systems cannot be considered as stand-alone, as they offer additional degrees of freedom to the energy system. The functional unit shall be the satisfaction of energy demand over a period of time.

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<sub>2</sub>-derived and conventional products will behave identically in all applications. However, as enhanced comparability is a major objective of these Guidelines, we recommend using mass for comparisons.

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

For **CO<sub>2</sub>-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 in such a way that the technical performance within the defined application of the products becomes comparable (*e.g., compare detergents based on their cleaning performance rather than on mass*).

The functional unit of **CO<sub>2</sub>-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 must 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 travelled via a specified vehicle/ship/aircraft*), since combustion properties may be different and thus comparability based on energy content is not guaranteed [43].

**Energy storage** enables delaying the use of electric energy after it is generated from sources of primary energy, thereby temporally decoupling electricity generation from consumption. In other words, electric energy that is generated at one time can therefore be stored in order to help meet demand at some later time [44]. Through temporally decoupling generation and consumption, energy storage offers additional degrees of freedom to operate electricity generation in a more efficient way and can thus lead to lower environmental impacts of the total energy system. However, potential impact reductions strongly depend on the dynamics of demand and supply through the energy system in which the energy storage operates, and the energy storage characteristics (*e.g., charge- and discharge-rated output*), power ramping capability, and the storage duration between charging and discharging. Due to the dynamic nature of energy systems with or without energy storage, the functional unit may not be defined as an amount of energy. Instead, the functional unit **shall** be defined as the satisfaction of energy demand over a period of time (*e.g., as a time series of annual energy demand with a temporal resolution of one hour*).

To compare energy storage systems that have different characteristics, they shall be compared against a baseline energy system lacking any storage capacity. In a second step, the environmental impacts of the energy storage alternatives can be compared.

The decision tree shown in Figure 3 determines the appropriate functional unit by answering up to three questions:

1. Is the subject of the study considered as a CCU product or an energy storage system?
2. If the subject of the study is a CCU product, is it chemically identical to the benchmark product or not?
3. Is the subject of the study intended to be used as a fuel or not?

There are other potential functional units that might be appropriate to very specific goals [45]. For example, defining the functional unit as “mass of CO<sub>2</sub> utilized” can be useful for comparing CCU to CCS [46, 47]. If the goal is to determine which technology makes most efficient use of renewable energy to reduce GHG emissions, then it could be meaningful to define the functional unit as “energy consumed” [26, 27]. Those types of functional units are beyond the scope of this document, but may be selected if appropriate.

## C.4.1.2 Provisions

Provisions C.2 - Functional Unit	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) A functional unit quantifying the technical performance of a product system or a service shall be defined unambiguously</li> <li>2) Excluded functions shall still be documented and reported</li> <li>3) For products with identical chemical structure and composition to their conventional counterparts, mass shall be used as a functional unit (<i>e.g., 1 kg of substance</i>)</li> <li>4) For fuels with identical chemical structure and composition to their conventional counterparts, the energy content shall be used (<i>e.g., 1 MJ of substance (LHV)</i>)</li> <li>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</li> <li>6) For fuels with different chemical structure and chemical composition to their conventional counterparts, the application shall be stated within the functional unit (<i>e.g., 1 kWh of electricity from combustion in gas turbine of type X</i>)</li> <li>7) For energy storage, the functional unit <b>shall</b> be defined as the satisfaction of energy demand over a period of time (<i>e.g., as an annual time series of energy demand at a temporal resolution of one hour</i>)</li> </ol>
<b>Should</b>	
<b>May</b>	<ol style="list-style-type: none"> <li>1) LCA studies may exclude additional functions that are beyond the study scope. Excluded functions <b>shall</b> still be documented and reported</li> </ol>

## 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 system boundary separates the product system from the technosphere and the ecosphere. The technosphere contains all other technical systems transformed by humans, whereas the ecosphere refers to the environment containing all other systems. Each product system has its own system boundary, but when conducting comparative studies these need to be analogous.

Flows that are exchanged between processes are called technical flows, whereas flows exchanged between processes and the environment are called elementary flows. Technical and elementary flows are gathered in the life cycle inventory (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 product systems are formed. As a result, the system boundaries for an LCA study of a simple product would need to encompass the entire global technosphere. 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, whereas other processes and flows are omitted (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 on environmental contribution; the latter is the most accurate cut-off criterion: *For example, highly toxic substances might make insignificant contributions to mass and energy balances, but may have major contribution in toxicity.*

Applying cut-off criteria reduces the completeness of a 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

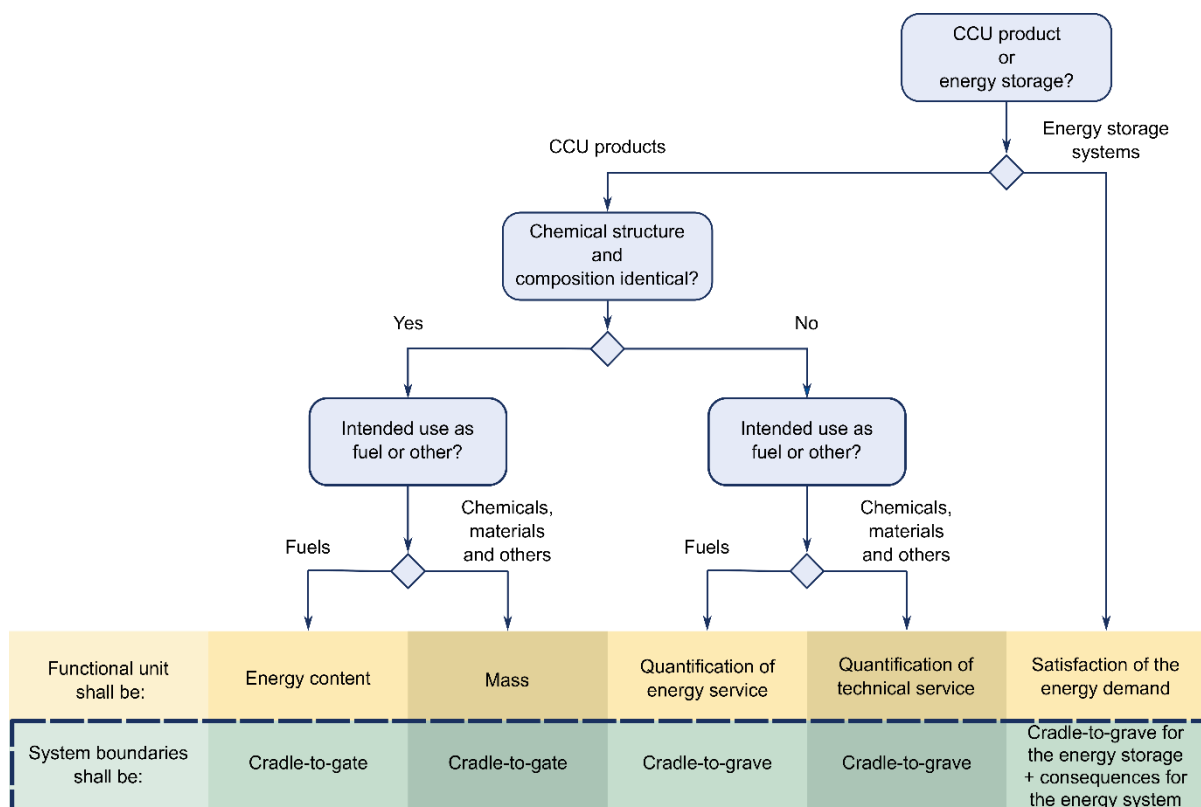


**Figure 4.** *The cradle-to-grave approach accounts for the entire life cycle of a product system. A cradle-to-gate study ends at the factory gate and does not account for any downstream environmental impacts.*

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 which the system boundaries only encompass the product system from extraction of raw materials to the final product leaving the factory gate (Figure 4). In fact, in some situations, it is impracticable to cover the entire life cycle (*e.g., if a product has numerous but unknown potential applications*). In those cases, the use of a cradle-to-gate approach and the associated limitations shall be stated unambiguously. The most prominent limitation is that a cradle-to-gate approach is not sufficient to assess whether a process is carbon- neutral or negative (C.7.1). Note that a cradle-to-gate assessment is only sufficient in cases where no large, structural changes are expected<sup>2</sup>. In the following, we derive a set of system boundaries for CCU technologies, which are in line with the functional units derived in C 4.1.1.

<sup>2</sup> 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 that is decommissioned annually, i.e., production plants that reach the end of their life span [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 occur. This might be the case if CCU technologies are deployed on a global scale and thereby trigger large-scale changes. The ILCD Handbook refers to this as the distinction between goal situation A and B.





**Figure 5: Decision tree for LCA of CCU b). Up to decision 2: system boundaries. For CCU products with identical chemical structure and composition to their conventional counterparts, a cradle-to-gate approach is sufficient. For CCU products that are not identical to their benchmark, the entire life cycle (cradle-to-grave) shall be compared to the benchmark. For energy storage systems, the system boundaries shall cover the storage system itself (cradle-to-grave) and all consequences of operating the energy system with addition of this storage system.**

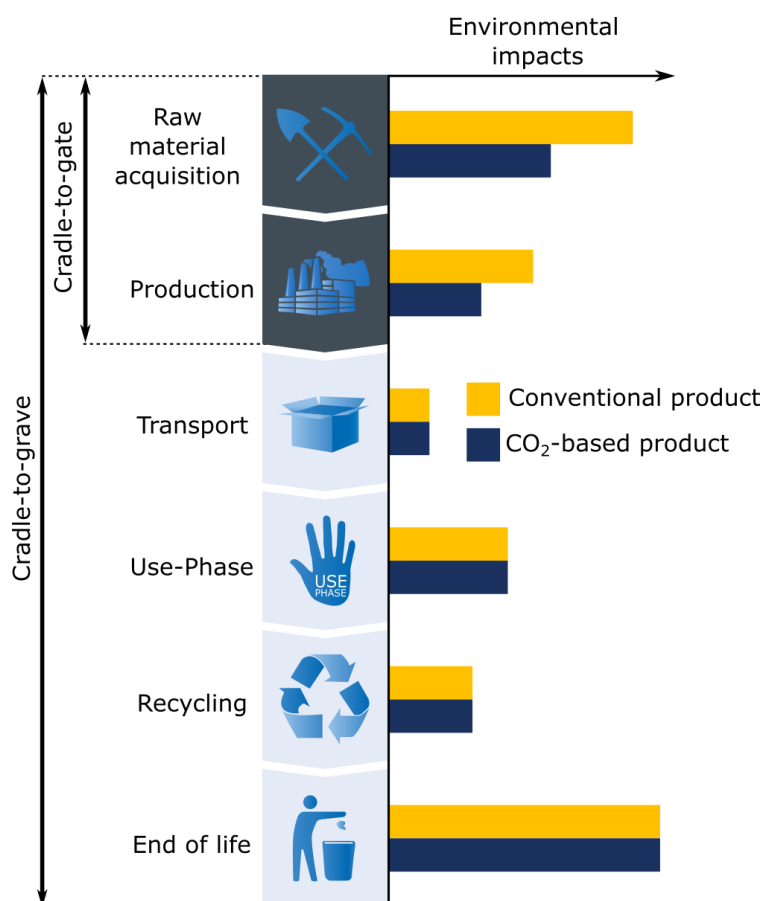
For **products and fuels with identical chemical structure and composition to their conventional counterparts**, a cradle-to-gate approach is sufficient, because: Since the products are chemically indistinguishable, both their downstream life cycle phases and environmental impacts will be identical (Figure 6).

System boundaries for **products with different chemical structure and composition to their conventional counterparts**, such as *CO<sub>2</sub>-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 in order to avoid problem-shifting from one life cycle phase to another (Figure 5).

For **fuels with different chemical structure and composition to their conventional counterparts**, a cradle-to-grave approach shall cover raw material acquisition; fuel production and transportation; plus the use phase and end-of-life, which often occur simultaneously during combustion. Omitting combustion can lead to qualitatively incorrect results, such as when different fuel types affect engine efficiencies and tailpipe emissions [43].

In some cases, omitting the combustion step might be necessary if the potential application is unknown (*e.g., in early stages of research and development*). Here, a cradle-to-gate approach **may** be applied for a preliminary LCA. In these cases, the results have limited validity and **shall** be interpreted with caution.





*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 therefore comparative studies only have to consider those phases.*

For comparison of **energy storage** options, the system boundaries **shall** cover the entire life cycle of the energy storage system (i.e., construction, operation, and decommissioning), and all consequences for the energy system (C.4.1.1). For marginal changes it might be sufficient to consider environmental impacts arising from the operation of the energy system. In other cases, the use of an alternative form of energy storage can lead to significant changes throughout the entire energy system, whereby construction etc. shall be accounted for. In every case, all consequences of operating the energy system when combined with the candidate storage system **shall** be included within the system boundaries.

The decision tree shown in Figure 5 determines appropriate system boundary units by answering two questions:

1. Is the subject of the study a CCU product or an energy storage system?
2. If the subject of the study is a CCU product, is it chemically identical to the conventional product or not?

The third question that was previously included in Figure 3 (*Intended use as fuel or other?*) is not relevant for defining the system boundaries; nevertheless, it is included in the decision tree to ensure a consistent layout, as it is relevant for the choice of functional unit.

### C.4.2.2 Upstream Environmental Impact from CO<sub>2</sub> Capture

CO<sub>2</sub> emitted to the environment is an elementary flow. Thus, captured CO<sub>2</sub> is often treated intuitively as a consumed emission ( $GW_{CO_2} = -1 \frac{kg_{CO_2e}}{kg_{CO_2}}$ ). However, captured CO<sub>2</sub> is a product of human transformation, and so consequently CO<sub>2</sub> is a technical flow and a chemical feedstock for CO<sub>2</sub> utilization. Thus, treating CO<sub>2</sub> as negative emission is usually incorrect, and so captured CO<sub>2</sub> must instead be treated like any other feedstock [12]. CO<sub>2</sub> sources **shall** be included within system boundaries as the supply of CO<sub>2</sub> leads to additional environmental impacts. Assessments **shall** comprise all process steps leading to environmental impacts, including CO<sub>2</sub> source, CO<sub>2</sub> purification, and transport, as shown in Figure 7.

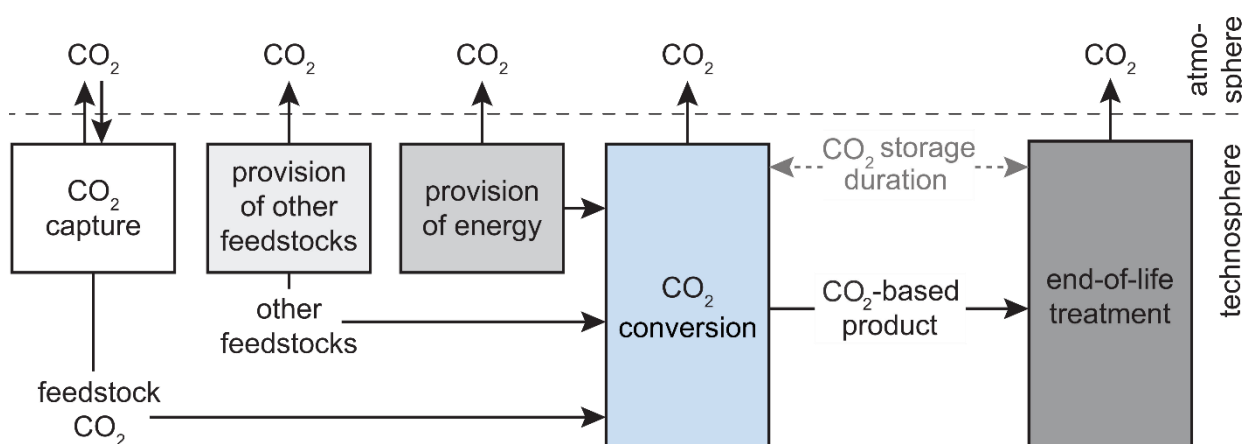


Figure 7. Schematic showing life cycle of CCU technologies from CO<sub>2</sub> source, supply of other feedstocks and energy to the end-of-life treatment. Environmental impacts must be considered during all life cycle stages. Adopted from [12].

### C.4.2.3 Provisions

Provisions C.3 - System Boundaries	
<b>Shall</b>	1) System boundaries shall be clearly defined and unambiguously described according to Figure 5
	2) System boundaries of all product systems to be compared shall be described
	3) CO <sub>2</sub> sources shall be included within the system boundaries, with all process steps, as the supply of CO <sub>2</sub> leads to additional environmental impacts
<b>Should</b>	
<b>May</b>	1) System boundaries other than those stated in Figure 5 may be applied if differences in downstream processes are not significant or if undertaking a preliminary study
	2) In early development stages, a cradle-to-gate approach may be applied for a preliminary LCA. In these cases, the results have limited validity and shall be interpreted with caution

### C.4.3 Life Cycle Inventory Modeling Framework and Solving Multi-Functionality

#### General Introduction

The life cycle inventory modeling framework defines how data are gathered and processed during a 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
- input and output systems (treatment of waste(s) and production of valuable product(s))

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

LCA methodology includes several choices concerning multi-functionality. The following methods are taken from the various standards [48–51] and guidelines [5, 52, 53]:

- 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

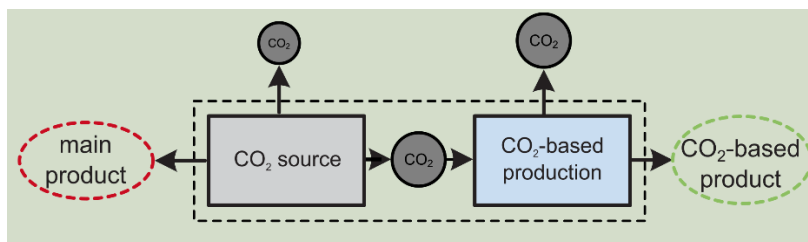
The system boundaries for LCA studies of CCU technologies start with acquisition of raw materials and end either at the factory gate or at the end of the product's life cycle (C.4.2).

During an LCA study, some 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, then inventory data specific to the process **should** be used. In other cases, this information might not be available, because products are purchased from a market (*e.g., electricity traded on 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 supply or demand induced by the CCU technology triggers large-scale structural changes. An example of a large-scale structural change is the installation of additional electrical power capacities in response to excessive electricity demand by a CCU technology, which could also affect production and consumption patterns in wider parts of the economy through changes in electricity prices. Such large-scale structural effects, however, might occur for a large-scale market introduction of CCU products. Nevertheless, assessing large-scale structural changes is typically beyond the scope of conventional LCA studies. The development of methodologies for this purpose, by integration of complex market models, is a topic of current research [46, 54, 55]. In these Guidelines, we focus on the scope of conventional LCA studies. Therefore, first, process-specific inventory data **shall** be used if available; Only otherwise **should** averaged market mixes be used as model inputs.

### C.4.3.2 Solving Multi-Functionality

Most CCU systems are multi-functional, because CO<sub>2</sub> sources often provide a main product in addition to CO<sub>2</sub> (Figure 8) [11]. For example, ammonia is produced by reacting hydrogen with nitrogen. Hydrogen can be co-produced with CO<sub>2</sub> in the steam-methane reforming process. Prior to the final stages of ammonia synthesis, CO<sub>2</sub> must be removed because it otherwise poisons the catalyst; consequently a pure CO<sub>2</sub> stream is extracted prior to ammonia synthesis but in most cases is emitted to the atmosphere. If this extracted CO<sub>2</sub> stream is captured rather than released, the main product ammonia and the co-product CO<sub>2</sub> are produced simultaneously (Figure 8). If the environmental impacts associated with the produced CO<sub>2</sub> stream need to be calculated, the total emissions of the system need to be split between the main and co-products.



**Figure 8. Stand-alone system analysis: Carbon capture from point source leads to the joint production of the CO<sub>2</sub>-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 can occur throughout the life cycle of CCU products. In general, the problem of multi-functionality is not specific to CCU, and 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 according to ISO 14044 and other guidelines. Subsequently, we demonstrate how the methods can be applied to a CO<sub>2</sub> source, since the problem of multi-functionality at the CO<sub>2</sub> source is at the core of most CCU processes.

### C.4.3.3 Hierarchy of Methods for Solving Cases of Multi-Functionality

Existing standards [48–51] and guidelines [5, 52, 53] rank methods for solving multi-functionality in a hierarchy, which **shall** be consistent with the stated goal definition. In the following, we present methods for solving multi-functionality according to the hierarchy given in the ISO standards and other guidelines.

1. First, check if multi-functionality can be solved by gathering individual process data and applying sub-division.
2. If sub-division 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 conflict with the initial research question, thereby requiring modification of the question.

If product-specific assessments are needed to answer the initial research question, the following hierarchy of allocation method shall be applied. Note that the results obtained via system expansion **shall** always be computed to assess the overall effect of introducing the CCU technology in addition to any product-specific assessments.

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

In the following, the alternative methods for solving multi-functionality are described and applied to account for the supply of CO<sub>2</sub>. For further information to account for the supply of CO<sub>2</sub> and detailed explanation, see Müller *et al.* [56].

#### C.4.3.3.1 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 for these smaller unit processes (*e.g., a factory with multiple products that derive from independent processes can be sub-divided into individual production lines*).

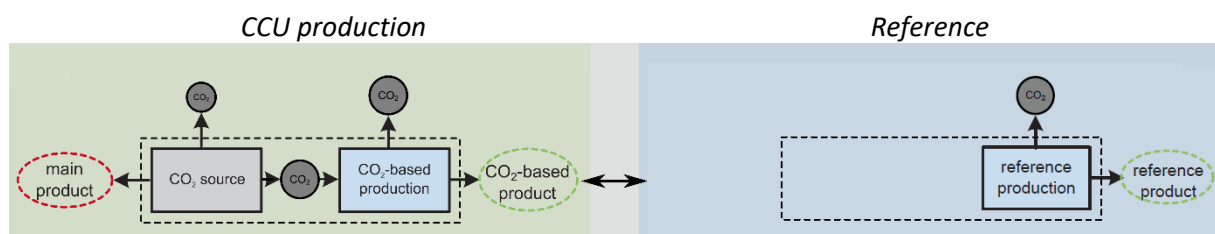
Cases where sub-division is applicable are not a problem of multi-functionality in a strict sense, but a problem of missing data. If these missing data can be gathered, multi-functionality can be fully resolved and thus, sub-division **shall** always be applied first. Sub-division **shall** be applied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

*Application to the CO<sub>2</sub> source:* Sub-division is not applicable to the CO<sub>2</sub> source, since CO<sub>2</sub> is always produced jointly with the main product.

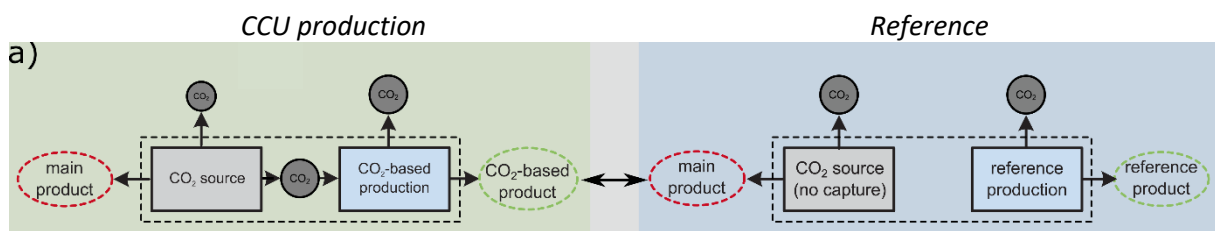
#### C.4.3.3.2 System Expansion

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

*Application to CO<sub>2</sub> source:* CCU processes are often multi-functional (*e.g., when the CO<sub>2</sub> 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 one needs to fulfil the same functional unit, and therefore the system boundaries and the functional unit of the product systems are revised. To compare a CCU process with two products (product of CO<sub>2</sub> source and product of CO<sub>2</sub> process) to a conventional system (Figure 9), the main product of the CO<sub>2</sub> source is added to the functional unit and the conventional system is expanded with the CO<sub>2</sub> source without CO<sub>2</sub> capture (Figure 10).



**Figure 9. Comparison of CCU production versus reference production: The CCU system produces a main product and a CO<sub>2</sub>-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<sub>2</sub> 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.**

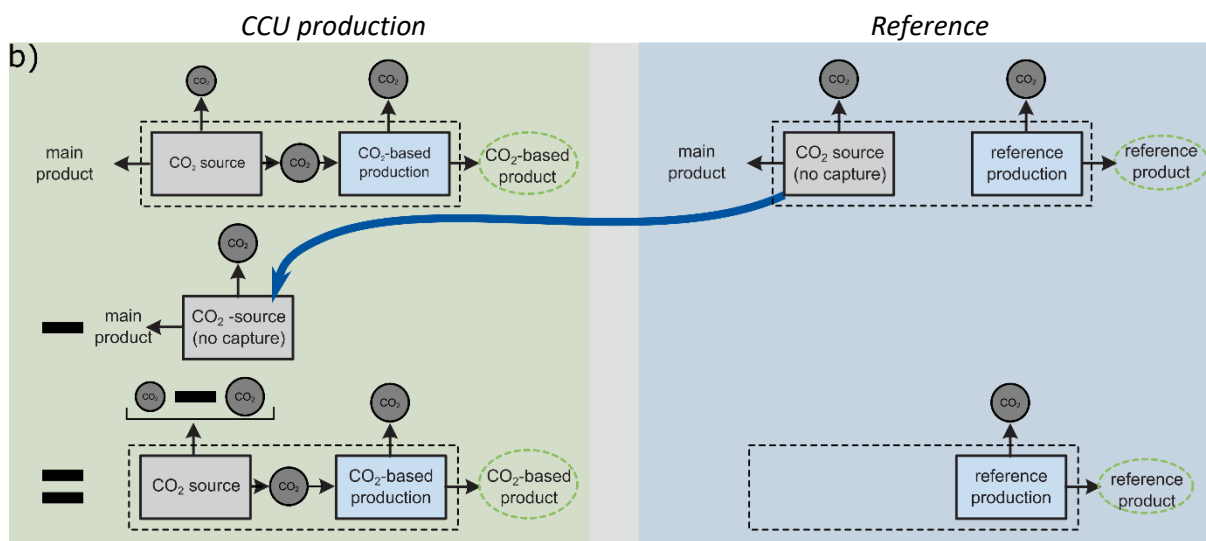
Note that a process used for system expansion (not in the case of CO<sub>2</sub> sources) might also be multi-functional, and so subsequent system expansion might be necessary. In theory, this process could extend to modeling the entire global technosphere. However, this endless chain of system expansion is usually interrupted by the defined cut-off criteria (C.4.2).

#### C.4.3.3.3 Substitution

Substitution does not include additional functions in the functional unit. Instead, a credit is given for the production of the co-product. The credit represents the environmental burdens avoided as a result of substituting the conventional production system that would otherwise have been used. 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) remain unchanged.

Similarly to the approach presented in Chapter C.4.3.1, 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<sub>2</sub> source:* For CO<sub>2</sub> sources, the substituted process is usually the same source but without capture (Figure 11). This assumption remains valid as long as not all CO<sub>2</sub> from this source is already fully utilized.

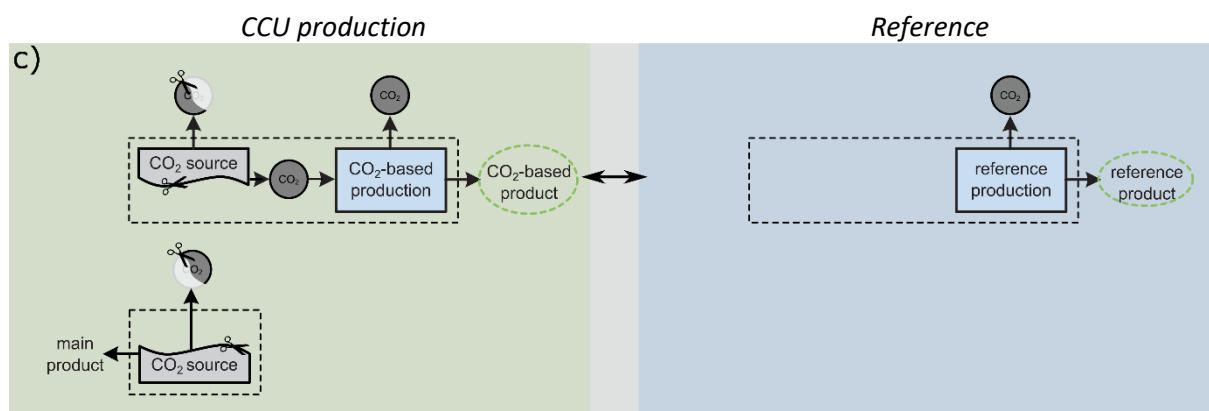


**Figure 11. Substitution: The production of the main product without carbon capture is avoided, and thus the CCU system is credited for the otherwise emitted CO<sub>2</sub>, but has to carry the burdens of purification, compression, and transportation of the CO<sub>2</sub>.**

Both approaches – system expansion and system expansion via substitution – are mathematically equivalent in a comparative LCA; however, the results, meaning, and interpretation of the results are not, because the system boundaries and functional unit are altered. System expansion via substitution can lead to negative values for environmental impacts (*e.g.*, *negative CO<sub>2</sub> emissions*), because by-products are credited. These negative values can be misinterpreted as implying that producing more of the product could offer infinite benefits to the environment. However, the effect of avoided environmental burdens is limited to the market capacity of the by-products and thus does not offer infinite benefits. Furthermore, these negative values for environmental impacts do not indicate that the production system takes up greenhouse gas emissions from the atmosphere, nor that natural resources are generated [57]. The negative values simply indicate that the production system has lower environmental impacts than the conventional production of all products and by-products through the conventional production. However, as a conceptual advantage, substitution conserves the causal interaction between processes by accounting for impacts in other life cycles.

## C.4.3.3.4 Allocation

Allocation partitions the inputs and outputs of the multi-functional process among the products or functions. The partition reflects an underlying physical causal, economic, or other non-causal physical relationship.



**Figure 12.** Allocation sub-divides the CO<sub>2</sub> sources into two processes and distributes the environmental burdens of the CO<sub>2</sub> source between the main product and the production of the feedstock CO<sub>2</sub> 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 the functional units agree.

## C.4.3.3.5 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 (*e.g., 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 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 then reflect this quantitative change of inputs and outputs<sup>3</sup>. Note that more than one relationship can be applicable within one process

*Application to CO<sub>2</sub> source:* A physical causality can be found by quantitatively changing the amount of main product and the product CO<sub>2</sub> 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<sub>2</sub>. Therefore, the amount of main product affects the inputs and outputs of the process. Varying the amount of product CO<sub>2</sub> changes the amount of CO<sub>2</sub> emitted, since captured CO<sub>2</sub> is no longer emitted, but inputs and outputs related to the capture process (*e.g., electricity for compression*) are also changed. Consequently, 1 kg of CO<sub>2</sub> provided by the CO<sub>2</sub> source leads to an emission reduction of 1 kg CO<sub>2</sub>-eq. and an increase of emissions related to the capture process. The result is identical to the substitution approach.

## C.4.3.3.6 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 the attributes of the product or functions. The most commonly applied attribute is the economic value of products or functions. Since the multi-functional process is artificially sub-divided, the physical causality

<sup>3</sup> The ILCD Handbook refers to this as “virtual sub-division.”



between processes is lost, i.e., products are now produced independently rather than jointly as in the previous case. In addition, the selection of the attribute is to some extent arbitrary.

*Application to CO<sub>2</sub> source:* The selection of a suitable product attribute to distribute the emissions of the CO<sub>2</sub> source among the main product and the CO<sub>2</sub> 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<sub>2</sub>. Energy is not a suitable attribute, since CO<sub>2</sub> does not contain any energy; more precisely, its lower heating value is zero. The economic value of CO<sub>2</sub> is uncertain, since the capture process has costs, the price of CO<sub>2</sub> might be positive, and thus economic allocation would attribute the product CO<sub>2</sub> with emissions of the CO<sub>2</sub> source. However, it can be argued that CO<sub>2</sub> has a negative economic value and is thus a waste stream that requires waste treatment. In this case, the CO<sub>2</sub> source has only one function, i.e., producing the main product, and has a technical waste flow, i.e., the concentrated CO<sub>2</sub> stream. The CO<sub>2</sub>-utilizing step would then be multi-functional in the sense that a CCU product is produced and the CO<sub>2</sub> waste stream is treated. As waste stream per se cannot carry any environmental burdens, the environmental impacts of the CCU-utilizing step would be allocated between the CCU product and the waste treatment [5]. As each applied criterion would significantly alter the environmental impact attributed to CO<sub>2</sub> and an objective selection of one allocation criterion is not possible, a sensitivity analysis **shall** always be performed.

#### C.4.3.4 Provisions

<b>Provisions C.4 - Life Cycle Inventory Modeling Framework and Solving Multi-functionality</b>	
	<p>1) If multi-functionality occurs within the defined system boundaries:</p> <p style="padding-left: 40px;">1) Sub-division shall be applied</p> <p>If not possible:</p> <p style="padding-left: 40px;">2) System expansion shall be applied</p> <p>If product-specific assessments are needed to answer the initial research question, the following allocation hierarchy shall be applied. Note that system expansion shall always be applied, and further product-specific assessment may be applied if necessary</p>
<b>Shall</b>	<p style="padding-left: 40px;">3) System expansion via substitution shall be applied. This step should be only in addition to system expansion</p> <p>If not possible:</p> <p style="padding-left: 40px;">4) Allocation shall be applied, first based on underlying physical causalities. This step should be only in addition to system expansion.</p> <p>If not possible:</p> <p style="padding-left: 40px;">5) Allocation using other underlying relationship(s) shall be applied additionally to system expansion. A sensitivity analysis of applicable criteria shall be conducted</p>
<b>Should</b>	
<b>May</b>	



## 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 collection is time consuming, it is beneficial to keep in mind the level of data quality that needs to 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 represent the true inventory of the process for which data are 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., using mass as a cut-off criterion might neglect substances that remain highly toxic at low concentrations*). Data measurements or process simulation have limited accuracy, and thus, data uncertainty is introduced with each collected data set. Methodological appropriateness and consistency refer to the selected modeling approach (*e.g., attributional or consequential*). In order to ensure consistency, modeling approaches should not be mixed. Note that this Guideline describes an attributional approach.

### C.4.4.1 Provisions

#### Provisions C.5 - Data Quality

**Shall** 1) It shall be stated which data are 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 the 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 standard [1, 4] and the PEF Guide [53]. Note that external review also allows studies to omit confidential information from the public report and can thereby protect intellectual property and commercially sensitive information.

### C.4.5.1 Provisions

Provisions C.6 - Special Requirements for Comparative Studies	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) Any study intended for external communication shall be reviewed</li> <li>2) For comparative studies or studies to be used in comparative assertions disclosed to the 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], ISO 14071 [58], and the GHG protocol [52]</li> </ol>
<b>Should</b>	
<b>May</b>	

## C.5 Life Cycle Inventory (LCI)

### General Introduction

In the life cycle inventory phase, the actual data are gathered and the product system is modeled according to the goal and scope definition. The modeling 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 C.4.2 and 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 of life cycle inventory in Chapter 7 (page 153ff.) [5]. See Chapter 4 (page 97ff.) of Baumann and Tillman for a practical introduction to constructing the flow chart, collecting data, and calculating environmental loads [8]. Also see Curran's handbook: Chapter 3 (page 43ff.) for an introduction to life cycle inventory and Chapter 5 (page 105ff.) for sourcing life cycle inventory [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: part 2a, Chapter 3 (page 41 ff.) [10].*

### C.5.1.1 Provisions

Provisions C.7 - Life Cycle Inventory (LCI)	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) System boundaries shall be described and represented in a flow chart</li> <li>2) Inventories shall be documented and reported, at least to external reviewers</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) All relevant unit processes with their relevant elementary and technical flows should be represented in the flow chart</li> </ol>
<b>May</b>	

## C.5.2 Estimation Methods of Bridging Data Gaps

During LCA studies, practitioners are often confronted with limited data availability; estimation methods have been developed to bridge such data gaps. 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,

second-law analysis is a useful tool for differentiating between feasible and unfeasible 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 on chemical processes is missing (*e.g., for feedstocks*) the Ecoinvent database 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 [59–61].

Jiménez-González *et al.* and Kim *et al.* provide a design-based method to estimate gate-to-gate inventory information when direct data are not available [62, 63]. The method defines transparent rules for data collection and provides several rules of thumb (*e.g., for estimating 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 from 0 to 4 MJ per kg for half of the organic chemicals and from -1 to 3 MJ per kg for half of the inorganic chemicals.

Bumann *et al.* provide a method for estimating gate-to-gate process energy consumption when no process engineering is available [64], which correlates the process energy demand with the energy index provided by Sugiyama *et al.* [65]. 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., reactants, products, co-products and by-products, reaction conditions, thermodynamic data*). From these data, an energy index is computed and used to estimate gate-to-gate energy consumption. The average deviation of this method is around 30%.

### C.5.2.3 Artificial Neural Networks

The environmental impacts of processes have been estimated from molecular descriptors of the desired product using neural networks [66, 67]. The resulting software tool, Finechem, 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 predictions for 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. This is a particular shortcoming for CCU technologies, which aim to substitute identical products, fuels, or materials.

### C.5.2.4 Provisions

Provisions C.8 - Estimation Methods	
<b>Shall</b>	1) If no other data are available, a best-case scenario based on stoichiometric schemes and thermodynamics shall be used to calculate potential environmental impact reductions
<b>Should</b>	
<b>May</b>	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 reference process has significant impact on the reduction potential of the assessed CCU technology, and must therefore be selected with care. In general, reference processes **shall** be market competitors of the CCU process, i.e., the marginal process. However, the identification of the marginal process might introduce complex market interactions, in particular if the process has more than one function. Therefore, the reference process **shall** be modeled as the average market mix if further information is missing and if no large-scale structural changes occur (C.4.3.1).

However, CCU technologies – particularly during early stages of development – do not compete with current technologies, since their market launch lies in the future. Instead, these CCU processes will compete with other future technologies. Thus, comparing CCU technologies in stages of early development to currently used processes does not reflect future market realities. Therefore, the time dimension is crucial for assessing the 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 for applying learning curves are described by Gavankar *et al.* [39] and Cespi *et al.* [68]. 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., changes in the energy supply due to higher shares of renewable energy*). Since GHG emissions are expected to decrease in future energy systems, the modified background processes impact the choice of technology when GHG emissions are constrained.

However, predicting future technologies is potentially beyond the scope and experience of many LCA practitioners and thus, if no reliable predictions of future developments are available, the current best available technology **should** be used as the reference technology. In this case, the metrics used to select the best available technology shall be clearly stated (*for CCU technologies the best available technology should be the one with the lowest GHG emissions<sup>4</sup>*). Note that the TRL of the reference process and the assessed technology might differ and thus, comparability is limited.

#### C.5.3.1 Provisions

Provisions C.9 - Selection of Reference Processes	
<b>Shall</b>	1) The reference process shall be the marginal process. If no marginal process can be identified, the market mix shall be assumed
<b>Should</b>	1) For processes in early stages of development, the current best available technology based on GHG emissions should be selected as the reference process. The related TRL and associated limitations in comparability shall be determined and reported
<b>May</b>	1) For processes in early stages of 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

<sup>4</sup> This concept fits the U.S. DOE Office of Fossil Energy recommendation for the “best-in-class” technology (Chapter 2.1.3.2) [69].

## 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 result from 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 endpoints. 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., dieback of coral reefs due to temperature rise, in turn resulting from enhanced radiative forcing caused by GHGs emitted 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; furthermore, they rely on the comparability of various types of damage done to the areas of protection (*e.g., malnutrition caused by drought, 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 by 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<sub>2</sub> 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 Centre [70] 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

A key driver for CCU is to lower both GHG emissions and 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 of CCU [3]. The introduction of CCU technologies might further affect a variety of environmental impacts, and so the holistic LCA approach aims to avoid problem-shifting from one impact category to another. Therefore, in order to avoid misleading decision making: impact categories **shall** not be omitted from LCA studies if they 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: There are numerous impact categories, and sometimes even multiple methods exist for one impact category. Furthermore, the uncertainty of impact assessment models varies according to the complexity of cause–effect chains and the

maturity of various methods. Consequently, different impact assessment models are used in practice, leading to differing LCA results.

The ‘International Environmental Product Declaration (EPD) System’ uses the impact assessment methodology provided by the Institute of Environmental Sciences (CML), University of Leiden, as a default for product category rules. To be in line with the EPD system, impact assessment **shall** use the most recent version of the CML methodology. At the time of publication (August 2020) the most recent version of CML is from August 2016. Additionally, if it is geographically more appropriate, a second set of methodologies **should** be applied in addition to CML, to ensure both comparability and geographical representativeness [71, 72]:

For Europe, the European Commission's Joint Research Centre (JRC) provides a selection of impact categories and methods that were defined through stakeholder dialogue involving LCIA model developers and LCA practitioners; the JRC recommendations **should** therefore be followed for Europe [6, 73]. Studies relevant to the United States **should** use the latest version of TRACI (currently version 2.1 as of autumn 2020), an impact assessment methodology by the US EPA [74].

Most impact assessment methods use a 100-year time horizon for global warming potential (GWP100). However, each greenhouse gas shows different behavior (*e.g., due to stability*), depending on the time horizon considered. Due to the urgency of climate change, a 20-year time horizon **should** also be considered (GWP20), with the most recent characterization factor as provided by the IPCC<sup>5</sup> [45, 75].

Note that life cycle impact assessment should be limited to midpoint indicators, because the level of uncertainty increases when utilizing endpoint indicators or single-point indicators. Also note that a detailed knowledge of impact assessment method is necessary to interpret and report results correctly (*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 Provisions

Provisions C.10 - Life Cycle Impact Assessment Methods	
<b>Shall</b>	<ol style="list-style-type: none"> <li>1) CML impact assessment methodology shall be used as a default</li> <li>2) LCA studies for CCU technologies shall analyze midpoints indicator categories</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>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. the latest version of TRACI</li> <li>2) GWP20 should be considered in addition to GWP100, as calculated in the latest IPCC report</li> </ol>
<b>May</b>	<ol style="list-style-type: none"> <li>1) Other categories or methods may be applied, but shall be justified, documented, and reported</li> </ol>

<sup>5</sup> The most recent version can be found in IPCC AR5. IPCC AR6 will be released in stages during 2021 and 2022.

## C.6.2 Temporary Storage of CO<sub>2</sub>

CCU products offer temporary carbon storage. Consequently, CO<sub>2</sub> emissions might be delayed and thus do not contribute to climate change during the period of storage. Therefore, temporary storage does not provide benefits that are additional to or independent of the impact on climate change. Temporary storage should only be considered quantitatively if this is explicitly required to meet the needs of the study goal (ILCD Handbook, p. 227).

The relevance of temporary storage depends on the class of CO<sub>2</sub>-based product or fuel considered:

For **CO<sub>2</sub>-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, as is the amount of carbon chemically bonded [54]. Therefore, the time between production and end-of-life treatment and the amount of CO<sub>2</sub> released during end-of-life treatment is identical. Thus, the emission time profiles are identical after factory gate (yellow and green lines in Figure 13) and there is no additional effect gained from storing CO<sub>2</sub>.

For **CO<sub>2</sub>-based products with different chemical structure and composition to their conventional counterparts**, emission time profiles are not identical (blue line in Figure 13), and thus temporary storage might offer climate benefits (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 again become identical.

For **CO<sub>2</sub>-based fuels with different 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.

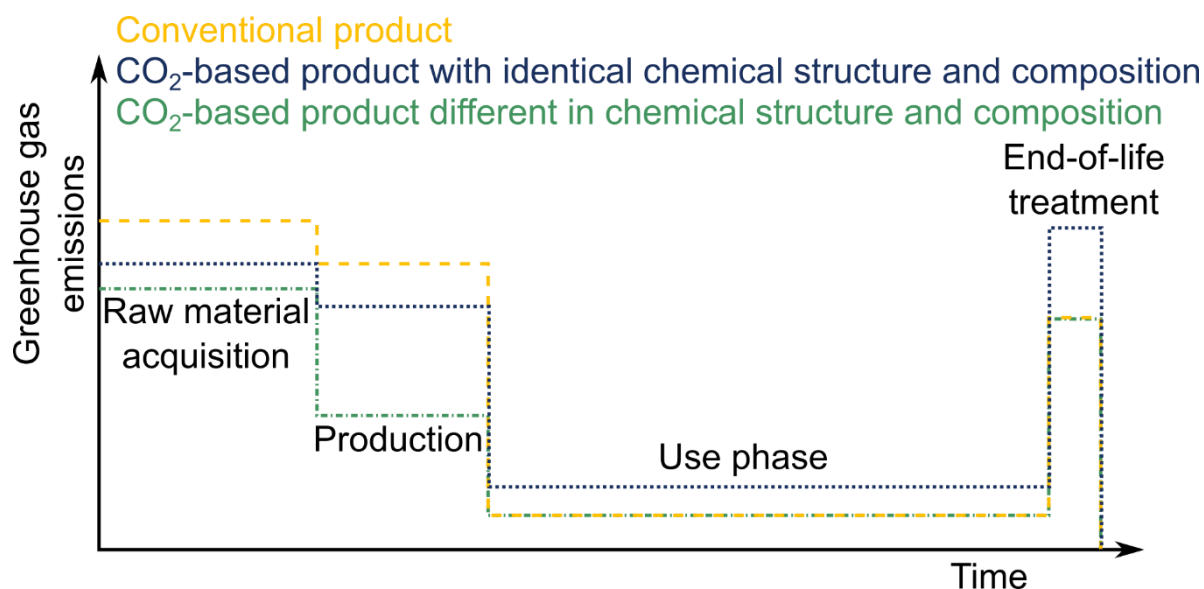
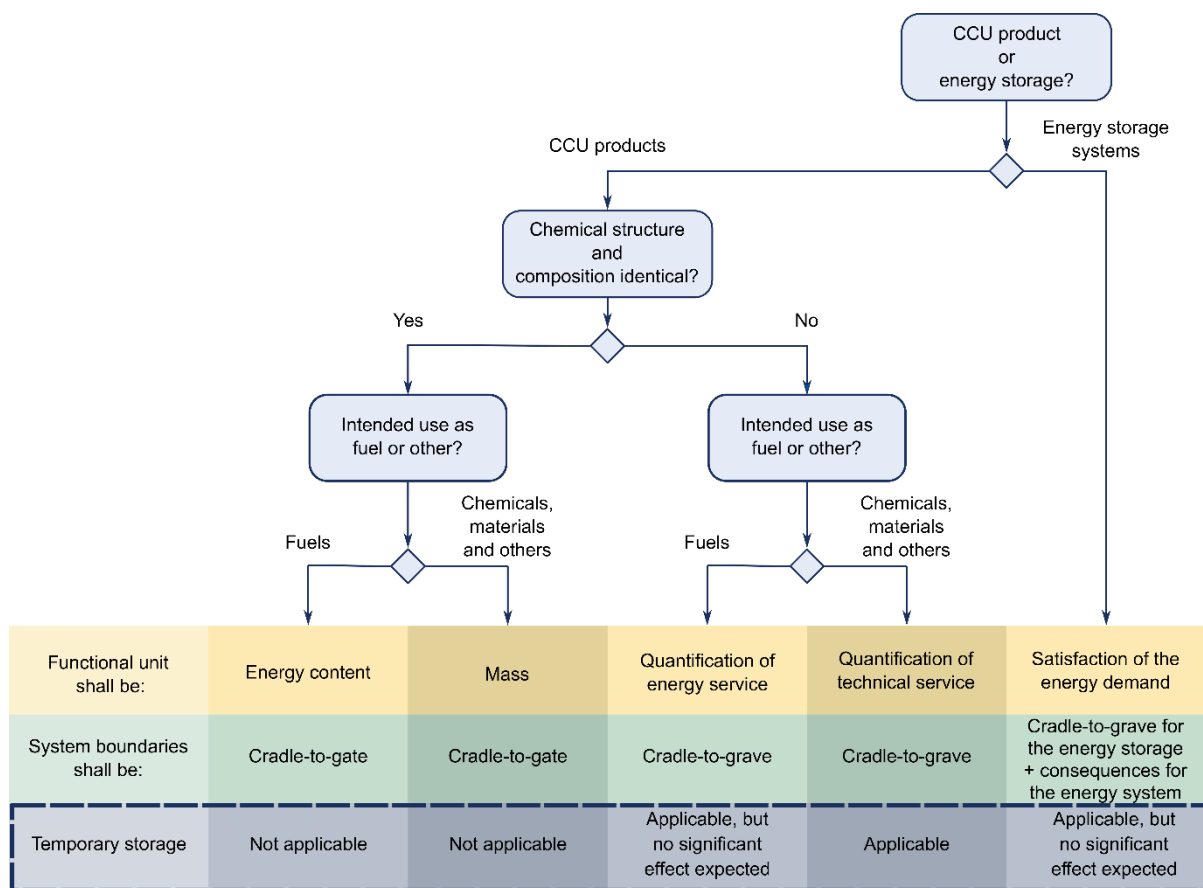


Figure 13: Emission time profiles for different products. CO<sub>2</sub>-based products with identical chemical structure and composition to their conventional counterparts have identical emission time profiles after production. CO<sub>2</sub>-based products with chemical structure and composition different from conventional counterparts can have different emissions during use phase and end-of-life treatment and also different life spans, resulting in different emission time profile.





**Figure 14. Decision tree for LCA of CCU c) up to decision 3: temporary storage. For CCU products with identical chemical structure and composition to their conventional counterparts, temporary storage is not applicable as this is not part of the system boundaries. For CCU products that are not identical to their benchmark, temporary storage is applicable, but especially for products with short storage durations, such as fuels, the effect is usually not significant.**

The effect of temporary CO<sub>2</sub> storage is known from biologically-based products, and methods have been developed to account for temporary storage [76–78]. 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 [79]. Furthermore, attempting to account for delayed emissions demonstrates the large uncertainties regarding future conditions (*e.g.*, *a future emission could be released at a point in time where the climatic system is even less stable than today*); as such, delayed emissions shall not be considered as beneficial for climate change mitigation [45]. To follow the established LCA principles, delayed emission **shall** not be discounted over time. Instead, emission time profiles, and the amount and duration of carbon stored **may** be reported as a separate item. Note that for permanent storage<sup>6</sup>, a discounting method is not needed because end-of-life emission never occurs and thus emissions are zero. If end-of-life emissions are zero, the effect of storage is therefore already considered.

<sup>6</sup> Permanent storage can be assumed if CO<sub>2</sub> is sequestered for 100,000 years.

To decide whether or not temporary storage might offer any climate benefit, we developed the decision tree shown in Figure 14 by answering a maximum of three questions:

1. Is the subject of the study a CCU product or a form of energy storage?
2. If the subject of the study is a CCU product, is it chemically identical to the conventional product or not?
3. If the chemical structure is not identical, is the subject of the study intended to be used as a fuel or not?

#### C.6.2.1 Provisions

<b>Provisions C.11 - Guideline Temporary Storage of CO<sub>2</sub></b>	
<b>Shall</b>	1) Delayed emission shall not be discounted over time as a default
<b>Should</b>	
<b>May</b>	1) If delayed emissions occur, an emission time profile of the conventional product and the CO <sub>2</sub> -based products with different chemical structure and composition may be reported. The amount and duration of carbon stored may be reported

## C.7 Life Cycle Interpretation

### General Introduction

The life cycle interpretation phase has two purposes:

- 1) Closing the feedback loop of the iterative steps of LCA studies, e.g., by evaluating the 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 the iterative steps of the assessment, 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 the gathered data are of insufficient quality, 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 answered satisfactorily. For this purpose, the completeness and consistency of the study is evaluated via qualitative methods (*e.g., expert opinions, 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, all conclusions drawn **shall** be based solely on the data quality, system boundaries, methodologies, and results presented in the assessment report.

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

*Further recommended reading:*

*See Chapter 4.5 of ISO 14044 [4] and Chapter 9 of the ILCD Handbook for more information on interpretation [5]. See Baumann and Tillman for practical introduction and guidance on the presentation of results [8]. See Laurent et al. for a review and detailed guidance [80].*

### C.7.1 Carbon-Neutral Products and Negative Emissions

CCU technologies consume CO<sub>2</sub> to produce value-added products. Thus, intuitively, CCU technologies might be regarded as technologies with potentially zero emissions or net-negative emissions.

CO<sub>2</sub> 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 release carbon previously consumed from the atmosphere.

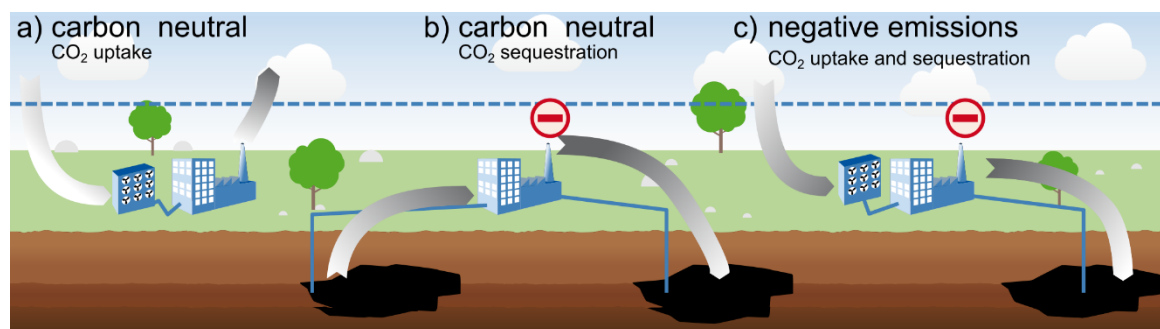
CCU technologies can theoretically be carbon-neutral over the entire life cycle:

- if CO<sub>2</sub> is captured from the atmosphere (via biogenic point sources or direct air capture) and the same amount of CO<sub>2</sub> is released at the end of life (Figure 15a)
- or if CO<sub>2</sub> is captured from fossil point sources and CO<sub>2</sub> is sequestered or permanently stored in the product (Figure 15b)
- and if all other GHG emissions are zero over the life cycle.

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

- if CO<sub>2</sub> is captured from the atmosphere (via biogenic point sources or direct air capture)
- and if CO<sub>2</sub> is sequestered or permanently stored in the product
- and if overall life cycle GHG emissions are lower than the amount of CO<sub>2</sub> fixed.

If the amount of atmospheric CO<sub>2</sub> capture and fixation during a process is equal to all fossil emissions over the life cycle of this process, the process is carbon-neutral.



*Figure 15. Case a) Carbon-neutral CO<sub>2</sub> uptake: CO<sub>2</sub> is taken from the atmosphere and the same amount is re-emitted during or after the product life cycle. Case b) Carbon-neutral CO<sub>2</sub> sequestration: Fossil carbon is taken from underground reservoirs and the embedded CO<sub>2</sub> is sequestered after the product life cycle. Cases a) and b) are only carbon-neutral if no emissions occur during the product life cycle. c) Negative emissions: CO<sub>2</sub> 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<sub>2</sub>-eq. per kg CO<sub>2</sub> taken up.*

In all other cases, CCU technologies have net-positive CO<sub>2</sub> emissions over the life cycle. Nevertheless, such emissions can be lower than for competing conventional processes (case d in Figure 16). In this case, the CCU process also contributes to climate change mitigation through substitution and hence is GHG-emission-reducing. Even though such processes lead to lower CO<sub>2</sub> emissions compared to the status quo, they are not carbon-negative. In particular, this also holds for GHG-emission-reducing processes with negative calculated values for CO<sub>2</sub> emissions obtained using substitution to solve multi-functionality. By applying substitution (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 entire life cycle. Therefore, negative CO<sub>2</sub> emissions obtained from substitution **shall** be clearly stated as an environmental benefit only in comparison with the benchmark technology and not as negative CO<sub>2</sub> emissions in absolute terms over the entire life cycle. Also, avoided CO<sub>2</sub> emissions and other environmental impacts from substitution **shall** be reported separately [57].

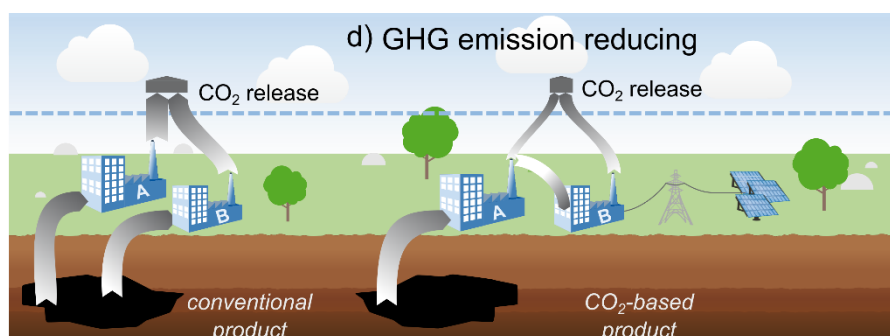


Figure 16. Case d) Greenhouse gas emission-reducing: CCU technologies can achieve lower CO<sub>2</sub> emissions than the status quo and thus may be considered as greenhouse gas (GHG) emission-reducing technologies.

### C.7.1.1 Provisions

Provisions 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 are of insufficient quality, either the model shall be refined or the goal and scope shall be adapted
	2) Conclusions drawn shall be based solely on the data quality, system boundaries, methodologies, and results
	3) Recommendations are a subjective interpretation of the conclusions and thus shall be based exclusively on the conclusions
	4) Negative emissions in cradle-to gate studies shall not be interpreted as CO <sub>2</sub> sinks if the life cycle does not end in permanent carbon fixation
	5) Emission reductions due to substitution effects shall be interpreted as environmental benefits and not as negative emissions
	6) Emission reductions due to substitution effects shall be reported separately
	7) The potential case (a–d) of a technology shall be clearly stated, to show whether a technology has the potential to be either carbon-neutral, carbon-negative, or emission-reducing
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 [81].

Parameters derived from imprecise measurements or estimations made by experts introduce parameter uncertainty. The definition of system boundaries, selection of processes, and impact assessment methods introduce model uncertainty. Uncertainty due to choices results, for example, from the determination of the functional unit or allocation criteria [81].

According to ISO 14040 and ISO 14044, the 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.

*Further recommended reading:*

*See Chapter 11 of the LCA4CCU report by Ramirez et al. for an overview of uncertainty analysis and related tools [45].*

In the following, methods for quantifying the impact of uncertainties are described and two levels of recommendation are provided. This section is adapted from Igos *et al.* [82]: 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.

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

### C.7.2.1 Basic Approach

In the basic approach, input variables **shall** be identified that have uncertainties with large implications for the uncertainty of the model output. For this purpose, a sensitivity analysis **shall** be carried out. Sensitivity analysis is a systematic procedure for estimating the implications for the study outcome of selecting alternative methods and data [4]. The most basic approach to sensitivity analysis is the one-at-a-time approach. In this approach, input variables **shall** be varied separately one after another to quantify the sensitivity of the model results to changes in 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 that have the largest influence on overall output uncertainty. If the variation of the input variables reveals weak points in 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 modeling approach **shall** be reviewed until the results are sufficient to answer the (re)defined goal of the study.

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 for 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<sub>2</sub>*). The production of those high-energetic reactants or the supply of energy can lead to high environmental impacts. Consequently, assumptions about the environmental impacts of these inputs have been identified as the major source of varying results in LCA studies of CCU technologies. Thus, the environmental impacts related to high-energetic reactants are often the key variables in studies of 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 1. The status quo is taken from the Energy Technology Perspectives report published by the International Energy Agency [83]. In a fully decarbonized industry the greenhouse gas emissions of the energy supply will be near-zero, while in a transition scenario the emissions will lie somewhere in between the status quo and that of fully decarbonized industry (*e.g., 50% of the current emissions*). Even though these scenarios are derived in a very simple manner and the scenarios will perform poorly for forecasting, valuable insights can be gained from this type of scenario analysis (*e.g., the dependence on clean energy supply can be shown*). Since the generation of scenarios can be time- and resource-intensive, scenarios for the supply of electricity, hydrogen, CO<sub>2</sub>, heat, and natural gas (as methane) for the European context are provided in the annex of this document (C.9.1.).

**Table 1. Example scenarios**

Input	Unit	Status quo	Transition	Full decarbonized
Electricity	kg CO <sub>2</sub> -eq /MJ	0.091 <sup>7</sup>	0.046	0

However, note that scenario analysis can suffer from ambiguity because the scenario definitions rely on the LCA practitioner and can hardly become an automated part of LCA calculations [84].

As an alternative to scenario analysis, threshold values can be calculated for key variables. 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, water electrolysis consumes 50 kWh of electricity per kilogram of hydrogen. To achieve lower greenhouse gas emissions than steam reforming of methane (10.7 kg CO<sub>2</sub>-eq per kilogram of hydrogen [80]), the GHGs emitted by supplying electricity for water electrolysis would need to be 0.214 kgCO<sub>2</sub>-eq per kWh electricity or less [80]. In this case, the threshold value of electricity supply for hydrogen from water electrolysis compared to the benchmark process steam-methane reforming of methane would be 0.214 kgCO<sub>2</sub>-eq per kWh electricity. For a sound interpretation, the calculated threshold values **should** lie within physical and thermodynamic limits.*

### C.7.2.2 Intermediate Approach

Based on the basic approach, the LCA practitioner **should** employ an intermediate approach to quantify the uncertainty of the model output, using uncertainty analysis. According to 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 in relation to the underlying decision process. Uncertainty analysis is usually carried out using stochastic methods (*e.g.,*

<sup>7</sup> Calculated from [83].

Monte Carlo simulation [85–88]) or perturbation theory (e.g., analytical uncertainty propagation [84, 89–93]).

In the intermediate approach, the Monte Carlo simulation is recommended since it is the most common method of uncertainty analysis and is integrated into 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 results are represented by a probability distribution and thus indicate the overall model uncertainty. The Monte Carlo method requires a large number of simulations in order to obtain representative results and can therefore be temporally and computationally demanding. Usually, 10,000 Monte Carlo sets are generated, but Wei Wei *et al.* showed that 1 million iterations might be necessary to achieve sufficiently accurate results [94]. In general, mathematical convergence of the results cannot be guaranteed [82]. Therefore, the number of Monte Carlo sets **should** be as large as possible, but at least 1,000 [82].

In comparative studies, Monte Carlo analysis **shall** not be carried out independently for each alternative, since the comparison of probability distributions can lead to inaccurate interpretations, i.e., a large overlap of two probability distributions might be misinterpreted as being inconclusive. Large overlaps can be a result of identical sensitivity of both systems to one parameter [95]. For example, if two hydrogen electrolysis methods (A and B) with different efficiencies are compared: The environmental impacts of A and B are both highly sensitive to the environmental impacts of the electricity supply, but are impacted in the same way. However, if assessed independently, overlaps can occur because a Monte Carlo set of A with low-impact electricity supply is compared to a Monte Carlo set of B with a high-impact electricity supply (Figure 17a). Here, the interpretation that both systems perform equally well is incorrect and can be avoided by a joint Monte Carlo simulation of the mathematical difference (e.g., ‘A minus B’) between both alternatives. A joint Monte Carlo analysis can show that the environmental impacts of alternative A are always lower than B in each Monte Carlo set, and that A is therefore clearly advantageous (Figure 17b).

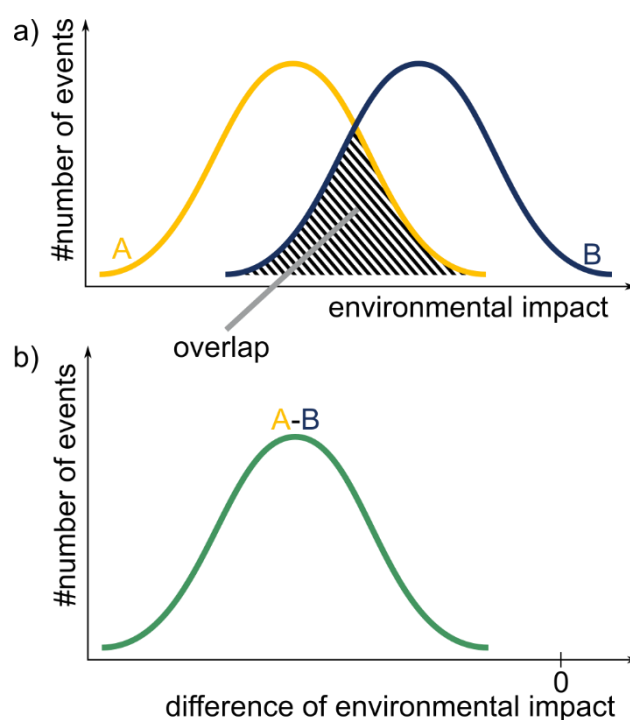


Figure 17. a) Results of an independent Monte Carlo analysis for alternatives A and B. b) Results of a joint Monte Carlo analysis of the difference (A-B) between technologies.



Therefore, different technologies **shall** be compared by means of a joint Monte Carlo simulation, which **shall** always be related to the same background system in order to ensure consistent results. For instance, the conventional synthesis of methanol requires large amounts of carbon monoxide and hydrogen, whereas the CO<sub>2</sub>-based production pathway requires large amounts of carbon dioxide and hydrogen. To ensure a fair comparison between both technologies, and thus a consistent result from the uncertainty analysis, the background production system of hydrogen must be the same for each individual Monte Carlo simulation step. For this reason, the use of aggregated processes in Monte Carlo analysis can be misleading (*since important variables in the foreground system cannot be varied in the background system*) and **should** therefore be avoided.

Uncertainty and sensitivity analyses are important for comparative studies, to identify whether calculated differences between 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 only that the study could not demonstrate any. Furthermore, note that ignorance, as an additional source of uncertainty, cannot be assessed by either uncertainty or sensitivity analysis “but may be revealed by qualified peer review” [5].

### C.7.2.3 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 [96]. Therefore, the results of the basic approach **shall** include parameters with high sensitivity and their effects on the overall model results. The results of the scenario analysis and calculated threshold values **shall** be reported separately from those of the sensitivity analysis. The intermediate uncertainty assessment approach **should** further 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.7.2.4 Provisions

Provisions C.13 - Uncertainty and Sensitivity Analysis	
<b>Shall</b>	<ol style="list-style-type: none"> <li>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 changes in the background system affect the technologies under study</li> <li>2) If variation of the input variables reveals weaknesses in 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 modeling approach shall be reviewed until the research question can be answered according to the defined goal</li> <li>3) If Monte Carlo analysis is applied for comparative studies, the analysis shall consider the alternatives within one joint Monte Carlo analysis</li> </ol>
<b>Should</b>	<ol style="list-style-type: none"> <li>1) The intermediate approach should be applied to quantify the uncertainty of the results</li> <li>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</li> <li>3) The standard scenarios provided in Annex C.9.1 should be used for scenario analysis</li> </ol>
<b>May</b>	

## C.8 Reporting

### General Introduction

ISO 14044 recommends: “The results and conclusions of the LCA shall be completely and accurately reported without bias to the intended audience.” Assumptions made regarding data and methods should be reported transparently 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/data cannot be published (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 recommended reading:*

*More details can be found in Chapter 5 of ISO 14044 [4] and in Chapter 10 of the ILCD Handbook [5].*

### C.8.1 CCU-specific Reporting

The following section provides a checklist for an executive summary. This checklist is derived from 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 (Annex 10.4) to provide easy access to the data used in the assessment. The main report shall report all assumptions, data used for calculations, methods, results, and limitations as transparently and in as much detail as possible. This is also important to help ensure reproducibility and full traceability.

Confidential information may be omitted from the main report to avoid breaches of confidentiality, and should be reported in a separate, confidential part available to the reviewing process. If confidential data are not disclosed to the public, this should be clearly stated, and then the relevant content redacted as necessary to avoid confidentiality issues.

### C.8.1.1 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 the public
- State unambiguous research question(s)
- State the classification of the assessed CCU technology

#### **Scope of the Study**

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

#### **Life Cycle Inventory and Life Cycle Impact Assessment**

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

#### **Interpretation**

- State any conclusions, recommendations, and limitations

### C.8.1.2 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 the 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 the study is preliminary
- State the commissioner of the study and other influential actors
- State the technology readiness level (TRL) of processes and sub-processes
- State the production or storage capacity
- State the review process and review experts, if any

#### Scope of the Study

- State the functional unit clearly and unambiguously according to the Guidelines; report any changes due to resolving multi-functionality
- State the performance characteristics, any omission of additional function in comparison, and how performance is measured (*e.g., products where chemical structure and composition differ from conventional counterparts*)
- State the system boundaries according to the Guidelines; state cut-off criteria; include a flow chart showing the system boundaries
- State any omitted life cycle stages and processes (*e.g., products where chemical structure and composition differ from conventional counterparts*)
- State relevant issues concerning data quality and assumptions
- State the method(s) used to resolve multi-functionality
- State the impact assessment methods
- State the data quality needs and how energy and material inputs/outputs are quantified
- State the software (and version) and data library (and version) used
- State the type of review and provide additional information about reviewers

### Life Cycle Inventory

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

### Life Cycle Impact Assessment

- Include the results of life cycle impact assessment
- State whether impact category coverage is reduced (*e.g., in the case of carbon footprinting*)
- If the results are reported on a relative basis, report this basis
- State whether delayed emissions occur: if so, include the emission time profile
- If applied, state the 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<sub>2</sub> sinks if the life cycle 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 the uncertainty and sensitivity analyses and report results separately
- Include a completeness check
- Include a consistency check
- State assumptions and limitations associated with interpretation of the results
- Include conclusions
- Include recommendations, if any

## C.9 Annex

### C.9.1 Description of Modeling Standardized Scenarios

The provided inventories were modeled using GaBi LCA software (Sphera Solutions, GmbH) and some of the inventories<sup>8</sup> were provided as a courtesy by Thinkstep [97]. The following section describes the modeling process. Note that the standardized data sets do not aim to accurately represent the status quo or the future. Instead, the use of standardized scenarios should help to avoid the need to generate unique scenarios for each individual LCA study; in addition, the standardized scenarios serve as a harmonized input, thereby allowing comparisons between technologies.

Four inventory data sets are provided, describing different scenarios:

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<sub>2</sub> supply in the high- or full-decarbonized scenarios, as in these scenarios fossil-fueled power plants will no longer be available as a CO<sub>2</sub> source. Instead, it is assumed that CO<sub>2</sub> is supplied by a direct air capture process. The selected technologies are listed in Table 2.

*Table 2: Selected Technologies for Scenarios*

	Status quo	Low-decarbonized	High-decarbonized	Full-decarbonized
<b>Hydrogen</b>	Steam-methane reforming	Alkaline electrolysis	Alkaline electrolysis	Alkaline electrolysis
<b>CO<sub>2</sub></b>	Coal-fired power plant	Coal-fired power plant	Direct air capture	Direct air capture
<b>Heat</b>	Natural gas vessel	Electrode vessel	Electrode vessel	Electrode vessel
<b>Natural gas (methane)</b>	Natural gas	Natural gas	Methanation	Methanation

#### C.9.1.1 Electricity

For present-day electricity generation, the mix of electricity production for the EU is taken from the GaBi database (EU-28: Electricity grid mix ts). For the low- and high-decarbonized scenarios, the mix of electricity

<sup>8</sup> LCIA results of the following processes are reproduced courtesy of Thinkstep: EU-28: Electricity grid mix ts, DE: Electricity from wind power ts EU-28: Heat ts, DE: Hydrogen ts.

production for the EU is modeled according to the 2°C scenario of the Energy Technology Perspectives report (published by the International Energy Agency) for the years 2030 and 2050 respectively [83]. The inventories for the electricity technologies are taken from the GaBi database [97]. 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 are available for the CCS technologies used. Therefore, electricity technologies with CCS are modeled as for conventional electricity technology, but greenhouse gas emissions from the IPCC WGIII AR5 are used instead of the greenhouse gas emissions stated in the original report [75]. 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) [97].

### C.9.1.2 Hydrogen

Hydrogen is either supplied by steam-methane reforming or by electrolysis. Currently, hydrogen is mainly produced by steam-methane reforming of hydrocarbons. Therefore, for hydrogen production under the status quo scenario a steam-methane reforming inventory is used (DE: Hydrogen ts). For all future scenarios, hydrogen generation via electrolysis is modeled based on an alkaline process [98]. The impact of the electricity demand for electrolysis is then calculated according to the energy scenario.

### C.9.1.3 CO<sub>2</sub>

For CO<sub>2</sub> supply, two sources are considered: capture from exhaust gases of a coal-fired power plant [99] 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 simply converts electricity to steam (95% efficiency). No other inventory was considered.

### C.9.1.5 Natural Gas

Natural gas is either supplied by the European natural gas network from the extraction of fossil natural gas or else by methanation of CO<sub>2</sub> and hydrogen.

The European natural gas network is modeled by weighting the national natural gas supply processes from the GaBi database according to their relative market volumes in Europe. The market volumes of the national gas markets are based on data from Eurostat and are assumed to remain constant over time [100]. The following assumptions are made in modeling the natural gas network:

- No data are available for the national markets of Malta and Cyprus. Thus, these countries are not considered in the EU natural gas mix.
- The GaBi database lacks national processes for Bulgaria, Croatia, the Czech Republic, Denmark, and Estonia [97]. The national market of these countries combined contribute less than 4% to the total European market and are therefore omitted here for simplicity.
- The market shares of the other countries have been adjusted accordingly to reach 100%.

The methanation process is modeled according Müller *et al.* [101].

## 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	<input type="checkbox"/> Sub-division <input type="checkbox"/> System expansion <input type="checkbox"/> System expansion via substitution <input type="checkbox"/> Virtual sub-division <input type="checkbox"/> Mass allocation	<input type="checkbox"/> Energy allocation <input type="checkbox"/> Economic allocation <input type="checkbox"/> Closed loop scenarios <input type="checkbox"/> Other (please specify)
INVENTORY	Data source	<input type="checkbox"/> Primary sources <input type="checkbox"/> Secondary sources <input type="checkbox"/> Stoichiometric data	<input type="checkbox"/> Process-modeling-based data <input type="checkbox"/> Mixes sources <input type="checkbox"/> Other (please specify)
	Energy sources (select all that apply)	<input type="checkbox"/> Grid mix <input type="checkbox"/> Power station with carbon capture <input type="checkbox"/> Wind <input type="checkbox"/> Solar	<input type="checkbox"/> Nuclear <input type="checkbox"/> Hydro <input type="checkbox"/> Future (see timeframes) <input type="checkbox"/> Other (please specify)
	Main sub-processes and TRLs	SUB-PROCESS	TRL TRL TRL TRL



	<b>Database &amp; software used</b>	
<b>ASSESSMENT</b>	<b>LCIA method</b>	<input type="checkbox"/> CML <input type="checkbox"/> ILCD recommendation: v. ____ <input type="checkbox"/> TRACI 2.1  OTHER IMPACT METHODS <input type="checkbox"/> .....  SINGLE CATEGORIES: <input type="checkbox"/> Climate change <input type="checkbox"/> CED <input type="checkbox"/> use TOX
	<b>Highlighted results</b> (graphical, text, or tabular format)	
<b>INTERPRETATION</b>	<b>Main conclusions</b>	
	<b>Sensitivity analysis</b>	<input type="checkbox"/> No <input type="checkbox"/> Yes (please specify below)

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