Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization (Version 2)

Technische Universität Berlin

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The University Of Sheffield.

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Foreword from the Global CO_2 Initiative

The urgency of required climate action was made clear unequivocally with the release of the latest IPCC report in February of 2022. 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 zero-carbon emissions power generation and broad-scale electrification, increased energy efficiency, and carbon-negative technologies.

The Global CO_2 Initiative, launched in 2016 during the meeting of the World Economic Forum with the goal of catalyzing innovative research in CO_2 utilization, seeks to get CO_2 capture and use recognized and implemented as a mainstream climate solution. The Global CO_2 Initiative's roadmap to a global market for CO_2-based products identified a trillion-dollar opportunity by 2030 for CO_2 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 negative 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 dioxide 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_2 Utilization, Version 1.0" in 2018.

Over the past four years, these Guidelines have been widely distributed and used, have been updated based on user input to Version 1.1, and have inspired an international collaboration to further harmonize LCA and TEA for CO_2 utilization, coordinated and funded by the Global CO_2 Initiative with EIT Climate-KIC support.

This revised and expanded version 2.0 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, the work of the International CCU Assessment Harmonization Group, and feedback from practitioners and users of LCA and TEA studies, have contributed to this updated version.

Version 2.0 includes new chapters on integrated assessments that combine LCA and TEA, how to assess early-stage technologies, and how to include social impact in LCA and TEA.

Separately from this new document, we are also providing an updated version of "Making Sense of Techno-Economic and Life Cycle Assessment Studies for CO_2 Utilization: *A guide on how to commission, understand, and derive decisions from TEA and LCA studies.*"

A new web resource, AssessCCUS, has been created to assist users with tutorials, templates, and useful links. We are grateful for support from the US Department of Energy to help us create this free resource.

We hope that this document will be useful to you and we invite feedback to help us produce future updates.

Global CO_2 Initiative, Ann Arbor, March 2022

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List of Abbreviations

AACE	Association for the advancement of cost engineering
AHP	Analytic hierarchy process
ANP	Analytic network process
BFD	Block flow diagram
CapEx	Capital expenditure
CAPM	Capital asset pricing model
CCS	Carbon capture and storage
CCU	Carbon capture and utilization
CEPCI	Chemical Engineering Plant Cost Index
CML	Institute of Environmental Sciences of the University of Leiden
CO_2	Carbon dioxide
COGM	Cost of goods manufactured
COGS	Cost of goods sold
DIN	Deutsches Institut für Normung
EBIT	Earnings before interest and taxes
EIA	Energy Information Administration
ELECTRE	Elimination Et Choix Traduisant la Realité
ETS	Emission trading system
EU	European Union
FCI	Fixed capital investment
FOAK	First of a kind
GHG	Greenhouse gas
GWP	Global warming potential
H_2	Hydrogen
IEA	International Energy Agency
IEAGHG	International energy agency greenhouse gas program
ILCD	International reference life cycle data
IPCC	Intergovernmental Panel on Climate Change
IRR	Internal rate of return
ISBL	Inside battery limits
ISO	International Organization for Standardization
JRC	European Commission's Joint Research Centre
LCA	Life cycle assessment
LCC	Life cycle costing
LCI	Life cycle inventory
LCOE	Levelized cost of electricity
LHV	Lower heating value
MADM	Multiple attribute decision making
MCDA	Multicriteria decision analysis
MODM	Multiple objective decision making
NGO	Non-governmental organization
NOAK	Nth of a kind
NOX	Nitrous oxides
NPV	Net present value
OAT	One at a time
OME	Oxymethylene ether
OpEx	Operating expenditure
OSBL	Outside/off-site battery limits
P&ID	Piping and instrumentation diagram
PEM	Proton-exchange membrane

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

PART A
General Assessment Principles

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Contents Part A

A.1 Introduction

In times of climate change, research on CO_2 utilization is gaining momentum in industry, academia, and policy spheres, leading to a vast number of promising technologies, for example in the fields of CO_2-derived chemicals, fuels, and minerals [1], [2]. The term 'promising technology,' however, reflects a subjective opinion on commercial and environmental viability but does not represent a systematic evaluation. Consequently, techno-economic assessment (TEA) and life cycle assessment (LCA) are essential methodologies for guiding research and development towards commercialization [2]. TEA is a methodology framework 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_2 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_2 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_2 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).

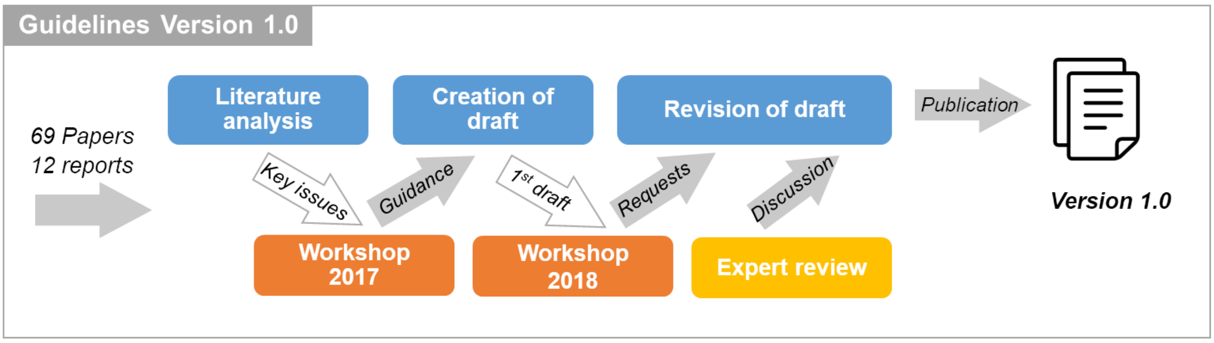

Figure 1. The process of creating the Guidelines document (version 1.0), involving literature analysis, draft creation and revision, involving stakeholder workshops and expert review

Version 1.0 of the Guidelines was revised with the continued participation of the CCU community. This updated version, named version 1.1, of the Guidelines was 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 Figures 2a). Version 2.0 of the guidelines builds on from version 1.1, adding new parts to the established guidelines covering early-TRL assessment, integrated TEA & LCA and a brief introduction to social LCA. Development of version 2 was handled partially in parallel with version 1.1 and continues the focus on communal participation through various engagement events (see Figures 2b).

Figures 2a & 2b. 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_2 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** ▪ Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization, Version 1.0 (2018) ▪ Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization, Version 1.1 (2020) ▪ Techno-Economic Assessment & Life Cycle Assessment Guidelines for CO_2 Utilization, Version 1.1 (2022) [THIS DOCUMENT] Peer-reviewed guideline articles ▪ Sick *et al*. (2019). The Need for and Path to Harmonized Life Cycle Assessment and Techno-Economic Assessment for Carbon Dioxide Capture and Utilization ▪ Zimmermann *et al*. (2020). Techno-Economic Assessment Guidelines for CO_2 Utilization ▪ Müller *et al*. (2020). A Guideline for Life Cycle Assessment of Carbon Capture and Utilization

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.

Table 2. List of publications closely connected to the Guidelines

Connected publications	**Publication for study commissioners and decision makers** ▪ Making Sense of Techno-Economic Assessment & Life Cycle Assessment Studies for CO_2 Utilization: A guide on How to Commission, Understand, and Derive Decisions from TEA and LCA studies, Version 1.0 (2020) ▪ Making Sense of Techno-Economic Assessment & Life Cycle Assessment Studies for CO_2 Utilization: A guide on How to Commission, Understand, and Derive Decisions from TEA and LCA studies, Version 2.0 (2020) **Worked examples for practitioners** ▪ Methanol Worked Examples for the TEA and LCA Guidelines for CO_2 Utilization (2018) ▪ Mineralization Worked Examples for the TEA and LCA Guidelines for CO_2 Utilization (2018) ▪ OME Worked Example for the TEA Guidelines for CO_2 Utilization (2019) ▪ A Guide to Goal Setting in TEA: A Worked Example Considering CO_2 Use in the Domestic Heating Sector (2020) ▪ Building an LCA Inventory: A Worked Example on a CO_2 to Fertilizer Process (2020) ▪ Interpretation of LCA results: A Worked Example on a CO_2 to Fertilizer Process (2020) ▪ Multi-Attributional Decision Making in LCA & TEA for CCU: An Introduction to Approaches and a Worked Example (2021) ▪ SNG Worked Example for the TEA Guidelines for CO2 Utilization (2021) **Workshop reports** ▪ Workshop on LCA/TEA for CO_2-based Products (2019) ▪ Towards a Common Understanding of LCA and TEA for CO_2 Utilization technologies: An Exchange Among Policymakers, Industry and Practitioners (2020)

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_2 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 six parts: Part A, **'General Assessment Principles'** introduces both TEA and LCA; Part B, the **TEA Guidelines**; Part C, the **LCA Guidelines**; Part D, the **Early-TRL Guidelines**; Part E, the **Integrated TEA & LCA Assessment Guidelines**; and Part F, an **Introduction to Social LCA** (see Figure 3). Figure 3 also schematically shows the organization of the guidelines where Part A provides a general introduction that acts as an overarching introduction. Parts B, C and F cover sit directly under part A addressing different aspects of impact assessment. Parts D and E are also guided by the principles in Part A, but can be seen as derivatives of the existing TEA and LCA guidance also, with Part D also feeding into Part E. Parts D and E deal with special application cases of the established methodologies and as such provide both contextual background and guiding principles for dealing with the subject matter.

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.

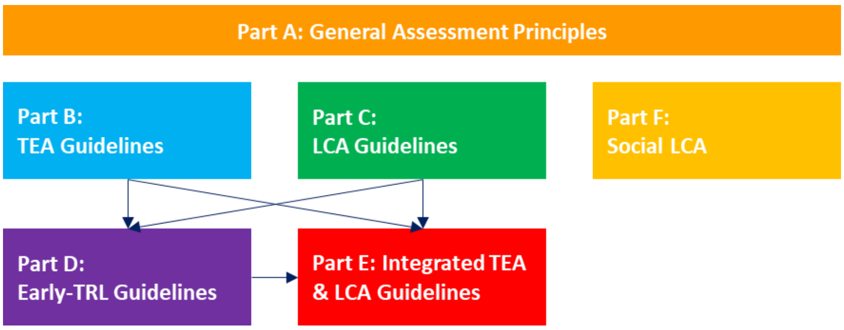

Figure 3. Structure of the TEA & LCA Guidelines document

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_2 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]	
Shall	1) Provision 1 2) Provision 2
Should	1) Provision 1 2) Provision 2
May	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_2) 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_2 that is potentially convertible to chemicals, fuels, and materials is much less than that currently emitted [1]. Furthermore, many CO_2-based products lie thermodynamically uphill; in other words, a large amount of energy is generally required to chemically reduce the CO_2. For other CCU technologies such as mineralization, no energy is required to convert the CO_2, 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)*.

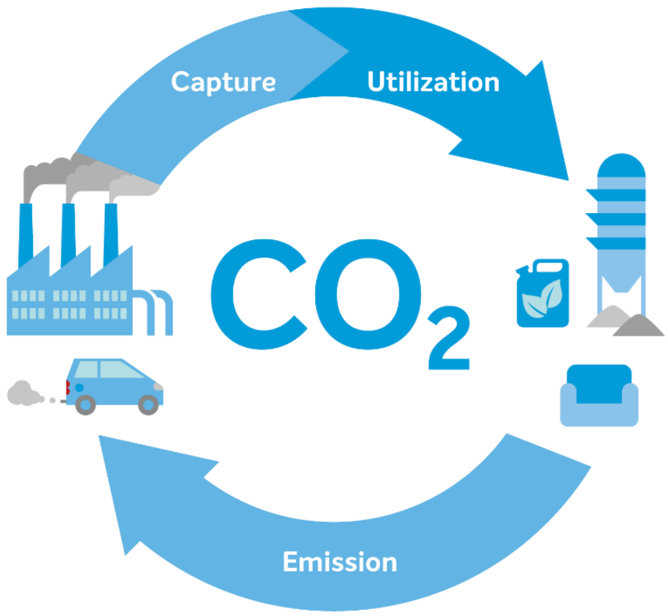

Figure 4. The CO_2 utilization cycle; Source: [1]

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_2 [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_2 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_2-based fuels that reduce nitrous oxide (NO_x) and soot emissions (see [19]).
- CCU technologies can even be carbon-negative if combined or integrated with CO_2 sequestration *(e.g., through mineralization)*.

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

- The vast majority of CCU processes have 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_2-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_2-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_2-based methanol vs. reference/benchmark gasoline for use as a drop-in fuel).*
- Energy storage systems *(e.g., CO_2-based methane that is stored and subsequently used for dispatchable electricity production).*

The 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_2 Utilization Today" by TU Berlin (2017) [1], the report "Putting CO_2 to Use" by the International Energy Agency (2019) [21], and the overview article "The Technological and Economic prospects for CO_2 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_2 Utilization" by the Global CO_2 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	**Research**	*Idea*	Basic principles observed and reported, opportunities identified, basic research translated into possible applications
2		*Concept*	Technology concept and application formulated, patent research conducted
3		*Proof of concept*	Applied laboratory research started, functional principle / reaction (mechanism) proven, predicted reaction observed (qualitatively)
4	**Development**	*Preliminary process development*	Concept validated in laboratory environment, scale-up preparation started
5		*Detailed process development*	Shortcut process models identified, simple analysis of property data, simulation of process and pilot plant using bench-scale information
6		*Pilot trials*	Pilot plant constructed and operated at low production rate, products tested in application
7	**Deployment**	*Demonstration & full-scale engineering*	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**	*Construction and start-up*	Products and processes integrated in organizational structure (hardware and software), full-scale plant constructed
9		*Continuous operation*	Full-scale plant audited (site acceptance test), turn-key plant, production operated over the full range of 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_2 generation and CO_2 capture are at deployment stage, CO_2 separation is at development stage, and the CO_2 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

Provisions A.1 - Technology Maturity	
Shall	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
Should	1) The TRL concept should be used to identify technology maturity 2) The TRL concept and its definitions should be clearly referenced or added to the report
May	

Integration of TEA and LCA

A.4.3 Introduction

When implementing new CO_2 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.4.4.1) 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.4.4 Types of TEA / LCA Integration

A.4.4.1 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.4.4.2 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.

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

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_2-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:

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

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 CO2-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.4.4.3 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 recommended 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.4.4.4 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.4.5 Alignment of TEA and LCA

A.4.5.1 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.4.5.2 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_2 hydrogenation within a renewable-power-to-liquid context in Germany?
- LCA goal: To compare the environmental consequences of producing methanol for use as a chemical feedstock in Germany, synthesized via two routes: the hydrogenation of CO_2 captured from a cement plant vs. methanol synthesized using the conventional steam-methane reforming process from natural gas.
- Integrated goal: How can a methanol production plant located in Germany, which uses wind energy for CO_2 hydrogenation, be optimized to maximize technological, economic, and environmental performance?

A.4.5.3 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_2 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_2 input flow *(e.g., by calculating the costs of CO_2 capture from the CO_2 source or by assuming CO_2 costs via a market price for CO_2)*. While system expansion can be applied when conducting TEA, it can cause complications involving detailed modelling and data collection for the CO_2-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.5 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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Figure 1 and Figures 2a&b were designed using resources from Flaticon.com.

PART B
TEA Guidelines

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Contents Part B

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).

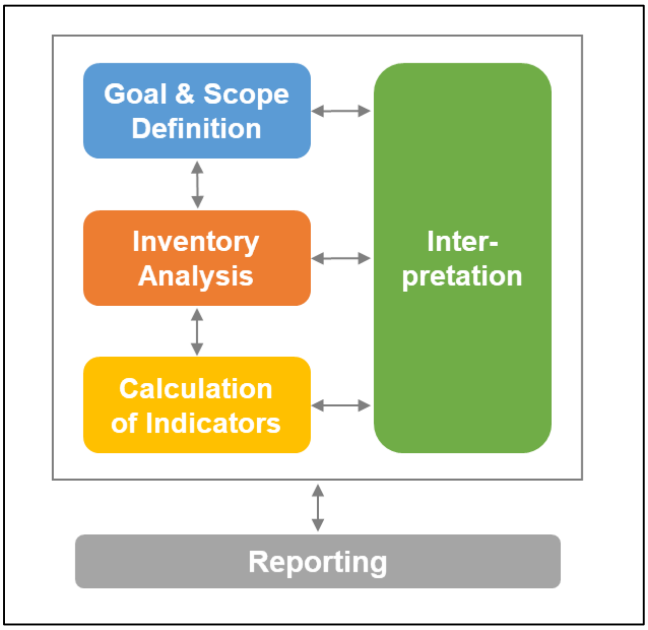

Figure 1. Phases of techno-economic assessment

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_2 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
R&D-perspective	Assessment of specific project(s) in research or development; either identification of major barriers and drivers (hot-spots) for a single project or comparison of various projects	▪ What are major cost and value drivers? ▪ What product performance characteristics have to be met? ▪ What aspects need to be worked on (next)? ▪ How does the current development state rank amongst alternatives? ▪ Do we fund CCU research and development of project X?	▪ *(Scientific) assessment of economic potential of product or technology* ▪ *Planning of next R&D steps or priorities* ▪ *Decisions on funding program*
Corporation-perspective	Analysis of projects in development and deployment; assessment of investment alternatives and comparison to existing processes; use of detailed process data is common	▪ How does the CCU product perform against current and upcoming benchmarks? ▪ Is the CCU product in a future scenario economically viable? ▪ How does the investment in a CCU product deployment / demonstration project / full-scale plant compare to alternatives?	▪ *Business case for new CCU plant* ▪ *Economic due diligence for investment in CCU start-up*
Market-perspective	Analysis of projects in development and deployment stages; focus on supply chains, effects of economic policy, the best use of resources, or the best way of obtaining a specific utility	▪ What are current states, favorable conditions, best practices, and necessary actions for regional CCU value chains? ▪ What regulatory clarification and support (type, timing, and budgets) is required for specific CCU products or services?	▪ *Local CO_2 supply chains* ▪ *National CO_2 regulations* ▪ *Comparing multiple product applications, comparing best resource use of CO_2, H_2, electricity*

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	
Shall	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
Should	1) The intended TEA perspectives (R&D, corporation, market) should be stated
May	

B.3.3 Assessment Scenarios

B.3.3.1 Introduction

Scenario analysis is the process of considering scenarios for evaluating potential future events. Scenarios are alternative – 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

Provisions B.2 - Assessment Scenarios	
Shall	1) Scenarios used shall be distinct and both physically and economically plausible 2) The base case scenario shall serve as a baseline for analysis, extending current trends 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 4) Scenarios used shall be developed in interaction with the stakeholders of the study 5) If TEA and LCA are integrated with high level of data alignment, the same set of scenarios shall be used
Should	1) Scenarios used should factors as necessary to account for potential temporal changes 2) Scenario assumptions and data should be provided via 'open access' 3) Scenarios featuring future, clean technologies should be considered
May	

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^2 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_2-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
Product application	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
Market segment	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)

Properties **CCU class**	**Substitutes** Chemical products	 Material products	 Fuels	 Energy storage systems	**Non-substitutes** All
Basis for comparison	Mass	Material performance	Energy	Storage performance	Service or performance provided
Functional unit	*e.g., mass, plant output*	*e.g., mass, plant output*	*e.g., energy, mass, plant output*	*e.g., energy, plant output*	Compare performance of new versus existing solutions
Reference flow	*e.g., 1 t methanol, 1.6 Mt/a plant output*	*e.g., 1 t concrete, 50 kt/a plant output*	*e.g., 1 MJ of* H_2*, 2.5 Mt/a diesel output*	*e.g., storing 1 MJ of electricity, 80 MWh battery*	*e.g., 1 t, 1 MJ, output of a plant*

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

Provisions B.3 - Definition of Product Systems and Functional Units	
Shall	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 2) The functional unit shall be defined based on the good judgement of the practitioner following these principles: 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 b. For products with a structure or characteristics different to benchmark products (non-substitutes), the functional unit shall be derived from the product performance 3) If the TEA study is conducted together with an LCA, the functional unit shall be consistent for both studies
Should	1) The definition of the product application should follow these principles: a. For products with a small number of applications, one typical application or a relevant application-mix should be defined 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 c. The product application should be defined specific to market segments 2) Corporate-perspective TEAs should include a description of at least one customer group and their needs
May	1) Multiple product applications may be assessed and compared against each other, following the provisions for each application individually 2) For products with a large number or unspecified applications, the functional unit may describe the output of a plant

B.4.3 Product System Elements and Boundaries

B.4.3.1 Introduction

For the purpose of this document, the term 'system element' describes a key activity of the product system, 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.

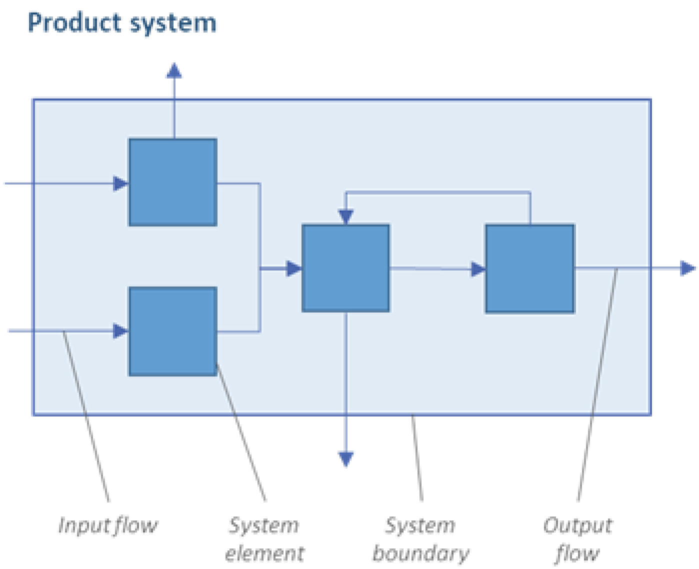

Figure 2. Example product system, showing elements, boundaries, and input & output flows

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_2 capture, methanol synthesis)*. If required by the assessment goal, the system elements **may** be further refined as unit operations *(e.g., reaction, distillation, adsorption, membrane filtration)* or even unit equipment *(e.g., pump, reactor vessel, rectification column).*

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_2 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_2 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_2 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]).

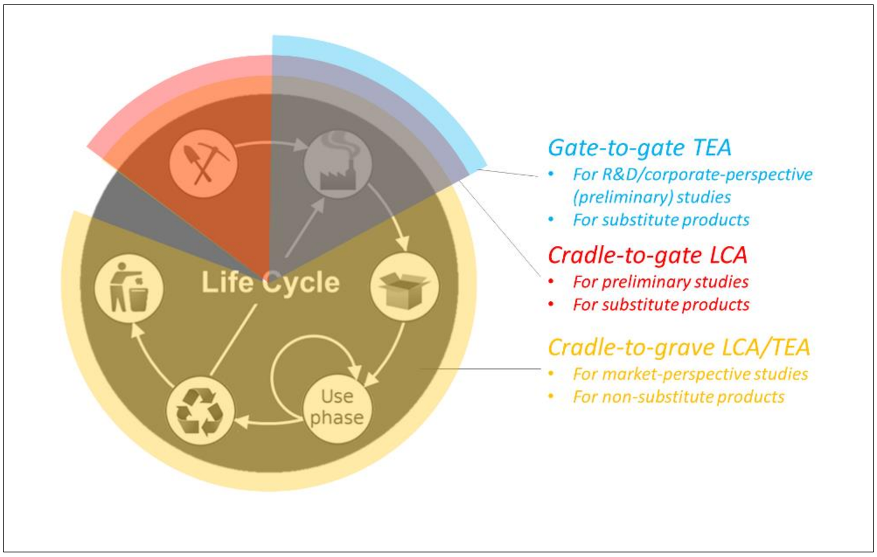

Figure 3. The scope of TEA and LCA in the product life cycle, adapted from [16]

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_2 capture, separation, and transport processes. Other common important upstream processes include H_2 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_2, H_2, or electricity are provided without charge. For example, if CO_2 can be used economically, the gain in value for the CO_2 consumer and the emitter will demand compensation; if CO_2 emissions are fiscally penalized, they create an additional burden for the emitter, and the CO_2 consumer will demand compensation for consumption.

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

Provisions B.4 - Definition of System Elements and System Boundaries	
Shall	1) Process units shall be used as the basis for system elements 2) The system boundaries shall be derived from the assessment goal and shall be consistent throughout the study 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 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 5) If an upstream process is excluded from the final system boundaries the reasoning shall be explained 6) Product systems, elements, and boundaries shall be presented in a graphical scheme and specifications for all input flows shall be described
Should	1) System elements should serve as the unit for accounting and recommendations 2) For non-substitute products, any gate-to-gate assessment should either include price–performance correlations or the boundaries should be extended to cradle-to-grave to include the impacts from the whole life cycle 3) Key CCU processes, such as CO_2 capture, separation, and transport, should be included in the assessment 4) For product systems with multiple functions, function dependencies should be taken into account
May	1) The system elements may be further refined as unit operations or even unit equipment 2) In case of an integrated assessment, cradle-to-grave boundaries may be used to align a TEA study with an LCA study

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_2-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	
Shall	1) Benchmark products and benchmark systems shall be selected and stated according to the product application and assessment goal 2) The currently most common or best-in-class products shall be selected as benchmark products; multiple benchmark products can be included
Should	1) Customer needs should be used to identify utility and competitive advantage 2) Benchmark products that are likely to become relevant in the future should be included
May	

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_2 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
Technical	Energy demand	*Heat demand, cooling demand, electricity demand, primary energy demand*
	Energy efficiency	*Lower heating value efficiency, higher heating value efficiency, energy/exergy efficiency, CO_2 capture penalty*
	Mass demand	*Mass demand of individual inputs, mass of CO_2 converted*
	Mass efficiency	*Atom economy, yield, percentage of CO_2 converted*
Economic	Processing effort	*Operational expenditure (OpEx)*
	Investment effort	*Capital expenditure (CapEx)*
	Product margin	*Market-derived margin for product, company-internal margin*
	Product volume	*Market volume for product, company-internal demand*
	Resource availability	*Market volume for feedstocks, company-internal availability of resources, number of suppliers*
	Profitability	*Profit, net present value, internal rate of return*
	Profit/cost per functional unit	*Cost per kg benchmark product equivalent, cost per km, cost per MJ stored*
Techno-economic	Technology maturity	*Technology Readiness Level (TRL) regarding market introduction (Horizon 2020 definition), company internal maturity rating*

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

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

B.4.6 Consistency and Reproducibility

It has been observed that consistency and reproducibility are challenging for CCU TEAs, and therefore it is suggested to follow the criteria of the ILCD Handbook [4], as summarized with minor adaptions 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	
Shall	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 2) Sufficiently consistent data regarding accuracy, precision, and completeness shall be applied 3) Inconsistencies shall be documented. If significant, the inconsistencies shall lead to the adaption of the goal or shall be taken into account for interpretation and reporting 4) All selected methods for calculating indicators shall be described clearly, including why they were chosen 5) Methods and method selection shall be documented a) *For public reports:* in an appropriate and transparent way that would enable another TEA practitioner to sufficiently reproduce the assessment and results b) *For confidential reports:* in a separate, confidential file that shall be made available to the critical reviewers in confidentiality
Should	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 2) The documentation should begin from the project start; documentation should be guided by reporting needs
May	1) The assessment may include suggested ways or techniques to avoid pitfalls in assessment procedures

B.5 Inventory 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).

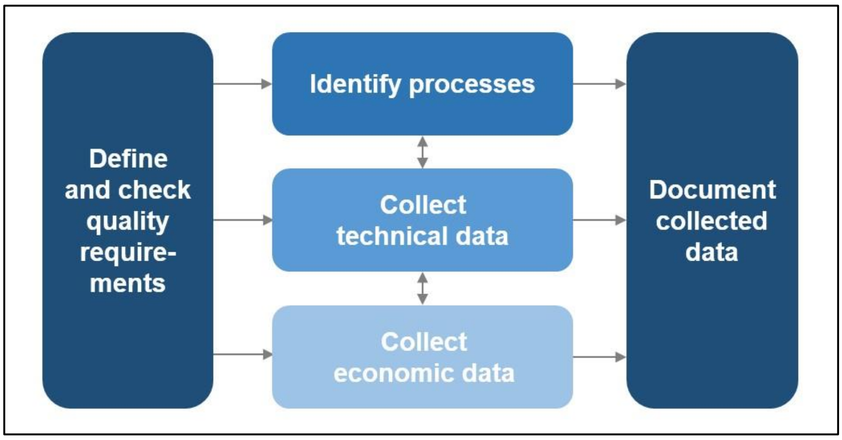

Figure 4. Five phases of TEA inventory creation

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_2 and other key inputs will be discussed in more detail within this chapter.

As a result, the inventory summarizes all relevant technical as well as economic parameters and assumptions of the product and benchmark systems, such as equipment, material and energy flows, transport or waste, and their assigned prices and market volumes. Additionally, information about the context (temporal, regional, economic) of the studied scenario 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_2 capture cost from data bases or literature reviews, average contents of typical steel plant flue gas streams, average transportation cost within a certain region, etc.)*
- ***Generic data:*** data that 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_2 capture cost or H_2 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

Provisions B.8 - Interim Quality Control and Approximations	
Shall	1) Quality requirements shall be defined for each collected data set according to the assessment goal 2) Data quality shall be checked and documented during data collection 3) Problems encountered in acquiring confidential data shall be clearly stated
Should	1) Data available at the corresponding technology maturity should be collected 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 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 4) Process-specific and primary data should be used with increasing maturity of the assessed process 5) Readily available generic or average data should be used from secondary sources where sufficiently representative
May	

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
Euro-Stat Prodcom database	Statistical data on manufactured goods	EU member states	Open
U.S. Bureau of Labor publications	Cost of operating labor	US	Open
IHS Markit	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
ICIS	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
Platts	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
Argus Media	Industry price data, market studies, business news	Worldwide and country-specific	Restricted
Alibaba	Industry price data	China	Open
US Energy Information Administration (EIA)	Energy and energy carrier prices	US	Open
UN Comtrade Database	Customs/trade data	Worldwide and country-specific	Open
Zauba Technologies & Data Services	Customs/trade data	India	Open
Alphasights	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_2 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].

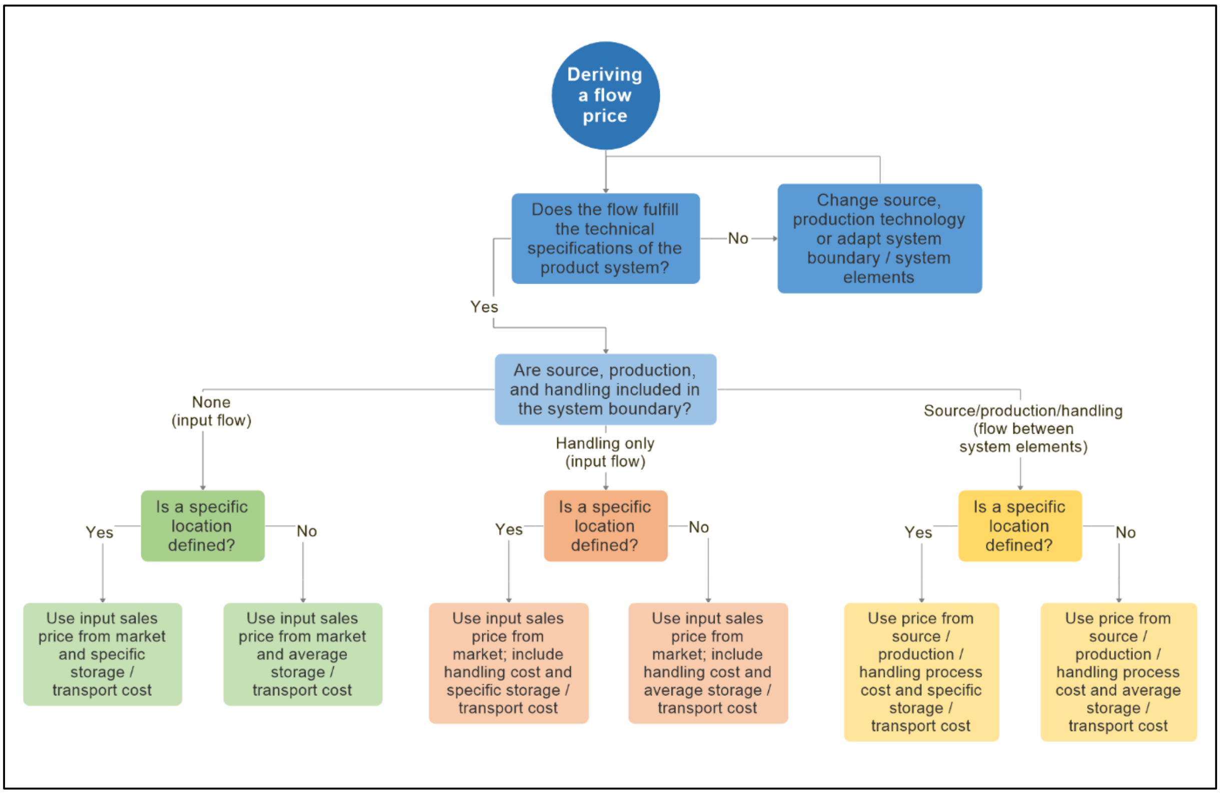

Figure 5. Deriving a flow price (as published in [28])

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

Provisions B.9 - Collecting Data	
Shall	1) Data collection shall be planned and prepared according to data requirements, selected methods and indicators, and overall assessment goal 2) The level of detail of the technical data shall follow the identified processes along the system elements 3) 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 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 5) Three consecutive factors shall be considered when deriving flow prices: a. Technical specifications: the technical specifications of the input flows shall match the requirements of the product system 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 c. Location: flow prices shall be further derived according to whether specific locations are defined for input source, transportation, and storage
Should	1) When collecting technical and economic data from different sources, harmonization should be carried out, which means maintaining uniformity and aligning assumptions 2) The quality of price data and the number of data sources should be adapted to technology maturity: a. In the early research and development stage, market-average price data should be used b. In the development stage, market-average price data that are date- and location-specific should be included c. In the deployment stage, process-specific data and primary sources should be used 3) Accessibility to the local value chain for both input material and product sales should be assessed
May	1) Regions or addressable market segments or market growth rates may be included to refine the estimation of market volumes

B.5.4 Deriving a CO_2 Price

B.5.4.1 Introduction

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

Typical pitfalls that TEA practitioners need to avoid when selecting CO_2 prices in TEA of CCU include:

- Assuming zero cost for CO_2
- Assuming emission trading price or emissions tax as CO_2 price
- Assuming greenhouse gas abatement cost instead of CO_2 capture cost (see following paragraph)

B.5.4.2 CO_2 Capture Cost and Greenhouse Gas Abatement Cost

In the following, the terms CO_2 capture cost and greenhouse gas (GHG) abatement cost are discussed in more detail. The amount of CO_2 captured states the amount of CO_2 emissions that is separated and available for further processing in a plant equipped with CO_2 capture technology. CO_2 capture cost (or cost of CO_2 captured) relates all resulting costs of the process to the amount of CO_2 captured *(e.g., cost/t$CO_{2\ captured}$)*. The costs include all operational and capital expenditures of capturing CO_2 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_2 equivalents, between a system with CO_2 capture and the benchmark system without CO_2 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_2 equivalents *(e.g., cost/t$CO_{2e\ abated}$)*. GHG abatement cost is a widely used measure from the field of CO_2 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_2 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_2 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_2 **Price**

The CO_2 price and its calculation or estimation strongly depend on the system elements in the product system, meaning whether CO_2 source, capture process, purification, compression, or transport are included or excluded from the assessment boundaries. If the CO_2 capture process is included in the system boundaries, the CO_2 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_2 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_2 emission streams and to consider average costs for capturing and compressing CO_2 at these plants as well as transporting the CO_2. In the case of high-purity CO_2 streams ready for use, capture is not relevant and instead compression and transport are the cost drivers. Note that commercial price quotes for CO_2 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_2 capture cost; if such information is unavailable, an explanatory statement **shall** be included.

B.5.4.4 Deriving CO_2 Costs from the Literature

Generally, when considering published data on CO_2 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_2 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_2 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_2 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_2 costs specific to CO_2 emission source, capture technology, time frame, and location
  - Literature reviews: Listing, analyzing, and comparing reported data on CO_2 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_2 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_2 Emission Sources and Costs

CO_2 cost generally differs depending on the selected CO_2 source, due to differing CO_2 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_2 streams as an input, others can utilize less pure CO_2 streams. Since purification requires additional efforts and has important impacts on costs, practitioners **should** select a CO_2 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_2-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_2 capture costs range between 5 USD and 180 USD per tonne of CO_2, or even higher for some sectors [29]–[32]. The open access EU Eurostats Prodcom database reports an average EU-28 market value for CO_2 of 0.078 Euros per kg of CO_2 in 2016 (division of the overall annual financial value of traded carbon dioxide by the annual sold volume in the EU-28 states in 2016) [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_2 sources is presented in Table 6.

Table 6. The range of CO_2 emitters in various sectors potentially providing CO_2 streams of differing purity

CO_2 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_2 price needs to be derived, otherwise a location-average CO_2 price is sufficient (see Figure 5 and B.5.3.2). Location-specific CO_2 prices are usually relevant for product systems including the source type, capture, and transport of CO_2 within the system boundaries, thus requiring data on locally available CO_2 emission sources. Location-average CO_2 prices are usually relevant for product systems excluding the specific source, capture process, and transport of CO_2 from system boundaries, thus requiring data on averaged CO_2 cost from regionally relevant sources with average assumptions about transport costs.

Practitioners **should** investigate the local proximity of the CO_2 source to the investigated utilization plant in relation to transport costs. In most cases the transportation of CO_2 is relatively costly, especially if there is no dedicated infrastructure, such as a pipeline system, in place. CO_2 transport cost will most likely decrease with closer proximity of the capture location to the utilization plant.

B.5.4.6 Regulation and CO_2 Price

As introduced in chapter B.5.4.1, the price for CO_2 flow cannot be derived based on prices of CO_2 emission certificates or taxes. Nevertheless, it is recommended that practitioners investigate the influences of regulations for CO_2 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_2 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_2 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_2 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_2 storage as an integral part in financing incentives *(e.g., ETS)*. Consequently, it is unclear to what extent CO_2 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_2 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_2 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_2 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_2 capture costs. In the case of literature values, it is not recommended to base the choice of emission source on the lowest CO_2 price available without critically reviewing the underlying sources and capture processes, as these might cause higher environmental burdens compared to alternatives. In the case of reported CO_2 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_2 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_2-related subsidies or penalties.

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

- Technologies: capture, compression, transport, and storage concepts; CO_2 concentrations, flow rates, flow conditions
- Prices: process-specific or average cost of CO_2 capture
- Limitations: regional restrictions, reference year, and applied transformation factors

B.5.4.8 Further Reading

An overview of CO_2 emission sources and reported CO_2 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_2 Price		
Shall	1)	CO_2 capture cost shall be reported; if such information is unavailable, an explanatory statement shall be included
	2)	Technological and economic assumptions shall be documented
Should	1)	The CO_2 source should be selected by considering CO_2 at the lowest purity and level of compression that is technically required by the process, and by the associated transportation requirements
	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.
	3)	Local proximity of the CO_2 source to the utilization plant should be investigated in relation to transport costs
May	1)	Regulatory adjustments (e.g., ETS) or cost-lowering mechanisms may be applied in additional scenarios except in the base case

B.5.5 Other Key CCU Inputs

B.5.5.1 Introduction

There is a considerable range of different key inputs for CCU technologies, besides CO_2, which will partly be introduced in the following chapters. Some typical CCU key inputs are electricity, hydrogen, mineral sources, fly ash, catalysts, fossil hydrocarbons, 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_2 is a decisive factor for profitability, which is why calculation or estimation of H_2 prices needs to be planned and executed carefully. Being strongly connected to energy input, H_2 generation can have both substantial economic and environmental impacts.

Typical pitfalls the TEA practitioner needs to avoid when deriving H_2 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_2 emissions in the CCU process
- Assuming free or negative electricity prices in the base case scenario
- Assuming H_2 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_2 production scales for particular technologies that are economically or technologically unfeasible
- Assuming an optimistic future scenario of H_2 generation as the base case

B.5.5.2.1 Present and Future H_2 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_2 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_2 or as a byproduct of other processes. So-called 'merchant' H_2 is produced off-site by a commercial H_2 supplier. An overview of current and future H_2 production technologies and estimated production costs can be found in technology roadmaps such as those provided by the International Energy Agency (IEA) [38]–[40]. The current predominant H_2 generation processes are listed in Table 7.

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

H_2 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_2 (calculated from the heat of formation) from fossil sources, biomass, or water differs considerably, being much lower for hydrocarbons than that for water electrolysis [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_2 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_2 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_2 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_2 production technologies.

Similar to the CO_2 price, the H_2 price needs to represent cost of production or a market price. It is of considerable importance to consider transportation and storage of H_2, as the energy required for compression and the safety requirements for storage need to be reflected in the attributed costs. H_2 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_2 production is included within system boundaries, the H_2 price need to be calculated based on the full location-specific process
- If H_2 production is excluded from system boundaries, the H_2 price need to be collected either from a supplier quote or a location-average estimate specific to the production route
- H_2 transport and storage need to be represented in the H_2 price, independent of their inclusion within system boundaries

In accordance with Guideline B.2, for the base case scenario, a current, mature H_2 generation process needs to be selected. In additional scenarios, future, low-carbon-footprint H_2 generation processes can also be considered for cost estimation. The scale and maturity of the selected H_2 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_2 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_2 generation utilization factor. If a specific electricity technology is selected *(e.g., for wind (onshore / offshore), photovoltaic, solar-thermal, nuclear, and other major low-carbon electricity generation technologies)*, 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_2 cost. If satisfactory data cannot be obtained to estimate the cost of producing H_2 from intermittent energy supply, then estimation based on LCOE by assuming reasonable full-load hours can be conducted. The price of H_2 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_2 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_2 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_2 input stream can be low, as the presence of impurities such as NO_x has no effect on the carbonation reaction. Costs for additional inputs such 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_2 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_2 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_2, 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_2 price estimation for different production routes can be found in various reports [38], [40], [41]. A general overview of H_2 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

Provisions B.11 - Other Key Inputs for CCU Technologies	
Shall	**Hydrogen as Input** 1) The scale and maturity of selected H_2 generation process shall be discussed regarding current and future technological and economic viability 2) Technological parameters and those for energy sources and electricity prices affecting hydrogen production costs shall be clearly documented **Electricity as Input** 3) If electricity from renewable sources is selected, then availability shall be discussed and temporal and regional contexts shall be documented
Should	**Electricity as Input** 1) Electricity from grid mix should be considered either in the base case or additional scenarios 2) Any electricity price in the base case should not be set at zero cost **Mineralization** 3) Preprocessing scenarios and their resulting energy demand as well as transportation scenarios should be assessed 4) The local regulatory context for compensation of industrial mineral waste treatment should be investigated **Further Inputs** 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 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
May	

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

Provisions B.12 - Documentation in Data Collection	
Shall	1) Relevant data, such as parameters, decisions, and assumptions, shall be documented for all scenarios, preferably throughout the collection process 2) Data shall be documented based on the functional unit and reference flow 3) Characteristics and limitations shall be documented – preferably at the beginning of the study 4) Parameters shall be documented in SI units, or else clear documentation and definitions shall be provided for all non-SI units utilized
Should	1) Data should be documented for each system element independently 2) Data quality should be documented throughout the data collection process 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
May	1) Data may be documented in absolute values 2) A conventional flow diagram, consisting of system elements together with mass and energy flows, may be extended by relevant TEA data

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_{CO2e})*. 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).

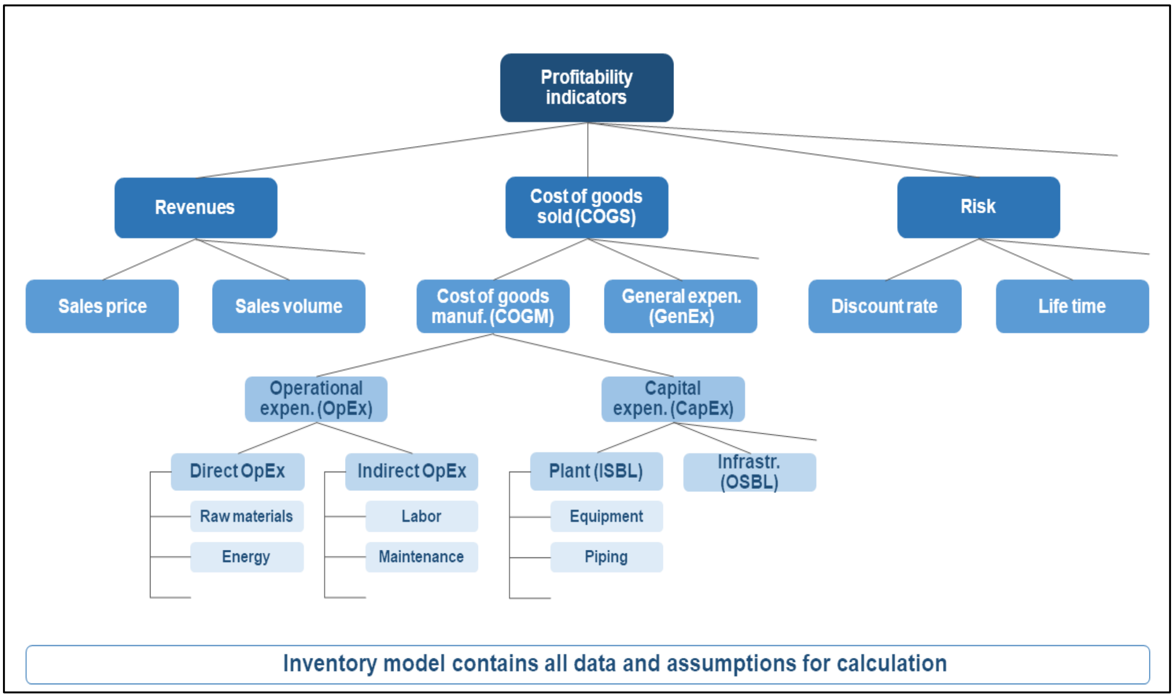

Figure 6. Calculation hierarchy for economic indicators, adapted from Buchner et al. [20]

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_2 capture, H2 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	
Shall	1) Methods that comply with the goal and scope of TEA shall be selected 2) Inventory data shall be linked to calculation of indicators 3) Calculation of indicators shall be conducted separately from inventory 4) If uncommon methods are used, motivation and explanation shall be stated 5) All assumptions, requirements, and adjacent estimates shall be stated 6) The equation employed and the reasons for choosing each indicator shall be presented 7) Calculations shall be conducted for the overall system as well as for each system element individually
Should	1) Results should be stored in a separate file from the calculation of indicators 2) Methods commonly used in the literature should be used 3) Methods that are as accurate as the available data permit should be selected, following the iterative approach
May	

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 adaptions 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 adaptions* [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

Technology maturity phases	Research	Development	Deployment
AACE Estimate Classes	**5 and 4**	**4 and 3**	**2 and 1**
Typical methods adapted from AACE	▪ Short methods ▪ Parametric techniques (low detail) ▪ Factored methods ▪ Cost transformation	▪ Component factored methods ▪ Parametric techniques (high detail) ▪ Inclusion of unit cost line items ▪ Cost transformation	▪ Unit cost line items (high detail or based on design quantities) ▪ Still undefined items: detail component factored methods (or “forced detail”)

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
- 'Nth 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	
Shall	
Should	1) At early to mid technology maturity 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 b. OSBL cost should be estimated in total as a factor applied to ISBL cost 2) At mid to high technology maturity, the cost scaling of the main components should be analyzed 3) At high technology maturity a. all CapEx items should be estimated independently b. OSBL should be estimated independently of ISBL 4) Components should be clearly assigned to either ISBL or OSBL 5) CapEx estimation should be conducted critically using multiple methods in parallel
May	1) If equipment specifications are required but cannot be derived, they may be assumed for economic calculations ('forced detail') 2) If CapEx is found to be of minor overall importance, the accuracy demands for CapEx estimation may be lowered 3) Contingency may be included in a CapEx estimate 4) Learning curve effects may be included to estimate NOAK plant CapEx

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_2, 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	▪ Based on stoichiometry, measured mass flows, or design/simulation	▪ Based on measured mass flows or design/simulation	▪ Based on measured mass flows or design/simulation
Energy, utilities & other variable OpEx	▪ Based on measured energy flows or design/simulation ▪ Factored estimation (based on material cost) ▪ Cost increments from similar plants	▪ Based on measured energy flows or design/simulation ▪ Cost increments from similar plants	▪ Based on measured energy flows or design/simulation
Fixed OpEx	▪ Simple factored estimation ▪ Cost increments from similar plants	▪ Detailed factored estimation ▪ Cost increments from similar plants	▪ Detailed factored estimation ▪ Separate calculation of fixed OpEx items
General expenses & freight	▪ Factored approach	▪ Factored approach or company-specific	▪ Company-specific
Main price data and sources	▪ Price data: market-average ▪ Sources: few, secondary	▪ Price data: market-average ▪ Sources: multiple, secondary	▪ Price data: process-specific ▪ Sources: few, primary (supplier quotes)

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

Provisions B.15 - Estimation of Operational Expenditure	
Shall	
Should	
May	1) If of minor importance, energy cost may be estimated as a share of the total raw material cost 2) If of minor importance, utilities or other variable costs may be estimated as a share of the total energy cost

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	
Shall	
Should	1) One indicator that normalizes profit to cost should be used 2) When the addressable market volume is derived, an absolute profit measure should be calculated 3) From later development stages onwards, NPV should be calculated 4) When applying dynamic indicators, an interest rate should be selected that represents the same risk profile as the projected technology 5) In later development and deployment, interest rates should be adapted to different financing instruments 6) When applying dynamic indicators, scenarios should be described in great detail
May	

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_{CO2e} / $t_{product}$ 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

Provisions B.17 - Normalization and Weighting	
Shall	
Should	
May	1) Normalization of results beyond the reference flow may be applied as an optional step, but only with great caution. If applied: a) Results have to be normalized for each indicator separately b) Reasons for selecting normalization and scaling criteria as well as initial, absolute indicator values must be documented 2) Weighting may be applied as an optional step, but only with great caution. If applied: a) Indicators with different dimensions must be normalized b) Indicators with the same dimension are recommended to be normalized c) Reason for weighting, weighting scheme, and the assigned weights, as well as initial, discrete indicator values have to be documented

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_2 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 bonds), 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].

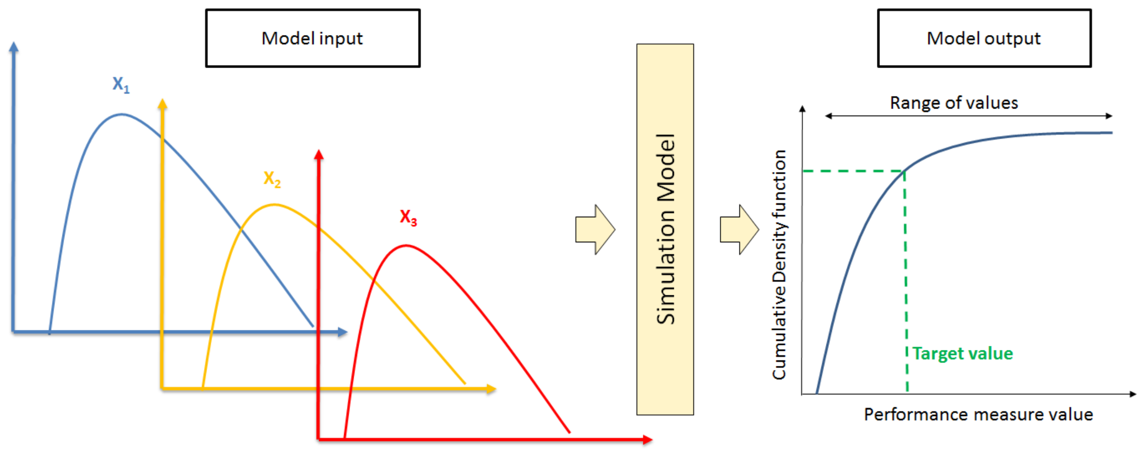

Figure 7. Simulating variable inputs to obtain probability distributions of a performance indicator

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_2 capture cost and CO_2 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., ±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].

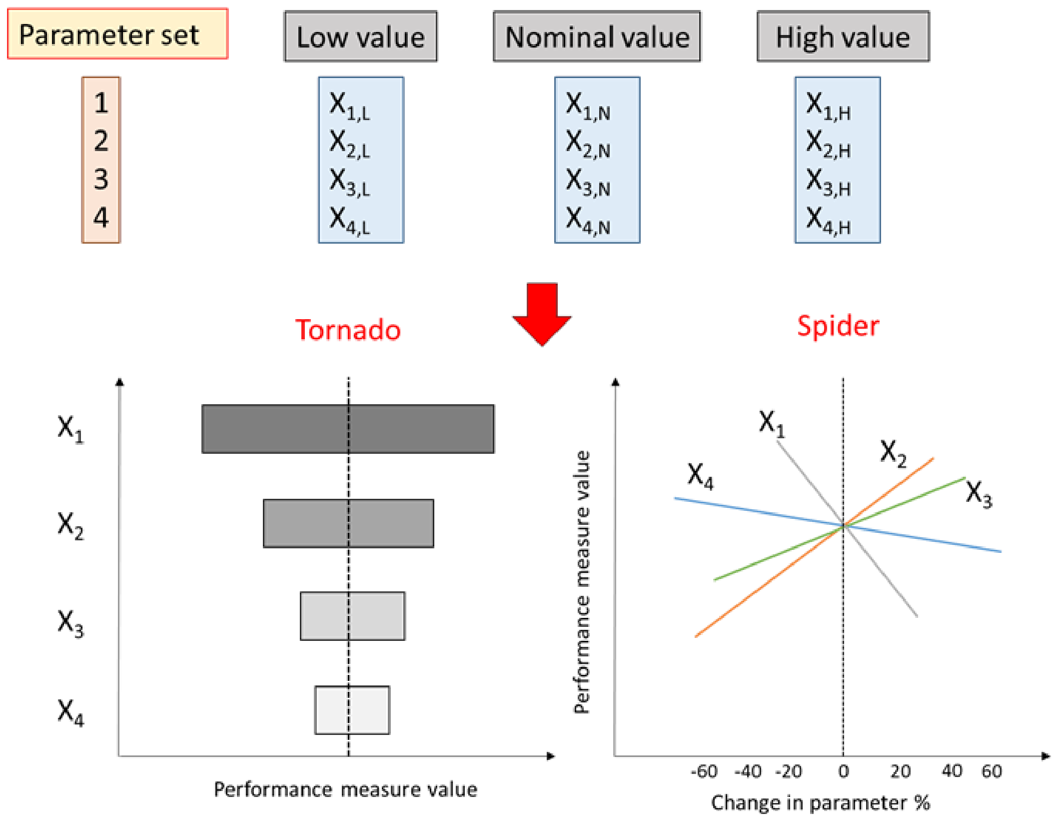

Figure 8. Visual representation of deterministic sensitivity analysis

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_2 capture, CO_2 conversion plant, H_2 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_2 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.

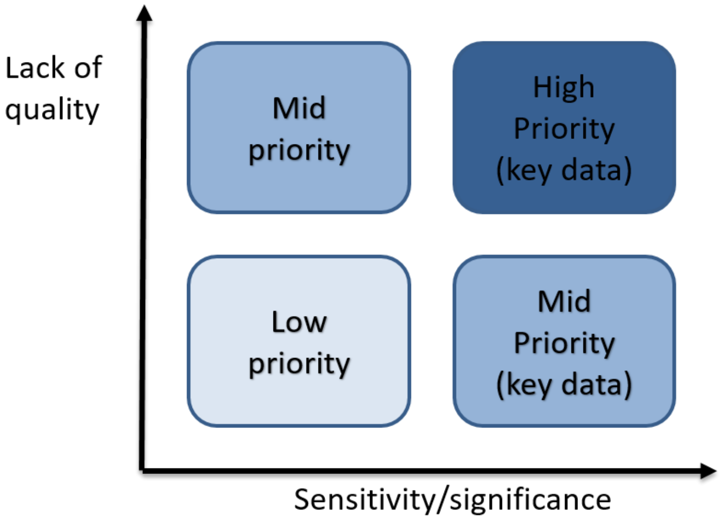

Figure 9. Priority setting for improving key data for inventory, adapted from [4]

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	
Shall	1) Conclusions, limitations, and a basis for recommendations with respect to the calculated results shall be provided 2) Uncertainty analysis shall be conducted and output uncertainty identified 3) Sensitivity analysis shall be conducted and key variables identified
Should	1) For the first assessment iteration, local sensitivity analysis should be conducted 2) To cover the whole parameter space, global sensitivity analysis should be conducted 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
May	1) Qualitative uncertainty analysis may be conducted in the research phase

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_2 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_2 input price, H2 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	
Shall	1) The interpretation of any indicators shall be conducted in compliance with their definition, especially according to its described limitations 2) Indicator values shall be compared to an alternative value 3) IRR shall be interpreted only together with respective indicators of absolute profitability
Should	1) The interpretation of indicators should involve absolute indicator results as well as the uncertainty ranges 2) Threshold analysis should be conducted for identified key variables
May	1) Risk preferences of practitioners may be documented for subsequent decision-making steps

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

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 Realité (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_2 conversion, undesirable side products, reactor temperature)*.

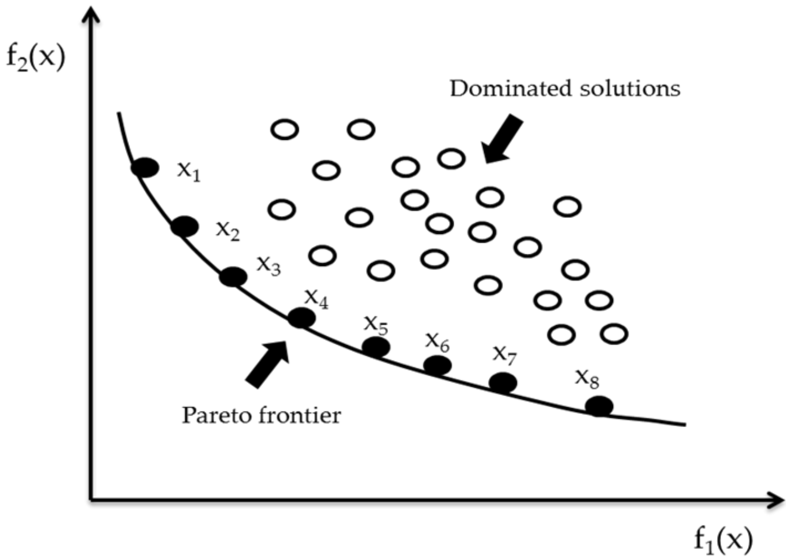

Figure 10. Potential range of solutions for a two-objective optimization problem showing the Pareto frontier

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

Provisions B.20 – Multi-criteria Decision Analysis		
Shall		
Should	1)	The whole spectrum of criteria relevant for decision making should be presented to decision makers
May	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 adaption 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_2 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_2 utilized in the process needs to be clearly stated in relative or absolute numbers. Moreover, it is essential to state that this amount does not correspond to the amount of 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_2 utilized refers to the amount of CO_2 that the process uses to produce the product. It is important to distinguish between CO_2 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_2 capture, H_2 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_2, hydrogen, electricity, minerals, fossil feedstocks, or catalysts
- ❑ State types and sources of data, including quality and confidentiality
- ❑ Report CO_2 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	
Shall	1) All phases of the study shall be covered in the TEA report 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 3) Indicator results shall be set in relation to uncertainties and sensitivities in the main report 4) Clear language shall be used in the TEA report
Should	5) If the provisions of this Guideline document were applied, conformity should be declared and for deviations an explanation provided 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 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 8) Reports should include a summary in written form (such as an Executive Summary) and a technical summary in table form 9) Findings for system elements as well as the whole product system should be reported to facilitate comparison with other studies 10) If economic incentives are included in the calculation, these **should** be clearly stated and their impacts clarified
May	1) LCA reporting principles may be applied in addition to TEA reporting, especially when conducting LCA and TEA in parallel 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 3) The Reporting Checklist may be used to ensure all aspects are covered

B.9 References

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B.10 Annex

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

CO_2 emissions (direct) industry, recent estimates from various years [Mt_{CO2}/year] [30]		CO_2 capture for combustion processes	CO_2 separation for all processes	*H_2 production*	*Electricity production*
Coal power plant (PP)	9 031	▪ Post-process	▪ 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_2 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	*Construction & start-up*	*Continuous Operation*
Description	Basic principles observed and reported, Opportunities identified, Basic research translated into possible applications *(e.g., by brainstorming, literature study)*	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
A *(e.g., CO_2 capture)*	Flue gas	t/h
	CO_2 input	t/h
	CO_2 capture	%
	Electricity consumption	MW
	…	
B *(e.g., Water electrolysis)*	Deionized water	t/h
	…	
C *(e.g., CO_2 conversion)*	CO_2 input	t/h
	…	
D *(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
Base year	Year	…
Location	-	
Location index for capital investment	-	
Currency	-	
Plant capacity	t/a	
Project lifetime	Years	
Operating time	Hours/year	
Construction period	Years	
Tax rate	%	
Equity/debt ratio	%/%	
Debt payment	Years	
Return on equity	%	
Cost of capital	%	
Salvage value	Currency	
Depreciation method	-	
Depreciation period	Years	
Material and utility prices		
Assumptions for market entry		…
Temporal and regional context		
Market limitations		
Other parameters		

Table 15. Technical summary table

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

PART C
LCA Guidelines

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SUPPORTED BY

Contents Part C

C.1 Introduction

C.1.1 General Introduction to Life Cycle Assessment

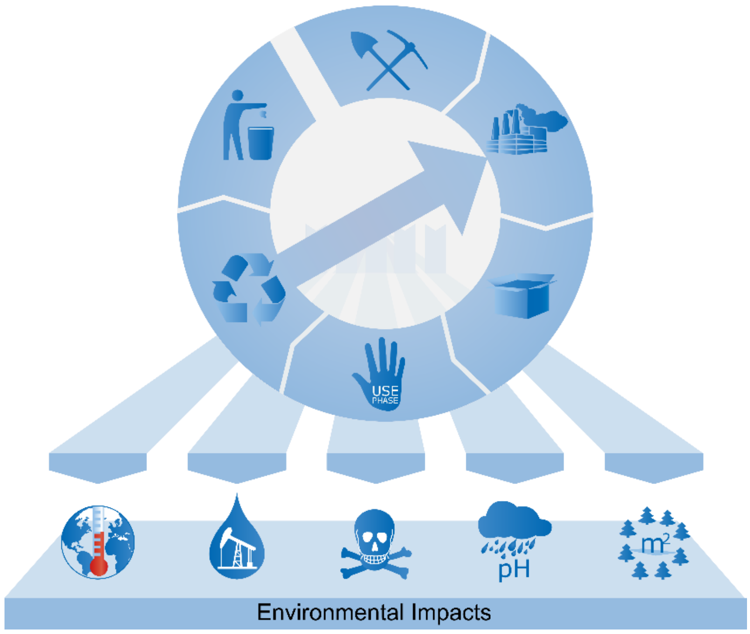

Figure 1. The holistic approach of life cycle assessment accounts for environmental impacts associated with all stages of a product's life cycle (central circle)

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[1]. 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

[1] 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.

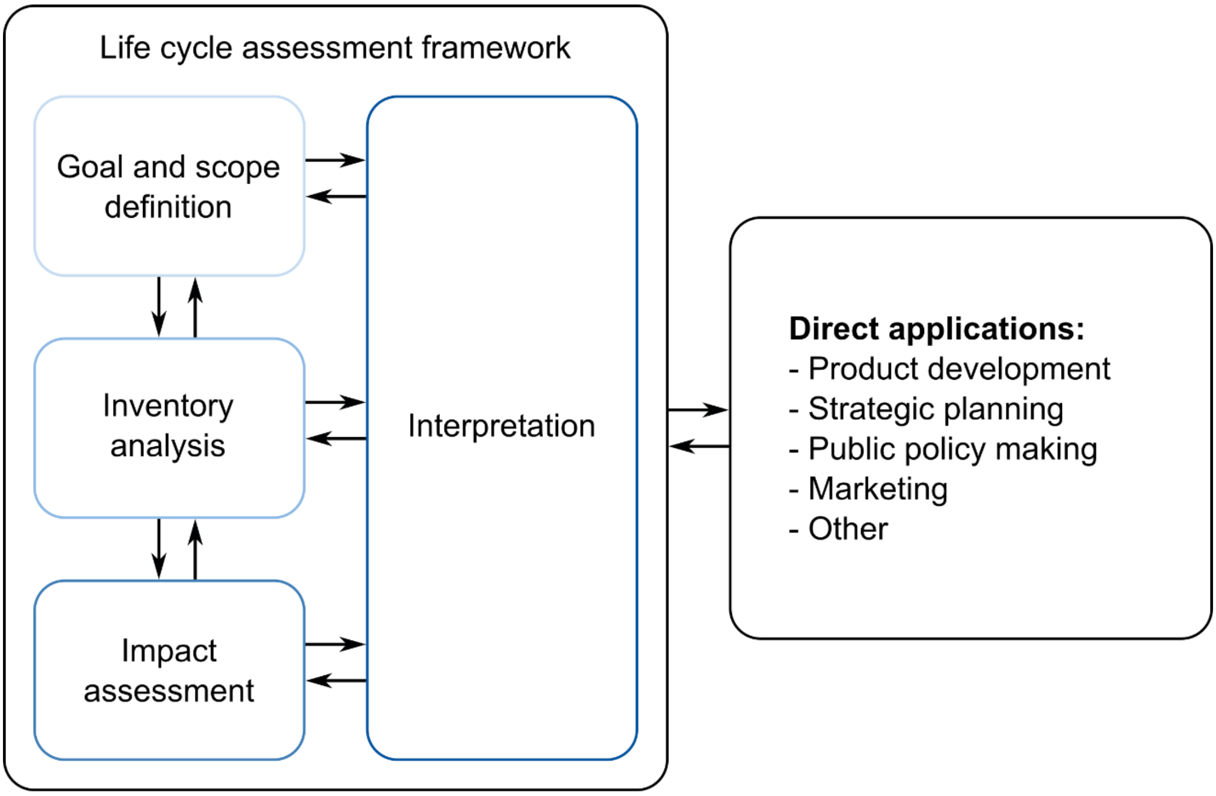

Figure 2. General framework for life cycle assessment [1]

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_2-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	
Shall	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
Should	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 **should** be reported and the reasons explained.
May	

C.4 Scope Definition

General Introduction

According to ISO 14040, “the scope should be sufficiently well defined to ensure that the breadth, depth and detail of the study are compatible and sufficient to address the stated goal.” In other words, it **shall** 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).

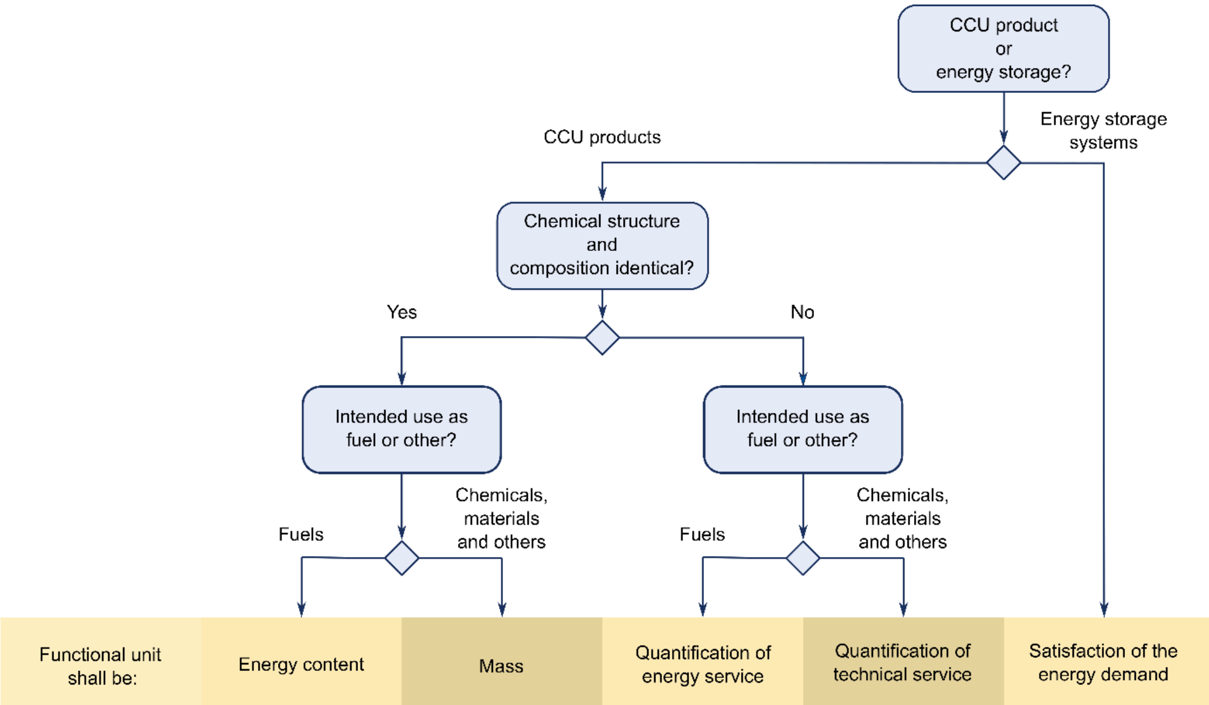

Figure 3. Decision tree for LCA of CCU: a) suitable functional unit. For calculation of the energy content, the lower heating value is recommended. If the respective chemical structures or compositions are not identical, define the functional unit in such a way that the performance is comparable for 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_2-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_2-based products with different chemical structure and composition** to their conventional counterparts, a generic functional unit cannot be defined. Instead, the functional unit **shall** be defined 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_2-based fuels with different chemical structure and composition shall** be defined with respect to the purpose of the fuel, i.e., energy services *(e.g., supply of electricity or heat)* or transportation of persons or goods. The functional unit 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_2 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	
Shall	1) A functional unit quantifying the technical performance of a product system or a service shall be defined unambiguously 2) Excluded functions shall still be documented and reported 3) For products with identical chemical structure and composition to their conventional counterparts, mass shall be used as a functional unit *(e.g., 1 kg of substance)* 4) For fuels with identical chemical structure and composition to their conventional counterparts, the energy content shall be used *(e.g., 1 MJ of substance (LHV))* 5) For products with different chemical structure and composition to their conventional counterparts, the function(s) and performance characteristics of the product system shall be stated clearly and an unambiguous, measurable functional unit quantifying the technical performance shall be derived 6) For fuels with different chemical structure and chemical composition to their conventional counterparts, the application shall be stated within the functional unit *(e.g., 1 kWh of electricity from combustion in gas turbine of type X)* 7) For energy storage, the functional unit **shall** be defined as the satisfaction of energy demand over a period of time *(e.g., as an annual time series of energy demand at a temporal resolution of one hour)*
Should	
May	1) LCA studies may exclude additional functions that are beyond the study scope. Excluded functions **shall** still be documented and reported

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[2]. 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.

[2] Following the ILCD handbook, this shall be assumed as long as the additional supply or demand of the production system under study does not exceed a threshold value of 5% of the annual market size of a supplied or demanded product. The threshold value of 5% refers to an estimated share of production capacity 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.

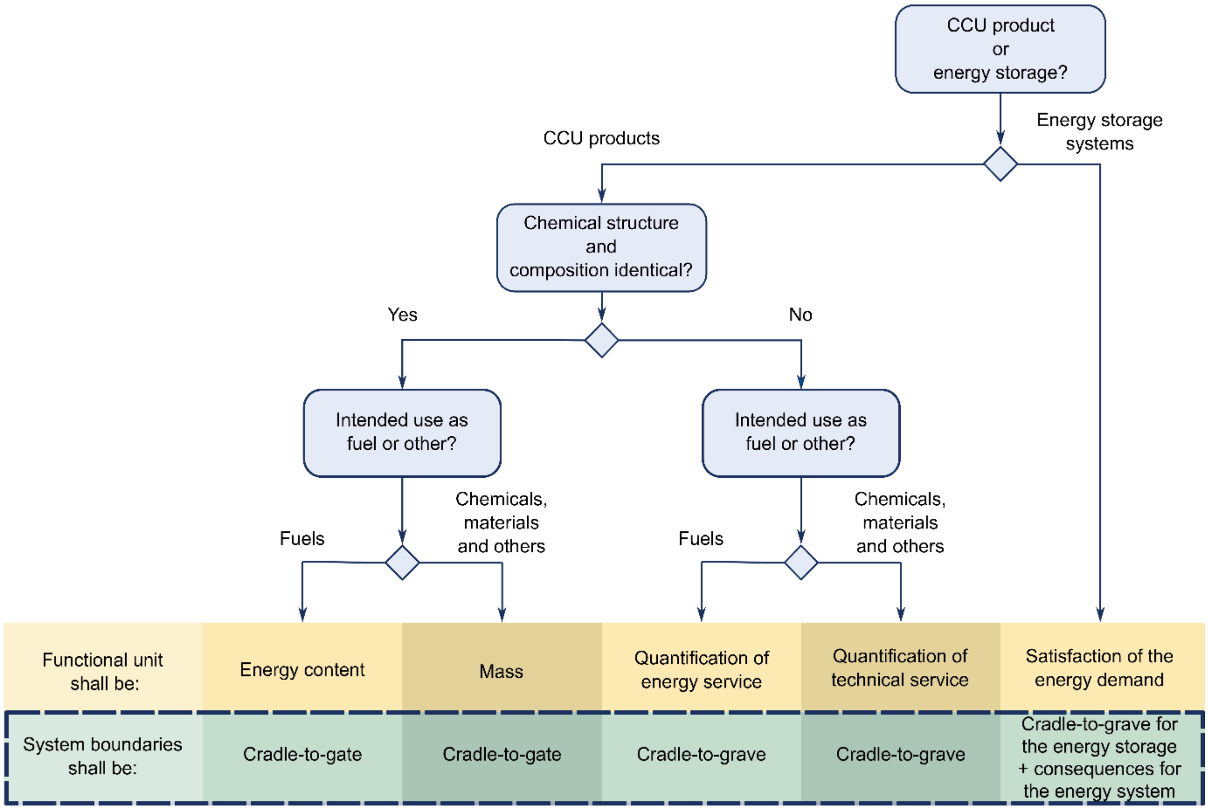

Figure 5: Decision tree for LCA of CCU b). Up to decision 2: system boundaries. For CCU products with identical chemical structure and composition to their conventional counterparts, a cradle-to-gate approach is sufficient. For CCU products that are not identical to their benchmark, the entire life cycle (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_2-based materials* *(e.g., consumer products)* **shall** cover the entire life cycle from cradle-to-grave. A cradle-to-gate approach is only applicable if differences in technical performance and end-of-life treatment do not differ significantly. In all other cases, materials perform differently and environmental impacts from downstream processes will not be identical. Therefore, LCA studies **shall** cover the entire life cycle 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.

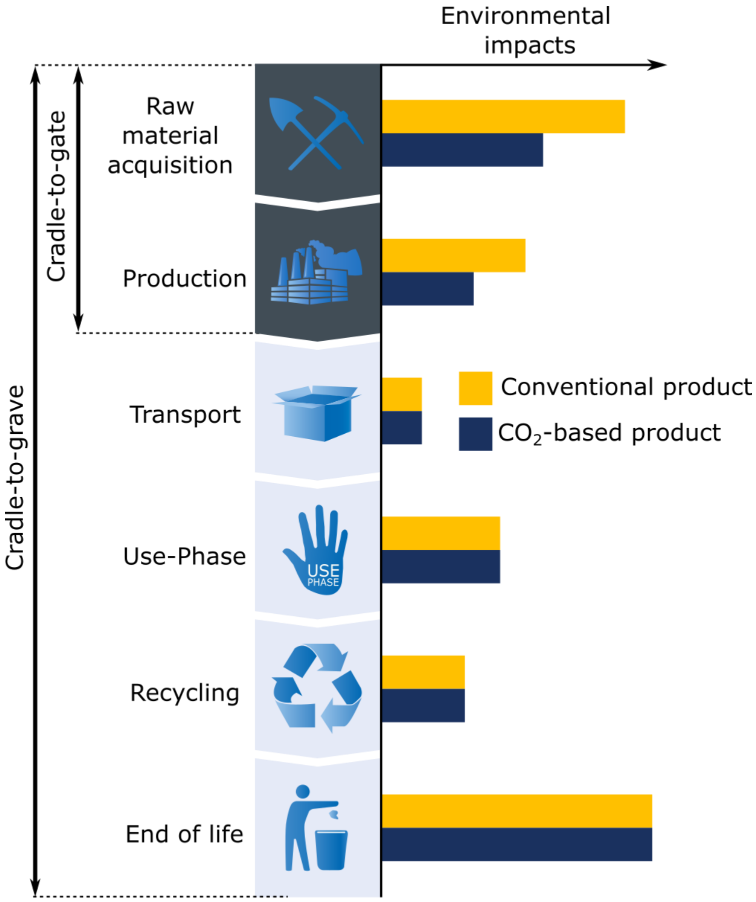

Figure 6. Comparison of environmental impacts for products with identical chemical structure and composition over the entire life cycle. Impacts only differ during raw material acquisition and production phases, and therefore comparative studies only have to consider those phases.

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_2 Capture

CO_2 emitted to the environment is an elementary flow. Thus, captured CO_2 is often treated intuitively as a consumed emission $\left(GW_{CO_2} = -1\frac{kg_{CO2e}}{kg_{CO2}}\right)$. However, captured CO_2 is a product of human transformation, and so consequently CO_2 is a technical flow and a chemical feedstock for CO_2 utilization. Thus, treating CO_2 as negative emission is usually incorrect, and so captured CO_2 must instead be treated like any other feedstock [12]. CO_2 sources **shall** be included within system boundaries as the supply of CO_2 leads to additional environmental impacts. Assessments **shall** comprise all process steps leading to environmental impacts, including CO_2 source, CO_2 purification, and transport, as shown in Figure 7.

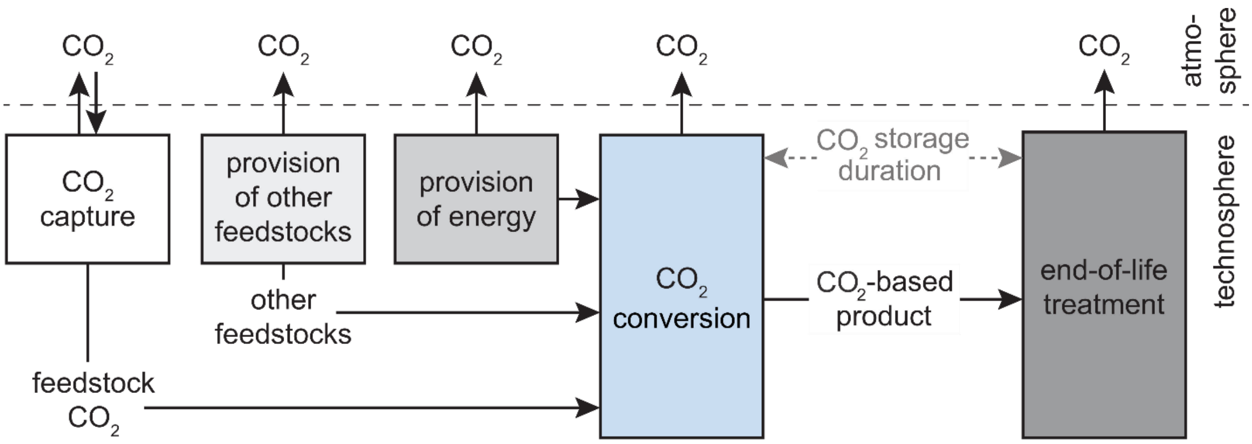

Figure 7. Schematic showing life cycle of CCU technologies from CO_2 source, supply of other feedstocks and energy to the end-of-life treatment. Environmental impacts must be considered during all life cycle stages. Adopted from [12].

C.4.2.3 Provisions

Provisions C.3 - System Boundaries	
Shall	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_2 sources shall be included within the system boundaries, with all process steps, as the supply of CO_2 leads to additional environmental impacts
Should	
May	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_2 sources often provide a main product in addition to CO_2 (Figure 8) [11]. For example, ammonia is produced by reacting hydrogen with nitrogen. Hydrogen can be co-produced with CO_2 in the steam-methane reforming process. Prior to the final stages of ammonia synthesis, CO_2 must be removed because it otherwise poisons the catalyst; consequently a pure CO_2 stream is extracted prior to ammonia synthesis but in most cases is emitted to the atmosphere. If this extracted CO_2 stream is captured rather than released, the main product ammonia and the co-product CO_2 are produced simultaneously (Figure 8). If the environmental impacts associated with the produced CO_2 stream need to be calculated, the total emissions of the system need to be split between the main and co-products.

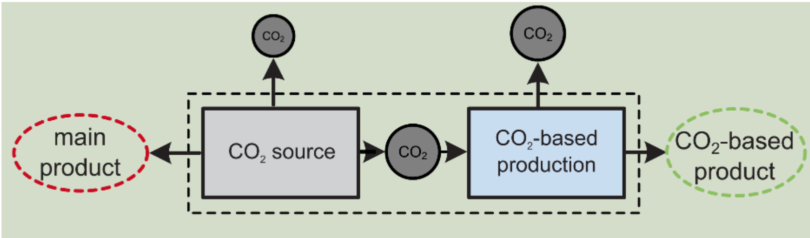

Figure 8. Stand-alone system analysis: Carbon capture from point source leads to the joint production of the CO_2-based product (functional unit, green-dashed line) and the main product of the point source

This problem is called multi-functionality. Other co-products or functions 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_2 source, since the problem of multi-functionality at the CO_2 source is at the core of most CCU processes.

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

Existing *s*tandards [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_2. For further information to account for the supply of CO_2 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_2 source: Sub-division is not applicable to the CO_2 source, since CO_2 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_2 source: CCU processes are often multi-functional *(e.g., when the CO2 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_2 source and product of CO_2 process) to a conventional system (Figure 9), the main product of the CO_2 source is added to the functional unit and the conventional system is expanded with the CO_2 source without CO_2 capture (Figure 10).

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

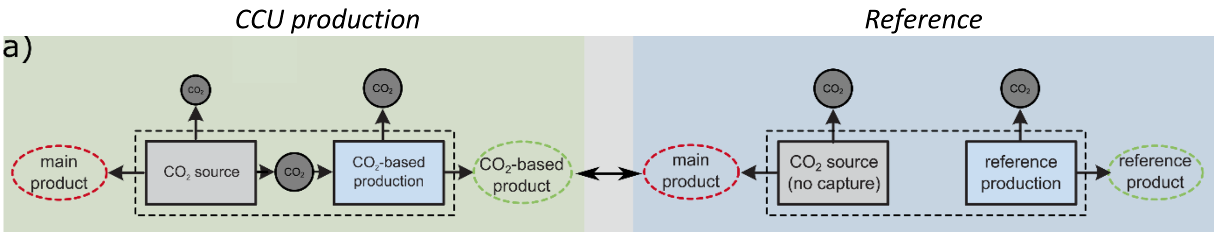

Figure 10. System expansion approach to compare a CCU production with a conventional production: The main product of CO_2 source is included in functional unit and the status-quo production system is expanded with the conventional production of the main product without carbon capture.

Note that a process used for system expansion (not in the case of CO_2 sources) 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 **shal**l be identified and used. In all other cases, a market-averaged process mix **shall** be assumed [5].

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

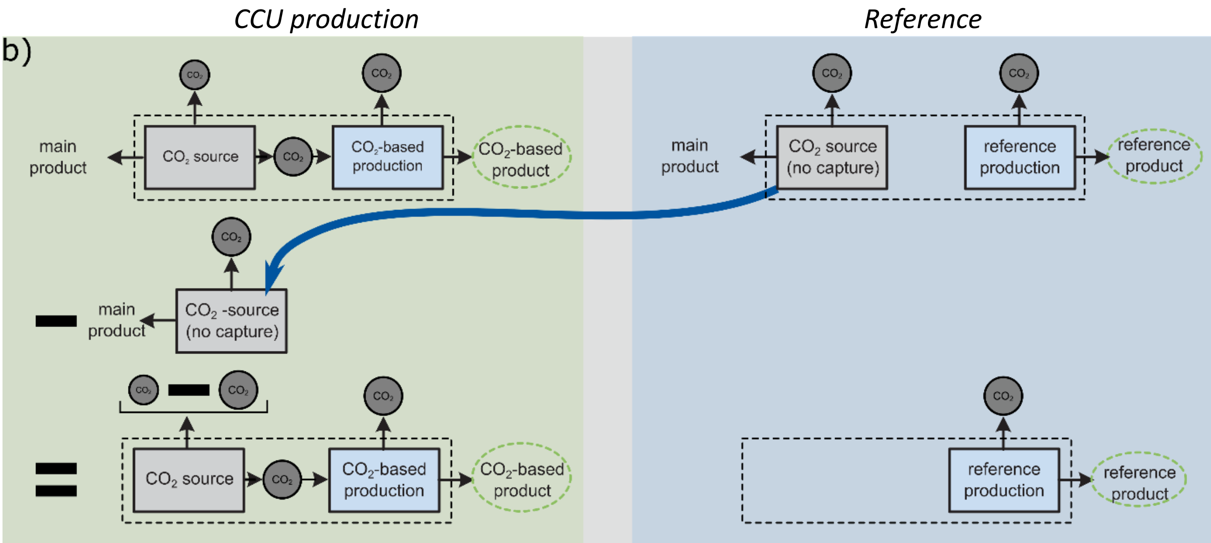

Figure 11. Substitution: The production of the main product without carbon capture is avoided, and thus the CCU system is credited for the otherwise emitted CO_2, but has to carry the burdens of purification, compression, and transportation of the CO_2.

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_2 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 trough 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.

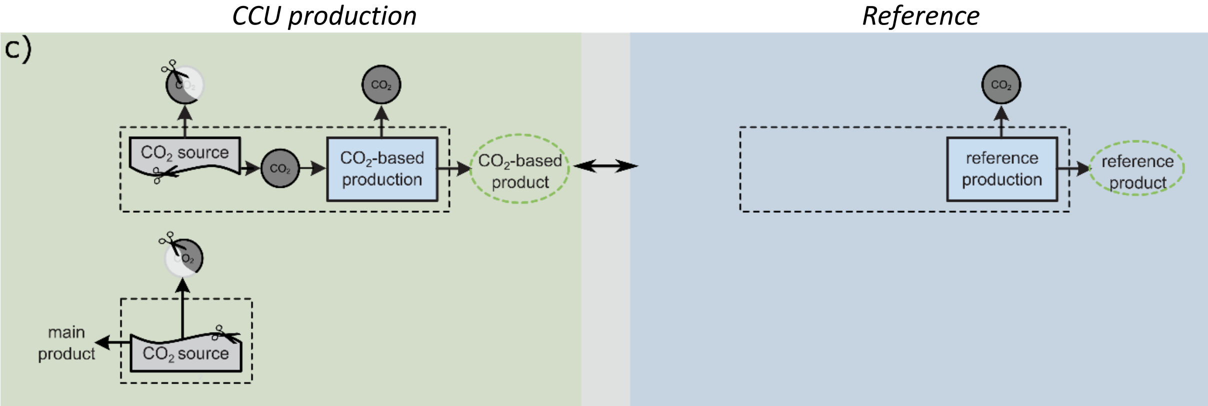

Figure 12. Allocation sub-divides the CO_2 sources into two processes and distributes the environmental burdens of the CO_2 source between the main product and the production of the feedstock CO_2 using underlying physical relationship or other relationship. The CCU production system becomes a mono-functional 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 than reflect this quantitative change of inputs and outputs[3]. Note that more than one relationship can be applicable within one process

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

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

[3] 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_2 source: The selection of a suitable product attribute to distribute the emissions of the CO_2 source among the main product and the CO_2 source can be difficult. Mass can be applied to all processes except power plants, since electricity has no mass and thus, all emissions would be distributed to CO_2. Energy is not a suitable attribute, since CO_2 does not contain any energy; more precisely, its lower heating value is zero. The economic value of CO_2 is uncertain, since the capture process has costs, the price of CO_2 might be positive, and thus economic allocation would attribute the product CO_2 with emissions of the CO_2 source. However, it can be argued that CO_2 has a negative economic value and is thus a waste stream that requires waste treatment. In this case, the CO_2 source has only one function, i.e., producing the main product, and has a technical waste flow, i.e., the concentrated CO_2 stream. The CO_2-utilizing step would then be multi-functional in the sense that a CCU product is produced and the CO_2 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_2 and an objective selection of one allocation criterion is not possible, a sensitivity analysis **shall** always be performed.

C.4.3.4 Provisions

Provisions C.4 - Life Cycle Inventory Modeling Framework and Solving Multi-functionality	
Shall	1) If multi-functionality occurs within the defined system boundaries: 1) Sub-division shall be applied If not possible: 2) System expansion shall be applied 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 3) System expansion via substitution shall be applied. This step should be only in addition to system expansion If not possible: 4) Allocation shall be applied, first based on underlying physical causalities. This step should be only in addition to system expansion. If not possible: 5) Allocation using other underlying relationship(s) shall be applied additionally to system expansion. A sensitivity analysis of applicable criteria shall be conducted
Should	
May	

C.4.4 Data Quality

General Introduction

Data gathered for the life cycle inventory **shall** have sufficient quality to answer the initial research question. Since data 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	
Shall	1) Any study intended for external communication shall be reviewed 2) For comparative studies or studies to be used in comparative assertions disclosed to 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]
Should	
May	

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)	
Shall	1) System boundaries shall be described and represented in a flow chart 2) Inventories shall be documented and reported, at least to external reviewers
Should	1) All relevant unit processes with their relevant elementary and technical flows should be represented in the flow chart
May	

C.5.2 Estimation Methods 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-Gonzáles *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	
Shall	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
Should	
May	1) Estimation methods may be applied to bridge data gaps. If applied, methods and assumptions shall be reported 2) Techniques to forecast future technology development may be applied. If applied, the forecast shall cover both the CCU and the reference technology and shall not exceed physical limitations

C.5.3 Selection of Reference Processes

The 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[4])*. 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	
Shall	1) The reference process shall be the marginal process. If no marginal process can be identified, the market mix shall be assumed
Should	1) For processes in 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
May	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

[4] 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_2 for climate change)*. All substances are normalized to the reference substance according to common mechanisms.

Further recommended reading:

For more details on impact assessment, please see "ILCD Handbook. Framework and requirements for life cycle impact assessment models and indicators" by the Joint Research 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[5] [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	
Shall	1) CML impact assessment methodology shall be used as a default 2) LCA studies for CCU technologies shall analyze midpoints indicator categories
Should	1) In addition to CML, a second, geographically more appropriate method should be applied. For Europe, JRC recommended methods should be used, and for the U.S. the latest version of TRACI 2) GWP20 should be considered in addition to GWP100, as calculated in the latest IPCC report
May	1) Other categories or methods may be applied, but shall be justified, documented, and reported

[5] 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 CO2

CCU products offer temporary carbon storage. Consequently, CO_2 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_2-based product or fuel considered:

For **CO_2-based products and fuels with identical chemical structure and composition to their conventional counterparts,** carbon storage does not offer any additional benefits since the product life is identical after leaving the factory gate for both products, as is the amount of carbon chemically bonded [54]. Therefore, the time between production and end-of-life treatment and the amount of CO_2 released during end-of-life treatment is identical. Thus, the emission time profiles are identical after factory gate (yellow and green lines in Figure 13) and there is no additional effect gained from storing CO_2.

For **CO_2-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_2-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.

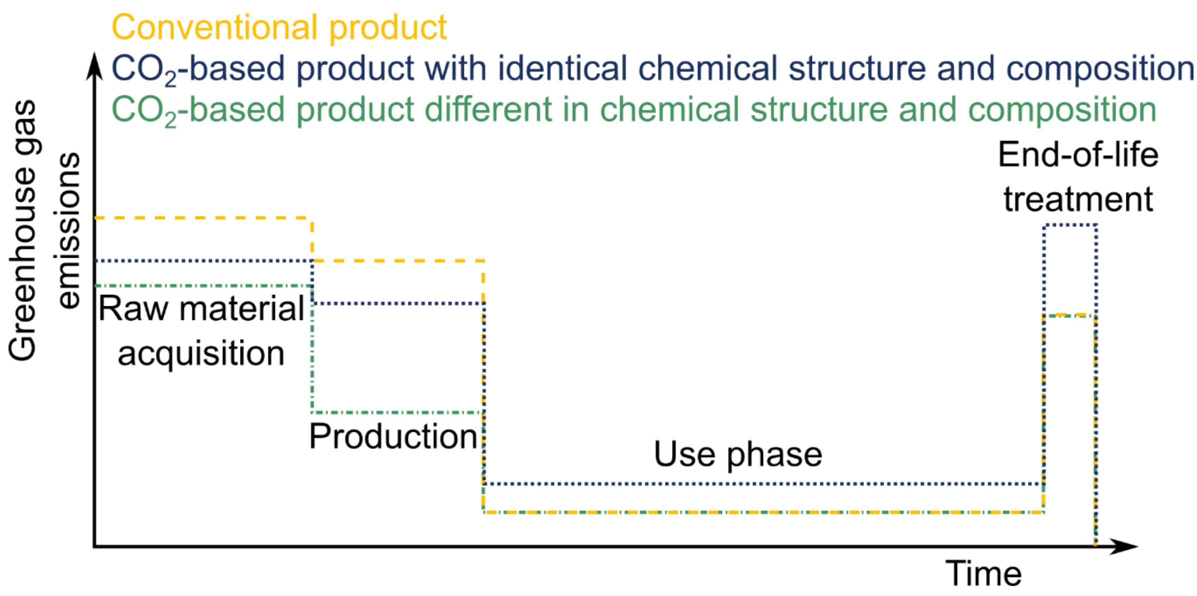

Figure 13: Emission time profiles for different products. CO_2-based products with identical chemical structure and composition to their conventional counterparts have identical emission time profiles after production. CO_2-based products with chemical structure and composition different from conventional counterparts can have different emissions during use phase and end-of-life treatment and also different life spans, resulting in different emission time profile.

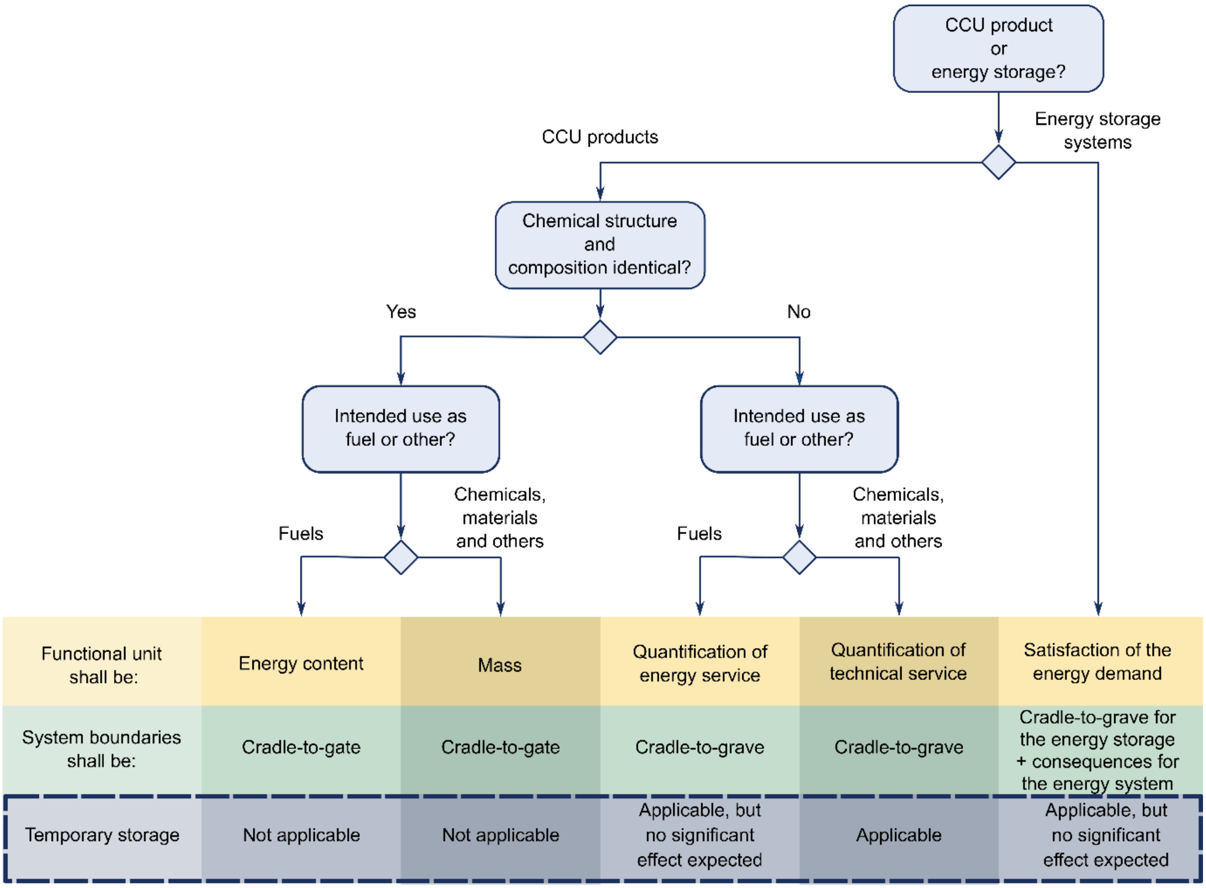

Figure 14. Decision tree for LCA of CCU c) up to decision 3: temporary storage. For CCU products with identical chemical structure and composition to their conventional counterparts, temporary storage is not applicable as this is not part of the system boundaries. For CCU products that are not identical 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_2 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[6], 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.

[6] Permanent storage can be assumed if CO_2 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

Provisions C.11 - Guideline Temporary Storage of CO_2		
Shall	1)	Delayed emission shall not be discounted over time as a default
Should		
May	1)	If delayed emissions occur, an emission time profile of the conventional product and the CO_2-based products 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_2 to produce value-added products. Thus, intuitively, CCU technologies might be regarded as technologies with potentially zero emissions or net-negative emissions.

CO_2 is usually considered to be captured from fossil or biogenic point sources or directly from the atmosphere via direct air capture. Fossil point sources release carbon previously stored in underground compartments, while biogenic point sources release carbon previously consumed from the atmosphere.

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

- if CO_2 is captured from the atmosphere (via biogenic point sources or direct air capture) and the same amount of CO_2 is released at the end of life (Figure 15a)
- <u>or</u> if CO_2 is captured from fossil point sources and CO_2 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_2 is captured from the atmosphere (via biogenic point sources or direct air capture)
- and if CO_2 is sequestered or permanently stored in the product
- and if overall life cycle GHG emissions are lower than the amount of CO_2 fixed.

If the amount of atmospheric CO_2 capture and fixation during a process is equal to all fossil emissions over the life cycle of this process, the process is carbon-neutral.

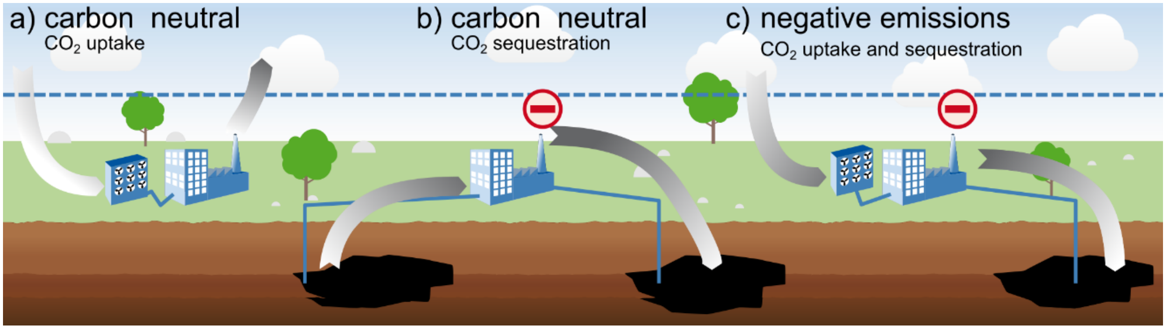

Figure 15. Case a) Carbon-neutral CO_2 uptake: CO_2 is taken from the atmosphere and the same amount is re-emitted during or after the product life cycle. Case b) Carbon-neutral CO_2 sequestration: Fossil carbon is taken from underground reservoirs and the embedded CO_2 is sequestered after the product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

In all other cases, CCU technologies have net-positive CO_2 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_2 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_2 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_2 emissions obtained from substitution **shall** be clearly stated as an environmental benefit only in comparison with the benchmark technology and not as negative CO_2 emissions in absolute terms over the entire life cycle. Also, avoided CO_2 emissions and other environmental impacts from substitution **shall** be reported separately [57].

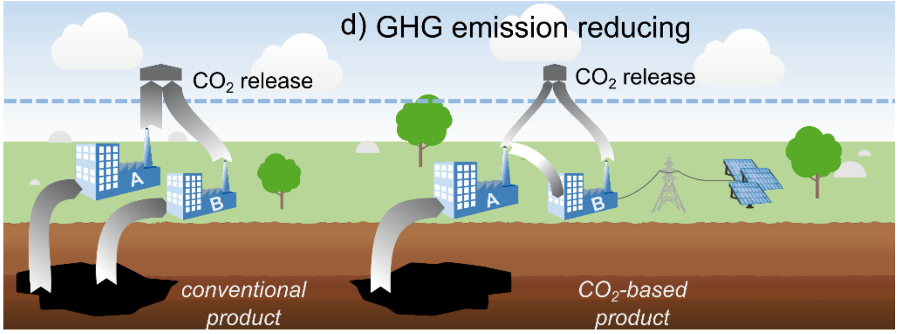

Figure 16. Case d) Greenhouse gas emission-reducing: CCU technologies can achieve lower CO_2 emissions than the status quo and thus may be considered as greenhouse gas (GHG) emission-reducing technologies.

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_2 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_2)*. 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_2, 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_2-eq /MJ	0.091[7]	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 CO2-eq per kilogram of hydrogen [80]), the GHGs emitted by supplying electricity for water electrolysis would need to be 0.214 kgCO2-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 kgCO2-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.,*

[7] 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).

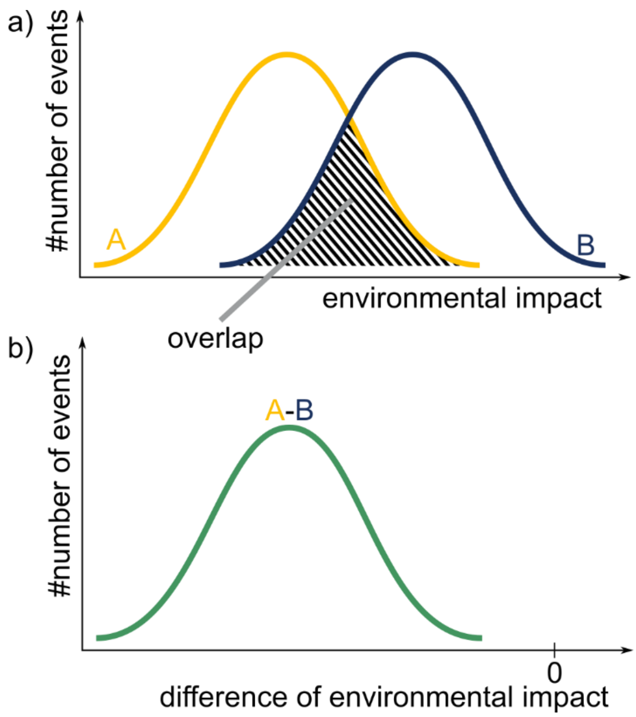

Figure 17. a) Results of an independent Monte Carlo analysis for alternatives A and B. b) Results of a joint Monte Carlo analysis of the difference (A-B) between technologies.

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_2-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	
Shall	1) As minimum requirement for uncertainty assessment, a basic uncertainty approach covering sensitivity analysis and scenario analysis shall be applied to identify key variables and to reflect how potential changes in the background system affect the technologies under study 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 3) If Monte Carlo analysis is applied for comparative studies, the analysis shall consider the alternatives within one joint Monte Carlo analysis
Should	1) The intermediate approach should be applied to quantify the uncertainty of the results 2) Aggregated processes should not be used for Monte Carlo analysis, since important variables in the foreground system cannot be varied in the background system 3) The standard scenarios provided in Annex C.9.1 should be used for scenario analysis
May	

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_2 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[8] 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_2 supply in the high- or full-decarbonized scenarios, as in these scenarios fossil-fueled power plants will no longer be available as a CO_2 source. Instead, it is assumed that CO_2 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
Hydrogen	Steam-methane reforming	Alkaline electrolysis	Alkaline electrolysis	Alkaline electrolysis
CO_2	Coal-fired power plant	Coal-fired power plant	Direct air capture	Direct air capture
Heat	Natural gas vessel	Electrode vessel	Electrode vessel	Electrode vessel
Natural gas (methane)	Natural gas	Natural gas	Methanation	Methanation

C.9.1.1 Electricity

For 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

[8] 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 IPPC 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_2

For CO_2 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_2 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	☐Sub-division ☐System expansion ☐System expansion via substitution ☐Virtual sub-division ☐Mass allocation	☐Energy allocation ☐Economic allocation ☐ Closed loop scenarios ☐Other (please specify)
INVENTORY	**Data source**	☐Primary sources ☐Secondary sources ☐Stoichiometric data	☐Process-modeling-based data ☐Mixes sources ☐Other (please specify)
	Energy sources (select all that apply)	☐Grid mix ☐Power station with carbon capture ☐Wind ☐Solar	☐Nuclear ☐Hydro ☐Future (see timeframes) ☐Other (please specify)
	Main sub-processes and TRLs	SUB-PROCESS	TRL TRL TRL TRL

	Database & software used		
ASSESSMENT	**LCIA method**	☐ CML ☐ ILCD recommendation: v.____ ☐ TRACI 2.1 OTHER IMPACT METHODS ☐...	SINGLE CATEGORIES: ☐ Climate change ☐ CED ☐ use TOX
	Highlighted results (graphical, text, or tabular format)		
INTERPRETATION	**Main conclusions**		
	Sensitivity analysis	☐No	☐ Yes (please specify below)

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PART D
Low-TRL Guidelines

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SUPPORTED BY

Contents Part D

D.1 Introduction

D.1.1 General Introduction to Early-stage Assessment

With growing interest in the potential of CCU, much research and development (R&D) effort is spent on novel CCU processes. R&D often starts from many basic ideas that initially lack technological maturity. However, R&D capacities are limited, and many early process ideas are likely to fail during development. To use R&D capacities efficiently, decision makers need to focus on environmentally and economically promising ideas as early as possible in the development pipeline. The sooner that unpromising options can be identified and discarded, the less time and effort are spent on them. Thus, it is vital to provide this decision support as early as possible in the development cycle, even if based on limited data.

LCA and TEA can support R&D decisions with insights into the environmental and economic potential of emerging CCU technologies. Parts B and C of these Guidelines provide CCU-specific recommendations for LCA and TEA to enable consistent and comparable studies. These methods are also applicable to low-maturity processes and **shall** be applied wherever possible. However, since the information available from R&D is limited during the early development stages, the outputs of LCA and TEA are also incomplete or subject to large uncertainties. For these reasons, there is a particular need for more guidance on how to perform LCA and TEA and interpret the results at early stages.

D.1.2 General Workflow of Accompanying LCA and TEA

While LCA and TEA of mature technologies aim to provide detailed information on economic and environmental aspects (e.g., for investment decisions or environmental product declarations), the review of research questions in chapter C.3.1 already revealed that most LCAs of CCU technologies also aimed to support decision making. The earlier a technology is assessed, the more important is rapid stakeholder support on R&D decisions, compared to the accuracy of results. Thus, in the early stages of R&D, the assessment time is often limited and close collaboration is essential – with direct feedback between researchers, process designers, decision makers, and LCA and TEA practitioners [3–5].

In this document, we present a general workflow, based on close cooperation of all involved groups, that aims to support the R&D process by means of LCA and TEA. This workflow considers that R&D is performed in a stage-gate process, where new information becomes available after each stage, and new decisions need to be made accordingly. In this document, we use the technology readiness level (TRL) concept as a measure of a technology's maturity and to define the stages in an exemplar stage-gate process. The TRL concept and the related TRLs are introduced in part A of these Guidelines and further described in chapter D.1.3.

The workflow of continuous support for R&D by LCA and TEA is visualized in Figure 1. The workflow starts after the first R&D stage (here TRL 1) and is designed as an iterative cycle that reoccurs at each stage. Thus, LCA and TEA need to be performed and refined iteratively throughout the entire R&D process in order to provide continuous guidance. The workflow assigns responsibilities and tasks either to R&D, or to LCA and TEA. The R&D tasks and responsibilities (shown in gray) are those of researchers, process designers, and decision makers, and are not explored further in this document. The LCA and TEA responsibilities and tasks can be divided into two steps: A first *Monitoring* step to inform Go/No-go decisions, and a second step to support upcoming R&D. The concept of *Monitoring* and *R&D support* is discussed in the Goal and Scope chapter.

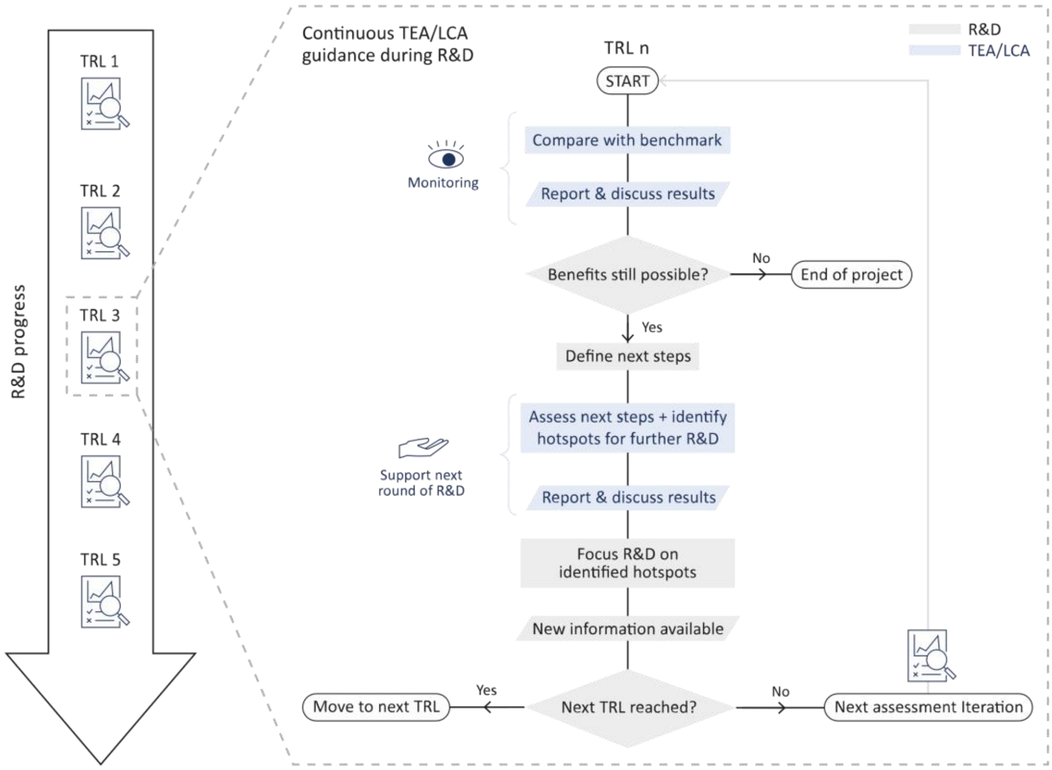

Figure 1 Workflow of LCA and TEA, continuously supporting research and development (R&D) at low TRLs. Illustrated for TRL 3.

The following questions are essential to understand the particular needs of early-stage assessments and are answered in this document:

1) What decisions are usually made during the early stages of R&D, and what information is usually desired/required from the LCA and TEA perspective to support this decision making? (chapters D.3 and D.4)
2) What data from R&D is usually available to LCA and TEA practitioners? How should LCA and TEA deal with missing data, and what decision support can LCA and TEA finally provide? (chapter D.5)
3) How can the results and uncertainties of these methods be communicated and discussed to avoid misleading decision support? (chapters D.7 and D.8)

D.1.3 Technology Readiness Levels (TRL) as a Measure of Technology Maturity

The general concept of technology readiness levels (TRL) to describe a technology's maturity is explained in part A.4. As part D focuses on particular challenges of early-stage assessments, we focus on TRL 1–5. The higher TRLs (6 to 9) are well covered in the recommendations presented in parts A and B, as TRL 6 requires a working pilot plant that provides sufficiently detailed information to follow the recommendations of part B and C. This sub-chapter describes TRL 1 to 5 as defined by Buchner *et al*. and used in the other parts of these Guidelines [8].

D.1.3.1 TRL 1 – Basic Idea

At TRL 1, only basic scientific principles are observed and reported, and opportunities are identified for applying the reported principles [8].The basic idea for a new process can either be to use a particular raw material, produce a new product, or provide a new production route for an existing product. CCU can be based on all three types of basic ideas, while the use of CO_2 as a raw material is, by definition, inherent to the CCU context. If an alternative is to be found for an established chemical production route, the main product is already defined, and therefore the primary task at TRL 1 is to select promising chemical reactions that might enable an alternative production route. If a new kind of product is to be found for a particular application, the primary task at TRL 1 is to select promising chemical products and the chemical reaction for their production.

At this stage, laboratory experiments have not yet started, and thus the available information derives solely from existing literature (if available) together with potentially promising theories and assumptions. However, the first iteration of LCA and TEA can already start to answer initial questions (e.g., do the candidate raw materials impose high impacts or costs? What information is available about the benchmark product?). The results from the first assessment can guide the development of a technology concept (TRL 2) and the selection of suitable chemical reactions.

D.1.3.2 TRL 2 – Concept

At TRL 2, the technology concept and product application are defined. A (set of) chemical reaction(s) is selected, and the number of reaction steps is identified [8]. Furthermore, R&D activities are planned, as laboratory work starts after TRL 2. At TRL 2, LCA and TEA can already assess whether the technology concept can potentially offer environmental or economic benefits, thereby also supporting decision making in R&D (e.g., help to identify hot spots for research or target values for reaction efficiency).

D.1.3.3 TRL 3 – Proof of Concept

At TRL 3, laboratory research has started, and the functional principle/reaction has been proven in laboratory-scale trials [8]. The concept has been tested in a laboratory environment, subsequently using the first amounts of synthesized product for further testing; First reaction characteristics (e.g., conversion, selectivity, and yield) have been measured. Often, the options for solvents and catalysts are identified and need to be compared. For process design, options for unit operations (e.g., separation by boiling points or by density) are found and can be compared and evaluated with LCA and TEA.

D.1.3.4 TRL 4 - Preliminary Process Development

At TRL 4, the proposed process concept is validated in a laboratory environment, and further development of the process has started. The feasibility of the reaction is confirmed through documented and reproducible (quantitative) experimental results. The reaction has been optimized for the chosen reactor type at a laboratory scale with regard to additives, catalysts, solvents, and by-products, and performance metrics such as conversion and selectivity. For process design, alternative process concepts have been evaluated, and unit operations are specified in detail (e.g., the use of rectification, sedimentation, or centrifugation). For the most promising process concepts, shortcut process models have been developed and can be used for LCA and TEA [8].

D.1.3.5 TRL 5 - Detailed Process Development

At TRL 5, a process flow diagram is developed, including mass and energy flows. Shortcut models can now be replaced by rigorous process models, and data on physicochemical properties are analyzed. The product properties are characterized and can be used to refine the process's functional unit and reference flow. The reaction engineering is specified in detail based on laboratory results, including kinetics, reactor types, product stability, and controllability mechanisms. Furthermore, appropriate materials are specified for process equipment according to the anticipated reaction conditions (e.g., temperature, pressure, and corrosion resistance). Ultimately, the process concept has been refined to the present stage based on laboratory experiments and simulations for each unit operation [8]. Based on the process concept, a pilot plant is planned and thus LCA and TEA should be considered when deciding whether to construct this plant. Assessments at this stage are fully covered by existing standards and guidelines, and must meet country-specific requirements for planning and building chemical pilot plants.

D.2 How to Read this Document

D.2.1 Aim and Scope of This Document

This document builds upon parts B and C of these Guidelines, which are based on the life cycle assessment ISO standards 14040 [14] and 14044 [15], the ILCD handbooks [16, 17], reference textbooks [18–21], and scientific publications [22, 23]. As a complementary part of the Guidelines, this document provides additional recommendations for LCA and TEA with the aim of supporting decisions during the early stages of R&D for novel CCU technologies. These additional recommendations respond to the needs of decision makers (e.g., researchers, process designers, and managers) and LCA and TEA practitioners for early-stage assessment. One major aspect is how to deal with limited availability of information (e.g., limited and/or poor-quality data). In this part of the Guidelines, LCA and TEA are considered together, as the information available at early stages (e.g., mass and energy flows) is relevant for both LCA and TEA. Both assessment types therefore face the same challenges, which are addressed in this part of the document. If necessary, questions are discussed that are specific to only TEA or LCA. The recommendations provided here are applicable to TEA, LCA, or combined assessments (see also part F) at early stages of development. The corresponding Guideline parts provide additional information and **should** be consulted for further details on TEA, LCA, and combined assessment.

D.2.2 Structure of This Document

Following parts B and C of these Guidelines, this document is structured in chapters following the phases of LCA and TEA:

1. Goal definition
2. Scope definition
3. Inventory analysis/Life Cycle Inventory
4. Calculation of indicators/Life Cycle Impact Assessment
5. Interpretation
6. Reporting

Each chapter provides a link to the corresponding parts B and C of these Guidelines and describes the challenges faced at low TRL, followed by recommendations on how to apply LCA and TEA to support R&D decisions at low TRL. In the inventory chapter, the recommendations are given for each TRL separately in the form of sub-chapters. Each chapter or sub-chapter concludes by providing a list of provisions that **shall**/**should**/**may** be performed.

These provisions are intended to enable LCA and TEA to support R&D for CCU processes at low TRL. For this purpose, the provisions are complementary but more specific and even more restrictive than the provisions of parts B and C.

There might be a need to add further tasks to those discussed in this document, if they are important for a specific case study. The present provisions do not exclude such additions. The provisions aim to support R&D decision making, which is usually done within an organization. Thus, the provisions are not suitable for producing comparative assertions disclosed to the public, as standardized for LCA in ISO 14040 and ISO 14044 for assessing mature technologies. Nevertheless, we believe there is a need for a consistent methodological core for LCA and TEA at early stages of research and development, which these Guidelines provide.

D.3 Goal Definition

General Introduction and Challenges

Defining the goal, which serves as the central research question, is key to every LCA and TEA and is explained in chapters B.3 and C.3. In general, the recommendations given in those chapters **shall** be considered for low-TRL assessments. However, technologies at the early stages of research and development are usually assessed within an organization and not disclosed to the public. Thus, the assessment focuses even more on supporting relevant decisions during the R&D process, as research questions are closely related to the maturity of a technology and need to be refined iteratively at each stage.

The main difference from the goals described in the previous chapters B.3 and C.3 is that in early-stage assessment the iterative process is not only due to the iterative nature of LCA but also due to the iterative development of the technology. During development, the assessment is iteratively enhanced to facilitate and steer upcoming research activities.

As described in chapter C3.1, comparative assessment between low-TRL and mature technologies can end up in "apple versus oranges" comparisons, since most reference technologies are mature and have been optimized for decades. In contrast, LCA studies on lab-scale processes can either under- or over-estimate environmental impacts. Thus, the limitations in data quality **shall** always be considered in comparative studies if a high-TRL technology is compared to a low-TRL technology (see Provisions A.1).

D.3.1 Defining Goals for Early-stage Assessments

D.3.1.1 Monitoring and R&D support

The R&D process involves multiple stakeholders, each of which are expected to have different requirements for the assessment. Here, we differentiate between two types of stakeholders and their respective requirements:

(1) Decision makers (e.g., management) and (2) R&D experts.

Managers typically seek to derive Go/No-go decisions and keep track of the current status, which requires *Monitoring* the project's status and potential. Monitoring needs to ensure that the chosen decision criteria do not overlook important effects, nor resolve one issue only to create other burdens (e.g., in other life cycle stages or impact categories). Thus, Monitoring requires comparing the assessed CCU technology to a benchmark technology (D.4.1.2.1). In contrast, R&D experts seek to identify the most promising options or which parameters are most relevant for the overall performance of the process under investigation, which can be supported by LCA and TEA (*R&D support*).

We identified research questions for each requirement that **should** be discussed with stakeholders in order to define the assessment goal. Discussing the goal definition ensures that the needs of decision makers are met, and also helps to manage their expectations, which might not match the available data [24]. The research questions are formulated to apply to all TRLs, while the assessment detail increases with TRL.

1) *Monitoring* current status and potential:

   a. Does the information available at the current R&D status/maturity level indicate a potential to reduce environmental impacts/costs compared to the benchmark?

   b. Could burdens be shifted to other impact categories or life cycle stages?

   c. Could costs be shifted, e.g., from CapEx to OpEx, causing long-term economic risks or benefits (e.g., use of a costlier but more selective reactant to avoid installing an additional separation unit)?

2) *R&D support*:

   a. Screening: What are the most promising process/product options, e.g., products, reactants, catalysts, reactors, separation units, solvents?

   b. Sensitivity analysis: What are the crucial parameters influencing these process options, e.g., recovery rates, reflux ratios, yield, and conversion?

   c. Scenario analysis: What are crucial external parameters influencing the process performance, e.g., heat and electricity supply, market prices of products, reactants, and auxiliaries?

   d. Break-even analysis: What is the worst value for each parameter, under which economic or environmental advantages are still possible (e.g., by one-at-a-time variation)?

The *Monitoring* step aims to assess a technology and its potential at its current state, to support Go/No-go decisions. Hence, *Monitoring* **should** be the first step of each assessment iteration (see D.1.2 and Figure 1).

After a Go-decision, the next tasks for R&D are defined. LCA and TEA offer a large set of methods, which can guide the definition and prioritization of tasks. All steps of *R&D support* **should** build upon the results of the *Monitoring* step. First, screening **should** be performed to discard inferior process/product options (e.g., products, reactants, catalysts, reactors, separation units, solvents) and narrow down the options that need to be considered in R&D. Second, the sensitivity to various parameters (e.g., composition of the CO_2 input stream, recovery rates, reflux ratios, yield, and conversion) of the remaining process options **should** be assessed to guide the focus of R&D towards the crucial parameters. At the same time, the sensitivity to external parameters (e.g., heat and electricity supply and market prices, or supply chains of products, reactants, and auxiliaries) **should** be assessed via scenario analysis. Furthermore, the minimum/maximum (break-even) values under which economic or environmental advantages become possible **should** be identified for each crucial parameter.

D.3.1.2 Limited Comparability

At early stages of development, data quality is generally low and results have a high or even unknown uncertainty, which limits the comparability of results [4]. Thus, early-stage LCA and TEA **shall** not be used for product declarations or to claim environmental or economic benefits. An additional challenge for comparing technologies at different readiness levels is the time horizon, as the technologies are likely to enter the market at different points in time. The time of market entry influences the expected learning process, leading to efficiency increases for technologies. Furthermore, the background scenario within which the technologies operate will change over time. Thus, a point of time **shall** be identified when the novel technology is expected to become operational.

D.3.1.3 Provisions

Provisions D.1 – Goal Definition	
Shall	1) The recommendations of chapters B.3 and C.3 **shall** be followed for low-TRL assessments. 2) Provisions A.1 **shall** be followed, and the limitations in data quality **shall** always be considered in comparative studies if a high-TRL technology is compared to a low-TRL technology. 3) LCA and TEA **shall** not be used for product declarations or to claim environmental or economic benefits from premature technologies. 4) A point of time **shall** be identified at which the novel technology is expected to be operational.
Should	1) The research questions provided for *Monitoring* and *R&D support* **should** be discussed with the stakeholders for the goal definition. *Monitoring* and *R&D support* **should** be applied within the iterative assessment workflow (D.1.2). 2) *Monitoring* **should** be the first step of each assessment iteration assessing a technology at its current state and supporting Go/No-go decisions. 3) *R&D support* **should** follow and build upon the *Monitoring* step. First, screening **should** be performed to discard inferior process/product options. Second, the sensitivity of parameters to the remaining process options and to external parameters **should** be assessed.
May	1) Problem-specific research questions **may** be added, if required by the stakeholders.

D.4 Scope Definition

General Introduction and Challenges

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." The scope definition is further described in chapter C.4, where more details are presented for:

- defining the functions, functional unit, and reference flows (C.4.1),
- system boundaries, requirements on completeness, and related cut-offs (C.4.2),
- the life cycle inventory modeling framework and co-product management (C.4.3),
- data quality requirements regarding technological, geographical, and time-related representativeness and appropriateness (C.4.4),
- and special requirements for comparative assessments (C.4.5).

The recommendations of chapters B.4 and C.4 **shall** be followed for low-TRL assessments. However, an early-stage assessment is often not intended for external communication, and thus the special requirements for comparative assessments (C.4.5) **may** be replaced by internal review and discussion with involved stakeholders.

At low TRL, the comparability of results is limited due to incomplete information. Moni *et al*. defined the following comparability challenges [25]:

- Functions of emerging technologies are often not comprehensively defined, and change with increased maturity.
- The emerging technology is not always functionally equivalent to existing alternatives.
- A direct comparison of emerging technologies is often difficult because of unclear co-product usages, disposal strategies, etc.

Thus, it is often difficult to define an appropriate benchmark technology for comparison, as the assessed CCU technology will be introduced into a future market, where other competing technologies might be available. Therefore, the benchmark involves high uncertainties and needs to be well defined in collaboration with R&D experts and management[26].

As these challenges have different implications depending on the goal of the assessment, this chapter provides recommendations for *Monitoring* (D.4.1) and *R&D support* (D.4.2) separately.

Assessments for low-TRL technologies **may** be simplified to quickly transform newly available data into LCA and TEA results. Different approaches for simplification exist, such as excluding indicators or parts of the inventory models, or substituting inventory data by aggregated background data. We recommend Beemsterboer *et al*. for further reading [27].

D.4.1 Scope Definition for *Monitoring*

General Introduction

Monitoring is the first step of each assessment iteration and aims to assess a technology at its current state, to support Go/No-go decisions, and to check whether the novel process still offers the potential to outperform the benchmark process.

D.4.1.1 Defining Functional Units and System Boundaries for *Monitoring*

For each *Monitoring* step during the iterative R&D process, the functional unit and system boundaries **shall** be refined with the involved stakeholder groups [28], as new information might suggest modifications of the functions and reference flows, or might add unit processes to the system boundaries [29]. If the functional unit is expected to change with increased maturity, multiple functional units **should** be defined to analyze the sensitivity of the assessment results to the choice of the functional unit [25, 30, 31]. Those multiple functions **may** be prioritized based on stakeholder engagement, or by conducting a series of assessments, showing the pros and cons for each function or market separately as described by Wender *et al*. [24, 32].

D.4.1.2 Defining the Benchmark Technology, Decision Criteria, and Inventory Modeling Framework for *Monitoring*

To reliably discard processes that do not provide the potential to outperform the benchmark technology, three key aspects **shall** be defined together with decision makers: First, an appropriate benchmark; second, relevant decision criteria; and third, modeling assumptions.

D.4.1.2.1 Benchmark Technology

The *Monitoring* step requires comparing the assessed CCU technology to another technology offering the same function ('benchmark technology' or 'reference process'), as the results must be considered within an appropriate context to support decision making. The benchmark technology must be chosen thoughtfully, as the choice can have a substantial influence on the comparative results (see also chapter C.5.3). Thus, the benchmark for comparison **shall** reflect the goal of the study, **shall** ensure functional equivalence, and **shall** reflect the technology that the assessed technology is expected to displace at the time of expected market entry [24], the so-called marginal-cost technology [33]. However, the future market situation remains uncertain, and the marginal-cost technology might change during technology development, e.g., it might be improved or itself fully substituted by an alternative technology. However, modeling the future development of markets is beyond the scope of LCA. Consequently, the estimated potential to reduce emissions or costs might be inaccurate. To avoid overestimation of environmental benefits the best available technology for reducing GHG emissions **should** be chosen, if the marginal-cost technology cannot be identified [33]. If more than one benchmark technology might be applicable, those benchmarks **should** be considered in a sensitivity analysis (D.7.2.2).

D.4.1.2.2 Decision Criteria

The decision criteria are based on the subjective preferences of decision makers. Thus, to identify a process as inferior, TEA- and LCA-related No-go criteria (e.g., specific target values for selected impact categories or economic indicators) **shall** be defined together with the decision makers. As CCU processes have the central goal of reducing GHG emissions, increasing the global warming impact compared to the benchmark **shall** be specified as a No-go criterion. Further impact categories and economic indicators **shall** be assessed and **should** be considered as decision criteria to avoid simply shifting environmental burdens or financial risks (see chapter D.6).

D.4.1.2.3 Modeling

The modeling framework for *Monitoring* **shall** – as an essential requirement – include an assumed best-case performance of the assessed CCU technology. If this assumed best-case is already inferior to the reference process in one or more of the defined No-go criteria, the CCU technology **shall** be discarded by decision makers. If the best-case performance does not lead to a No-go decision, more realistic modeling assumptions **should** be considered in the inventory generation to assess the sensitivity to modeling assumptions. Chapter D.5 provides more details on estimating inventory data for the best-case performance and the integration of more realistic assumptions.

The recommendations on dealing with multifunctionality described in C.4.3 **shall** be applied. At low TRLs, the CO_2 source – and thus, the additional functions of the overall system – might not be identified. In this case, all eligible CO_2 sources **shall** be considered and compared. Müller *et al*. provide further information on dealing with multifunctionality when comparing different CO_2 sources [34].

D.4.1.3 Data Quality Requirements for *Monitoring*

The recommendations on data quality requirements described in C.4.4 **shall** be followed. Low-TRL assessments inherently face challenges of lower data quality. Thus, the resulting limitations **shall** be clearly stated and explained to the decision makers. All assessed technologies and benchmarks **shall** be modeled with the same background data.

D.4.1.4 Provisions

Provisions D.2 – Scope Definition for *Monitoring*	
Shall	1) The recommendations of chapters B.4 and C.4 **shall** be followed for low-TRL assessments. However, an early-stage assessment is often not intended for external communication, and thus the special requirements for comparative assessments (C.4.5) **may** be replaced by internal review and discussion with involved stakeholders. 2) The **functional unit** and **system boundaries shall** be refined with the involved stakeholder groups at each *Monitoring* step. If the functional unit is expected to change with increased maturity, multiple functional units **should** be defined to analyze the sensitivity of the assessment results to the choice of the functional unit. *3)* The benchmark for comparison **shall** reflect the goal of the study, **shall** ensure functional equivalence, and **shall** reflect the technology that the assessed technology is expected to displace at the time of expected market entry [24]. 4) TEA- and LCA-related No-go criteria (e.g., specific target values for selected impact categories or economic indicators) **shall** be defined together with decision makers. Increased global warming impact relative to the benchmark **shall** be included as a No-go criterion. Further impact categories and economic indicators **shall** be assessed and **should** be considered as decision criteria to avoid simply shifting environmental burdens or financial risks (see chapter D.6). 5) The modeling framework for *Monitoring* **shall** – as an essential requirement – include an assumed best-case performance of the assessed CCU technology in order to discard inferior processes. If the best-case performance does not lead to a No-go decision, more realistic modeling assumptions **should** be considered in the inventory generation as described in chapter D.5. 6) The recommendations on dealing with multifunctionality described in C.4.3 **shall** be applied. If the CO_2 source is not yet identified, all eligible CO_2 sources **shall** be considered and compared. 7) The recommendations on data quality requirements in chapter C.4.4 **shall** be followed. The limitations of low data quality **shall** be clearly stated and explained to decision makers. All assessed technologies and benchmarks **shall** be modeled using the same background data.
Should	1) The best available technology in GHG emissions **should** be chosen, if the marginal-cost technology cannot be identified [33]. If more than one benchmark technology might be applicable, those benchmarks **should** be considered in a sensitivity analysis.
May	

D.4.2 Scope Definition for *R&D Support*

General Introduction

If the decision is made to proceed with R&D, the next steps in R&D are planned. Here, research experts might envision a set of alternatives for the process design and decide what experiments or studies to perform next. To focus their research efforts, they need to know the hot spots for improvement of the overall process performance. With increasing maturity, the alternatives become more detailed (e.g., from the choice of reactants and catalysts, to the reactor design, to specific unit processes and their detailed optimization). LCA and TEA can provide support by reducing the set of alternatives and by identifying the environmentally/economically most relevant parameters to consider. *R&D support* builds upon the previous *Monitoring* step, while the focus shifts from comparing the current state against a benchmark towards modeling and comparing different alternatives for the process design.

D.4.2.1 Defining Functional Units and System Boundaries for *R&D support*

The functional unit and system boundaries **should** be carried over from the previous *Monitoring* step. However, they **may** be reduced when comparing alternatives **if comparability between alternatives is guaranteed** (e.g., the impacts of changing one unit process or its parameters if both unit processes have the same functionality).

D.4.2.2 Steps to Perform LCA and TEA for *R&D Support*

The benchmark process and decision criteria **should** be taken from the previous *Monitoring* step. In *R&D support*, the comparison with the benchmark process is necessary to avoid selecting inferior process alternatives.

In line with the goal of the study, the following steps **should** be performed:

1) A screening of alternatives **should** be performed, using the available information for each alternative and best-case assumptions
2) For promising alternatives, a sensitivity analysis **should** identify the parameters/choices that have the strongest influence on environmental and economic performance
    a. Sensitivities to process-related parameters
    b. Sensitivities to external parameters = Scenario analysis
3) A one-at-a-time break-even analysis **should** be performed on those parameters that strongly influence performance

These steps apply to the choice of alternatives for reactants, catalysts, or unit operations, to identify parameters that need to be defined next and to assess external factors (e.g., energy mix, CO_2 price, etc.) influencing the results.

The screening step is useful if different alternatives have been identified and need to be compared (cf. A.4). Screening builds upon the inventory modeled for the previous *Monitoring* step and adds available information about each alternative being considered to develop the process further. As in the *Monitoring* step, unpromising alternatives can be discarded to reduce the effort invested in conducting more detailed sensitivity or break-even analysis.

The break-even analysis can be performed for each decision criterion, and investigates under which circumstances the investigated process would perform equally to the benchmark process [35]. A break-even analysis is performed for one parameter at a time and is therefore subject to the uncertainties of the other parameters. Screening, sensitivity analysis, and break-even analysis are explained in chapter D.7.2.

D.4.2.3 Data Quality Requirements for *R&D Support*

The data quality requirements described for *Monitoring* **shall** be met. As the focus of R&D changes with increasing maturity, the necessary support from LCA and TEA changes and more detailed methods for estimating missing input data and modeling the system are needed. Chapter D.5 provides further details on the LCI generation for each TRL.

D.4.2.4 Provisions

Provisions D.3 – Scope Definition for *R&D Support*	
Shall	1) The recommendations of chapters B.4 and C.4 **shall** be considered for low-TRL assessments. However, an accompanying assessment is not intended for external communication, and thus the special requirements for comparative assessments (C.4.5) **may** be replaced by internal review and discussion with involved stakeholders. 2) The recommendations on data quality requirements described in C.4.4 **shall** be followed. Low-TRL assessments inherently face challenges of lower data quality. Thus, the resulting limitations **shall** be clearly stated and explained to decision makers. All assessed technologies and benchmarks **shall** be modeled using the same background data. 3) The recommendations on dealing with multifunctionality described in C.4.3 **shall** be applied. If the CO_2 source is not yet identified, all eligible CO_2 sources **shall** be considered and compared.
Should	1) The functional unit and system boundaries **should** be carried over from the previous *Monitoring* step. 2) The benchmark process and decision criteria **should** be taken from the previous *Monitoring* step. 3) A screening of alternatives **should** be performed, using the available information for each alternative and best-case assumptions. 4) For promising alternatives, contribution and sensitivity analysis **should** identify the parameters/choices with the strongest influence on environmental and economic performance. 5) A one-at-a-time break-even analysis **should** be performed on parameters that strongly influence performance.
May	1) The functional unit and system boundaries **may** be reduced when comparing alternatives **if comparability between alternatives is guaranteed** (e.g., the impacts of changing one unit process or its parameters if both unit processes have the same functionality).

D.5 Life Cycle Inventory (LCI)

General Introduction

In the Life Cycle Inventory phase, the inventory data are gathered, and the production system is modeled according to the goal and scope definition. For technologies with low technology readiness levels (TRL), data can often not be measured or obtained from existing databases. Thus, assessments of low-TRL technologies rely on estimating missing data to answer a research question. The research question can be related to either *Monitoring* or *R&D support*. Estimation methods differ in terms of their necessary input data and the type and uncertainty of the output data. Chapter C.5.2 provides a basic overview of estimation methods, as missing data is not only an issue of low-TRL processes.

This chapter provides TRL-specific recommendations for estimation methods, as the applicability of estimation methods depends on the available information and thus on the maturity of a technology. Therefore, this chapter is structured by TRL of chemical processes, as in Buchner *et al.* [8].

D.5.0 General Recommendations and Structure of This Chapter

LCA and TEA **shall** be conducted in a manner closely related to the process design in order to avoid redundant work and ensure consistency. A commonly applied hierarchy for process design was proposed by Douglas and subsequently refined [36, 37] (Figure 2). The process design hierarchy reflects well the order in which data become available at low TRLs.

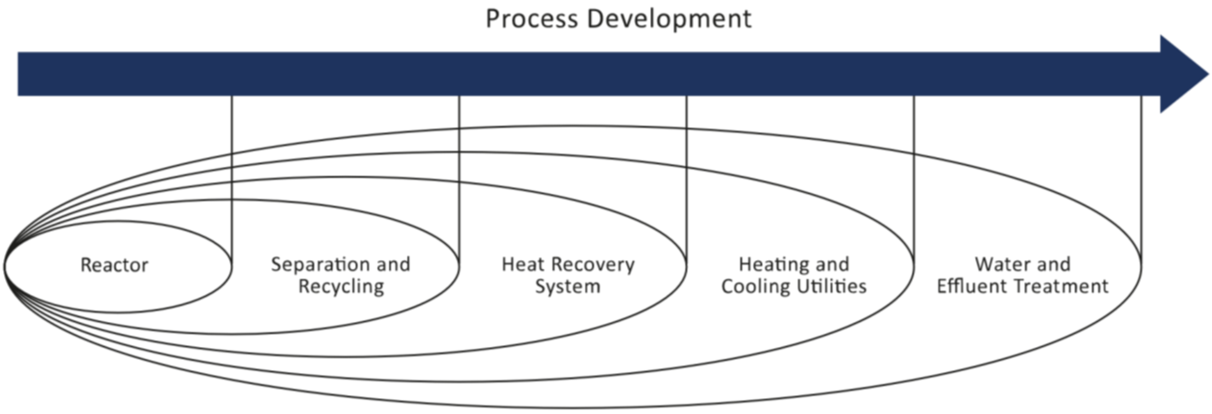

Figure 2 Onion model of chemical process design adapted from Smith [37]. Chemical process design starts with the reaction and gradually adds more details of the process, such as the separation and recycling system and the heating and cooling system. Finally, the heating and cooling utilities and the water and effluent treatment are included. The order of information availability fits the TRL concept used in these Guidelines.

Wherever inventory information is missing, estimation methods **shall** be utilized until the process design provides more detailed data [12]. The conditions associated with the information (e.g., data source, data quality, limitations) **shall** always be determined and communicated to decision makers.

In the following, we provide a short description of the available information at each TRL (1–5), including a simplified block flow diagram. Based on the available information, we present a general approach to apply estimation methods, and provide a set of tables summarizing applicable estimation methods for the four key aspects of an inventory: Mass flows, energy flows, emissions to and resources from the environment, and equipment costs. At the end of each TRL sub-chapter we discuss general limitations regarding data quality and give recommendations for dealing with these limitations.

When calculating the capital costs of chemical processes, the estimation is commonly classified into five levels, each of increasing accuracy [38]:

- Order-of-magnitude estimation
- Study estimation
- Preliminary estimation
- Definitive estimation
- Detailed estimation

The five levels given above correspond to the five estimation classes defined by AACE [39, 40]. Behind each term there are several methods that provide results that are comparable for a given level of quality. The choice of methods is based on the availability of input data, the objectives of the evaluation, and their advantages and disadvantages (see references in the following tables); i.e., the methods can be grouped according the quality of their results.

D.5.0.1 Provisions

Provisions D.4 – Life Cycle Inventory (LCI)	
Shall	1) LCA and TEA **shall** be conducted in a manner closely related to the process design, in order to avoid redundant work and ensure consistency. 2) Wherever inventory information is missing, estimation methods **shall** be utilized until the process design provides more detailed data. The conditions associated with the information (e.g., data source, data quality, limitations) **shall** always be determined and communicated to decision makers.
Should	
May	

D.5.1 TRL 1 - Idea

D.5.1.1 Available Information

At TRL 1, the chemical reaction and the reaction steps are either unknown or not yet selected. Information might (or might not) be available for the primary raw materials and target product. At the same time, essential information for LCA and TEA is still missing at this stage (e.g., the necessary amounts of raw materials, involved auxiliaries, and the target product's detailed composition).

Chemists might provide a list of potential reactions, and LCA and TEA **should** screen those reactions based on the reaction stoichiometry, if already available. The use of stochiometric calculations is discussed at TRL 2 (D.5.2) where it becomes generally applicable.

Figure 3 provides a simplified block diagram to summarize the information available for a process at TRL 1.

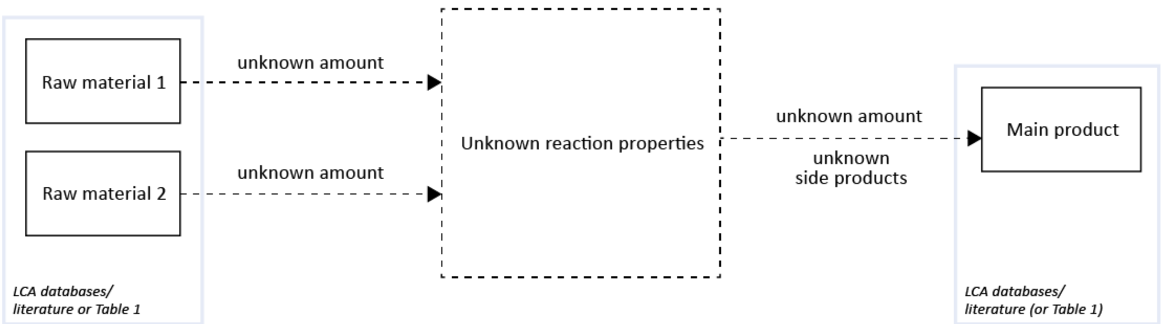

Figure 3 Simplified block flow diagram including available information at TRL 1. Unknown or likely unknown flows are shown as dashed lines. At this TRL, either the main product or the raw materials might be unknown; A list of possible reactions might exist. The blue boxes refer to those tables summarizing related estimation methods.

D.5.1.2 Recommendations for LCA and TEA at TRL 1

Starting at TRL 1, TEA can provide price information on raw materials and products. LCA can assess whether raw materials with high environmental impacts are involved. For alternative routes for an established product, LCA can determine whether the environmental impacts of the conventional process are high, indicating a reduction potential. Besides gathering this information on the materials and products, the focus is on selecting an appropriate benchmark for future *Monitoring* (see chapter D.4.1.2.1).

Missing information about the cradle-to-gate environmental impacts of raw materials **shall** be gathered from internal or external LCA databases or literature. If information about a background or benchmark technology is readily available within the company or from its partners, this information **should** be included. If no information is available in LCA databases, molecular structure-based models (MSM) **may** be used for the initial estimation of cradle-to-gate life cycle impacts [41]. Textbox 1 provides general information about MSM and their limitations. Table 1 provides examples of MSM[1].

For this Guidance, the focus is on MSM used to estimate cradle-to-gate impacts of chemicals. MSM are widely used for the prediction of physical and thermodynamic properties and have also been applied to reduce the necessary inputs for LCIA characterization models, such as toxicity characterization for emitted substances [42–44].

MSM **should** only be used for first predictions of life cycle impacts where background data are missing (e.g., raw materials) if the process route of these raw materials is expected to be of minor importance to the foreground system [41]. When using MSM, the limitations described in Textbox 1 **shall** be considered. Most importantly, the data used for training and testing the model **shall** be comparable to the molecule of interest. Furthermore, the results are often limited to a small set of impact categories. The limitation in impact categories restricts the possible environmental tradeoffs that can be considered at this stage.

> Excurse: **Molecular structure-based models for LCIA**
>
> Molecular structure-based models (MSM) in LCA can be trained to predict impact categories from a set of molecular descriptors (physical–chemical properties of the target chemical). The models can be set up from a variety of methods, e.g., artificial neural networks (ANN), decision trees from clustering, classification, or multi-linear regression. When **choosing a model**, the data used for training and testing the model **shall** be comparable to the molecule of interest. For **input data,** molecular descriptors can be taken from standard tables or from property databases such as SPRESI [1], ChemSpider [2], PubChem [6], or NIST [7].
>
> **Limitations:** The MSM are limited in their field of application and their prediction accuracy. Many models do not provide any process-specific information. However, combined models exist using process indicators in addition to the molecular structure [9, 10]. Usually, MSM are not designed to be further disaggregated for a contribution analysis, as they streamline the LCA approach without estimating separate LCI data.
>
> When using MSM, the quality of the training data is of key importance, as an MSM cannot overcome the limitations of the training data sets used [11].
>
> **Further reading:** Parvatker and Eckelman, 2019 and Kleinekorte *et al.*, 2020 [12, 13]

Textbox 1: Molecular structure-based models

The EstiMol Database (https://www.ifu.com/en/umberto/estimol/) **may** be used, before choosing an MSM that needs to be self-adapted from the literature, as EstiMol provides benefits known from databases (e.g., reproducible results and ease of use). The choice of an estimation method depends on the investigated molecule, the desired impact categories (and the related prediction accuracy), and the accessibility of data

[1] Note that the review of these models was conducted in 2020, and the field is evolving quickly. The joint SETAC NA and ACLCA interest group on LCA (https://www.setac.org/members/group.aspx?id=90710) is currently investigating the leveraging of new technologies in LCA, including machine learning tools for LCI and LCIA predictions; Results are expected in Q4 of 2022.

and tools. Combined models **may** be used if the range of necessary process indicators can already be assumed.

For TEA, only a qualitative estimation of costs can be performed, e.g., comparing the prices of raw materials with that of the target product when produced via benchmark technology. For this purpose, cost/price data for the raw materials and benchmark products **shall** be collected. The raw material price can usually be gathered from market data. Public and/or restricted sources offer secondary cost data for raw materials (statistical or industrial data), such as the Euro-Stat Prodcom database, IHS Markit, Alibaba, etc.[2] These sources typically focus on specific countries or regions. Given the limited availability of data for technologies with low TRLs, the assessments at TRL 1 are mainly conducted qualitatively. Hence, the main task of the assessment is often to identify critical factors that affect the production route. Generally applicable methods are not available for TEA due to the variety of possible process concepts. For a TEA, the structure of the process, combining synthesis and separation steps, is more important than the molecular structure of the product. A block flow diagram can provide the first representation of a process, indicating its level of complexity and necessary equipment. Cost estimations that apply shortcut methods also require this representation for new chemical processes, but such information is usually unavailable at TRL 1.

Table 1 Molecular structure-based models, sorted by year of publication. The heading (in the blue box) includes the reference and the missing data to be estimated. The impact categories for which a method is not recommended are shown in brackets. The table further includes information about the necessary input data, training data, prediction accuracy, accessibility of data to use the method, implementation effort, and recommendations for using the method.

Kleinekorte, 2019 [10]: 17 ReCiPe v1.08 (H) midpoint categories	
Input	• Set of 6 descriptors chosen by the ANN for each impact category out of 185 potential descriptors in total, consisting of 178 molecular descriptors (e.g., physical and chemical properties) and 7 process descriptors as proposed by Patel *et al*., e.g., the concentration of each component at the reactor outlet (calculated assuming ideal phase and chemical equilibrium) or the sum of the environmental impacts of the reactants [45]
Method and training data	• ANN with a training set of 63 organic chemicals from the Gabi Database (https://www.gabi-software.com/databases/gabi-databases) • Each impact category is covered in a separate ANN
Prediction accuracy	• Of training data set based on leave-one-out: • Coefficient of determination (R^2) up to 0.64 (for marine ecotoxicity) and around 0.3 for 7 environmental impact categories such as climate change. The 9 remaining impact categories had an R^2 less than 0.2
Accessibility of data	• Underlying data are not available from open sources
Implementation effort / limitations	• Available upon request from the authors
Recommendations	• This ANN can predict trends for process-/pathway-specific cradle-to-gate impacts for different process routes for an organic chemical and can be used to compare process routes if experts provide the missing information. • At TRL 1, the process descriptors rely on expert opinions or assumptions, which must be verified as soon as more specific information is available

[2] Table 5 of chapter B.5.3.3 and the GCI website (https://assessccus.globalco2initiative.org/tea/databases) list and briefly explain more sources and useful databases.

Karka, 2019 [9]: Classification of bio-based products to low, medium, or high impacts: ReCiPe and CED methods (23 metrics in total)	
Input	• 30 predictor variables (molecular descriptors of the FineChem tool and process indicators as proposed by Sugiyama and Patel [45, 46])
Method and training data	• Classification-based decision trees for each impact category, based on 91 study systems as training data (bio-based processes)
Prediction accuracy	• 4–9% classification error for published best-performing decision trees
Accessibility of data	• Provided in the supplementary information of publication
Implementation effort / limitations	• Low effort if using published best-performing decision trees (published for 6 impact categories: human health, total score ReCiPe, cumulative energy demand (CED), water depletion, marine eutrophication, and climate change)
Recommendations	• Applicable for bio-based processes • Decision trees might *support R&D decisions* when deciding on feedstocks, reactions, and process concepts. Not recommended for *Monitoring*. • At TRL 1, the process-related variables rely on expert opinions or assumptions, which must be verified as soon as specific information is available
Calvo-Serrano, 2019 [47]: CED, GWP, (COD, BOD5, TOC), Eco-indicator 99 (EI99)	
Input	• 15 molecular descriptors, 12 thermodynamic properties, and surface charge density distributions of molecules (σ-profiles taken from COSMO-RS)
Method and training data	• Multi-linear regression, based on the data set presented by [48]; outliers and molecules removed where no thermodynamic properties are available, resulting in 83 data points [49] • 7 data sets added for conventional pesticides
Prediction accuracy	• Relative errors in the range 20–44%, while prediction errors exceeded 700% for: chemical oxygen demand (COD), biological oxygen demand (BOD5), and total organic carbon (TOC)
Accessibility of data	• COSMO-RS σ-profiles [50] need to be calculated by quantum mechanics tools or provided by COSMO-file database • Authors used COSMOtherm software [51] (version C3.0, release 17.01) with the parametrization: BP_TZVP_C30_1701 (BP86 as DFT-functional and defTZVP as a basis set for quantum mechanical calculation of σ-profiles) • Bell *et al.* provide a freely available COSMO database for academic and noncommercial users [52]
Implementation effort / limitations	• The final prediction models are provided in the supplementary information. • The same settings for quantum mechanical calculations must be applied for comparable σ-profiles.
Recommendations	• Recommended only for predicting CED, GWP, and EI99 [47] • Check whether the target molecule lies within the min and max values presented in the supplementary information

Song, 2017 [11]: CED, global warming (IPCC 2007, 100a), acidification (TRACI 2.0), and three end-point impact categories: Eco-indicator 99 (I,I, total) (EI99), ecosystem quality (Impact 2002+), and human health (Impact 2002+)	
Input	• Molecular descriptors such as functional groups (calculated using Dragon 7 https://www.chm.kode-solutions.net/products_dragon.php, which is no longer available)
Method and training data	• ANN trained with a total of 166 chemicals (wide range) from ecoinvent database [53–55]: 10 as test set, 16 as a validation set, the rest for training
Prediction accuracy	• On testing dataset: Coefficient of determination (R^2) 0.45–0.87 (0.48 for climate change) and mean relative error (MRE) 30–65%. • The applicability domain characterizes the confidence level of outputs • Highest uncertainties for global warming and human health
Accessibility of data	•Access to the ecoinvent database is necessary • Dragon 7 is no longer available. However, the authors recommend using an open-source alternative to calculate molecular descriptors (Mordred) by Moriwaki *et al*. [56]
Implementation effort / limitations	• High effort, as the method must be self-implemented, and the model must be fitted to newly calculated molecular descriptors
Recommendations	• Check if molecules are within the range of training data
Wernet, 2009 [57] -> FineChem Tool: CED, (GWI, Eco-indicator 99 (EI99), electricity use, heat use)	
Input	•Molecular weight • Information on chemical structure such as number of functional groups, the numbers of several specific atoms (O, N, and halogens), and number of aromatic or aliphatic rings
Method and training data	• 392 data sets for petrochemicals initially (process data from industry (296) and the ecoinvent database v2.01 [54] (96)); averaging data sets for the same products reduced the number of individual sets to 338; • An average European electricity mix was used in the background
Prediction accuracy	• Mean values of 30 test sets based on leave-one-out: Coefficient of determination (R^2) between 0.41 (GWP) and 0.69 (EI99) and mean relative error (MRE) 20.7–94.6% in all estimated impact categories • Provides standard deviations to approximate uncertainties
Accessibility of data	• Available as EstiMol Database (https://www.ifu.com/en/umberto/estimol/)
Implementation effort / limitations	• Low effort if EstiMol database is used • Electricity and heat use for exothermic reactions are likely to be overestimated [57]
Recommendations	• Recommended for initial screening if background data are missing • Check if the predicted impacts are within the range of training data. If one or more predicted impact is outside the training data range, EstiMol does not recommend using any predicted impact for that molecule (https://www.ifu.com/en/umberto/estimol/) • Use only for petrochemicals without Br or I, not more than four F atoms, and not more than one S or P atom (https://www.ifu.com/en/umberto/estimol/)

D.5.1.3 Provisions

Provisions D.4.1 – Inventory – TRL 1	
Shall	1) Information about the raw materials **shall** be gathered from internal and external LCA databases or literature. 2) Cost/price data for the raw materials and benchmark products **shall** be collected for TEA. 3) The limitations (e.g., unknown stoichiometry, risk of burden-shifting due to missing impact categories) **shall** be reported. 4) If impact categories are omitted due to missing information, all omitted criteria **shall** be listed, the reasons for omission explained, and potential impacts on results discussed. 5) If molecular structure-based models are used, the data used for training and testing the model **shall** be comparable to the molecule of interest.
Should	1) If information about a background or benchmark technology is readily available within the company or from partners, this information **should** be included. 2) To guide further research, alternative chemical reactions **should** be screened if available.
May	1) If no information about life cycle impacts is available, molecular structure-based models **may** be used to estimate cradle-to-gate life cycle impacts. Ensure that the data for training and testing the model are comparable to the molecule of interest, and be aware of the limitations (e.g., the field of application, prediction accuracy) (see Textbox 1). Molecular structure-based models **should** only be used for first predictions of life cycle impacts where background data are missing (e.g., raw materials). 2) The EstiMol database **may** be used before choosing an MSM that needs to be adapted from literature. 3) Combined models **may** be used if the range of necessary process indicators can already be assumed.

D.5.2 TRL 2 – Concept

D.5.2.1 Available Information

At TRL 2, the stoichiometry of the selected main reaction(s) is available and can be used to build up an initial, basic reaction model. The reaction phase (e.g., gas or liquid) and the general type of CO_2 utilization technologies (e.g., thermochemical reaction [T], electrochemical reaction [E], or biochemical reaction [B]) [58] have been identified. The number of reaction steps and the unit operation classes (e.g., separation) are identified but might still be changed during R&D. All available information is still based on literature and assumptions, and therefore needs to be validated in a laboratory environment to reach TRL 3. Figure 4 provides a simplified block flow diagram to summarize the available information for a process at TRL 2.

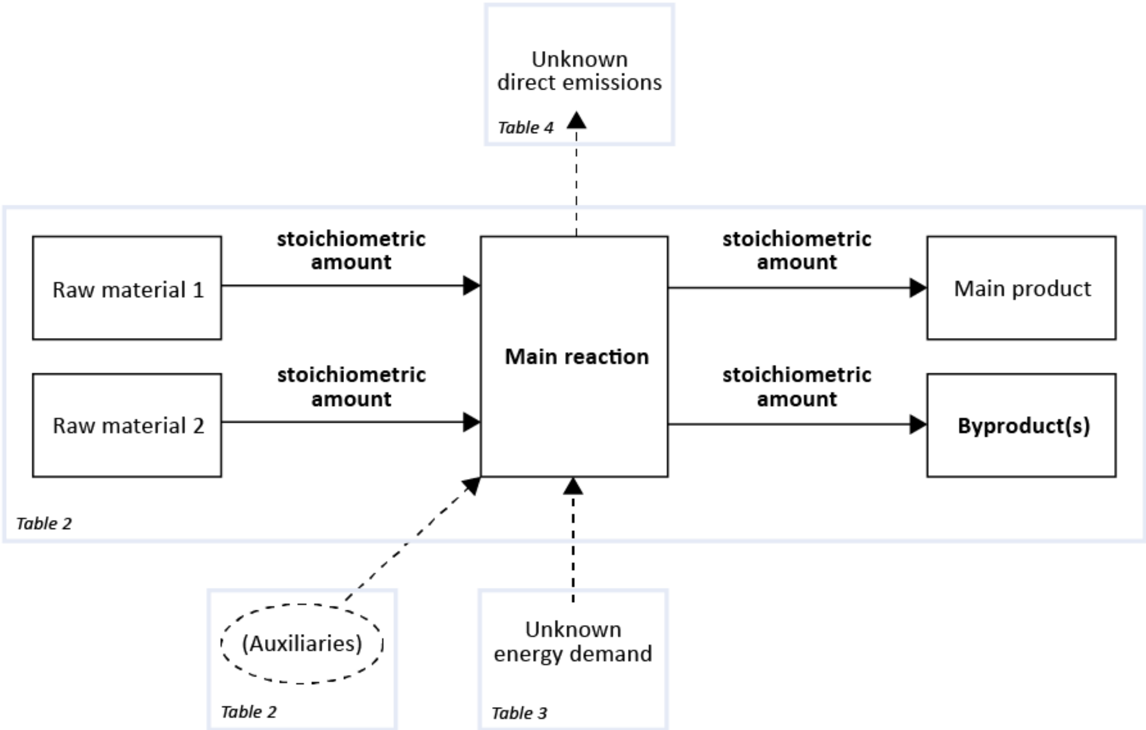

*Figure 4 Simplified block flow diagram including available information at TRL 2. Unknown or likely unknown flows are shown as dashed lines. Newly available information is shown in **bold** typeface. The reaction stoichiometry of the main reaction and possibly occurring by-products are known at this stage. The blue boxes refer to those tables summarizing related estimation methods.*

D.5.2.2 Applicable Estimation Methods

At TRL 2, information about the reaction step(s) is available. Therefore, the assessment model **shall** focus on the reaction unit. For the reaction unit, the efficiency according to the mass flow (usually yield), the heat and energy demand, and direct emissions to the ecosphere **shall** be considered. In addition, the separation can be included as a pseudo-unit assuming perfect separation without the necessity of a recycling flow and neglecting energy demand for separation [46, 58].

D.5.2.2.1 Mass Flow

A stoichiometric approach **shall** be used to calculate the mass flows within the reaction step as described in Textbox 2. Stoichiometric calculations for the mass flows can be further refined by adding information about the yield. If information about side reactions, auxiliaries, wastes, or product losses is missing, either proxy values can be used or respective flows can be excluded, depending on the assessment goal:

1. Goal: *Monitoring*:

Unknown mass flows **may** be omitted if the assessment goals are to monitor the process performance compared to a benchmark and exclude inferior reaction pathways. The omission of unknown mass flows leads to a lower bound of environmental impacts and costs. If this lower bound indicates that a No-go criterion will be exceeded (e.g., equal or higher impacts/costs than the benchmark), the process route **shall** be discarded.

2. Goal: *R&D Support*:

If the assessment goal is to guide upcoming R&D (e.g., by identifying hot spots for further research via contribution and sensitivity analysis), the omission of unknown mass and energy flows might be misleading. As a starting point for including missing information, expert opinions **should** be used to define ranges, or estimates **should** be made based on heuristics (Table 2).

D.5.2.2.2 Process Energy Demand

The gate-to-gate process energy demand can be estimated using either the minimum energy demand for the reaction step or using a proxy value (Table 3). The calculation of minimum energy demands allows for the *Monitoring* of different reaction pathways. However, as energy-related information is only available for the reaction step, further process steps such as separation are not considered, and thus the overall energy demand is usually underestimated.

Proxy values can provide quick estimations of the overall process energy demand and **should** be used as a starting point for sensitivity analysis or break-even analysis. Proxy values can be based on expert opinions or averaged chemical industry values. However, averaged values do not reflect information about the reaction and the process. The energy demand for separation can vary significantly, so that a ranking based only on the energy required for the reaction step and addition of proxy values is insufficient.

Excurse: **Stoichiometric calculations**

For each reaction step, mass and energy balances can defined based on the stoichiometric equation of the reaction. While mass balances are defined by the stoichiometric equation, the relation of stoichiometry to actual energy demand is very limited, as only the difference between the energy content of raw materials and products is considered when calculating the reaction enthalpy.

Input data: If the reaction stoichiometry is not provided by the researchers, the stoichiometric equation can be taken from existing chemical databases (e.g., ChemSpider SyntheticPages [2], Ullmann's Encyclopedia of Industrial Chemistry [59], NIST [7], e-EROS [60], Reaxis [61], or Organic reactions [62]) or predicted through retrosynthesis [63].

Limitations: A stoichiometric calculation is limited to the estimation of mass flows, but omits that a reaction might happen in separate steps necessitating additional auxiliaries, e.g., solvents. Furthermore, the calculation does not include information about the kinetics and chemical equilibrium. Often, one or more reactants are provided in excess to shift the equilibrium towards the desired product. Furthermore, side reactions can occur, leading to additional side products. Those side reactions are often unknown at TRL 2. The reactants in excess and the additional side products usually are separated from the main product and recycled in the process, which is omitted for the stoichiometric approach. Thus, the stoichiometric calculations **underestimate the necessary mass flows** to produce a certain amount of product.

Textbox 2 Stoichiometric calculations

D.5.2.2.3 Direct Emissions

Direct emissions, which are calculated from gate to gate, to the environment are difficult to foresee at low TRL. The overall direct emissions result from the process itself (e.g., emissions from incineration) and from fugitive emissions at all unit processes due to small amounts of leakage. Fugitive emissions of unit processes are usually calculated indirectly by closing the mass balance of the process rather than being measured directly. As the mass balances themselves need to be estimated at low TRL, it is even more challenging to estimate direct emissions. A common and straightforward approach used in the literature is to assume that a fixed factor of the raw materials is directly emitted (Table 4). Emission factors can be used to estimate emissions to air or water. These emission factors might not reflect the emissions of the final process but can be used in a contribution analysis to identify hot spots. The results can support process designers in preventing direct emissions.

The following tables provide a literature overview of methods for estimating mass and energy flows at TRL 2. Table 2 provides heuristics for the yield and gate-to-gate water consumption to estimate the mass flows at TRL 2. Table 3 provides averaged values and methods to estimate the gate-to-gate process energy demands. Table 4 provides an overview of various fugitive emission factors used in the literature. Furthermore, a method is listed for calculating emissions to water based on the yield and fugitive emission factors [64].

Table 2 Heuristics to estimate mass flows available at TRL 2. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s), and recommendations on when and how to use the estimation method.

Mass flow Weidema *et al.*, 2013; Althaus *et al.*, 2007; Hischier *et al.*, 2005 [53, 55, 64]	
Input	• Stoichiometric reaction equation
Underlying assumption(s)/ limitation(s)	• Yield = 95% • No side reactions or auxiliaries considered
Recommendations	• Check plausibility with experts • Use for missing background data • Use for an initial contribution and completeness analysis if no other expert opinion is available • Use to guide R&D if information about yield is missing
Water consumption: 24 $kg_{water}/kg_{product}$ Hischier *et al.*, 2005 [64]	
Input	• Amount of product
Underlying assumption(s)/ limitation(s)	• Average value of around 1.500 chemical products. • Based on the environmental report of a chemical plant site of several chemical production companies in Germany (Gendorf, 2000) • Not specific to chemicals or process routes • Does not reflect the water consumption for major CCU inputs such as H_2 or CO_2
Recommendations	• Use the latest Gendorf report to update the average water consumption: As of 2020, 24 $kg_{water}/kg_{product}$ is still applicable [65] • Check plausibility with experts • Use for an initial contribution and completeness analysis if no other expert opinion is available • Use for missing background data

Table 3 Estimation methods for the gate-to-gate process energy demand, available at TRL 2. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s), and recommendations on when and how to use the estimation method.

Minimum energy demand for the reaction step Roh *et al.*, 2020 [58]	
Input	• Minimum ΔH_R at standard conditions [Thermochemical conversion] • Gibbs free energy change [electrochemical or biological conversion]
Underlying assumption(s)/ limitation(s)	• Calculates minimum energy demands as a lower bound • Does not account for the actual conditions of the reactor
Recommendations	• Use minimum energy demand for *Monitoring*
Gate-to-gate steam consumption High (3–16 $kg_{steam}/kg_{product}$) or low (0–1 $kg_{steam}/kg_{product}$) [medium becomes available at TRL 3] Pereira *et al.*, 2018 [66]	
Input	• Information about the reaction mechanism + amount of product
Underlying assumption(s)/ limitation(s)	• Based on statistical models, such as probability density functions (PDF) and classification trees • Assuming that energy demand is mainly driven by reaction type, while reactants, solvents, etc., are neglected • Training data: 250 data points calculated based on information *'provided by nine industry partners in Switzerland, Germany, France and the United States'* using a previously described approach [67] • Limited to batch process • Steam considered at 6 bar • Classification to low or high steam consumption was successful only for 9 out of 17 test data points; 2 data points were overestimated, 6 data points were underestimated • A predicted range for high steam demand (3–16 kg_{steam}) might not provide sufficient decision support in practice
Recommendations	• Only applicable to batch processes • Check plausibility with experts
Gate-to-gate energy demand: Electricity demand: 1.2 $MJ/kg_{product}$ and Heat demand: 2 $MJ/kg_{product}$ Althaus *et al.*, 2007[55]	
Input	• Amount of product
Underlying assumption(s)/ limitation(s)	• Average value of around 1,500 chemical products. Based on the information from the environmental report of a chemical plant site of several chemical production companies in Germany (Gendorf, 2000) • Not specific to chemicals or process routes • Does not reflect energy demands for major CCU inputs such as H_2 or CO_2. However, these inputs are available in the energy scenarios of these Guidelines

Recommendations	• Compare to the latest Gendorf report to update the energy demands[3] • Check plausibility with experts • Use for an initial contribution and completeness analysis if no other expert opinion is available • Use for missing background data
Gate-to-gate process energy demands **Kim and Overcash, 2003 [68]**	
Input	• Amount of product
Underlying assumption(s)/ limitation(s)	• Findings from modeling 86 chemical processes [69]: (see table below) • The standard deviation is presented in brackets. Both data sets show a large standard deviation due to the variety of chemical processes. Note that a normal distribution was assumed by the authors, while a lognormal distribution might better reflect the data as the modelled results do not show negative values • Where byproducts are produced, an allocation on mass basis is applied • Facility energy, or energy for waste treatment are excluded
Recommendations	• Check plausibility with experts • Use for an initial sensitivity analysis considering the provided standard deviations to assess for uncertainties

Energy carrier	Organic chemicals	Inorganic chemicals
Electricity [$MJ/kg_{product}$]	0.6 (±0.98)	1.9 (±5.1)
Steam [$MJ/kg_{product}$]	7.7 (±14)	3.6 (±8.2)
Heating fuel [$MJ/kg_{product}$]	0.15 (±0.5)	1.5 (±3.2)
Potential energy recovery [$MJ/kg_{product}$]	−1.6 (±−1.9)	−2.0 (±−5)

Table 4 Factors to estimate direct emissions to the environment, available at TRL 2. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Averaged gate-to-gate emissions to air **Hischier *et al.*, 2005 [64]**	
Input	• Amount of input materials
Underlying assumption(s)/ limitation(s)	• 0.2% of input materials as gate-to-gate emissions • $emissions_{air} = 0.002 * \left(\frac{1}{yield}\right) * stochiometric\ reactants$ • Generic value with no validation presented
Recommendations	• Check plausibility with experts • Use for missing background data

[3] As of 2020, 2.1 $MJ_{electricity}/kg_{product}$ and 3 $MJ_{heat}/kg_{product}$ are reported. Nevertheless, we recommend still using the values above, because the 2020 report neglects intermediate products staying within the chemical park, which does not reflect gate-to-gate demands for single processes [65].

Gate-to-gate emissions to air for worst- and best case Geisler *et al.*, 2004 [70]	
Input	• Amount of input materials
Underlying assumption(s)/ limitation(s)	• Worst case (0.1%) = maximum emission rate of considered processes • Best case (1 x 10^{-5}%) based on EU-Technical Guidance document (chosen two magnitudes smaller to represent best case) • Specialty chemicals produced in batch processes in a large Swiss chemical site
Recommendations	• Limited to batch processes • Check plausibility with experts
Gate-to-gate emission factors to air (TRL 2 for main reactants, TRL 3 for auxiliaries) Jiménez-González *et al.*, 2000 [69]	
Input	• Amount of each chemical present in the process
Underlying assumption(s)/ limitation(s)	• Emission factors only depend on boiling point: ○ < 20°C (gas) -> 0.5% ○ 20 - 60°C -> 2% ○ 60 - 120°C -> 1% • Rule of thumb with no validation presented
Recommendations	• At TRL 2, fugitive emission factors can be applied to the main reactants and products • Check plausibility with experts • Use as a conservative assumption for the foreground system in an initial contribution and completeness analysis and to guide further R&D
Averaged gate-to-gate emissions to water Hischier *et al.*, 2005 [64]	
Input	Amount of water, yield, and fugitive emissions
Underlying assumption(s)/ limitation(s)	All additionally needed reactants due to imperfect yield are assumed to be emitted either to air or to water. Does not consider treatment of waste flows such as incineration or waste-water treatment No clear calculation presented; we assume the following calculation: $emissions_{water} = additionally\ required\ reactants - emissions_{air}$ $\Leftrightarrow emissions_{water} = \left(\frac{1}{yield} - 1\right) * stochiometric\ reactants - emissions_{air}$
Recommendations	**Should** be used as a realistic worst-case assumption to investigate the requirements for waste-water treatment

D.5.2.3 General Limitations and Recommendations for LCA and TEA at TRL 2

When comparing different process routes, one estimation method **should** be applied consistently. The applied estimation method, its underlying assumptions, and limitations **shall** be clearly described.

To calculate a lower bound for discarding inferior pathways, unknown input mass flows **should** be omitted, and a yield of 100% and the minimum energy demand **should** be assumed. The lower bound of mass and energy flows does not provide a realistic estimate and **shall not** be mistaken as an achievable case, as environmental impacts and costs are underestimated. The results **shall** be reported as an unachievable lower bound, and the limitations **shall** be discussed to avoid misinterpretation.

Special attention is required when calculating the minimum energy demand for exothermic reactions, as those reactions often result in negative energy demands. The amount of excess heat **shall** be reported but assumed to be waste heat to prevent overestimating benefits, as the temperatures and excess heat usability are unclear at TRL 2. If excess heat is a planned side-product of the novel process, the heat **should** be included in the functional unit, and the system boundaries of the benchmark technology **should be** expanded accordingly.

To calculate mass and energy flows for *R&D support*, initial assumptions for missing mass and energy flows are necessary. These initial assumptions **should** be taken from expert interviews, if possible. Otherwise, Table 2, Table 3, and Table 4 provide an overview of averaged values used in the literature. As a default for yield and water demand, assumptions from Hischier *et al.* and Althaus *et al.* **should** be used as listed in Table 2 [55, 64]. The average gate-to-gate process energy demands described by Kim and Overcash **should** be used as default, as presented standard deviations reflect a wide variety of chemical processes and can be used for sensitivity analyses [68]. For some reactions, average energy demands might be lower than thermodynamically achievable. Thus, the average values **shall** be compared to the minimum energy demand (e.g., calculated from ΔH_R) and discussed with experts.

To estimate direct emissions, emission factors proposed by Jiménez-González *et al.* **should** be used as conservative assumptions to identify those chemicals for which fugitive emissions need to be avoided [69]. These emission factors are likely to overestimate fugitive emissions, as pollution prevention methods are neglected, and unit process-specific emission rates described later (cf. Table 13) indicate lower overall emissions.

The default values **shall** be discussed with experts to refine the initial inventory. Another estimation method **may** be chosen from Table 3 or Table 4 if considered more plausible for the investigated process(es).

If information about **background data** (e.g., for the raw materials) is missing, molecular structure-based assumptions or other proxies **should** be replaced by more detailed data as soon as possible. If the raw materials are chemicals with known reaction stoichiometries, their cradle-to-gate impacts **should** be modeled according to the ecoinvent database [53–55]: Assuming a yield of 95%, fugitive emissions of 0.2%, an averaged electricity demand of 1.2 MJ/$kg_{Product}$ (+ Heat demand: 2 MJ/$kg_{product}$) and an averaged impact for construction of the chemical plant [53, 55, 64]. The provisory inventory (with background data from molecular structure-based models and the ecoinvent approach) **should** be subject to a contribution analysis. All flows with relevant contributions (e.g., more than 5%) **should** be modeled in more detail as soon as possible.

In general, it is impossible to tell if the concept is economically viable at TRL 2 as techno-economic indicators (e.g., production costs, net present value) strongly depend on the process design which is not defined yet. However, TEA can estimate the OpEx based on the calculated mass and energy flows using available cost/price data and compare them on a semi-quantitative level [41]. Decisions **shall** take into account that comparisons of cost/price data for the raw materials and products cannot reflect the true costs of the process and hence **shall** only be used for qualitative guidance. At TRL 2, No-go decisions **should** be made for process alternatives based on limited and too expensive raw materials. Also, unpredictable developments in raw material costs might result in a No-go decision for the particular option.

D.5.2.4 Provisions

Provisions D.4.2 – Inventory – TRL 2	
Shall	1) At TRL 2, the assessment model **shall** focus on the reaction unit. For the reaction unit the efficiency according to the mass flow (usually yield), the heat and energy demand, and direct emissions to the ecosphere **shall** be considered. 2) The stoichiometric reaction equation **shall** be used to calculate the mass flows within the reaction step as described in Textbox 2. 3) Based on the stoichiometric equation, a best case **shall** be modeled for *Monitoring*. If this lower bound indicates equal or higher impacts than the benchmark, the process route **shall** be discarded. 4) Exclusions of side reactions, auxiliaries and wastes, heating and cooling demand, or product losses **shall** be reported and discussed. 5) If exothermic reactions lead to a negative energy demand, the excess heat **shall** be reported separately but assumed to be waste heat in order to prevent the overestimation of benefits. If excess heat is a planned side-product of the novel process, the heat **should** be included in the functional unit and the system boundaries of the benchmark technology expanded accordingly. 6) Decisions **shall** take into account that comparisons of cost/price data for the raw materials and products cannot reflect the true costs of the process and hence **shall** only be used for qualitative guidance.
Should	1) When comparing different process routes, one estimation method **should** be applied consistently. The applied estimation method, and its underlying assumptions and limitations, **shall** be clearly described. 2) To calculate a lower bound for discarding inferior pathways, unknown mass flows **should** be omitted, a yield of 100%, and a minimum energy demand **should** be assumed. To avoid misinterpretation, the results **shall** be reported as an unachievable lower bound, and the limitations **shall** be discussed. 3) Initial assumptions for mass and energy flows for guiding R&D **should** be taken from expert interviews, if possible. Otherwise, 95% yield and 24 $kg_{water}/kg_{product}$ water demand **should** be assumed and the gate-to-gate energy demands **should** be estimated as proposed by Kim and Overcash [68]. The estimated values **shall** be discussed with experts to refine the initial inventory and **shall** at least be higher than the minimum energy demand [58]. Another estimation method **may** be chosen from Table 3 or Table 4 if considered more plausible for the investigated process(es). 4) Averaged gate-to-gate emissions to water **should** be used as a realistic worst-case assumption to investigate the requirements for waste-water treatment. 5) Background data from molecular structure-based models **should** be replaced by more detailed data as soon as possible. If the raw materials are chemicals with known reaction stoichiometries, their cradle-to-gate impacts **should** be modeled according to the ecoinvent database [53–55]. The preliminary results **should** form part of the contribution analysis, and all flows with relevant contributions (e.g., more than 5%) **should** be modeled in more detail as soon as possible [41].
May	

D.5.3 TRL 3 – Proof of Concept

D.5.3.1 Available Information

At TRL 3, the first laboratory data are available. These data include information about the catalyst(s), yield of the main reaction, and the target product's physical and thermodynamic properties. In addition, occurring side reactions and resulting by-products are detected at this TRL. The target values for yield, conversion, and selectivity are defined based on the experiments and might vary for different solvents and catalysts. Furthermore, the mass balance is usually closed for the reaction step.

On the process-design side, a simple block flow diagram is available, and options for unit operations can be compared. The operation mode of the reactor and process (batch or continuous production) is identified. Figure 5 provides a simplified block flow diagram to summarize the available information for a process.

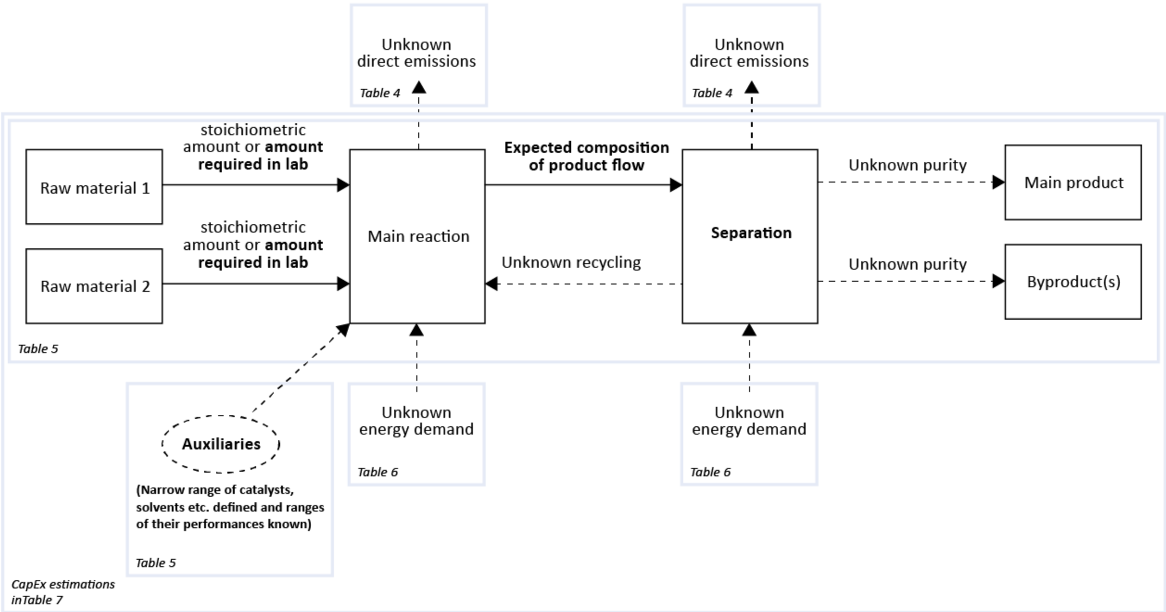

*Figure 5 Simplified block flow diagram including available information at TRL 3. Unknown or likely unknown flows are shown as dashed lines. Newly available information is shown in **bold** typeface. At this stage, initial lab data are available, and target values for the reaction performance are defined.*

D.5.3.2 Applicable Estimation Methods

At TRL 3, the reaction step(s) can be modeled in more detail (including first measurements for selectivity, conversion and yield, ranges of reaction conditions, and options for auxiliaries, solvents, and catalysts). In addition to the reaction step, the separation and its related mass flows and energy demands can be assessed. For missing information on yield, number, and mass of solvents and utilities for solvent recycling, Geisler *et al.* provide best-case and worst-case default values (Table 5) [70].

At TRL 3, first information about unit operations is available, which allows calculating minimum energy demands for single unit operations in addition to methods estimating the overall process energy demands. The energy demands for separation in the laboratory cannot be compared to those of a full-scale process, as the separation techniques might differ and laboratory-scale separation is not optimized for energy efficiency [71]. Therefore, Table 6 provides an overview of methods to model energy demands for equipment typically used in scaled-up processes.

Information is still not available for direct emissions. Thus, the same estimation methods **should** be applied as in previous TRLs (Table 4). If more chemicals (e.g., additional reactants, solvents, and catalysts) are known, they **should** be included.

From TRL 3 onwards, it is possible to conduct quantitative estimation of capital costs based on the block flow diagram. Typically, only a general process flowsheet is created, without showing the exact types of equipment used, specification of equipment, energy & material flows, etc. An order-of-magnitude estimation of CapEx can be conducted to check the feasibilities of considered production routes (Table 7) when a similar production exists. The cost estimate is obtained by applying scaling factors, which are adjustment factors based on production capacity, to the known CapEx of previously constructed plants.

Table 5 Best- and worst-case assumptions related to mass flows, available at TRL 3. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumptions and limitations of the method, and recommendations on when and how to use the estimation method.

Best- and worst-case assumptions for yield, number and mass of solvents, and solvent recycling Geisler *et al.*, 2004 [70]	
Input	• Reaction equation, solvent type (water or organic), side-product(s), reaction phase
Underlying assumption(s)/ limitation(s)	• Default values based on data for a Swiss chemical site • Averaged solvent proxy • Limited to batch processes and specialty chemicals
Recommendations	• Recommended to estimate mass flow ranges for fine and specialty chemicals produced in batch processes

Table 6 Estimation methods related to the energy demand of the gate-to-gate process or single unit operations, available at TRL 3. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method. Newly available estimation methods and changes in methods compared to TRL 2 are highlighted in ***bold*** *typeface.*

Minimum energy demand for reaction step Roh *et al.*, 2020 [58]	
Input	• Minimum ΔHR at suggested conditions [thermochemical conversion] • Electric power based on the applied voltage and measured current density [electrochemical conversion]
Underlying assumption(s)/ limitation(s)	• Calculates minimum energy demands as the lower bound • Does not include energy demand for heating the reaction medium
Recommendations	• Use minimum energy demand for Monitoring
Energy for separation and recycling Roh *et al.*, 2020 [58]	
Input	• Composition of the product stream, properties of components (e.g., boiling points) and ΔH_{mixing}
Underlying assumption(s)/ limitation(s)	• Minimum separation work, energy demand for pressurizing vapor feed streams
Recommendations	• Recommended for *Monitoring*
Energy demand for reactor Parvatker and Eckelman, 2019 [12]	
Input	• Mass and heat capacity of reaction medium (concentrations of components), temperature difference, enthalpy of reaction
Underlying assumption(s)/ limitation(s)	• Basic process calculations based on Towler and Sinnott [5] • Does not consider the integration of unit processes
Recommendations	• Use for comparisons of different process routes

Energy demand for distillation Parvatker and Eckelman, 2019 [12]	
Input	• Mass flows, specific heat capacities and temperatures for feed, top product, and bottom product; reflux flow; top product enthalpy of vaporization; relative volatility
Underlying assumption(s)/ limitation(s)	• Basic process calculations based on Towler and Sinnott [5] • Assumes constant relative volatility • Assumes perfect efficiency (100%) of heating system • Does not consider the integration of unit processes
Recommendations	• Limited applicability, as assumptions about the mass flows are necessary at TRL 3 • Can be applied if information becomes available during R&D before reaching TRL 4
Energy demand for dryer Parvatker and Eckelman, 2019 [12]	
Input	• Mass and heat capacity of the feed stream; the temperature difference between boiling point and feed temperature
Underlying assumption(s)/ limitation(s)	• Basic process calculations, based on Towler and Sinnott [5] • Does not consider the integration of unit processes • Does not account for the mass of solvent to evaporate and the efficiency of heating
Recommendations	• Use for comparisons of different process routes • Limited applicability, as assumptions about the mass flows are necessary at TRL 3 • Can be applied if information becomes available during R&D before reaching TRL 4
Overall steam consumption ranges High (3–16 kg $_{steam}$/kg$_{product}$), **medium (1–3 kg $_{steam}$/kg$_{product}$)** or low (0–1 kg $_{steam}$/kg$_{product}$) Pereira *et al.*, 2018 [66]	
Input	• Reaction mechanism identified **+ distillation (y/n)**
Underlying assumption(s)/ limitation(s)	• Based on statistical models such as probability density functions (PDF) and classification trees. Assuming that energy demand is mainly driven by reaction type, while reactants, solvents, etc. are neglected • Training data: 250 data points calculated based on information *'provided by nine industry partners in Switzerland, Germany, France, and the United States'* using a previously described approach [67] • Limited to batch process, steam considered at 6 bar • A predicted range from 3 to 16 kg$_{steam}$ might not provide sufficient decision support in practice • Classification to low, **medium,** or high steam consumption was successful only for 6 out of 17 test data points; 7 data points were overestimated; 4 data points were underestimated
Recommendations	• Use only for batch processes • Check plausibility with experts

<table>
<tr><td colspan="2">Gate-to-gate energy demand for background processes:
Electricity 1.2 MJ/$kg_{product}$ and Heat demand: 2 MJ/$kg_{product}$
Althaus et al., 2007 [55]</td></tr>
<tr><td>Input</td><td>• Amount of product</td></tr>
<tr><td>Underlying assumption(s)/ limitation(s)</td><td>• Averaged value of around 1,500 chemical products. Based on environmental reporting data from one integrated chemical park in Germany (Gendorf, 2000)
• Not specific to chemicals or process routes
• Does not reflect energy demands for major CCU inputs such as H_2 or CO_2. However, these inputs are available in the energy scenarios of these Guidelines</td></tr>
<tr><td>Recommendations</td><td>• Use the latest Gendorf report to update energy demands [65]
• Check plausibility with experts
• Use for an initial contribution and completeness analysis, if no other expert opinion is available and if the calculated energy demands for all considered unit processes does not exceed the averaged values presented here
• Use for missing background data</td></tr>
<tr><td colspan="2">Best- and worst-case assumptions for utility inputs (energy carriers, cooling water, and inert gas)
Geisler et al., 2004 [70]</td></tr>
<tr><td>Input</td><td>• Reaction equation, solvent type (water or organic), side-product(s), reaction phase</td></tr>
<tr><td>Underlying assumption(s)/ limitation(s)</td><td>• Default values based on data for a Swiss chemical site
• Averaged solvent proxy
• Limited to batch processes and specialty chemicals</td></tr>
<tr><td>Recommendations</td><td>• Recommended to estimate utility input ranges for fine and specialty chemicals produced in batch processes</td></tr>
<tr><td colspan="2">Gate-to-gate process energy demands
Kim and Overcash, 2003 [68]</td></tr>
<tr><td>Input</td><td>• Amount of product</td></tr>
<tr><td>Underlying assumption(s)/ limitation(s)</td><td>• Findings from modeling 86 chemical processes [69]:
<table>
<tr><td>Energy carrier</td><td>Organic chemicals</td><td>Inorganic chemicals</td></tr>
<tr><td>Electricity [MJ/$kg_{product}$]</td><td>0.6 (±0.98)</td><td>1.9 (±5.1)</td></tr>
<tr><td>Steam [MJ/$kg_{product}$]</td><td>7.7 (±14)</td><td>3.6 (±8.2)</td></tr>
<tr><td>Heating fuel [MJ/$kg_{product}$]</td><td>0.15 (±0.5)</td><td>1.5 (±3.2)</td></tr>
<tr><td>Potential energy recovery [MJ/$kg_{product}$]</td><td>-1.6 (±-1.9)</td><td>-2.0 (±-5)</td></tr>
</table>
• The standard deviation is presented in brackets. Both data sets show a large standard deviation due to the variety of chemical processes. Note that a normal distribution was assumed by the authors, while a lognormal distribution might better reflect the data as the modelled results do not show negative values
• Where byproducts are produced, an allocation on mass basis is applied
• Facility energy or energy for waste treatment are excluded</td></tr>
<tr><td>Recommendations</td><td>• Check plausibility with experts
• Use for an initial sensitivity analysis considering the provided standard deviations to assess for uncertainties</td></tr>
</table>

Table 7 Estimation method for capital cost, available at TRL 3. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Order-of-magnitude estimation Peters, Timmerhaus, and West, 1991 (Chapter 6), Towler and Sinnot (Chapter 6) [5, 38]	
Input	• Capital costs of existing plant and scaling factors
Underlying assumption(s)/ limitation(s)	• The assessed production routes are similar to existing plants, and costs can be estimated from those for reference plants based on capacity • The six-tenths rule (see Equation 5-1) is applied • When an entire novel production technology is investigated, such assessment is not applicable
Recommendations	• Can be used to estimate capital costs • Using the 'order-of-magnitude' method to estimate capital cost results in an uncertainty range of ±30–50% [5]

D.5.3.3 General Limitations and Recommendations for LCA and TEA at TRL 3

At TRL 3, LCA and TEA can support the choice of reaction conditions, solvents, and catalysts. Furthermore, LCA and TEA can provide an initial contribution analysis of the planned process steps for reaction and separation to the overall impacts/costs. For this purpose, the model of TRL 2 **shall** be further refined by new information available (e.g., more detailed reaction conditions; options for unit operations).

To compare different reaction designs, the separation and its related mass flows and energy demands **shall** be considered in addition to the reaction step. To estimate the minimum mass flows at TRL 3, a perfect separation with sharp splits and complete recycling of all involved components **should** be assumed while wastes are neglected. These assumptions represent the lower boundary for input flow demands, and the sensitivities to these assumptions **shall** be analyzed to guide further R&D activities. To understand the range of the assumptions, process design experts **should** be involved. In addition, experimental data for separation (e.g., mass fractions before and after the separation step, chemical/physical properties used for separation) **may** be considered in defining the range, if available. However, laboratory results **shall** be considered with caution, as they often rely on small-scale batch experiments that have limited data reliability for large-scale continuous processes.

To calculate the minimum energy demand for reaction and separation, the approach described by Roh *et al.* **should** be applied [58]. More detailed calculations described by Parvatker and Eckelman **should** be applied to enhance the model if additional information becomes available [12]. The limiting information for calculating the energy demand of the separation is often the composition of the feed stream to the separation unit. If chemists provide no other information on the composition after the reaction step, the chemical equilibrium at expected reaction conditions (temperature, pressure, initial composition of reactants) **may** be used to estimate the composition before the separation step. The equilibrium constant K can be calculated from the reactions standard Gibbs energy ΔG_r° and the reaction temperature T [72].

The presented estimation methods for the energy demand of a unit operation [12, 58] are based on best-case assumptions (e.g., ideal properties, neglecting inefficiencies) and are likely to underestimate the real energy demands of each unit operation. Thus, these methods **should** be used to calculate a lower bound of environmental impacts/costs and discard unpromising options (e.g., solvents or process routes). However, no heat integration is considered yet, and cooling is usually neglected at TRL 3. Thus, the energy demands for heating might even be lower than estimated and so the potential for energy recovery **should** be estimated. For this purpose, Jiménez-González *et al.* recommend preparing a table of all heating and cooling demands and to use simple efficiency rules [69]. If no other information is available, hot streams **should** be assumed to leave the process after being cooled to room temperature.

As in the previous case of TRL 2, emission factors proposed by Jiménez-González *et al.* **should** be used to identify those chemicals for which fugitive emissions need to be avoided [69] (cf. D.5.2.2.3). If more chemicals (e.g., additional reactants, solvents, and catalysts) are known, they **should** be included.

An order-of-magnitude estimate for the capital cost **should** be given when the proposed process is similar to plants built before. This method assumes that the same set of equipment will be used, and the costs only vary as time and capacity change. Therefore, both the effects of capacity (e.g., six-tenths rule [73]) and time (e.g., Chemical Engineering Plant Cost Index (CEPCI) [74]) **shall** be considered when applying factors to the cost data of reference plants. Most commonly the six-tenths rule can be used, which uses a cost exponent of 0.6 when scaling up or down the cost of a reference plant to estimate the capital cost of a new plant. More specific estimations for the exponents of some processes or unit operations **should** be used as available in the literature [5, 73, 75].

$$C_{new} = C_{old} \left(\frac{Q_{new}}{Q_{old}}\right)^n \quad , \text{n = 0,6} \qquad (5\text{-}1)$$

Where C_{new}: capital cost of a new plant

C_{old}: capital cost of a previously constructed plant

Q_{new}: capacity of a new plant

Q_{old}: capacity of a of a previously constructed plant

C_{new} then needs to be multiplied by indices such as CEPCI to be updated in terms of time.

According to AACE International, an accuracy of ±30–50% is typically expected for an 'order-of-magnitude' cost estimation [40]. However, most CCU processes are rather novel, in which case capital costs cannot be estimated at TRL 3 since no reference values are available.

D.5.3.4 Provisions

Provisions D.4.3 – Inventory – TRL 3	
Shall	1) The model used in TRL 2 **shall** be further refined by newly available information (e.g., more detailed reaction conditions; options for unit operations) 2) To compare different reaction designs, the separation, and its related mass flows and energy demands **shall** be considered in addition to the reaction step, as further explained in the recommendations. 3) The effects of both capacity and time **shall** be considered for the order-of-magnitude estimation of the capital cost.
Should	1) When comparing process routes, one estimation method **should** be applied consistently. The applied estimation method, its underlying assumptions, and limitations **shall** be clearly described. 2) The minimum energy demands of single unit operations **should** be calculate to provide a lower bound of environmental impacts/costs and discard unpromising options (e.g., solvents or process routes). First, the minimum energy demand for reaction and separation **should** be calculated as explained by Roh *et al.* [58]. As a next step, the more detailed calculations summarized by Parvatker and Eckelman [12] **should** be applied when required data become available. As no heat integration is considered yet, the energy demands for heating might even be lower than estimated, and the potential for energy recovery **should** be estimated, assuming that all streams leave the process at room temperature. 3) Direct emissions **should** be estimated as proposed by Jiménez-González *et al.* [69]. The proposed emission factors are conservative assumptions to identify those chemicals for which fugitive emissions need to be avoided. All known chemicals **should** be included. 4) Background data from molecular structure-based models **should** be replaced by more detailed data as soon as possible. The preliminary results **shall** be subject to contribution analysis, and all flows with expected relevant contributions (e.g., more than 5%) to the mass, energy, and costs of the process **should** be modeled in more detail as soon as possible [41]. 5) When the proposed process is similar to previously constructed plants, an order-of-magnitude estimate of capital cost **should** be given.
May	1) If the composition after the reaction step is unknown, the chemical equilibrium at expected reaction conditions **may** be used to estimate the composition before the separation step.

D.5.4 TRL 4 - Preliminary Process Development

D.5.4.1 Available Information

At TRL 4, further experiments have been conducted to optimize the reaction and broaden the application spectrum of the target product. Laboratory data are now available for the conversion, selectivity, involved additives, catalysts, solvents, and by-products.

On the process design side, an enhanced block flow diagram is available, including equipment/apparatus types and mass flows. The process concept has been validated in the laboratory, and the ranges are identified for all characteristic operating conditions (pressure, temperature, concentrations). Relevant kinetic and thermodynamic parameters are available to describe the unit operations from experiments or literature/databases. Based on those parameters, the amount of energy needed has been estimated by process design for all unit operations. In addition, the costs for utilities **may** be estimated if adequate data are available. Figure 6 provides a simplified block flow diagram to summarize the available information for a process at TRL 4.

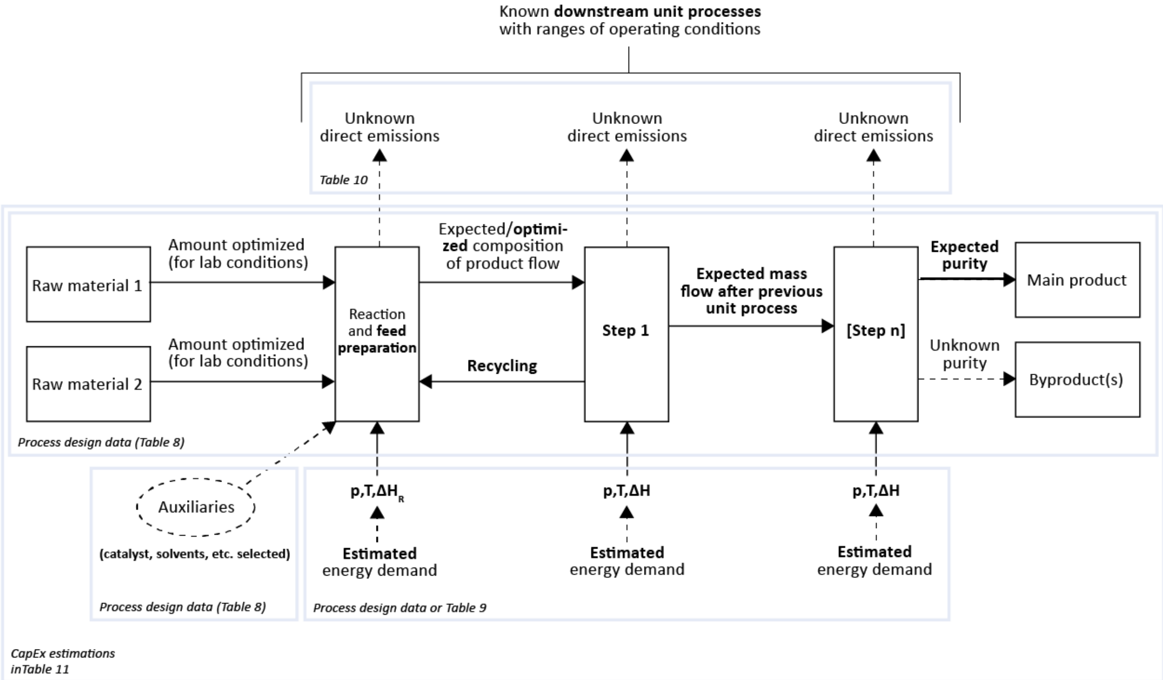

*Figure 6 Simplified block flow diagram including available information at TRL 4. Unknown or likely unknown flows are shown as dashed lines. Newly available information is shown in **bold** typeface. At this point, the reaction conditions are optimized and unit processes identified.*

D.5.4.2 Applicable Estimation Methods

Shortcut models from process design already provide information on the foreground production system. Thus, LCA and TEA practitioners **shall** use data from process design for the mass flows (Table 8) and estimated energy demands. However, the actual demands for solvents, additives, and catalysts strongly depend on the final process's recycling steps and might change with increasing TRL. Thus, close cooperation between LCA and TEA practitioners and experts from the R&D department is necessary to avoid omitting relevant decision-making aspects.

If LCA and TEA practitioners do not have access to the information about mass and energy flows, these must be obtained via advanced process calculations, as explained by Parvatker and Eckelman [12]. The mass flows on a unit-operation level can be calculated based on conversion, selectivity, auxiliaries, and thermochemical equilibrium. Table 9 provides advanced calculation methodologies for the energy demands of single unit operations.

Regarding fugitive emissions, the available information is sufficient to estimate emissions to air on a unit process level (Table 10). The two available methods use average emission factors provided by the U.S. Environmental Protection Agency [76] and can be further enhanced with additional information if already available.

Given a block flow diagram that contains more information regarding equipment, mass flows, etc., a study or preliminary estimate **should** be provided for the capital cost of the major equipment (see Table 11) [38, 39]. The factor methods can be used to calculate the cost of each piece of equipment identified at TRL 3. The size of the equipment is roughly estimated based on experimental data. Given the purchased equipment cost, the Lang factor method [77] or Hand factor method [78] can be used to estimate the total capital cost of a plant, which is done by multiplying the total equipment cost by a constant, i.e., the Lang factor or Hand factor. The Lang factor is selected according to the general type of the plant, while Hand factors are selected for different equipment types. The cost estimates of alternative processes **should** be compared to each other to check their respective economic viability.

In the following tables, the estimation methods becoming available at TRL 3, and changes in methods compared to the previous TRL, are highlighted in **bold** typeface. The estimation methods for single unit operations presented at TRL 3 are no longer listed here, as those methods are assumed to be already used for previous calculations. Moreover, the data available at TRL 4 allow for more detailed calculations once the process design has started.

Table 8 Material flow data available at TRL 4. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Mass flows as calculated for process design	
Input	• Data provided by process designers
Underlying assumption(s)/ limitation(s)	• The preliminary process design requires detailed information about the mass flow • No additional calculations by LCA and TEA practitioners are necessary
Recommendations	• Iteratively discuss the results with process designers and ensure that data can be used for LCA and TEA

*Table 9 Estimation methods related to the energy demand of the gate-to-gate process or single unit operations, available at TRL 4. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method. Newly available estimation methods and changes in methods compared to TRL 3 are highlighted in **bold** typeface.*

Gate-to-gate steam consumption ranges High (3–16 $kg_{steam}/kg_{product}$), medium (1–3 $kg_{steam}/kg_{product}$), or low (0–1 $kg_{steam}/kg_{product}$) Pereira *et al.*, 2018 [66]	
Input	• Reaction mechanism identified + distillation (y/n) + **reaction temperature and time (+ PMI) (+steam demand for distillation)**
Underlying assumption(s)/ limitation(s)	• Based on statistical models, such as probability density functions (PDF) and classification trees. Assuming that energy demand is mainly driven by reaction type, while reactants, solvents, etc., are neglected. • Training data: 250 data points calculated based on information *'provided by nine industry partners in Switzerland, Germany, France, and the United States'* using a previously described approach [67] • Limited to batch process; steam considered at 6 bar

	• A predicted range from 3 to 16 kg_{steam} might not provide sufficient decision support in practice • Classification to low, **medium,** or high steam consumption (*+ information about steam demand*) was successful for 11 (*14*) out of 17 test data points; 3 (*2*) data points were overestimated; 3 (*1*) data points were underestimated
Recommendations	• Use only for batch processes, and compare the results with the total energy demand calculated on a unit operation basis • Check plausibility with experts
Energy demand for a liquid batch reactor Piccinno *et al.*, 2016 [71]	
Input	• Mass of feed, c_p, ΔT, $ΔH_R$, surface area of reactor, thermal conductivity of insulation, thickness of insulation, time
Underlying assumption(s)/ limitation(s)	• Basic process calculation for a liquid batch reaction, based on the energy demand for heating of the reactor • Does not consider the integration of unit processes • Expert opinions on surface area, and insulation [79] might be necessary if process models do not provide information
Recommendations	• Use for *Monitoring* and comparisons of different process routes (*R&D support*)
Energy demand for distillation Piccinno *et al.*, 2016 [71]	
Input	• Mass flow of feed, averaged c_p of feed, ΔT, mass flow of distillate, heat of vaporization of distillate (MJ/kg), minimum reflux ratio, and efficiency indicator
Underlying assumption(s)/ limitation(s)	• Basic process calculations, based on Underwood *et al.* [80] and empirical data provided by Capello *et al.* [81] • Reflux ratio calculated based on the relative volatility, and mole fractions of light boiler in feed and distillate • Does not consider the integration of unit processes • Expert opinion needed at least for efficiency parameters
Recommendations	• Use for *Monitoring* and comparisons of different process routes (*R&D support*)
Energy demand for drying Piccinno *et al.*, 2016 [71]	
Input	• Mass flow of feed, c_p, ΔT (feed temperature and boiling temperature), heat of vaporization of solvent (MJ/kg), efficiency indicator
Underlying assumption(s)/ limitation(s)	• Omits heat-sensitive solids, for which less heating demand but higher demand for vacuum pumps would be necessary • Does not consider the integration of unit processes • Expert opinion needed at least for efficiency, here assumed between 0.3 and 1
Recommendations	• Use for *Monitoring* and comparisons of different process routes (*R&D support*)
Energy demand for pumping Piccinno *et al.*, 2016 [71]	
Input	• Mass flow, height difference, pump efficiency
Underlying assumption(s)/ limitation(s)	• Further assumptions based on Vauck and Müller [82] • Does not consider the integration of unit processes • Expert opinion needed at least for the efficiency; Piccinno *et al.* assume an efficiency between 0.7 and 0.85
Recommendations	• Use for *Monitoring* and comparison of different process routes (*R&D support*)

Energy demand for pressurizing Perry *et al.*, 1997 [79]	
Input	• Number of compressor stages, c_p of gaseous fluid, temperature; pressure before and after compression
Underlying assumption(s)/ limitation(s)	• Ideal fluid, isentropic compression, completely inter-cooled after each compressor stage • Expert opinions are needed at least for the efficiency; Perry's Chemical Engineers' Handbook suggests high efficiencies for axial compressors (85–90%) and slightly lower efficiencies for centrifugal compressors (78–83%)
Recommendations	• Use for *Monitoring* and comparisons of different process routes (*R&D support*)

Table 10 Module-specific estimation methods for emissions to the environment, available at TRL 4. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Hybrid framework for fugitive emission estimation Ng *et al.*, 2017 [83]	
Input	• Process modules (TRL 4); mass and energy balances in process modules (TRL 5); piping and instrumentalization (TRL 7)
Underlying assumption(s)/ limitation(s)	• Based on Hassim *et al.* (see below): • Based on US EPA emission rates [76] • Applied to three stages: conceptual design, preliminary design, and final design • Fugitive emissions, **tank emissions, venting, etc**. • No differentiation between product classes and risk levels • Likely overestimates for dangerous (toxic, explosive, …) substances, since these are subject to stricter regulations [84–87]
Recommendations	• Use to calculate fugitive emissions of process modules
Fugitive emission rates and local concentrations Hassim *et al.*, 2010 [88]	
Input	• Process modules (TRL 4); mass and energy balances in process modules (TRL 5); piping and instrumentalization (TRL 7)
Underlying assumption(s)/ limitation(s)	• Based on US EPA emission rates [76] • Applied to three stages: conceptual design, preliminary design, and final design • Limited to fugitive emissions • No differentiation between product classes and risk levels • Likely overestimates for dangerous (toxic, explosive, …) substances, since these are subject to stricter regulations [84–87]
Recommendations	• Framework by Ng *et al.* (see above) **should** be preferred, as more emission types are included • Can be used for risk assessment in R&D, as local concentrations are considered

Table 11 Estimation methods for capital cost, available at TRL 4. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Study estimation for capital costs Peters, Timmerhaus, and West, 1991 (Chapter 6) [38]	
Input	• Capacity measure or sizes, reference cost data, and approximate layout of a list of major equipment, multiplying factors for quantifying capital costs
Underlying assumption(s)/ limitation(s)	• The equipment cost is related to the unit capacity • The capacity of assessed equipment must be within the range of reference capacity.
Recommendations	• Lang or Hand factor method **may** be used to estimate capital costs • The accuracy of study cost estimation falls within the range -20 to +40% [38]
Preliminary capital cost estimation Peters, Timmerhaus, and West, 1991 (Chapter 6), Towler and Sinnot (Chapter 6) [38, 39]	
Input	• This estimation requires more accurate sizing of equipment than that used in the study estimation. The layout of each piece of equipment is determined considering piping, instrumentation, and electrical requirements
Underlying assumption(s)/ limitation(s)	• The equipment cost is related to the unit capacity • The capacity of assessed equipment must be within the range of reference capacity.
Recommendations	• Lang or Hand factor method **may** be used to estimate capital costs • Accuracy of preliminary cost estimation is within the range ±20–30% [38, 39] • Preliminary estimation is recommended for the comparison between different processes

D.5.4.3 General Limitations and Recommendations for LCA and TEA at TRL 4

The advanced process calculations presented in Table 9 help to estimate the energy demand of relevant unit operations. However, possible heat integration of units/processes is not considered. Thus, the overall environmental impacts and costs might be overestimated if the final process can use waste heat or provide steam for other processes. Scenario analysis **should** be applied to assess the sensitivity of the process's environmental performance to changes in energy source (see also chapter D.7.2.2). The standard scenarios provided as supplementary material to these Guidelines **should** be applied for this purpose. Many CCU processes are energy-intensive, and renewable low-carbon electricity is likely a limiting factor for full-scale introduction of CCU processes [89]. Thus, the energy source **shall** be clearly defined, and **shall** be discussed if the chosen energy source can deliver the amount of energy needed for the process. This discussion **may** be supported by an analysis of other technologies that might compete for the same energy source, to ensure that it is used where it can achieve the highest environmental and economic benefits [90].

The estimation methods for fugitive emissions (Table 10) do not differentiate between different chemical classes and neglect different risk classes. Thus, the estimation methods likely overestimate the emissions of dangerous (toxic, explosive, …) chemicals, since those are subject to stricter regulations on a national level and necessitate low-emitting equipment and instrumentalization [84–87]. However, the hybrid framework for fugitive emission estimation proposed by Ng *et al.* **should** be applied to identify where such equipment or instrumentalization is necessary to avoid high environmental impacts [83].

A study estimation of capital cost is essentially calculated based on knowledge of the major items of equipment, while the preliminary estimate of capital costs requires more accurate sizing of equipment than that used for the study estimation. When the primary purpose of estimating capital costs is to compare alternative options to make a Go/No-go decision or even to approve budgets, practitioners **should** select the preliminary estimation method.

D.5.4.4 Provisions

Provisions D.4.4 – Inventory – TRL 4		
Shall	1)	LCA and TEA practitioners **shall** use data from process design for the mass flows and estimated energy demands, and discuss available data with experts to avoid omitting relevant decision-making aspects.
	2)	The energy source **shall** be clearly defined, and **shall** discuss whether the chosen energy source can deliver the amount of energy needed for the process. This discussion **may** be supported by an analysis of other technologies that might compete for the same energy source, to ensure that it is used where it can achieve the highest environmental and economic benefits [90].
Should	1)	Scenario analysis **should** be applied to assess the sensitivity of the process's environmental performance to changes in energy source. The standard scenarios provided as supplementary material to these Guidelines **should** be applied for this purpose.
	2)	When comparing process routes, one estimation method **should** be applied consistently. The applied estimation method, its underlying assumptions, and limitations **shall** be clearly described.
	3)	The hybrid framework for fugitive emission estimation proposed by Ng *et al.* [83] **should** be applied to identify where low-emitting equipment or instrumentalization is necessary to avoid high environmental impacts.
	4)	When comparing process routes, preliminary estimates for capital costs **should** be calculated and, meanwhile, the accuracy **should** be indicated.
	5)	A rough estimation of the operating cost **should** be carried out, including raw material and energy demands and fixed OpEx costs based on study or preliminary estimation.
May	1)	The Lang factor or Hand method **may** be used for the estimation of capital cost [77, 78].

D.5.5 TRL 5 - Detailed Process Development

At TRL 5 the *Monitoring* step via LCA and TEA is essential, as a Go or No-go decision for building a pilot plant is required to continue the R&D project. Building and running a pilot plant is associated with high costs and relevant environmental impacts. To avoid building a pilot plant for a process that is ultimately found to be unsustainable, the assumption of a best-case performance is no longer sufficient at this stage. Instead, realistic and even pessimistic assumptions **shall** be considered, and uncertainties **shall** be included in the model to assess the possible range of plant operation. Pessimistic assumptions can be taken from worst-case expectations within a realistic set of conditions.

When supporting R&D, contribution analysis followed by sensitivity analysis **shall** be conducted to identify significant issues for plant construction (e.g., material choice, choice of location, and the pilot plant's operational range). Both contribution analysis and sensitivity analysis **should** be combined with background scenario analyses. First, a contribution analysis **shall** be conducted to reveal the main contributors to the overall process performance. If a unit process or life cycle stage (e.g., plant construction) contributes significantly (e.g., top x contributors, or above y% contribution) in an expected future scenario, this contributor **shall** be subject to sensitivity analysis [91]. A sensitivity analysis can evaluate the influence of decisions (e.g., for materials) on the overall performance.

D.5.5.1 Available Information

At TRL 5, few remaining alternative process concepts are evaluated in detail, and property data are obtained on a laboratory or mini-plant scale. The required product properties are detailed. Therefore, the reference flow that fulfills the functional unit can be refined, particularly for novel products. At this point, a complete, quantitative model description of the reaction system's kinetic behavior is available and can be used for process simulations [8]. Additionally, the effects of equipment/apparatus dimension parameters (e.g., catalyst loading, bed void, gas hourly space velocity, etc.) on reactions can be tested in the laboratory for certain chemical reactions.

On the process-design side, a process flow diagram, including mass and energy flows of single unit operations, is available and based on experiments and models from process designers. The process models for planning the pilot plant and final process can be used for LCA and TEA. The compositions of all mass flows are known from such models, and the required form of energy for each unit operation is specified. Thus, foreground data already provide a high level of detail but are not yet measured at the operating scale. However, some information might still be unavailable (or lack detail) for a full assessment (e.g., detailed emissions, catalysts durability, solvent degradation, detailed waste-treatment, and the supply chains for the entire life cycle). Figure 7 provides a simplified block flow diagram to summarize the available information for a process at TRL 5.

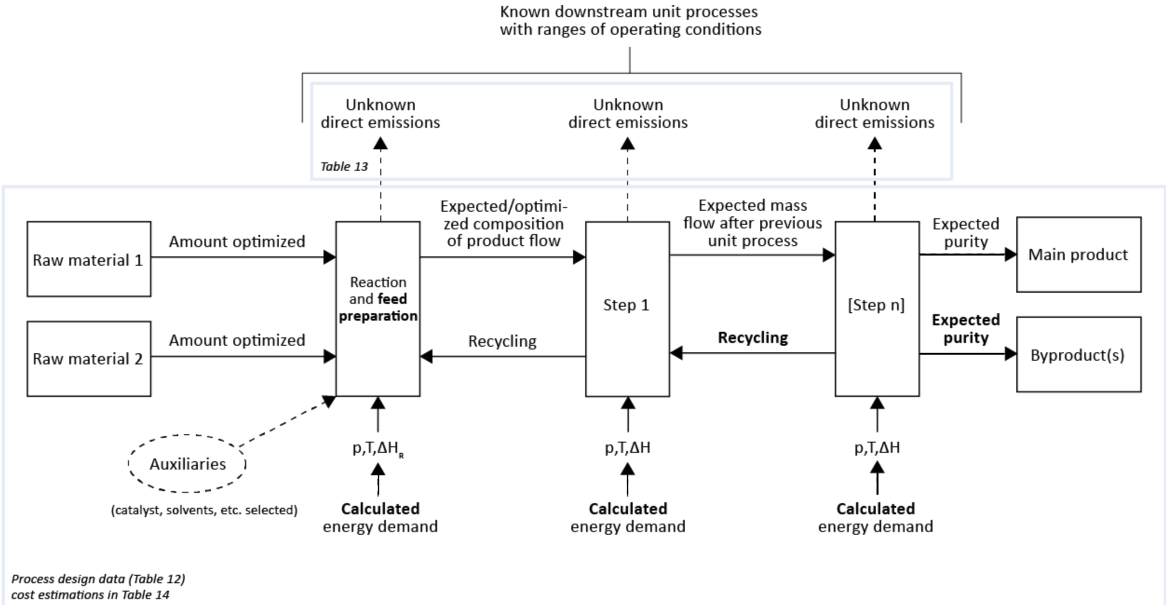

*Figure 7 Simplified block flow diagram including available information at TRL 5. Unknown or likely unknown flows are shown as dashed lines. Newly available information is shown in **bold** typeface. At this point, a process flow diagram is available, including all mass and energy flows (for generalization, here still a block flow diagram is shown to visualize available information).*

D.5.5.2 Applicable estimation methods

At TRL 5, TEA and LCA **shall** use available data from process design. The data quality and uncertainty **shall** be discussed with process designers and chemists, including related limitations for the assessment. As mass and energy flows are known, no estimation methods for mass and energy flows are necessary if process designers and TEA and LCA practitioners cooperate closely (Table 12). If not available from process design, advanced process calculations **may** still be applied, as described for TRL 4.

Fugitive emissions still are not based on measured data or process simulation and need to be estimated on a process module level (Table 13). All estimation methods for fugitive emissions suggested here are based on average emission factors provided by the U.S. Environmental Protection Agency [76]. At TRL 5, additional information (e.g., detailed mass and energy balances of process modules) are available and **shall** be included for a more detailed assessment. Additional information about the fugitive emissions **shall** be added when available (e.g., emission factors from piping and instrumentalization or field measurements).

At this level, a more detailed capital cost estimation, called a definitive estimation [5, 38, 39] , **should** be conducted given preliminary specifications for all the equipment, utilities, instrumentation, etc. (Table 14). The definitive estimation is based on almost complete data for the analyzed processes just before finalized equipment specifications are determined.

A common technique for estimating equipment costs at TRL 5 is the module costing method, which relates the costs to the purchased cost of equipment operated at base conditions. The deviation from the base conditions is corrected by using the cost factor reflecting the specific equipment type, pressure, and materials used. At TRL 5, the costs for other items and the equipment **shall** be considered individually (e.g., installation, piping, insurance, contingency, etc.). Typically, these costs are estimated by applying cost multiplying-factors to the total cost of the equipment. Ultimately, the sum of all costs gives an estimate for total capital cost. Two sets of cost factors are required at TRL 5, i.e., the correction factors for equipment cost estimation, and multiplication factors for estimating bare module costs. Practitioners **shall** select these factors by referring to the literature, based on their experience and expertise. Operating costs (variable & fixed) **may** also be estimated, given the material and energy flows, assumed costs for labor, maintenance, etc., and fixed capital investment.

Table 12 Material and energy flow data available at TRL 5. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Mass and energy flows as calculated for process design	
Input	• Detailed data (e.g., process flow diagram) from process design
Underlying assumption(s)/ limitation(s)	• The detailed process development requires detailed mass and energy balances. • No additional calculations by LCA and TEA practitioners are necessary.
Recommendations	• Iteratively discuss the results with process designers and ensure that data can be used for LCA and TEA

Table 13 Module-specific estimation methods for emissions to the environment, available at TRL 5. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s), and recommendations on when and how to use the estimation method. Newly available estimation methods and changes in methods compared to TRL 4 are highlighted in bold typeface.

Emission factors for storage emissions, process vent emissions, fugitive emissions Smith *et al.*, 2017 [92]	
Input	• Number of pumps [mass flow of light boiler (vapor pressure above 0.3 kPa)/ heavy (vapor pressure below 0.3 kPa at 20°C) liquids]; number of compressors; number of valves for light and heavy liquids and gas; yearly operating hours -> simplification: approximated equipment numbers for typical unit operations
Underlying assumption(s)/ limitation(s)	• Average emission factors based on data from US EPA • No differentiation between product classes and risk levels • Likely overestimates for dangerous (toxic, explosive, …) substances, as those substances are subject to stricter regulations [84–87]
Recommendations	• TRL 6 or higher -> simplified approach at TRL 5

Hybrid framework for fugitive emission estimation Ng *et al.*, 2017 [83]	
Input	• Process modules (TRL 4); **mass and energy balances in process modules (TRL 5)**; piping and instrumentalization (TRL 7)
Underlying assumption(s)/ limitation(s)	• Based on Hassim *et al.* (see below): • Based on US EPA emission rates [76] • Applied to three stages: conceptual design, preliminary design, and final design • Fugitive emissions, tank emissions, venting, etc. • No differentiation between product classes and risk levels • Likely overestimates for dangerous (toxic, explosive, …) substances, as those substances are subject to stricter regulations [84–87]
Recommendations	• Use to calculate fugitive emissions of process modules
Fugitive emission rates and local concentrations Hassim *et al.*, 2010 [88]	
Input	• Process modules (TRL 4); **mass and energy balances in process modules (TRL 5)**; piping and instrumentalization (TRL 7)
Underlying assumption(s)/ limitation(s)	• Based on US EPA emission rates [76] • Applied to three stages: conceptual design, preliminary design, and final design • Limited to fugitive emissions • No differentiation between product classes and risk levels • Likely overestimates for dangerous (toxic, explosive, …) substances, as those substances are subject to stricter regulations [84–87]
Recommendations	• The framework by Ng *et al.* (see above) **should** be preferred, as this includes more emission types • Can be used for risk assessment in R&D, as local concentrations are considered

Table 14 Estimation method for cost, available at TRL 5. Each method is highlighted in a blue box, followed by information about the necessary inputs for calculation, the underlying assumption(s) and limitation(s) of the method, and recommendations on when and how to use the estimation method.

Definitive cost estimation Peters and Timmerhaus (Chapter 6) [38]; Towler and Sinnot (Chapter 6) [5]	
Input	• *Capital cost:* • Detailed specifications for all equipment, utilities, instrumentation, electrical and off-site facilities/equipment • Multiplying factors for quantifying direct and indirect capital cost and cost index • *Operating cost:* • Based on mass & energy balances or results from simulation, market-average price data

Underlying assumption(s)/ limitation(s)	• Equipment cost is related to unit capacity, and operating cost is estimated based on assumptions regarding fixed capital investment • Market-average estimate • Hight uncertainties lie in the selection of multiplication factors
Recommendations	• Aim for an accuracy of definitive estimation (±10–15%), to support decisions on building the pilot plant [5]

D.5.5.3 General limitations and recommendations for LCA and TEA at TRL 5

TEA and LCA can support further process development by analyzing the sensitivity to criteria that are relevant for the overall performance of the process (e.g., the operational range of pilot plant, catalyst recovery and demand, energy demand and energy source for each unit operation, process stability, and related maintenance efforts). To enhance the assessment quality, uncertainties of mass and energy flows **shall** be included in the assessment if known. The overall quality of assessment and decision support are highly dependent on the degree of cooperation between process designers and TEA and LCA practitioners. The importance of close collaboration increases with maturity and becomes crucial at TRL 5 at the latest, as the data quality and required assessment detail at TRL 5 exceed those of results based on estimation methods.

The estimation methods for fugitive emissions still rely on averaged data. Thus, the recommendations **shall** be followed as provided for TRL 4. The estimated emissions help identify where such equipment or instrumentalization is necessary to avoid high environmental impacts.

D.5.5.4 Provisions

Provisions D.4.5 – Inventory – TRL 5	
Shall	1) Realistic and even pessimistic (worst-case expectations from research and process design) assumptions **shall** be included in the model together with uncertainties, to mitigate the risk of building a pilot plant for a process that ultimately is found to be unsustainable. 2) LCA and TEA **shall** use available data from process design, and discuss the quality and uncertainty of available data and related limitations for the assessment with process designers and chemists. Additional information that becomes available at TRL 5 (e.g., mass and energy balances and fugitive emissions of process modules) **shall** be included for a more detailed assessment. 3) Contribution analysis followed by sensitivity analysis **shall** be conducted to support decisions on plant construction (e.g., material choice), choice of location, and the pilot plant's operational range. 4) For estimating fugitive emissions, the recommendations **shall** be followed as provided at TRL 4.
Should	
May	1) Advanced process calculations **may** still be applied, as described for TRL 4, if sufficient data are not available from process design.

D.5.6 TRL 6 and Higher – Pilot Trials and Deployment

Starting with TRL 6, measured pilot-plant data and process simulations are available. Thus, sufficient inventory information is available to follow full LCA principles described in parts A, B, and C of these Guidelines. However, the following limitations remain: Lack of direct measurements for fugitive emissions, long-term stability and degradation, and changes due to learning.

From TRL 6 onwards, the detailed estimation of the capital cost (also known as contractor's estimate [5]) **shall** be provided to decide whether or not to commence plant construction. This requires complete design information for the process and all related utilities in order to obtain vendor quotes for all equipment. Furthermore, more accurate estimates for operating costs **shall** be provided.

D.5.6.1 Limitations

Direct measurements for fugitive emissions might be missing. Thus, if no better data for direct emissions are available, the module-specific estimation methods described in Table 13 **should** be used to account for missing data.

The development and deployment of the process in a real working environment often lead to adjustments, while integration and further optimization might enhance performance. To reflect such enhancements, technology learning curves **may** be applied early on [93–95].

Before reaching TRL 6, process design often takes a purely technical point of view without considering equipment availability. As a result, practitioners are likely to encounter situations where the estimated sizes or desired equipment specifications are not available from commercial vendors when detailed estimates are examined. Then, practitioners **shall** either communicate with equipment suppliers to check whether it is possible to acquire tailored equipment or else redesign the equipment or operating conditions. In the latter case, iterative process design is inevitable, since the types of equipment might need to be changed or the production route might even need to be split into multiple parallel processes so that the equipment currently available on the market can meet the production demand. Consequently, both the environmental and economic metrics could deviate from the initial simulation results. Hence, it is recommended that practitioners collect commercial data on major equipment or communicate with potential suppliers as early as possible in order to avoid unnecessary repetition of work.

D.5.6.2 Provisions

Provisions D.4.6 – Inventory – TRL 6 and Higher	
Shall	1) LCA and TEA **shall** use available data from process design and discuss the quality and uncertainty of available data and related limitations for the assessment with process designers and chemists. Additional information that becomes available **shall** be included for a more detailed assessment. 2) The assessment **shall** follow the provisions in parts A, B, and C of the Guidelines, as detailed inventories are available from measured pilot plant data and process simulations. 3) From TRL 6 onwards, the detailed estimation of the capital and operating costs **shall** be provided to decide whether or not to commence construction of a commercial-scale plant.
Should	1) If no better data for direct emissions are available, the module-specific estimation methods described in Table 13 **should** be used.
May	1) Technology learning curves **may** be applied early on, to reflect further optimization due to learning.

D.6 Calculation of Indicators and Life Cycle Impact Assessment

General Introduction

After the collection or calculation of inventory data, the performance indicators are calculated in a separate phase. In LCA, this phase is called Life Cycle Impact Assessment (LCIA). For combined assessment, indicators of LCA and TEA **may** be put in relation at the end of this phase (see chapter F.6).

For TEA, the provisions introduced in part B **shall** first be applied. For low-TRL CCU technologies in particular, TEA indicators **shall** be selected and calculated based on the data available at each TRL (D.6.1). As TRL increases the selected TEA indicators **shall** be calculated with updated data and extended scope. Zimmermann *et al.* propose a framework and recommend a set of indicators that **may** be used for assessing the CCU system at different TRLs [96]. If practitioners define new indicators, the definitions and equations **shall** be documented and explained.

For LCIA, the recommendations provided in chapter C.6 **shall** be applied, as technology maturity affects neither the LCIA methods nor the interpretation of temporary CO_2 storage. In particular, LCIA **shall** account for all impact categories to avoid burden-shifting, which might be of particular importance for emerging technologies, as the relevance of impact categories might change over time. Note that the calculation of environmental impacts introduces additional uncertainties into the assessment. Given the high uncertainties of inventory data during the early stages of R&D, the resulting overall uncertainties could thus mean that interpretations of the results are meaningless. Furthermore, LCIA might suffer from missing characterization factors if novel materials are involved in a CCU process (D.6.2).

D.6.1 Dependence of TEA Indicators on TRL

As stated in chapter B.6, practitioners **shall** select calculation methods that comply with the specified goal and scope of the study. In general, all provisions for indicator calculation introduced in B.6 **shall** be applied.

Zimmermann *et al.* found that the indicators used to assess CO_2 utilization remain non-standardized [97]. Furthermore, it is challenging to conduct TEA for CO_2 utilization technologies with low TRLs, as no widely used framework can provide sufficient guidance. In recent years some researchers have attempted to build up frameworks for LCA and TEA based on TRLs. Thomassen *et al.* proposed the Environmental Techno-Economic Assessment (ETEA) framework for prospective green technology assessment [98]. In this framework, LCA and TEA are used alongside TRLs to classify assessment methods. Zimmermann *et al.* proposed a so-called Efferi framework to assess CCU technologies at low TRLs from the perspectives of efficiency, feasibility, and risk [96]. Schoubroeck *et al.* developed a novel techno-sustainability assessment (TSA) framework for emerging technologies [99].

The assessment approaches for chemical engineering also adopt the concept of stages concerning technology maturity [38, 39], which is also mentioned in chapter D.5.0. Nevertheless, as Zimmermann *et al.* point out, the defined development stages of chemical R&D do not precisely match the concept of TRLs [97]. Given the high uncertainty and limited data availability at low TRLs, not all commonly used TEA indicators can be estimated at all TRLs. Therefore, when TRL is assigned to TEA indicators, two questions need to be addressed: 1) what indicators can be calculated at each TRL (selection)? and 2) what methods can be used to calculate the indicators (calculation)? In other words, the selection and calculation of TEA indicators are intrinsically bound with data availability and further with TRL. The TEA indicators **shall** be selected and calculated based on the data available at each TRL. This sub-chapter matches the calculation of TEA indicators to TRLs (TRL 1 to 5) and provides guidance on the selection and calculation of the indicators.

At TRL 1 only basic scientific principles and potential applications are reported, as described in chapter D.1.3.1. Even the chemical reaction is not defined, and therefore access to data is very limited. As a result, it is impossible to calculate either technical or economic TEA indicators. Hence, qualitative assessment (e.g., comparing raw material prices, heating values of products, products' chemical composition, etc.) **should** be conducted at this level. Given the qualitative assessment, practitioners **should** derive recommendations for technology pathways [100].

At TRL 2, the technology pathway and application have been conceived, and stoichiometric reactions have been selected accordingly for the proposed CCU system. At this stage only ideal reactions are considered, and therefore kinetic limitations, as well as side reactions, are neglected. As a result, quantitative TEA indicators such as mass and energy conversion efficiencies **should** be calculated according to stoichiometry. For instance, in the Efferi framework proposed by Zimmermann *et al.* three indicators are introduced to assess CCU systems from a TEA perspective: 1) mass efficiency, 2) energy efficiency, and 3) value efficiency [96]. More specifically, mass efficiency indicates to what extent the analyzed reactions produce the targeted products, with a value of zero meaning no targeted products are produced, and a value of one meaning that only the targeted products are produced. In terms of energy efficiency, a commonly used TEA indicator, the sum of higher heating values (HHV) of the products and output energy are compared to the sum of the HHVs of the reactants and input energy. The result, ranging between zero and one, refers to how much energy from the reactants and input energy is retained in the products. The third indicator (value efficiency) measures how much monetary value has changed in the reaction process. In a similar form to the energy efficiency calculation, value efficiency is estimated as a ratio of the weighted price of all the outputs to that of the inputs. A value efficiency of less than one indicates that the outputs (products, energy) are of less value than the inputs (reactants, energy) [96].

In general, any indicators selected by the practitioners at TRL 2 can be used in the later stages but **shall** be calculated with updated data inputs and extended scope. At TRL 3, experimental laboratory data are available, and thus more accurate information about the reactions is obtained (e.g., reactions kinetics, side reactions, etc.). Therefore, the selected indicators **should** be calculated based on the reactions observed in the experiments rather than on ideal reactions. Similarly, at TRL 4 & 5, the indicators **should** be calculated based on the validated process.

As the production concept has been validated at TRL 3, it is possible to estimate the capital expenditure (CapEx with an order-of-magnitude approach (see D 5.4)). Nevertheless, the prerequisite for this approach is that a similar production technology has been constructed previously. The cost data obtained from that benchmark technology can then be used to estimate the CapEx of the proposed system via cost transformation. Typically, this case does not apply to CCU production systems due to their novelty, and practitioners must wait until TRL 4 or higher to conduct CapEx estimation

From TRL 4 onwards, more accurate methods for estimating CapEx can be applied. Chapter B.6 sorts methods for CapEx at different stages of technology maturity (see Table 8 in chapter B.6). Buchner *et al.* [101] also sort CapEx estimation methods according to TRL, and state that the given TRL for each method is the 'earliest recommended TRL for the application'. The same principle applies to the estimation of operational expenditure (OpEx). OpEx can be estimated from TRL 2 onwards. Items including the energy and utility cost can be roughly estimated according to reaction enthalpy, or else **may** be omitted at early stages. It can be calculated more accurately with increasing TRL when the configuration of each piece of equipment is determined via simulation or experiments [101].

For both CapEx and OpEx, the number of cost items that can be calculated increases with higher TRL, and thus the accuracy improves. According to AACE [102], an accuracy of ±30–50% is expected for order-of-magnitude estimation at TRL 3, improving to ±5–10% for the detailed estimation, which is usually conducted at TRL 5 or 6. Figure 8 shows which cost items can be estimated at a given TRL. As described above, only qualitative assessment can be conducted at TRL 1, Hence, this is not reflected in the figure.

Profitability indicators, another set of significant TEA indicators, are difficult to calculate at early TRLs, as the market is uncertain. Practitioners can refer to chapter B.6.5 for commonly used profitability indicators. As stated in B.6.5, at TRL 1–3, practitioners **should** normalize the profit to cost, in order to display and compare the profit potential of analyzed systems. From TRL 4 onwards, profitability indicators – be they static indicators (e.g., payback time, etc.) or dynamic (e.g., net present value (NPV), etc.)) – can be calculated but are still restricted because the future market is not yet well understood. From later development stages (TRL 5 and above), dynamic indicators such as NPV **shall** be calculated (see B.6.5) to serve as a structural basis for later stages. Practitioners **may** not calculate profitability indicators at early TRLs unless sufficient market information and data are available.

As discussed above, at each TRL, practitioners can decide which indicators to calculate as long as they address the three core aspects of TEA, i.e., mass, energy, and profit/cost. Practitioners **may** use the indicators and methods introduced in the proposed frameworks (Efferi [96], ETEA [98], etc.) to analyze CCU systems at early TRLs. If practitioners employ new indicators that are not commonly used in the TEA community, these indicators **shall** be defined, clearly explained, and equations given.

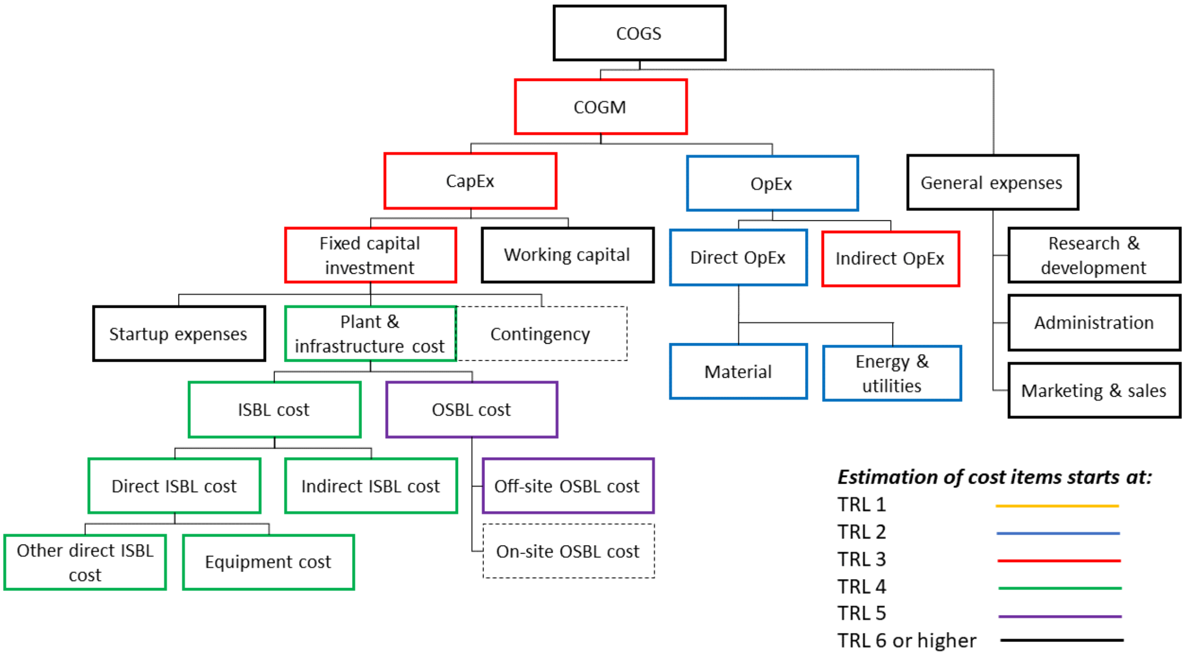

Figure 8 Cost estimation and TRLs. Adapted from Buchner et al. [101]

D.6.1.1 Provisions

Provisions D.5 – Calculation of Indicators for TEA	
Shall	1) All of the provisions introduced in chapter B.6 concerning the calculation of indicators **shall** be applied. 2) TEA indicators **shall** be selected and calculated based on the data available at each TRL. 3) As TRL becomes higher, the selected TEA indicators **shall** be calculated with updated data and extended scope. 4) TEA indicators that practitioners themselves define **shall** be clearly explained, and equations **shall** be given.
Should	1) At TRL 1, qualitative assessment **should** be conducted and recommendations for technology pathways **should** be derived. 2) From TRL 2 onwards, quantitative assessment **should** be carried out.
May	1) TEA indicators proposed in published frameworks **may** be used as shortcut at low TRL. 2) Profitability indicators **may** not be calculated at low TRLs.

D.6.2 Novel Materials and Their Environmental Impacts

CCU processes might utilize or produce novel materials, e.g., for the capture of CO_2 or during reaction and processing. For these novel materials, it is unlikely that any characterization method is available [24]. Thus, practitioners **shall** check whether the novel material is characterized in the applied LCIA method. Missing characterization factors **shall** be clearly stated in the reporting, and the relevance of missing characterization factors **should** be evaluated according to the ILCD handbook (chapter 6.7.4) by assuming a conservative value or realistic worst case [91]. This assumption **may** be based on chemical, physical, or other similarity to other elementary flows contributing to the same impact category [91]. The ILCD handbook recommends attempting to obtain a more accurate and precise value for the missing characterization factor. However, deriving high-quality characterization factors is unrealistic for most assessments, as deep expert knowledge is required [24, 91, 103]. In practice, practitioners must often accept the omission of particular characterization methods and **shall,** as a minimum requirement, report these and their implications for the assessment quality [24]. Practitioners **may** estimate preliminary characterization factors based on expert opinions, literature reviews, lab experiments, molecular structure-based impact prediction models (e.g., quantitative structure-activity relationship (QSAR) models [104, 105]). In this case, practitioners **shall** report and explain the limitations of such preliminary characterization factors.

D.6.2.1 Provisions

Provisions D.6 – Life Cycle Impact Assessment		
Shall	1)	The recommendations provided in chapters C.6 **shall** be applied.
	2)	LCIA **shall** account for all impact categories in order to avoid burden shifting.
	3)	LCA practitioners **shall** check and report whether characterization factors are missing in the chosen LCIA methodology.
Should	1)	The relevance of missing characterization factors **should** be evaluated, assuming a conservative value or realistic worst case (e.g., based on chemical, physical or other similarity to other elementary flows contributing to the same impact category) [91].
May	1)	Practitioners **may** estimate preliminary characterization factors based on expert opinions, literature reviews, lab experiments, molecular structure-based impact prediction models (e.g., quantitative structure-activity relationship (QSAR) models [104, 105]). In this case, practitioners **shall** report and explain the limitations of such preliminary characterization factors.

D.7 Life Cycle Interpretation

General Introduction

The (life cycle) interpretation phase has two main objectives: 1) to evaluate the gathered inventory data and indicators during the iterative steps of an assessment and check whether they are sufficient to answer the initial research question; and 2) to evaluate the results for deriving robust conclusions and potential recommendations that are well balanced with the results of the TEA, since only economically viable processes and products justify further consideration.

The interpretation is of particular importance within the iterative steps of assessments that accompany R&D. Each assessment iteration is intended to already provide support, following the iterative improvements during R&D. In contrast, a full assessment of a mature technology provides recommendations and conclusions only at the very end of the study, while the iterations during full assessment only evaluate which gaps need to be closed in order to answer the initial goal. In contrast, a low-TRL technology assessment evaluates the potential of a technology and guides the ongoing research, and data become available stepwise. Low-TRL assessments **shall** not be used to claim carbon neutrality, carbon negativity, or GHG emission reduction, nor do they demonstrate profitability.

In the interpretation phase, different requirements are placed on *Monitoring* and *R&D support* to fulfill specific interpretation tasks. For *Monitoring,* general quality checks, such as a completeness check and a consistency check, are central and **shall** be applied as a minimum requirement for interpretation. For *R&D support,* more detailed investigations regarding sensitivities and scenarios are required. General information on sensitivity analyses and their relation to uncertainty analysis is available in chapters B.7 and C.7. Detailed descriptions of each analysis step for LCA are available in chapter 9 of the ILCD Handbook and Laurent *et al.* [35, 91]. Chapter 12 of the ILCD Handbook provides detailed information on the general data quality concept and data quality measures.

D.7.1 Interpretation for *Monitoring*

First, the best case is modeled and compared to the benchmark, following the provisions for comparative studies in chapters B.7 and C.7. If the assessed process already performs worse than the benchmark in one or more decision criteria (D.4.1.2), the process **shall** be discarded (Provisions D.4.1.4). In this case, the following interpretation steps **may** be performed qualitatively to ensure no mistakes have been made during the assessment.

D.7.1.1 Completeness Check

For low-TRL assessments, it is obvious that information is incomplete. However, to understand the reliability of an assessment, it is critical to understand how complete the inputs used for the assessment are. The earlier in the R&D an assessment is performed, the more difficult it is to approximate the completeness of a study. Thus, the completeness check **shall** consider all known and expected unknowns (e.g., missing downstream units, missing auxiliaries, etc.) and include expert opinions on the most likely flows in order to approximate the 100% completeness value. The completeness check requires discussing missing information with R&D experts and is a chance to agree on the next key information to be provided to further evaluate the process. Note that a completeness check requires expert opinions for the most likely values, in contrast to the estimated best-case values used to answer the *Monitoring* goal. Thus, the completeness check helps to put the *Monitoring* results into context. This context helps decision makers if a No-go decision is under debate (e.g., if the performance under best-case assumptions is not substantially better than the benchmark, or if the number of alternatives is to be reduced further).

If expert opinions are not available, averaged values from the chemical industry **may** serve as an initial approximation (see methods presented in Table 2, Table 3, and Table 4 in chapter D.5.2.2). In early-stage assessment, the completeness check **should** not be used to argue for neglecting flows, as the approximated contribution is not accurate enough to justify a cut-off.

D.7.1.2 Consistency Check

The consistency check is performed to verify that the assumptions, methods, and data are applied consistently throughout the assessment and are in accordance with the goal and scope definition [15]. Thus, this check is required for *Monitoring* and *R&D support*, as both types of studies have individual assessment goals and underlying assumptions.

The provisions given in this document aim for maximum consistency. However, poor data quality can also result in a lack of consistency in two ways: 1) Assumptions and inventory estimation methods used for different unit processes of one technology are likely to vary, since the level of detail for each unit process depends on the current state of R&D; and 2) Data quality and method choices between alternative technologies are likely to vary, as technologies might not be at the same TRL. Thus, comparisons of alternative processes **shall** be performed only on the same TRL, even if one process option is already more advanced. An exception is the comparison of the assessed CCU process with the benchmark system, which is a necessary step in *Monitoring* and *R&D support* and must accept limitations.

Differences in data quality between unit processes or between processes is an inherent issue of R&D and cannot be resolved. However, the consistency check **shall** identify and document all differences in data quality, to reflect possible limitations for the goal and scope of the study. The assumptions and inventory estimation methods used for an assessment might differ in the level of detail for separate unit processes (e.g., more detailed modeling of the reaction than the separation steps). Therefore, the consistency check **shall** ensure that the underlying assumptions do not contradict each other or the goal and scope of the study (e.g., best-case assumptions for the *Monitoring* goal). To avoid contradictory assumptions, the consistency check **shall** be discussed with process design experts.

The difference in data quality between the benchmark process and the CCU process under assessment must be accepted and **shall** be clearly documented, stating the limitations in comparability between different TRL. The *Monitoring* and the *R&D support* goals and related provisions reflect the lower data quality compared to the benchmark process. Besides the inconsistency in data quality, all other inconsistencies (e.g., methodological choices, use of background data, LCIA methodology, etc.) **shall** be avoided by following the provisions of parts B, C and F of these Guidelines.

D.7.1.3 Additional Requirements

Further analyses, such as sensitivity and contribution analysis, **may** be performed additionally if required by the goal of the *Monitoring* study. Those analyses might, for example, be necessary if a Go/No-go decision needs to be drawn beyond the No-go criteria (e.g., if the best-case assumptions lead to results close to a No-go criterion). Additional analyses become more important with increasing TRL, as the number of processes to be assessed is reduced and the assessment goals become more ambitious. The provisions given in chapter D.5 reflect these additional requirements and **shall** be followed. Contribution analysis can be used, for example, to identify the relevance of background data compared to the foreground process and thus assess the relevance of supply chain optimization. Sensitivity analysis can help place the *Monitoring* results within a broader context and support decision making, for example by identifying the influence of process scale or other uncertain factors on the overall performance.

D.7.1.4 Provisions

Provisions D.7 – Interpretation for *Monitoring*	
Shall	1) Low-TRL assessments **shall** not be used to claim carbon neutrality, carbon negativity, or GHG emission reduction. 2) A completeness check and a consistency check **shall** be applied as a minimum requirement. 3) The completeness check **shall** consider all known and expected unknowns (e.g., missing downstream units, missing auxiliaries, etc.) and include expert opinions on the most likely flows, to approximate the 100% completeness value. If expert opinions are not available, averaged values from the chemical industry **may** serve as an initial approximation (see methods presented in Table 2, Table 3, and Table 4, in chapter D.5.2.2). 4) The consistency check **shall** identify and document all differences in data quality in order to reflect possible limitations for the goal and scope of the study. The consistency check **shall** ensure the underlying assumptions do not contradict each other or the goal and scope of the study (e.g., best-case assumptions for the *Monitoring* goal). To avoid contradictory assumptions, the consistency check **shall** be discussed with process design experts. All other inconsistencies (e.g., methodological choices, use of background data, LCIA methodology, etc.) **shall** be avoided by following the provisions of parts B, C and F of these Guidelines. 5) Comparison of process alternatives **shall** be performed only on the same TRL.
Should	1) In early-stage assessment, the completeness check **should** not be used to argue for neglecting flows, as the approximated contribution is not accurate enough to justify a cut-off.
May	1) If a process will be discarded, the interpretation steps **may** be performed qualitatively. 2) Additional analyses, such as sensitivity checks, **may** already be performed in the *Monitoring* step if required by the goal of the *Monitoring* study. The provisions given in chapter D.5 reflect these additional requirements and **shall** be followed.

D.7.2 Interpretation for *R&D support*

The assessment for *R&D support* builds upon the previous *Monitoring* step and includes additional information necessary to answer the goal of the study. The previously performed completeness check might have revealed missing information for *R&D support* and **shall** be updated when new information is added. Before conclusions for *R&D support* can be drawn (e.g., from screening or sensitivity analyses), another consistency check **shall** be performed (see D.7.1.2) to check whether the system boundaries, functional unit, inventory data, and assumptions reflect the goal and scope of *R&D support*.

D.7.2.1 Screening of Alternatives

In the early stages of R&D, the degrees of freedom are typically high, and researchers must consider a large set of alternatives (e.g., products, reactants, catalysts, reactor types, separation units, solvents, etc.). An essential task is to narrow down the alternatives and find the best-fitting solutions. LCA and TEA can support this task by performing a screening assessment (see also chapter A.6). First, each alternative **shall** be assessed considering a best-case performance. The best-case performance is calculated and assessed analogously to the previous *Monitoring* step but additionally includes those options that are not yet fixed.

If a process alternative requires additional input products or waste treatment, those requirements **shall** be included in the assessment.

Second, the remaining alternatives **may** be directly compared to each other on the same TRL. For a direct comparison, more realistic assumptions than the previous best-case assumptions **shall** be defined in cooperation with R&D experts. Those realistic assumptions **shall** account for uncertainties to the best of current knowledge. In the case of a direct comparison, the results are highly dependent on the quality of the data and models used, and are subject to high uncertainties. Thus, special attention **shall** be paid to ensuring robust evaluation by means of completeness, sensitivity, and consistency checks, and drawing conclusions. When drawing conclusions at an early stage, often no clear preference for one alternative can be identified because the large general uncertainties are likely to mask relatively small differences between alternatives. According to the ILCD handbook, insignificant differences **shall** not be misinterpreted either by claiming the equality of the alternatives or by over-interpreting single aspects to make up differences.

As introduced in the last chapter, a shortcut method such as the Efferi framework [96] can be used to provide specific guidance at each maturity level, forming a robust and easy-to-use assessment method for early-stage CCU technologies, facilitating comparisons and allowing clearer Go/No-go recommendations for reduced assessment effort. Shortcut studies compare many alternatives at a low-level of detail, in contrast to full-scope studies that compare a few technology alternatives at a high level of detail.

The advantage of using shortcut indicators is that recommendations can be made requiring less data and effort; the disadvantage is a less detailed and therefore less thorough assessment. Zimmermann *et al*. apply shortcut indicators for TEA in this assessment framework to provide recommendations for decisions with sufficient certainty in an environment with many unknowns, such as early-stage R&D projects [96]. While shortcut indicators seem suitable in early-stage assessments or screening assessments, practitioners **should** avoid using them for assessing late-stage projects and when detailed data are available.

D.7.2.2 Dealing with Uncertainty Using Contribution, Sensitivity Analysis, and Break-even Analysis

For low-TRL assessments, it is common that not all physico-chemical processes are yet fully understood, and therefore the assessment results typically include substantial uncertainties. Hence, especially for low-TRL assessments, it is essential to tackle these inherent uncertainties. To do so, it is important to know where these uncertainties arise. For low-TRL assessments we encounter uncertainties in the model assumptions, in the data, as well as in the scenarios employed. Hereby, we must distinguish between uncertainties and variability in low-TRL assessments: uncertainty of an input arises, for example, from assumptions used in the inventory (e.g., emissions from the electricity grid in 2030), whereas input variability arises when there is a choice of multiple differing values for an input (e.g., present day electricity grid emissions in either France or Germany). While low-TRL assessments often display high variability (e.g., the deployment location of the technology is not yet known), thorough reporting of the chosen assumptions and results, together with scenario analysis, can clarify these challenges. To tackle uncertainties for low TRL, a thorough uncertainty analysis is needed.

Uncertainties for low-TRL assessment can be assigned to four categories [4]: 1) ‘risk’ — known system parameters and known probabilities, 2) ‘uncertainty’ — known system parameters but unknown probability distributions, 3) ‘ignorance’ — unknown system parameters and unknown probability distribution, and 4) ‘indeterminacy’ — future development is inherently undetermined. For mature technologies, ignorance and indeterminacy are usually negligible and therefore global methods of uncertainty analysis (e.g., via Monte Carlo analyses) are recommended, as described in chapter B.7 and C.7. Nonetheless, low-TRL assessments include all four categories of uncertainty and hence only local uncertainty methods (e.g., one-at-a-time sensitivity analysis) as described in chapter B.7 and C.7, combined with a scenario analysis, **shall** be applied. In the following we describe the specific steps which **shall** be taken when analyzing uncertainties in low-TRL assessments.

Before performing a local sensitivity analysis, contribution analysis **shall** be performed to identify significant unit processes or inventory data. Unit processes and inventory data that make high contributions **shall** be further assessed by a local sensitivity analysis. Local sensitivity analysis can be used to evaluate process-related parameters and external factors (also known as scenario analysis) and to identify their influence on overall economic or environmental performance. To combat the ignorance and indeterminacy present in low-TRL assessments (following the local sensitivity analyses, where via contribution analysis selected input variables are varied over a selected interval, e.g., ±15% of the initial value), a scenario analysis **shall** be performed. This defines multiple plausible future scenarios (e.g., optimistic, mid, pessimistic) to grasp the entire potential input space, and the low-TRL assessment is performed for each scenario. The scenario analysis **shall** include both model-specific variables (e.g., reaction yield) as well as external variables (e.g., market prices or grid emissions). In order to define these scenarios a panel of stakeholders (likely with differing perspectives) **may** be consulted.

Unit processes and inventory data that make a large contribution, and particularly those process parameters and external factors with high influence on the overall performance (e.g., costs or environmental impacts), **shall** be suggested as focal points for further R&D.

Furthermore, for focal parameters, practitioners **may** calculate break-even points at which a performance indicator is equal to the benchmark. Break-even points can be calculated for all parameters and performance indicators (e.g., for each economic indicator or impact category). The break-even points **should** be calculated for the No-go criteria defined in the scope of the study.

The clear communication of inherent uncertainties is important for both sensitivity and uncertainty analysis particularly for low-TRL assessments. While uncertainties are inevitable in these assessments, R&D decisions can only be taken if the uncertainties and limitations of the calculations are known. TEA and LCA practitioners **shall** report the determined focal points, and the results of local sensitivity analysis (e.g., as spider web plots or tornado plots) as well as the scenario analysis. For comparative studies the results of sensitivity as well as scenario analyses **should** be reported together, thereby facilitating comparisons in order to inform R&D decisions. Additionally, to tackle potential variabilities in the outputs, variable inputs (e.g., choice of location for the assessment) **shall** be communicated clearly.

D.7.2.3 Provisions

Provisions D.8 – Interpretation for *R&D Support*	
Shall	1) Low-TRL assessments **shall** not be used to claim carbon neutrality, carbon negativity, or GHG emission reduction. 2) The completeness check performed in the previous *Monitoring* step might have revealed missing information for *R&D support* and **shall** be updated when new information is added. 3) Before conclusions for *R&D support* can be drawn (e.g., from screening or sensitivity analyses), another consistency check **shall** be performed (cf. D.7.1.2) to check whether the system boundaries, functional unit, inventory data, and assumptions reflect the goal and scope of *R&D support*. 4) For screening, each alternative **shall** first be assessed considering a best-case performance. 5) Insignificant differences **shall** not be misinterpreted either by claiming the equality of the alternatives or by over-interpreting single aspects to make up differences. 6) Before performing a sensitivity analysis, contribution analysis **shall** be performed to identify significant unit processes or inventory data. A sensitivity analysis **shall** further assess those unit processes and inventory data that make large contributions. 7) Unit processes and inventory data with a large contribution, and particularly those process parameters and external factors with high influence on the overall performance (e.g., costs or environmental impacts), **shall** be suggested as focal points for further R&D. 8) Both contribution and local sensitivity analysis **shall** be performed together with uncertainty analysis as described in chapters B.7 and C.7. 9) A scenario analysis **shall** be performed 10) All results of the contribution, sensitivity as well as scenario analysis **shall** be communicated clearly to ease R&D decision-making processes.
Should	1) For comparative studies, the results of sensitivity and scenario analyses **should** be reported together in order to ease the comparison for R&D decisions.
May	1) After initial screening, the remaining alternatives **may** be directly compared to each other. In case of a direct comparison, more realistic assumptions **shall** be defined based on current information, in cooperation with R&D experts, to account for uncertainties. Special attention **shall** be paid to ensuring robust evaluation by completeness, sensitivity, and consistency checks, and drawing conclusions. 2) For focal parameters, practitioners **may** calculate break-even points at which a performance indicator is equal to the benchmark. The break-even points **should** be calculated for the No-go criteria defined in the scope of the study. 3) A panel of stakeholders **may** be consulted when defining the scenarios to be analyzed.

D.8 Reporting

General Introduction

Early-stage assessments are conducted for the purpose of deriving decisions, and thus, reporting the results to decision makers is a central element. To accompany R&D, the LCA and TEA practitioners are in constant dialogue with researchers, developers, and all relevant decision makers.

Ideally, the recommendations for reporting provided in chapters B.8 and C.8 **shall** be applied wherever possible, and exceptions **shall** be explained. However, these recommendations are made to prepare a final report, while the internal reporting for *Monitoring* and *R&D support* is done iteratively and as a dialogue. Often, time is limited mainly when numerous parallel assessments are conducted and explained to management and R&D experts. Thus, the reporting must be tailored to the audience and represent the current state of knowledge. The requirements for internal reporting **shall** be discussed with the audience when first agreeing on the goal and scope of the study, in order to manage stakeholders' expectations. If low data quality does not allow sufficient completeness or consistency to answer the research question, stakeholders and practitioners **shall** adapt the goal to the available data or pause the study until research and development have filled the data gaps [24].

An additional challenge is the missing external review, usually ensuring consistent assessment quality. This challenge becomes even more relevant as the assessments are conducted parallel to the R&D progress, which can take several years. Thus, each reporting step **shall** be documented to keep track of the assessment status. A technical summary **should** be used for this documentation to enable a quick overview. Furthermore, a critical review **may** be conducted internally, e.g., by other LCA or TEA practitioners or R&D experts.

The workflow recommended in this part of the Guidelines **may** be adjusted to the individual needs of a research project. Further information is available in the 'Making Sense Report' [106].

D.8.1 Reporting for *Monitoring*

The *Monitoring* report is intended for decision makers and **should** be aligned to them in terms of readability. The recommendations and checklists for an executive summary provided in chapters B.8 and C.8 **should** be followed for reporting. The reporting **may** take the form of a presentation allowing for direct questions and answers, on condition that all recommendations for good reporting are applied. Particular attention **shall** be paid to explaining the completeness and consistency of the study, the underlying assumptions, and uncertainties. The influence of these aspects on the results **shall** be discussed. The results **shall** be communicated as preliminary results representing an unachievable best-case as an upper boundary of performance. While No-go decisions can be derived from consistent best-case assumptions, those assumptions do not provide realistic estimations of the future performance and cannot guarantee any benefits.

As the *Monitoring* results are reported iteratively, the changes since the last report **should** be highlighted in order to use the reporting time efficiently. The reporting allows discussing required changes to the goal and scope for the next iteration, which **should** be further detailed at the next stage-gate.

D.8.2 Reporting for *R&D Support*

The report for *R&D support* is intended for technical experts (e.g., researchers and process designers) and **should** be aligned to them in terms of readability. The requirements of the *Monitoring* report **shall** be applied for reporting the screening results. A technical summary and additional data sheets **should** be added to the report for full transparency of the underlying assumptions and the inventory data used. The recommendations and checklists for reporting the results of contribution, sensitivity, and break-even analysis provided in chapters B.8 and C.8 **should** be followed.

The necessary close collaboration between R&D experts and LCA & TEA practitioners requires inputs and discussion at several assessment phases. To avoid misinterpretations of intermediate discussions as reporting, the reporting **should** be performed separately from those discussions.

D.8.2.1 Provisions

Provisions D.9 - Reporting	
Shall	1) The individual provisions of Guideline parts B and C **shall** be applied wherever possible, and exceptions **shall** be explained. 2) The requirements for internal reporting **shall** be discussed with the audience when agreeing on the goal and scope of the study in order to establish expectations. 3) If low data quality does not allow sufficient completeness or consistency to answer the research question, stakeholders and practitioners **shall** adapt the goal to the available data or pause the study until research and development have generated the missing data [24]. 4) Each reporting step **shall** be documented to keep track of the assessment status. A technical summary **should** be used for this documentation to enable a quick overview. 5) Particular attention **shall** be paid to explaining the completeness and consistency of the study, the underlying assumptions, and uncertainties. The influence of these aspects on the results **shall** be discussed. 6) If best-case assumptions are applied, the results **shall** be communicated as preliminary results representing an unachievable best-case as an upper bound of performance.
Should	1) The *Monitoring* report is intended for decision makers and **should** be aligned to them in terms of readability, following the recommendations and checklists for an executive summary (B.8 and C.8) 2) The report for *R&D support* is intended for technical experts (e.g., researchers and process designers) and **should** be aligned to them in terms of readability. A technical summary and additional data sheets **should** be added to the report for full transparency of the underlying assumptions and the inventory data used. 3) To avoid misinterpretations of intermediate discussions as reporting, the reporting **should** be performed separately from those discussions.
May	1) A critical review **may** be conducted internally, e.g., by other LCA or TEA practitioners or R&D experts. 2) The reporting **may** take the form of a presentation allowing for direct questions and answers, on condition that all recommendations for good reporting are applied. 3) The workflow recommended in this part of the Guidelines **may** be adjusted to the individual needs of a research project.

D.9 References

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PART E

Integrated TEA & LCA Guidelines

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SUPPORTED BY

Contents Part E

E.1 Introduction to Integrated TEA and LCA

E.1.1 An Introduction to the Concept of Integrated Assessment

The earlier chapters of this guideline document outline concepts for assessing the environmental and economic impacts of CCU-related technologies, products, and services. Both TEA and LCA offer insight into singular dimensions of the broader concept of sustainability, and the outputs from each can be utilized to answer a broad range of research questions as outlined in Parts B and C [1].

Whilst assessing impacts within a singular dimension is useful, it does have one obvious limitation – one-dimensional studies do not capture the impacts associated with the other pillars of sustainability. A TEA study can predict whether a product could feasibly compete in the market space, but it offers no insight into whether it offers better or worse environmental performance than an existing market-dominant product. A similar analogy can be drawn for LCA: A comparative study can show a reduction in environmental impact for a new product when compared to a market-dominant option, but offers little direct insight into whether the product can compete economically.

The appeal of integrated economic and environmental assessment is clear: Assessing in both dimensions allows stakeholders to assess, analyze, and interpret results in a more holistic manner. Not only are the one-dimensional indicators made available, but new opportunities arise at the intersection of both dimensions. Concepts such as combined eco-enviro indicators can help strengthen reporting and decision making, for example by allowing for the exploration of trade-offs.

The concept of eco-enviro indicators is one that should be familiar, at least in part, to many within the CCUS community: Both the cost of carbon avoided and the cost of carbon abated are frequently seen examples that have percolated through to a wider audience.

However, whilst the advantages of integrated TEA and LCA assessment are numerous, there remain numerous pitfalls and methodological challenges. This chapter aims to address these by providing additional guidance to those looking to conduct integrated assessments. 'Additional' is a keyword in this regard; prior to reading the current chapter on integrated assessments, it is advised that practitioners familiarize themselves with the individual TEA (Chapter B) and LCA (Chapter C) guidelines, since those form the basis for this present chapter. Here, integrated assessments are treated as a special sub-class of LCA & TEA studies (see Section E.1.3 for more details), and as such this guidance is given in addition to, or in amendment of, the existing best practices outlined.

As a final note: these guidelines consider specifically the integration of TEA and LCA, and should not be confused as providing guidance for integrating other combinations of environmental or economic impact assessment tools. Integrated economic and environmental impact assessment can be applied to a broad range of goals/research questions, not all of which are suitable for integrated TEA and LCA studies. The following section explores this concept, providing a suggested use-case for integrated TEA and LCA; and whilst other use-cases may exist, care should be taken to identify whether these could be better addressed by other integrated study combinations (e.g., integrated LCC & LCA).

Furthermore, this chapter pays little attention to the third sustainability dimension (society): Those interested in incorporating social impact assessment are advised to read the social-LCA guidance found in section F, in combination with other external sources [2][3][4].

E.1.2 Defining TEA & LCA and What This Means for Integrated Assessment

With both TEA and LCA discussed as individual studies in earlier chapters of this guideline document, a brief reminder is included here of the definitions for both study types:

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" uncovering the cost of manufacturing and potential 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, or for assessing cost drivers on key inputs into the production phase.

Life cycle assessment (LCA) accounts 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.

What does this mean for integrated assessment?

Both TEA and LCA are methodological frameworks, and in the case of these guidelines both follow the same structure. However, they are used for assessing different aspects of (potentially) the same product or service (for brevity, both are subsequently referred to as 'product').

For TEA the focus of assessment is to analyze economic impact: determining costs & potential market opportunities for one or multiple stakeholders. Typically, the stakeholder is the producer of a given product or group of products, however the above definition does leave some possibility for considering other groups (e.g., users, or the 'market perspective') or for considering other perspectives (see section B.3.2 for more details). However, care should be taken to not confuse LCC with TEA, particularly in the use & disposal phases. These methodologies are similar but aim to address different perspectives and goals.

For LCA the focus of assessment is to analyze environmental impact: determining the impact associated with consuming natural resources and emitting pollutants. Unlike TEA, LCA is always conducted on a holistic basis and addresses interactions with the environment across the whole life cycle of the product, from 'cradle to grave' – with the notable exceptions of 'cradle-to-gate' studies, which can be utilized under specific circumstances (see LCA guidelines section C.4 for more detail).

The applications of TEA and LCA within CCU are considered in earlier chapters, with typical research questions listed for both (B.3.2 for TEA, C.3.1 for LCA and D.3.1 for early TRL assessment). These research questions (and the associated study perspectives) show typical use cases for these studies within CCU, thus a reasonable first question to ask for integrated assessment is: *Are there any valid use cases for integrated TEA and LCA assessment for CCU?*

Arguably, TEA (regardless of perspective) provides insight into factors that impact 'internal' costs – defined here as the financial/economical costs to a specific stakeholder or group of stakeholders (for example, if more than the production phase is considered). These range from identifying major cost drivers in the research phase, to investigating economic viability in development or deployment phases, to assessing the impacts that regulatory frameworks (taxes, policy initiatives, etc.) have on whether a technology is deployable at the highest TRLs. All of these study types consider impact factors in which internal cost estimations are vital for answering the central research question.

For LCA, it can be seen that the studies provide insight into 'external' costs – defined here as the indirect impact that the activity incurs. For LCA in particular, the external costs considered are determined by the assessment methodology used but are generally environment focused (i.e., excluding social impacts, with this typically covered by other studies such as social life cycle impact assessment (S-LCA)).

Thus, one obvious use case arises immediately: integrated TEA and LCA can be used to combine internal and external cost impacts for a given CCU technology, product, or service, and well aligned integrated studies allow for the comparison of these impacts across differing scenarios, technologies, and products.

This use case forms the basis and justification for this guidance chapter but, as previously stated, it is not assumed to be the only viable use case.

Specific research questions derived from this use case can be found in the goal definition section (section E.3), which address specific applications within this broader scope.

E.1.3 The Structure for Integrated Studies

Upon determining that there is a use case for integrated assessment, a second question arises: *Is there a valid methodology for integrated assessment?* In other words, can the studies be utilized together to meet the identified use case? Whilst the rest of this chapter provides detailed guidance on the more detailed 'phase-by-phase' aspects of an integrated methodology, the present section will outline the broader basis for developing an integrated study.

Given the intention of this chapter to provide guidance on integrated TEA and LCA studies, a decision was made to ensure that the individual methodologies are preserved when conducting the constituent studies. In other words, the LCA component used in an integrated study should remain capable of standing alone and being ISO-compliant, as outlined in the earlier chapter, while necessitating only minimal changes to its core structure (e.g., removing reference to economic impact); and the TEA study/studies used should remain compliant with the guidance outlined in Chapter B. Schematically, this concept is captured in Figure 1, where the core concepts of the life cycle thinking are maintained and combined with those of TEA to create something that is 'greater than the sum of its parts' through enabling additional insight and analysis in the form of two-dimensional assessment.

The intention to preserve the methodologies also allows for the utilization of existing TEA and LCA studies in an integrated assessment – albeit with a need to rework certain phases to incorporate a broader, multi-dimensional approach.

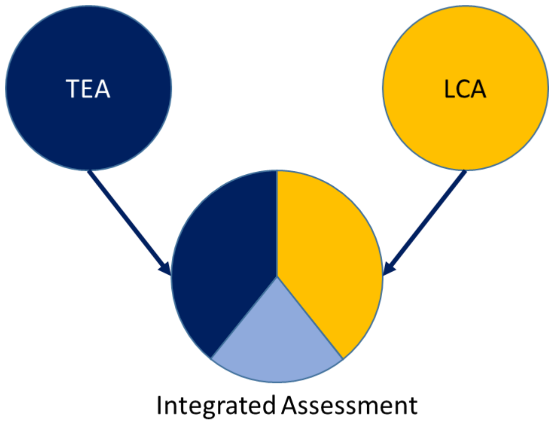

Figure 1 – Concept schematic for integrated assessment

With this in mind a proposed structure for integrated TEA and LCA assessments is proposed and captured in Figure 2, one that is derived in part from ISO 14045 (Eco-efficiency assessment of product systems) [5] due to the similar nature and target outcomes. Whilst this guidance chapter does not meet all the requirements of ISO 14045, many of the same guiding principles are used throughout the following subchapters. A unified approach is taken to handling goal and scope definition, whilst the inventory and impact assessment for the constituent TEA and LCA parts are handled in parallel (albeit with significant overlap in some places, such as the use of the same technical data in the inventory) but with a focus on ensuring consistency and alignment between the two. Combined impact assessment, such as the development of eco-enviro indicators, is then handled holistically, with interpretation an ongoing task throughout the study.

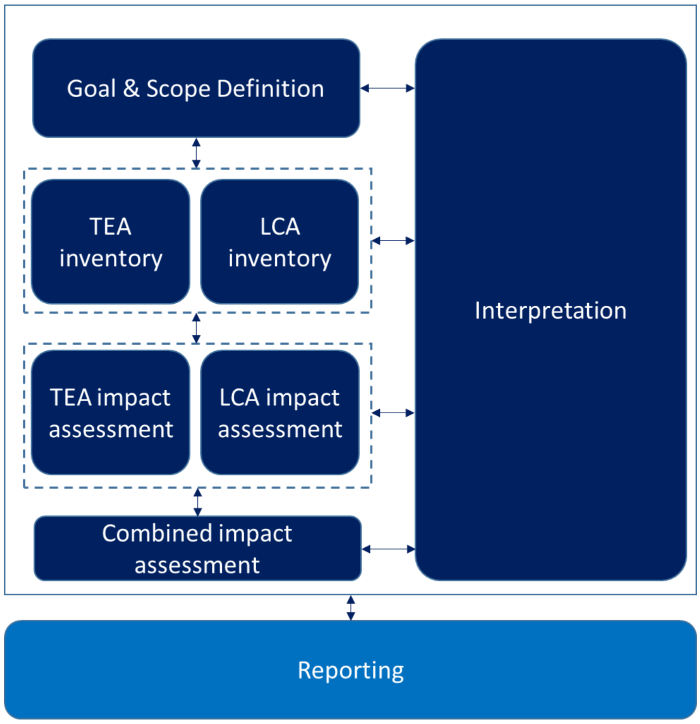

Figure 2 – Proposed structure of integrated TEA and LCA assessment

E.1.4 Overview of Existing Guidance

This guidance part frequently refers to the guidance and provisions outlined in the prior parts, with an intention to minimize the repetition of existing guidance. As such, it is highly recommended that readers familiarize themselves with the prior TEA and LCA parts. For a quick point of reference, Figures 3 and 4 below outline where specific provisions can be found in each chapter.

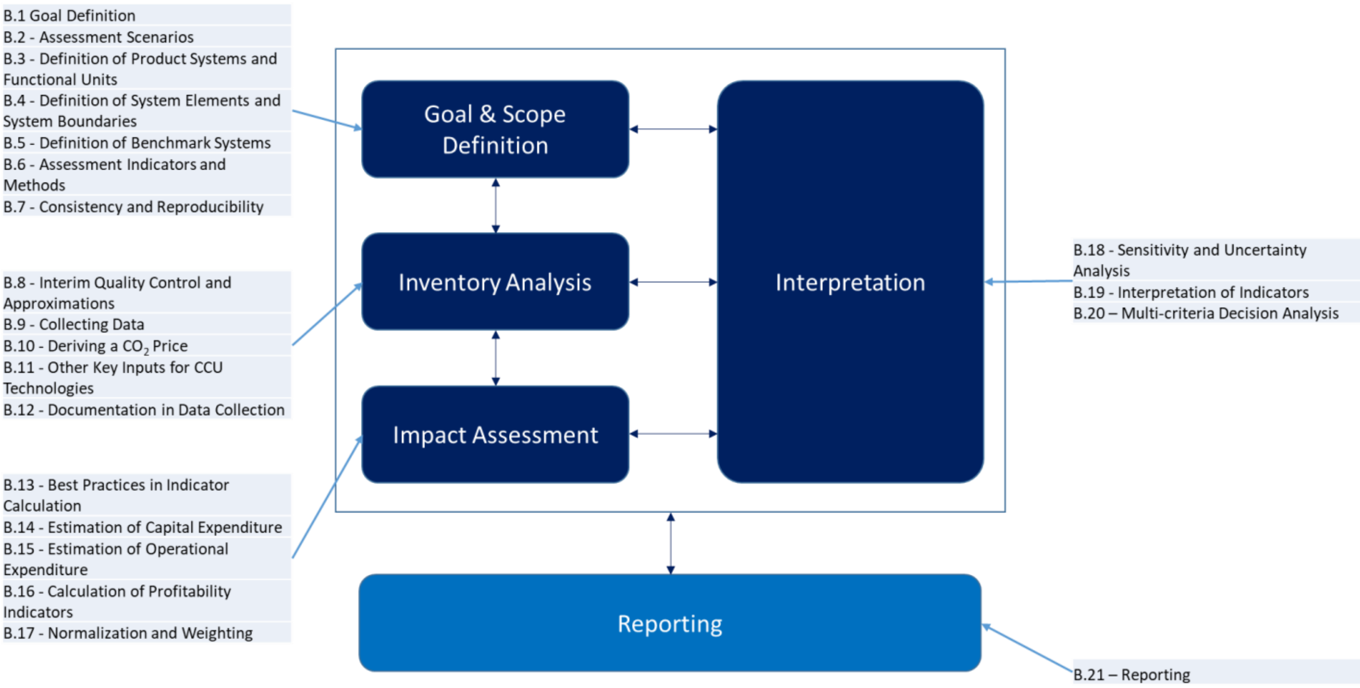

Figure 3 – Overview of TEA chapter provisions

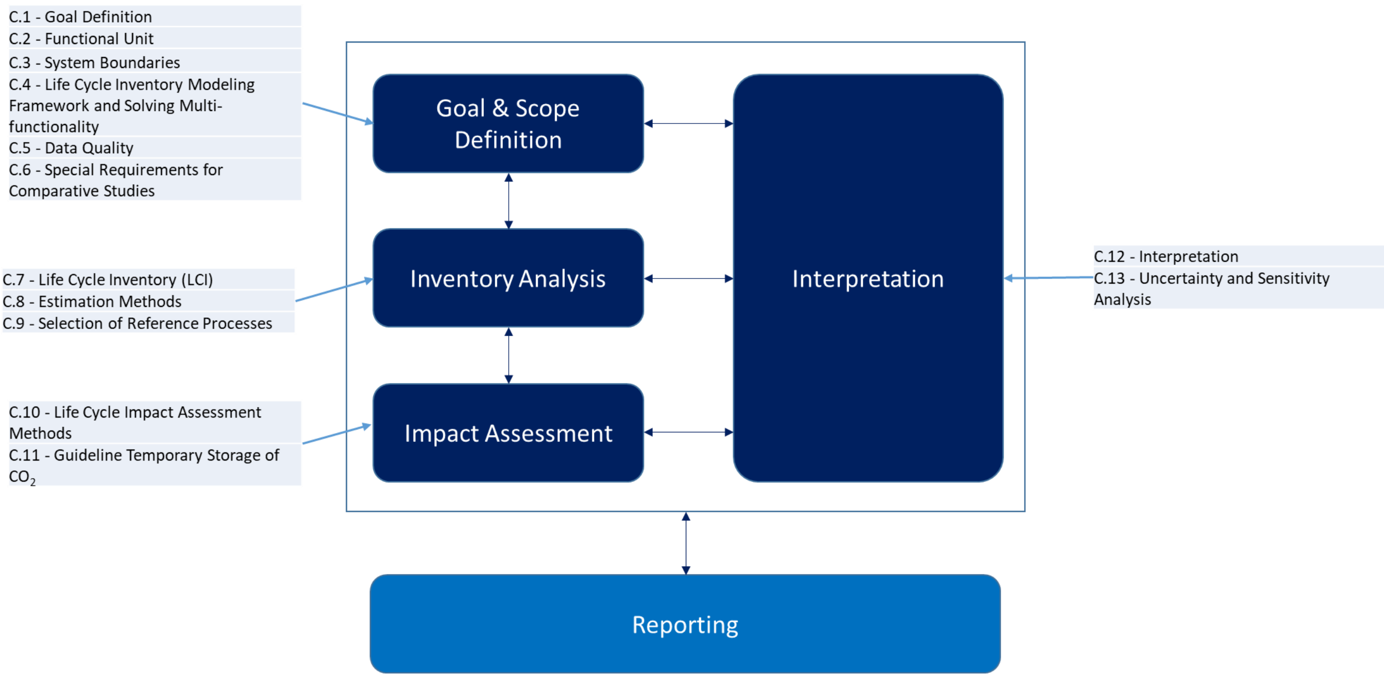

Figure 4 – Overview of LCA chapter provisions

E.2 How to Read This Document

E.2.1 Aim and Scope of Part E

This document builds upon parts B and C of the Guidelines last updated in version 1.1 of these guidelines [1], which are based on the ISO 14040 [6] and 14044 [7] standards for life cycle assessment, the ILCD handbook [8], various other books and scientific papers referenced throughout these parts. References in this part are also made to ISO 14045 [5]. As a complementary part of the Guidelines, this document provides additional recommendations for TEA and LCA that aim to support integrated TEA and LCA studies. These additional recommendations respond to the needs of TEA and LCA practitioners wishing to answer research questions best suited to integrated TEA and LCA, but with some consideration to the requirements of a broader range of stakeholders including decision makers (e.g., researchers, process designers, and management).

E.2.2 Structure of This Document

Analogous to parts B, C and D, this chapter is structured to address each phase of the TEA and LCA process, with the addition of a chapter that addresses the use of multi-criteria decision analysis within the interpretation phase:

1. Goal definition
2. Scope definition
3. Inventory analysis
4. Calculation of indicators
5. Interpretation
6. Interpretation: Multi-Criteria Decision Analysis
7. Reporting

Each chapter refers to the guidance outlined for TEA and LCA in the earlier chapters, before providing additional guidance of specific interest to those conducting integrated studies. As with previous parts, provisions will be captured in a list of **shall**/**should**/**may** provisions to be performed periodically. Look out for tables with the following style:

Provisions E.X - [topic]	
Shall	1) Provision 2) Provision
Should	1) Provision 2) Provision
May	1) Provision 2) Provision

E.3 Goal Definition

General Introduction and Challenges

For both TEA and LCA the definition of the goal is a key aspect and starting point of any study, as explained in Chapters B.3 and C.3. This extends to integrated assessment, and as such the recommendations given in those chapters **shall** be considered when conducting the individual studies to be used in an integrated study. In general, provisions B.1 and C.1 are well aligned and thus the guidance outlined there provides a solid basis for developing the goal of an integrated study.

However, some specific aspects need to be considered when setting an integrated assessment goal. Primarily the goal for an integrated assessment **shall** refer to both economic and environmental aspects. Furthermore, the goal chosen **shall** be suited to combined TEA and LCA; if this is not the case, changes can be made to either the goal/research question or to the studies used in the integrated assessment (e.g., there are instances where life cycle costing may be a more appropriate assessment technique).

E.3.1 Goal Definition Overview

The first step in conducting an integrated study is to identify the study goal, addressing the research question that provides the impetus for the commencement of the study. Given that individual TEA and LCA studies focus on questions of techno-economic and environmental impacts respectively, an integrated TEA/LCA study will naturally feature both a techno-economic and an environmental aspect. The proceeding section explores some example integrated research questions that can be addressed in more detail.

As discussed in prior sections, there are some practical challenges to utilizing existing TEA and LCA studies in the production of an integrated study, among which the setting of a suitable goal is one area of necessary focus. An existing TEA/LCA study will obviously not contain a goal statement that is fit for the purpose of an integrated study, and therefore those wishing to utilize an existing study will have to decide upon how best to incorporate this with their intended integrated goal.

As a suggested approach, an integrated study goal **may** be drafted prior to considering the use of an existing TEA or LCA study. This goal statement can then be compared to that of the existing TEA or LCA study, if there is sufficient alignment between the two on the relevant economic/environmental criteria, it **may** be feasible to use the subsequent parts of the study (inventory, calculation of indicators, and aspects of the interpretation) directly in the integrated study. If this is not the case, it **may** be more appropriate to only utilize parts of an existing study. For example, a practitioner may wish to use an existing study of a CO_2 to X plant based in the US as part of an integrated study located in Europe. The existing mass balances and plant efficiencies etc. may remain valid for use, allowing these to be reproduced in the new, combined inventory. However, the impact associated with energy use may differ and thus require updating, thereby invalidating the pre-existing indicator calculations (these will need to be recalculated for the new integrated study). Reviewing the intended goal and the desired level of alignment/accuracy will help inform the best plan of action.

In terms of specific guidance for writing combined goals, the natural starting point is to review the existing guidance for TEA and LCA.

A review of the provisions for goal setting in TEA (provisions B.1) and LCA (provisions C.1) shows that the guidance in goal setting is consistent across both study types. In both sets of provisions, the 'shall' addresses the need to: state the study context; the intended application; the target audience; the commissioners & authors of the study; and any limitations on usability. Naturally, it follows that integrated study goals **shall** also follow this approach, as also seen in ISO 14045, thereby allowing for clear communication of the study's aims and other relevant information.

In the TEA section, additional guidance is provided on 'perspectives,' with these used to frame groups of differing yet common goal-related questions and objectives. Each perspective is stated to serve differing groups of stakeholders with differing areas of focus. Given that this directive is included to help communicate the intended goal of the study, an integrated goal **should** also state the perspective where possible.

Wunderlich et al. [9] found in their review of integrated TEA and LCA assessments that in many cases the goal statement did not explicitly cover both an environmental and an economic objective. Such a failing is problematic in two ways: First, an incomplete goal statement makes the iterative approach followed in these types of study difficult to complete; second, the written goal statement is a form of communication between the practitioner recording their study and the reader of the report. In other words, an incomplete or ill-defined goal statement leaves open the potential for error in either the completion or later analysis of a study. Therefore, an integrated goal statement **shall** explicitly state both an economic and an environmental component.

In response to this, an integrated goal **should** state which types of integration (detailed in section A.5.2) are to be deployed: qualitative, discussion-based integration; combined indicator-based integration; and/or preference-based integration.

Finally, even if a goal statement covers both an economic and an environmental aspect, consideration **shall** be given to ensuring that an integrated TEA and LCA study is the most appropriate format for achieving the stated goal. To aid with this, the following section explores the concept of an integrated TEA and LCA research question in more detail.

E.3.2 Integrated Assessment Research Questions

E.3.2.1 Research Questions in TEA and LCA for CCU

It is stated, and evidenced, in the TEA and LCA chapters that these methodologies can be used to answer many different types of question. The LCA guidance presents four 'most common research questions' (as derived from a literature review), from which some parallels can be drawn within the TEA 'common goal-related questions' (see sections C.3.1 and B.3.2.2.3 for more details). The common themes in both are explored within Table 1.

Table 1 – Common themes in TEA/LCA assessment goals for CCU

Thematic Element	LCA Guidance	TEA Guidance
Comparisons to a benchmark or other emerging alternative	Covered in the 1st common research question	Covered in the R&D and corporation perspectives
Hot-spotting (identifying major factors contributing to overall performance, through contribution analysis)	Covered in the 2nd common research question	Covered in the R&D and corporation perspectives
Best use of a constrained resource (e.g., pure CO_2 or renewable energy)	Covered in the 3rd common research question	Covered in the market perspective
Product certification/declarations	Covered in the 4th common research question	Not explicitly covered – product declarations are typically environmentally focused
Development or assessment of policy support for technology deployment	Not explicitly covered	Covered by market and corporation perspectives

E.3.2.2 What Does This Mean for Integrated Studies?

The common themes addressed in TEA and LCA studies for CCU appear to remain consistent in the limited published examples of integrated assessment as shown in recent publications [9][10]. This is to be expected, given that many of these themes tie directly to the realities of CCU:

- CCU technologies in general aim to be 'disruptive' technologies that displace existing routes to deliver the same functionality but ideally at a competitive price point and with a lower environmental impact. Consequently, there is a need for comparative studies; without comparison against benchmark technologies or other alternatives, it can be difficult to quantify sufficient performance in the metrics of interest – be they economic or environmental, or a combination of both for an integrated study
- The CCU field is dominated by processes and technologies in the TRL 3 to 8 range, with a general focus on identifying developmental pathways to full scale deployment. Whilst benchmarking provides some insight into performance against an alternative, it can lack the granularity needed to derive decisions regarding research direction. Beyond this, comparative studies at low TRLs carry significant risk of comparing emerging technologies against established and optimized ones, which may lead to poorly informed decision making. Therefore, whilst comparisons against a benchmark may be beneficial, in many cases understanding which elements contribute to the overall performance may be of equal or greater value. Further details on this can be found in Chapter D (the low-TRL guidance chapter) and in the paper produced by the International CCU Harmonization Group on this subject [11]. It is here where contribution analysis can be of assistance for adding this granularity, providing details on how different elements of the process contribute to the overall result in a given indicator
- The use of constrained resources is common in CCU technologies, such as low-fossil carbon electricity and high-purity CO_2. With such resources there is often a focus on attempting to maximize the economic return and/or the reduction in environmental impact for their use. Assessing alternative routes that offer these best returns can be bolstered by TEA, LCA, or integrated assessment

All three of the above themes fit with the proposed use case (discussed in the Introduction of this chapter) for integrated assessment within CCU. Each of the three cases can benefit from integrated assessment, where analysis of the combined eco-enviro performance and an understanding of potential trade-offs between the two offers additional insight. Taking the above and considering integrated studies in particular:

For comparative studies, being able to assess likely performance against both an economic and environmental benchmark/alternative allows for a more detailed analysis of performance to be considered. Figure 5 shows how performance in both 'dimensions' can be compared against a benchmark or alternative. The 'better–better' and 'worse–worse' performance quadrants are easy to interpret, but the remaining two present challenges, especially when no obvious Pareto improvements are available (a Pareto improvement here being defined as the ability to improve performance in one category without making another category worse).

Specifically, these issues can be posed as questions: *Is better performance in one dimension worth an offset in the other?* And *how much better does the performance in one dimension have to be to offset poorer performance in the other?* Given the multi-criteria nature of this problem, no singular answer can be given; instead, it a necessitates a subjective choice that will impact decision making.

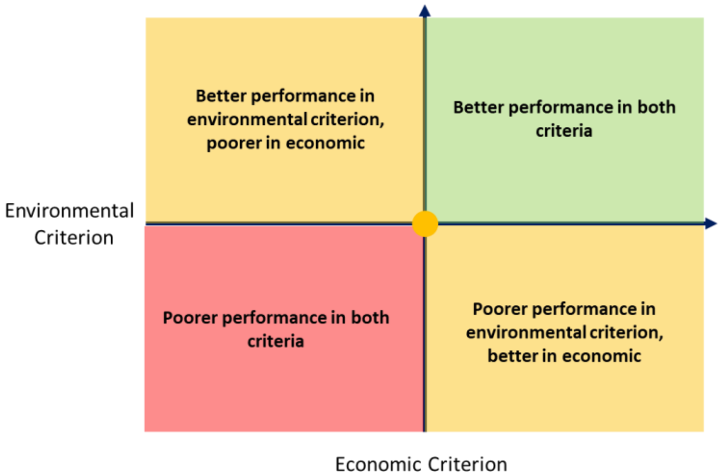

Figure 5 – Performance matrix for comparison against an alternative or benchmark process (orange dot)

An integrated assessment can help quantify the scale of this trade-off (or trade-offs if multiple assessment indicators are considered), providing additional decision support if required when assessing against the benchmark/alternative. It should be noted that, for CCU, when comparing against a current market-dominant benchmark or other emerging alternative, poorer environmental performance by a candidate CCU counterpart is likely to be undesirable regardless of potential economic gains. Therefore, in most cases the focus is likely to be on the inverse scenario: assessing whether there is sufficient improvement in environmental performance to offset potentially poorer economic efficiency.

Contribution analysis within integrated assessments offers the potential to identify if there are any contributors that are both economic and environmental hotspots, with this potentially helping to strengthen decisions made on research direction for example. Contribution analysis is discussed within the TEA, LCA, and low-TRL chapters and so is not extensively discussed here, but the same basic principle can be applied: 'unit processes within the product system that are shown to be significant contributors shall be suggested as focal points for further R&D.' With the consideration of both economic and environmental dimensions there is an added complexity in determining an apparent 'order of priority' for this focus. Implementing multi-criteria decision analysis (MCDA) in the interpretation of the study may offer some advantages here.

When considering constrained resources, integrated assessment can offer the benefit of ensuring that use of these resources is optimized with regard to both environmental and economic aspects. Once again, decision making is made more complex in multi-dimensional studies by the need to determine the 'optimal' use case. As in the above case, MCDA can help the practitioner/study commissioner in determining a preference or preferential order.

E.3.2.3 Example Research Questions

The following research questions are derived from their counterparts in the LCA; these questions **may** be used or other alternatives may be proposed.

In addition to this, the prior chapter on low-TRL assessment lists a number of research questions for the 'monitoring' and 'R&D support' activities outlined in that chapter. In many cases it may be beneficial to apply integrated TEA and LCA during these low-TRL assessments.

Table 2 – Transforming common LCA research questions into integrated TEA and LCA ones

LCA common research question	**Proposed integrated research question**
Is a CCU-based product or service environmentally beneficial compared to the same product or service derived from fossil carbon sources?	How does the economic and environmental performance of a CCU product or service compare to its fossil carbon-derived counterpart?
Where are the environmental hot spots for technology improvement to reduce environmental impacts in the life cycle of a CCU product/process?	What impact does addressing environmental hotspots for technology improvement have on the economic performance of a CCU product/process?
What is the environmentally preferred CCU technology to make best use of a scarce resource, e.g., renewable energy?	What is the preferred CCU technology when trying to maximize economic return & minimize environmental impact to make best use of a scarce resource?
Low-TRL assessment research question	**Proposed integrated research question**
Monitoring example question Does the information available at the current R&D status/maturity level indicate a potential to reduce environmental impacts/costs?	Does the information available at the current R&D status/maturity level indicate a potential to reduce environmental impacts and costs? Are there any relationships between the two that warrant further investigation?
R&D support (screening) example question What are the most promising process/product options, e.g., products, reactants, catalysts, reactors, separation units, solvents?	Applicable in given form; however, it may be worthwhile stating that 'promising' in this sense would involve both economic and environmental considerations

E.3.2.4 Provisions

Provisions E.1 – Goal: Definition	
Shall	3) The goal **shall** follow the provisions outlined in the guideline rules C.1 particularly with respect to: state the study context; the intended application; the target audience; the commissioners & authors of the study; and any limitations on usability 4) The goal statement **shall** explicitly state both an economic and an environmental component 5) Consideration **shall** be given to ensuring that an integrated TEA and LCA study is the most appropriate format for achieving the stated goal.
Should	3) The goal **should** also state the perspective (R&D, corporate, market) where possible 4) The goal **should** state which types of integration are to be deployed: qualitative, discussion-based integration; combined indicator-based integration; and/or preference-based integration
May	3) The goal **may** be drafted prior to considering the use of an existing TEA or LCA study, and where possible elements of the existing study **may** be used 4) The goal **may** address one of the research questions provided, or an alternative can be used if required

E.4 Scope Definition

General Introduction and Challenges

ISO 14040 states that the scope of an LCA study needs to '*be sufficiently well defined to ensure that the breadth, depth and detail of the study are compatible and sufficient to address the stated goal*' and this approach also holds for integrated studies. As established in Chapters B (TEA guidance) and C (LCA guidance) the scope **shall** describe the conditions and assumptions under which the results are valid. For integrated studies, these assumptions and conditions (namely functional unit, product system, and reference flow) **shall** be consistent across both the TEA and LCA constituent studies in addition to the resultant combined assessment. The product system boundary for an integrated study **shall** be consistent with that of the constituent LCA. Dependent on the study goal and the product system, the constituent TEA **may** draw additional internal boundaries when necessary, e.g., when there is a need to demarcate asset ownership and the implications this has for economic calculations.

E.4.1 Scope Overview

After setting a study goal, attention can be turned to outlining a study scope. In the prior TEA and LCA, scope definition covers a range of activities that define and describe key aspects of the study; with the TEA chapter adopting and modifying existing LCA practices for economic assessment. In doing this a certain amount of symmetry can be seen between the two methodologies, however, significant challenges remain with regard to integrating both into a singular structure that does not invalidate existing methodologies or limit their capacity to address the stated study goal.

For integrated studies the tasks that fall within scope definition remain the same as those outlined in the LCA chapter, with these requirements derived from ISO 14040 and the ILCD handbook. The following aspects need to be described or defined:

- The product system or process to be studied, its function, functional unit, and reference flow
- System boundaries, completeness requirements, and related cut-offs
- Co-product management approach to be taken
- Inventory data requirements
- Additional requirements for comparative and externally published studies

Additionally, for the TEA element, assessment indicators are chosen during the scope phase. To mirror this, techno-economic indicators and combined eco-enviro indicators **shall** be selected in accordance with the goal during the scoping phase of integrated assessments. When the product system has been determined, a block diagram of the system **shall** be drawn; at this point, detailed labelling of elementary flows is not necessary. The selection of indicators and the block diagram **shall** be agreed upon by all relevant stakeholders.

As stated earlier in this chapter, the intention within these guidelines is to maintain the integrity of the LCA element of an integrated study, which means ensuring methodological compliance with the relevant standards and guidance. The intention of this integrated methodology for CCU assessment is based on the concept of exploring how financial or economic choices may impact the broader environmental scope. There is no point in developing so-called 'sustainable' CCU technologies that damage the environment. This needs to be kept in mind by both the practitioner and other stakeholders when determining what is captured within the product system boundary. Additional guidance on this matter can be found in section E.4.3.

E.4.2 Product System, Functional Unit, and Reference Flow

The definitions of product system, functional unit, and reference flow remain consistent with those established in LCA, covered in the relevant chapter (C.4.1). Thus, the product system **shall** contain all the processes relevant to the integrated assessment, and a functional unit that quantifies the technical performance of the whole system **shall** be defined unambiguously. For a combined assessment the functional unit used needs to be consistent throughout all study aspects. The TEA and LCA chapters provide guidance on how to define reference flows that make up this function unit, and the guidance therein remains valid here. Should additional details be required, section C.4.1.1 provides a simple decision tree, but for completeness:

- Comparisons made on fuels with identical chemical structure and composition **shall** be made on an energy content basis
- Comparisons made on non-fuels with identical chemical structure and composition **shall** be made on a mass basis
- Comparisons made on fuels with a non-identical chemical structure and composition **shall** be made on quantification of an energy service
- Comparisons made on non-fuels with a non-identical chemical structure and composition **shall** be made on quantification of a technical service
- Comparisons of energy storage systems **shall** be made on a basis that satisfies the energy demand over a period of time

The TEA guidelines discuss product applications explicitly; here, an assumption is made that all product applications will fall within one of the above categories, provided that a suitable and specific description of the service can be made. With sufficient specificity the desire to compare '*high-quality products with other high-quality products*' can be met, thus any product application needs **should** be discussed in sufficient detail within the scope and captured within the relevant reference flow.

E.4.2.1 Provisions

Provisions E.2 – Scope: Product System, Function Unit, Reference Flow	
Shall	1) The product system **shall** contain all the processes relevant to the integrated assessment 2) A functional unit that quantifies the technical performance of the whole system **shall** be defined unambiguously 3) The decision tree in section C.4.1.1 **shall** be consulted for the determination of a suitable reference flow (see text above for a summary of options)
Should	1) Any product application needs (e.g. a want to compare 'high quality products to other high quality products) **should** be discussed in sufficient detail within the scope and captured within the relevant reference flow
May	

E.4.3 System Boundaries, Completeness Requirements, Related Cut-Offs, and Solving Multi-Functionality

The system boundary defines which processes and life cycle stages are needed to fulfill the function as defined by the functional unit, and thus are part of the analyzed product system. The product system boundary delineates what is included within the product system and what is not, with input and output flows between the technosphere and the ecosphere (elementary flows from the ecosphere, releases to the ecosphere and product/technical flows from and to the technosphere).

The approach to handling the function unit remains largely the same – if multiple reference flows are captured in the functional unit the relationship between these flows **shall** be defined by the practitioner with respect to the physical properties of the system (i.e., if a tonne of methanol is to be part of the functional unit, the amount of the symbiotic product should be derived from the emission factor for the product and the amount of CO_2 needed to produce the methanol).

The approach to setting the product system boundary in integrated assessment is consistent with that used in TEA and LCA, and this also extends to identifying which phases of the product life cycle are included for assessment (e.g., cradle to gate or cradle to grave).

When considering a stand-alone TEA study there are valid CCU cases in which gate-to-gate boundaries can be applied; however, assessing on this basis within an LCA study is not recommended due to the potential for misinterpretation and misrepresentation of the broader product life cycle.

So what drives this difference? The answer to this question lies in what a gate-to-gate study achieves, namely the analysis of performance within a single 'value added' process within the entire life cycle. Linking together singular processes as part of a large value chain, as is done in cradle-to-gate or cradle-to-grave studies, provides significantly more insight into the burdens and particular hotspots associated with the production, use, and disposal of a product. The goals of an LCA study cannot typically be met by considering such a limited scope.

However, in TEA it is perfectly feasible to be interested in a narrower part of the value chain, such as a singular 'value added' process. This is reflected both in the goals frequently set for these studies, especially in the R&D or corporate perspectives, and in the indicators often selected. For TEA, determining that a unit process or a series of unit processes controlled by a singular stakeholder (e.g., the owner of a chemical plant) is economically viable provides a useful conclusion. For most cases, if one or more unit processes are shown to be economically unviable through gate-to-gate studies then questions can be raised over the viability of the entire supply chain as modelled.

This means that in order to preserve compliance with the ISO standard for the constituent LCA, any integrated assessment **shall** operate on either a cradle-to-gate or cradle-to-grave basis. The LCA guidance provides a simple flowchart for determining which of these two alternative system boundaries **shall** be applied (see Figure 5 in Chapter C.4.2 for more details).

Preserving the validity of the constituent LCA is a priority in these guidelines for integrated assessment. Failure to preserve the methodology introduces the risk of misrepresenting the product system, resulting in poor interpretation and leading to the potential to arrive at conclusions that do not accurately address the intended study goal.

This then poses questions for how to handle the constituent TEA elements of an integrated study, with this ultimately decided by the goal. If the economic aspect of the study goal naturally aligns in scope with the environment aspect, for example if the standalone TEA and LCA to assess the individual goal aspects would require the same system boundary and constituent unit processes, then the established methodology for dealing with multifunctional products systems **shall** be followed. For example, a broader 'market perspective' TEA may be interested in determining economic viability for a CCU process across the whole supply chain and this would align with a cradle-to-gate/grave LCA. The majority of mono-functional CCU processes (e.g., those that use direct air capture for a CO_2 source) are also likely to fall within this category.

Further details can be found in section C.4.3.2, but in summary the hierarchy of methods for solving multi-functionality is:

1. Sub-division
2. System expansion
3. System expansion via substitution
4. Allocation on underlying physical causalities
5. Allocation on other underlying relationships (e.g., value)

However, in many cases the economic aspect of an integrated study goal will not align with that of the environmental aspect. For example, the integrated study goal may only concern determining how economically viable a specific unit process is, rather than the entire cradle-to-gate (or grave) system. This is common in CCU where new technologies can be inserted into existing supply chains, and where the new technology may not necessarily be owned by the same stakeholder who owns the symbiotic CO_2-producing plant. Thus, the intended integrated study goal could be to assess the economic viability of the inserted CCU process whilst also assessing how this changes the broader environmental impacts of the product system.

Even if this is the case the entire product system outlined for the LCA **shall** be assessed, and the ways in which the economic performance & techno-economic aspects of this are handled will likely depend on the data available to the practitioner. Here the challenge likely becomes one of dealing with variable granularity in data for each unit process within the system. A balance must be found between assessing system-wide economic performance with that of the specific unit process/processes of interest (analogous to foreground and background in LCA).

In general, modelling the techno-economic performance of the entire product system in detail will likely be the most ideal solution. The benefits to this more granular approach are clear: a better understanding of the technical and economic performance of the whole system and the relationships that exist between the sub-systems (e.g., what impact does resolving an upstream 'hotspot' have on a downstream unit process). But this requires data, much of which may not be readily available. For LCA, existing databases provide a basis for assessment – one in which the relationship between technical performance and environmental impact is well described.

For TEA, there is no equivalent dataset, and many aspects that drive a production cost or a minimum selling price to break even are specific to a given plant/product system or unit process. Whilst not ideal, local/regional 'free on board' market prices for products, co-products, and by-products provide a reasonable proxy for costing flows that cannot be modelled in detail. In this sense, an assumption is made that price is at least in part a function of cost and that long-term operation of a unit process is generally only viable if it is economically sustainable (e.g., that the production cost of goods sold does not exceed the sales revenue).

There are clear limitations to this approach:

- Whilst related, market prices are not production costs, and market forces are complex and differ from product to product
- Using a market price prevents detailed techno-economic analysis of the specific unit process of interest, and this will impact the interpretation and conclusions of the study. How impactful this is will depend on the study goal
- The relationship between additional costs for dealing with by-products (e.g., carbon taxes, treatment of wastes such as fly ash) and the impact this has on production costs for products and co-products cannot be explored in detail without sufficient cost modelling, leaving it relatively obscure. Qualitative analysis may be possible, but no detailed quantitative breakdown will be available

For example, considering CCU specifically, products that are not a long-term carbon sink will still likely oblige the product system to pay associated carbon taxes (if applicable) and this then becomes a cost to be allocated between the existing products and co-products and the new CCU product. Alternatively, long-term storage in mineralization products likely sees the avoidance of such taxes, and the resulting benefit of lower costs would then require allocation between the existing products and co-products and the new CCU product.

How these potential changes impact local market prices for all products and co-products will depend a multitude of factors that may be difficult to accurately analyze within the scope of a study. The scale of the product system analyzed versus the scale of the market for each product is anticipated to be of importance here. In most cases it is likely that the scale of the market is vastly greater than that of the product system and that market prices are not impacted by the implementation of the CCU product system investigated. This simplifies the problem somewhat, leaving only the change in economic burden/benefit to be assigned between the unit processes as determined by the practitioner.

With this in mind the following guidance is provided:

In many cases it may not be feasible or desirable to model the entire economic performance of the product system in great detail. At this point, cut-offs for detailed economic modelling **may** be identified; if used, these **shall** be described and clearly stated in the limitations of the study. Where these cut-offs are drawn will likely be influenced by the goal, the study perspective, and the relevance of costs versus prices for the stakeholder of focus (i.e., how the flow impacts their internal costs).

All reference flows in the functional unit **shall** have a monetary value reported, either calculated or derived from other data sources when cut-offs are used.

E.4.3.1 Visual Representations of the Schemes Discussed Above

This section aims to illustrate some of the scenarios described above for ease of interpretation. A system is proposed for the production of methanol, coupled with a CO_2-producing industry, with the functional unit comprising of methanol and a product.

Comparison Case

The comparison case system is shown in Figure 6, with the production of the unspecified product and methanol considered as standalone processes. The blue border denotes the system boundary, and the purple border denotes detailed economic modelling.

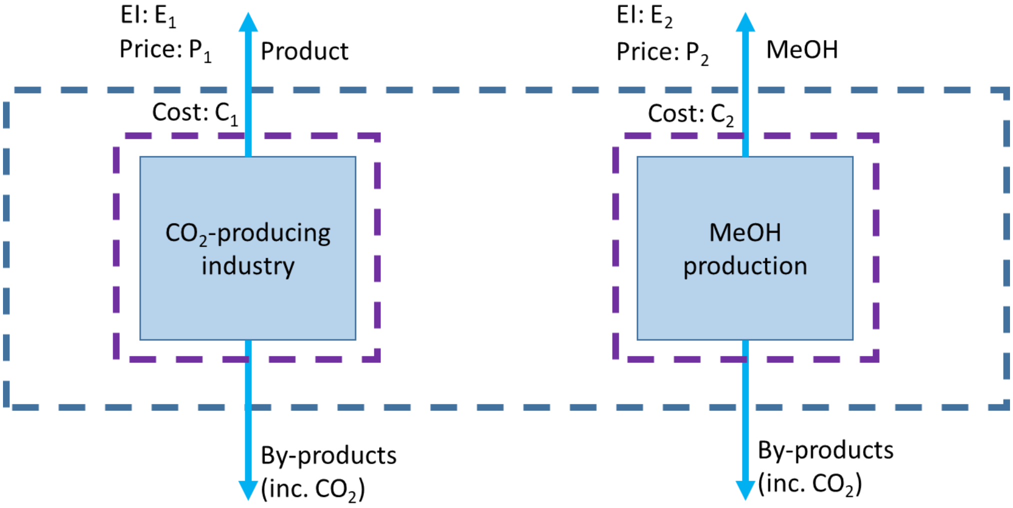

Figure 6 – Comparison case system diagram

For each flow in the functional unit an associated environmental impact (EI) is calculated, a market price (P) is stated, and some representation of production cost (C) is calculated. From this a number of relationships can be drawn:

Environmental impact for the entire functional unit = $E_1 + E_2$

Production cost for the entire functional unit = $C_1 + C_2$

Market value of the functional unit = $P_1 + P_2$

Profit derived from the sale of the functional unit = $P_1 + P_2 - C_1 - C_2$

Ideal CCU Case: System Expansion

A schema for the CCU system in which the entire product system has full alignment between the detailed economic and environmental modelling is given below in Figure 7 (i.e., complete system expansion).

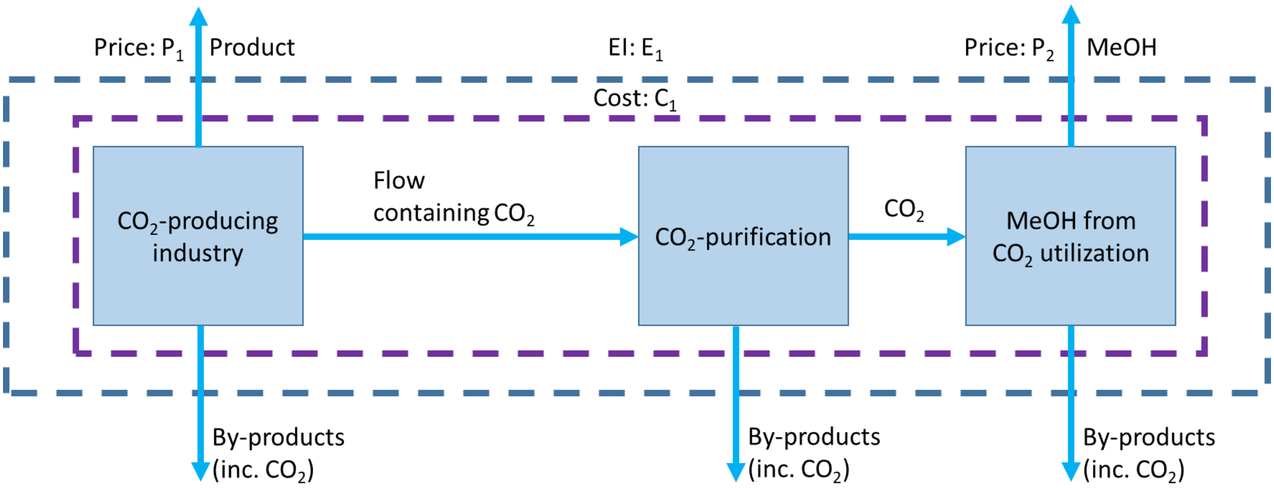

Figure 7 – CCU product system with full alignment in assessment scope

This is the preferred approach for handling multifunctional product systems, as this allows for the most detailed modelling of both economic and environmental performance across the entire product system.

The whole system is modelled and a singular cost (C_1) and an associated set of environmental impacts (EI_1) are calculated. This system expansion approach is the most objective available [12], due to its avoidance of allocation of any kind. In the above form the system can:

- Easily be compared directly against the reference system in terms of total cost & total environmental impact
- The impacts of changes made to minimize EI or C can be investigated without the need for assumptions with regards to allocation
- Identify whether the whole system is profitable

The only real disadvantage to the system as modelled above is that impacts are calculated on a whole-system basis, which may be problematic if the whole product system is not owned or operated by the same stakeholder. Demonstrating reduced environmental impact and economic viability in the product system is beneficial but the distribution of this may be of great interest to the specific stakeholders.

However, if required, this can be handled by allocating costs and environmental impact across the reference flows in the functional unit. If allocation is used to divide the whole system impacts and costs between stakeholders/products this **shall** be done in addition to determining the whole system performance.

Alternative CCU Case: Allocated System

The final approach illustrated is the alternative approach, in which only part of the system contains detailed economic modelling. Here, a method for compensating with monetary flows is provided for situations when production costs for the symbiotic CO_2 producing industry cannot be calculated. Figure 8 shows a schema for this scenario.

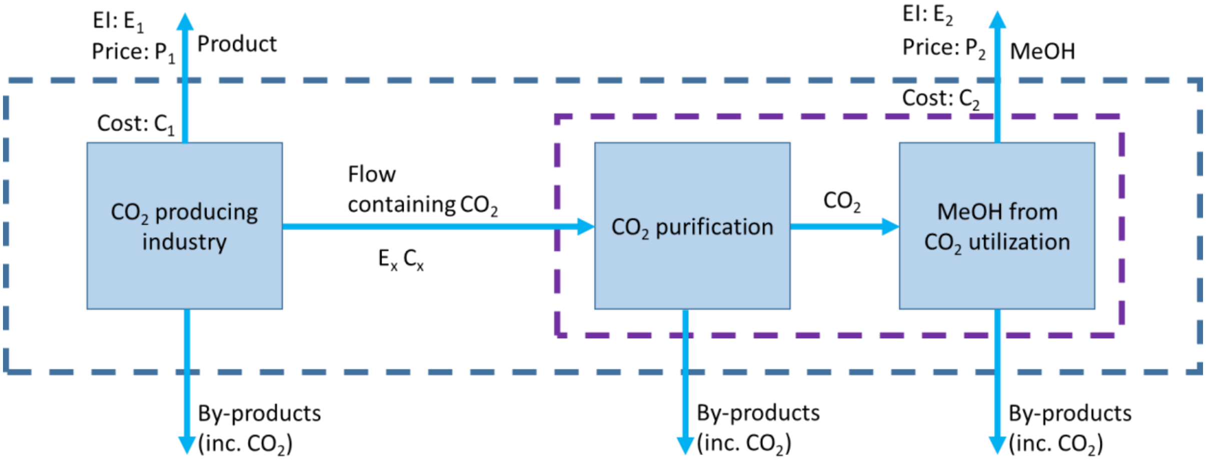

Figure 8 – CCU product system with limited alignment between detailed economic and environmental assessment scope

Rather than providing economic oversight of the whole system, the focus shifts to a singular unit process (or sub-set of these). The functional unit still requires monetary values for all functional flows, but these are now taken to be relative to the CCU plant:

- The cost of producing the symbiotic product for the CCU plant is assumed to be P_1 , i.e., the price required to purchase this from the market
- CO_2 is now treated as a co-product and can be assigned a price and/or allocated some of the environmental impact from the CO_2-producing industry (E_x and C_x); these values will be embedded in the costs and environmental impact profile for the CCU product
- For the purpose of quantitative analysis, changes in the product system should only be considered for the parts of the product system (in this case the CCU unit process) that can be altered by the 'stakeholder of focus'

The relationships described in the comparative case can still be applied here, with the added condition of: $P_1 = C_1$, which narrows the detailed economic picture that of the CCU and CO_2 capture unit processes.

E.4.3.2 Provisions

Provisions E.3 – Scope: System Boundaries, Completeness Requirements, Related Cut-Offs and Solving Multi-Functionality	
Shall	1) Flows **shall** be defined by the practitioner with respect to the physical properties of the system 2) Any integrated assessment **shall** operate on either a cradle-to-gate or cradle-to-grave basis 3) The system boundary applied (cradle to gate or cradle to grave) **shall** be determined as handled within LCA as shown in the decision tree in section C.4.2.1 4) If the economic aspect of the study goal naturally aligns in scope with the environment aspect, for example if the standalone TEA and LCA to assess the individual goal aspects would require the same system boundary and constituent unit processes, then the established methodology for dealing with multifunctional products systems **shall** be followed as detailed in section C.4.3.2 5) The entire product system **shall** be assessed, with costs/monetary values provided for all flows in the functional unit, even if cut-offs for detailed economic modelling are used 6) If allocation is used to divide the whole system impacts and costs between stakeholders/products this **shall** be done in addition to determining the whole system performance
Should	
May	1) Cut-offs for detailed economic modelling **may** be identified; if used, these **shall** be described and clearly stated in the limitations of the study

E.4.4 Selection of Indicators

For an integrated assessment, four broad classifications of impact assessment indicators can be considered: environmental, technical, economic, and combined.

Selecting appropriate indicators is also a task handled in the scope phase. For LCA there is typically little discussion to be held on the selection of indicators, with the mid-point (and end-point if required) indicators typically determined through the selection of an impact assessment method. Guidance on selecting an impact assessment method for LCA can be found in Chapter C.6.1 (where CML is determined to be the default methodology, but additional, geographically appropriate methods may also be applied).

The TEA guidance provides an introduction to both technical and economic indicators (see Table 4 in the TEA guidelines within section B.4.5.2 for common CCU examples).

Technical performance indicators provide insight into the performance of the product system as a whole and also specific unit processes within, if required. These indicators influence both economic and environmental indicators, which is something to keep in mind throughout the study – for example, the 'technical-environmental' and 'technical-economic' need to maintain the same technical basis (e.g., the same energy demand for a given unit process), as failure to do this can result in serious errors during later phases.

Within TEA, economic indicators are typically more variable than the already mentioned environmental ones, with their selection largely determined by the study goal and scope; This approached can be also be applied to integrated studies.

Technical, economic, and environmental indicators **shall** be selected to best suit the needs of the study, with this defined by the study goal and scope.

The final class of indicators to consider are combined indicators, and these **may** be selected if deemed beneficial in achieving the study goal. Here, combined indicators are taken to typically be a combination of an economic and an environmental dimension. No definitive approach is given within these guidelines for the selection of combined indicators; Practitioners can pursue any avenue they deem viable on the basis that:

- If used, all combined indicators **shall** be explained in detail, and the method to calculate these communicated clearly

E4.4.1 Eco-Efficiency Principles for Combined Indicators

Whilst no definitive approach is given, this section is dedicated to exploring the development and deployment of combined indicators that draw from the concepts outlined in eco-efficiency. A more detailed introduction to the concepts of eco-efficiency can be found in the relevant ISO standard (ISO 14045 [5]), in a range of other publications [13][14][15][16], and in various publications that use the concept of eco-efficiency to derive indicators, measures, or frameworks [17][18][19]. On the largest of scales, eco-efficiency can be applied to the activities of nations in economy-wide assessments, however the initial driver for its development was as a tool for the business sector. In both cases the base concept remains the same: generate more goods and services whilst using fewer resources and generating less waste and pollution [20]. Thematically, this concept ties neatly with that of CCU and the broader circular economy; with a general goal of producing more whilst extracting fewer resources.

ISO 14045 defines eco-efficiency as:

(An) *aspect of sustainability relating the environmental performance of a product system to its product system value*

The required 'environmental performance' can be determined through LCA or other environmental impact assessment methods that use 'life cycle thinking.' 'Product system value' is a broader term within the guise of the ISO standards, where value can encompass functional, monetary, esthetic, or other aspects.

This definition of system value leads to an equally broad scope for the development of indicators within the bounds of the ISO; with the definition of an eco-efficiency indicator being '(a) *measure relating environmental performance of a product system to its product system value.*'

With the general principles defined, attention can now be turned to applying these to the specific case of integrated TEA and LCA for CCU.

ISO 14045 states that LCIA can be used to determine environmental performance, with the usual caveat that weighting **shall** not be used for comparative eco-efficiency assertions made publicly.

TEA indicators can be used to determine a monetary value for the product system value. For the purpose of eco-efficiency, monetary value can be expressed in a range of terms: costs, prices, willingness to pay, added value, profit, and future investment are all valid examples. Not all of these can be readily determined from the calculation of TEA indicators; and the suitability of others will depend largely on the specific assessment. The measures of cost, price, and profitability are discussed earlier within the Scope section – which of these indicators are selected to represent product system value will depend on the particular assessment and the intended goal.

The quantification of eco-efficiency within the scope of the ISO standard is also relatively open, with the condition that eco-efficiency **shall** be determined by relating the results of the two assessments according to the goal and scope.

With this in mind, eco-efficiency type indicators **should** be selected to meet the needs of the goal and scope – providing that the pre-requisite environmental and economic performance indicators can be calculated for the product system.

A common (but not the only) way of deriving eco-efficiency is to consider the ratio between system value and environmental impact:

$$Eco\ efficiency = \frac{Product\ system\ value}{Environmental\ impact} \qquad \text{(Equation 1)}$$

The environmental impact used can be a singular mid-point indicator (e.g., global warming), an end-point indicator, or a weighted overall score (albeit with the latter not to be used for public assertions as stated above).

It can be seen that eco-efficiency can be improved by either increasing product system value or decreasing environmental impact. If a ratio is to be used, the eco-efficiency indicator **shall** be structured in a way that maintains the condition that a larger value for eco-efficiency consistently equates to a more eco-efficient system.

Given that eco-efficiency indicators are always comparative; normalization is also frequently applied against an identified reference point. When normalizing performance, the '**shall**' provision above is a necessary consideration, and how this is structured will depend on what 'improved performance' means for a given indicator:

- If production costs are to be used, an improvement in system value would see a decrease in production cost for the functional unit. This will see the numerator in the eco-efficiency ratio (shown in equation 1 above) increase, and should be structured as: $\frac{Production\ cost_{reference}}{Production\ cost_{assessed}}$
- If system value is determined by profitability the inverse will be true – greater profit would increase system value, and so the inverse structure should be used: $\frac{System\ profit_{assessed}}{System\ profit_{reference}}$
- For environmental quantities (specifically in this case environmental impacts), a decrease in numerical value would see an improvement in performance for the functional unit. This will see the denominator in the eco-efficiency ratio (Equation 1) decrease, and should be structured as: $\frac{Environmental\ impact_{assessed}}{Environmental\ impact_{reference}}$

E4.4.2 Assessing Cost Trade-Offs as Indicators

Calculating relative costs is not a new concept within CCU or CCS. Assigning a cost to carbon avoided and cost of carbon abated have been discussed extensively in various literature sources [21][22][23], and provide some contextual background for assessing cost trade-offs.

As with the eco-efficiency indicators discussed in the prior section, trade-off indicators are calculated on a comparative basis and **shall** be selected with reference to the goal and scope. A general form can be derived, with two indicators (X and Y) for two comparative cases (1 and 2):

$$Change\ in\ X\ per\ change\ in\ Y = \frac{X_1 - X_2}{Y_2 - Y_1}$$

X and Y can be any indicator, but for integrated eco-enviro indicators one indicator from each of the TEA and LCA set **shall** be selected.

This type of indicator has been introduced elsewhere in these guidelines (see A.5.2.2) in the form of GHG abatement costs, and further discussion on these indicators can be found there.

E.4.4.3 Provisions

Provisions E.4 – Scope: Selection of indicators		
Shall	1)	Technical, economic, and environmental indicators **shall** be selected to best suit the needs of the study, with this defined by the study goal and scope
	2)	If weighting is applied to indicators, weighted results **shall** not be used for comparative assertions on any type of indicator
	3)	If eco-efficiency type indicators are used, eco-efficiency **shall** be determined by relating the results of the two assessments according to the goal and scope
	4)	If a ratio is to be used, the eco-efficiency indicator **shall** be structured in a way that maintains the condition that a larger value for eco-efficiency consistently equates to a more eco-efficient system
	5)	Trade-off indicators are calculated on a comparative basis and **shall** be selected with reference to the goal and scope
	6)	For integrated eco-enviro indicators one indicator from each of the TEA and LCA set **shall** be selected
Should	1)	Eco-efficiency type indicators **should** be selected to meet the needs of the goal and scope
May	1)	Combined indicators **may** be selected if deemed beneficial in achieving the study goal. If used, all combined indicators **shall** be explained in detail, and the method used to calculate these communicated clearly

E.4.5 Additional Requirements for Comparative Studies

The section 'Special Requirements for Comparative Studies' in the LCA guidance provides two basic principles that **shall** be adhered to, namely:

- 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.

For integrated studies, a study **shall** only be compared with others that employ the same boundaries for detailed economic and environmental modelling. If eco-efficiency-type indicators are to be used and communicated publicly, an eco-efficiency profile **shall** be determined by relating the LCIA profile to the product system value.

E.4.5.1 Provisions

Provisions E.5 – Scope: Additional Requirements for Comparative Studies	
Shall	1) Any study for external communication **shall** be reviewed 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 3) For integrated studies, a study **shall** only be compared with others that employ the same boundaries for detailed economic and environmental modelling 4) If eco-efficiency-type indicators are to be used and communicated publicly, an eco-efficiency profile **shall** be determined by relating the LCIA profile to the product system value
Should	
May	

E.5 Integrated Assessment Inventory

General Introduction and Challenges

For integrated assessment, the inventory phase is a primarily a merger of the inventory processes outlined in the individual study types, albeit with significant overlap with regards to some data points such as technical data. Thus, there are also some additional requirements to ensure sufficient data alignment across multi-faceted entries.

The inventory phase for both TEA and LCA sees the gathering of data and the modelling of the product system in accordance with the needs of the defined goal and scope. The data-gathering requirements for both TEA and LCA are well described in earlier chapters, and these principles **shall** be adhered to.

Integrated studies **shall** state the degree of precision required for alignment between data used in each constituent study. Where possible the data provided for the constituent economic and environmental aspects of the inventories **should** consider data that provide a consistent approach to temporal, locational, and technical performance (e.g., market average, 'best in class') aspects; deviations from this **shall** be clearly stated and explained.

Should there be a need to estimate data, a consistent methodology **shall** be used (and clearly explained in the report) across both the environmental and economic dimensions of the inventory. Further details on estimating data are provided in chapter D.5 of the low-TRL guidance part.

E.5.1 Inventory Overview

'The emissions and resources consumed linked to a specific product are compiled and documented in a Life Cycle Inventory' – ILCD Handbook.

After the goal has been defined and the scope of the study established, attention can turn to building an inventory for the study. As with TEA and LCA, the data requirements will be informed by the decisions made in the previous phases (goal and scope) of the study.

Whilst the focus in the preceding goal & scope phases is to fully integrate the approach, the inventory and the calculation of TEA/LCA indicators pose a different challenge. Here and in the calculation of indicators, much of the methodology can continue in 'parallel' – albeit with checks across both parts to ensure that methodological choices remain consistent. To clarify: 'Parallel' is used here to dictate that the methodologies described in the prior chapters remain mostly as described – environmental data are collected or estimated, validated, and recorded as described in the LCA chapter; and techno-economic data follow the same pattern. An integrated inventory can be seen as a merger of the required TEA and LCA inventories, with the data requirements defined within the scope. Ultimately whilst inventory building remains parallel there are some areas of significant overlap (e.g. technical data that may be of use in both TEA and LCA) – ensuring consistency in these areas can only strengthen the reliability of the outputs of the study and any conclusions drawn or recommendations made.

This approach mirrors, to a degree, that seen in ISO 14045 for eco-efficiency analysis – where environmental impact and product system value assessments are undertaken in parallel after determining a singular goal and scope.

With this amalgamation, the main challenge to inventory building also carries over from the constituent studies: the need to ensure a consistent methodological approach to data across the entire inventory. This challenge is not necessarily more complex to handle for an integrated study, but it does introduce a broader dataset to manage (technical, economic, and environmental).

E.5.2 Data Quality Goals & Product System Mapping

Whilst the methods can be considered in parallel, there are some tasks that only need to be completed once. In the scope definition phase, the system boundary and relevant unit processes are identified; as a minimum requirement a flow chart of the product system **shall** be included here in the inventory. Preferably, a more detailed flow chart **should** also be completed and included, showing representations of all relevant flows (both mass and energy); this flow chart **may** also include reference to other data points deemed of interest to the intended audience (e.g., monetary values for flows such as CO_2 or H_2).

Data quality goals **shall** also be reported, with reference to temporal, geographical, technological, and completeness requirements included. These requirements **shall** also specify a minimum acceptable level of correlation between environmental and economic aspects for the system or for specific elements within the system. This **should** be done with reference to a relevant pedigree matrix for data quality, such as those found in [24][25]. Failure to meet these data quality requirements requires revision of the goal and scope, or further data collection.

E.5.2.1 Provisions

Provisions E.6 – Inventory: Data Quality & Product System Mapping		
Shall	1)	A flow chart of the product system **shall** be included in the inventory that shows the system boundary and relevant unit processes
	2)	Data quality goals **shall** also be reported, with reference to temporal, geographical, technological, and completeness requirements included
	3)	The completeness requirements **shall** also specify a minimum acceptable level of correlation between environmental and economic aspects for the system or for specific elements within the system. This **should** be done with reference to a relevant pedigree matrix for data quality.
Should	1)	A more detailed flow chart **should** also be completed and included, showing representations of all relevant flows (both mass and energy)
May	1)	The flow chart **may** also include reference to other data points deemed of interest to the intended audience (e.g., monetary values for flows such as CO_2 or H_2)

E.5.3 Bridging Data Gaps with Estimation Methods

When using estimation methods to bridge data gaps, a consistent methodology **shall** be used across both the economic and environmental aspects. A consistent methodology in this case will cover both the approach used for estimating data and for the drawing of boundaries between unit processes.

Details on employing second law analysis, gate-to-gate inventory estimation, and artificial neural networks as estimation methods are provided in the LCA guidance and in the low-TRL guidance (see chapter D.5 for more details). These methods allow for estimation of technical performance, with this then used in part as a basis for generating the relevant economic and environmental data entries. If required, details on how to estimate the price of CO_2 or other key inputs (e.g., H_2) are provided in the TEA part (see chapters B.5.4 and B.5.5).

A problem unique to integrated studies is the potential to have scenario- / site- / deployment-specific data for either the economic or environmental aspect of the inventory but not the equivalent for the other aspect. For example, it is possible that a company may be willing to share environmental data on an input–output basis treating the plant as a 'black box' but may be more restrictive in its sharing of relevant economic/financial data. It is possible that data could be completely withheld, or only provided on a limited basis (e.g., aggregated costs in place of a detailed breakdown), potentially leading to problems for detailed modelling and investigating hotspots, for example.

If complete data are not provided (e.g., for confidentiality reasons) this **shall** be clearly stated, with clear reference to what data are provided and what are taken from other sources or estimations. Any generic data used **should** preferably be of similar temporal, geographical, and technological stature. If generic data are paired with site-specific data, this **shall** be clearly reported and the impacts **should** be investigated within the interpretation phase through sensitivity and uncertainty analyses.

E.5.3.1 Provisions

Provisions E.7 – Inventory: Bridging Data Gaps with Estimation Methods		
Shall	1)	When using estimation methods to bridge data gaps, a consistent methodology **shall** be used across both the economic and environmental aspects
	2)	If complete data are not provided (e.g., for confidentiality reasons) this **shall** be clearly stated, with clear reference to what data are provided and what are taken from other sources or estimations
	3)	If generic data are paired with site-specific data, this **shall** be clearly reported and the impacts **should** be investigated within the interpretation phase through sensitivity and uncertainty analyses
Should	1)	Any generic data used **should** preferably be of similar temporal, geographical, and technological stature
May		

E.5.4 Selecting a Benchmark Process or Technology

For comparative studies selecting a benchmark process or technology for the basis of comparison is an important methodological choice. Selecting an incorrect benchmark can lead to interpretation issues which may impact the outputs of the study. This methodological choice is just as important for integrated TEA and LCA as it is for singular dimensional studies.

However, little space will be dedicated in this part to discussing recommended guidance, due to the significant detail that can be found in parts B, C and D. Table 3 summarizes the recommendations made in earlier parts, and the recommended benchmark **should** be selected with regards to the maturity of the product system assessed.

Deviations from the recommended benchmark **should** be explained in the report.

Table 3 – Suggested reference case basis for CCU technologies of varying TRLs

Technology Readiness	Recommended Benchmark
TRL 1–4 (Concept/Lab)	As suggested in Part D of these guidelines: BIC GHG
TRL 5–6 (Prototype/scale-up)	As suggested in Part D of these guidelines: BIC GHG
TRL 7–8 (Demonstration/FOAK)	As suggested in Parts B and C: Marginal Cost
TRL 9 (Commercial/NOAK)	As suggested in Parts B and C: Marginal Cost

Definitions for both of the classifications are given below:

- **Best-in-Class (BIC) Technology** – Best-in-class technology is defined as the *process* or *product* with superior performance. BIC can be used as benchmark against which the *process* or *product* investigated is compared. Note that BIC can be defined according to environmental, economic or technical criteria
- **Marginal Cost** – Cost relative to one additional unit of production, that is the cost of producing one more unit of a good. Also defined as *Cost increment or Incremental cost*

Table 3 states a preference for using GHG as the BIC defining criteria for CCU studies, if an alternative definition is used this **shall** be stated and one consistent selection **shall** be used across the whole assessment. However, given that an integrated study considers both economic and environmental aspects it is feasible that some alternative criteria could be considered.

A strong preference for GHG is given here as the overarching aim of CCU is to reduce GHG emissions and selecting any other BIC classifier may risk misalignment with this goal. If marginal cost is used as the benchmark, a consistent definition of the marginal cost **shall** be defined and applied across all study aspects.

E.5.4.1 Provisions

Provisions E.8 – Inventory: Selecting a Benchmark Process or Technology	
Shall	1) If an alternative to GHG emissions is used as a 'best in class' classifier this **shall** be stated and one consistent selection **shall** be used across the whole assessment 2) If marginal cost is used as the benchmark, a consistent definition of the marginal cost **shall** be defined and applied across all study aspects
Should	1) A benchmark **should** be selected with regards to the maturity of the product system assessed: - For TRLs 1 to 6 'best in class' **should** be used as the benchmark - For TRLS 7 to 9 'marginal cost' **should** be used as the benchmark 2) Deviations from the recommended benchmark **should** be explained in the report
May	

E.6 Impact Assessment for Integrated Studies

General Introduction and Challenges

The impact assessment phase sees the computation of the assessment indicators using the data collected in the inventory. The prior TEA and LCA impact assessment guidelines outline how single-dimension indicators **shall** be calculated.

All CAPEX and OPEX calculations **shall** clearly state which system elements are considered within the bounds of each, ensuring that all of the product system is captured within the overall CAPEX and OPEX aggregations. To prevent misrepresentation, comparisons of CAPEX and OPEX **shall** only be carried out in situations where both the assessed and the comparison case use the same modelling approach

For integrated studies additional 'eco-enviro' indicators **may** be considered if required to achieve the intended study goal. The selection and derivation of these indicators will have already been reported clearly within the scope. If used, combined indicators **shall** be calculated using indicators that have a common basis for measurement.

Normalization and weighting **may** also be considered at this stage, although the necessity of this is likely to be decided by the goal statement and intended study outputs.

E.6.1 Impact Assessment Overview

In the impact assessment phase, the data captured in the inventory are used to calculate the impact assessment indicators selected in the scope. As with the inventory in the prior sections, some elements of indicator calculation can be seen as parallel tasks: LCA and TEA indicators can be calculated using the relevant inventory data and established methods, following the guidance provided in the prior chapters. With this in mind, TEA and LCA indicators for combined assessments **shall** be calculated within the bounds of the guidance already provided in earlier chapters.

For some studies, calculating a range of single-dimension indicators will provide sufficient results to meet the goal of the study in the interpretation phase. Examples could include studies in which the economic and environmental impacts are only to be explored qualitatively, or those in which attributional MCDA approaches are to be used in the interpretation phase. In other situations, combined 'eco-enviro' indicators **may** be considered if required to achieve the intended study goal.

E.6.1.1 Deriving CAPEX and OPEX for the Product System

The two approaches presented in section E.4.3.1 for handling expanded product systems employ different approaches to calculating OPEX and CAPEX.

In the expanded system approach, CAPEX and OPEX are calculated with respect to the whole product system and the functional flows. This can be presented on a whole-system basis, or in a disaggregated form if required.

In the allocated approach, economic modelling is taken on a basis relative to a singular unit process or group of unit processes, with the other reference flows 'purchased' at market price. Here CAPEX modelling will only cover what is captured within the detailed TEA model. The cost of purchasing the other reference flows is an operational one, but **may** be considered on a disaggregated basis separately from the OPEX calculated within the TEA model.

Two provisions are derived from the above:

- All CAPEX and OPEX calculations **shall** clearly state which system elements are considered within the bounds of each, ensuring that all of the product system is captured within the overall CAPEX and OPEX aggregations
- To prevent misrepresentation, comparisons of CAPEX and OPEX **shall** only be carried out in situations where both the assessed and the comparison case use the same modelling approach

E.6.2 Combined 'Eco-Enviro' Indicators

Practitioners may wish to proceed with the calculation of combined 'eco-enviro' indicators. Here, a broad definition is taken in which an 'eco-enviro' indicator is deemed to be any indicator derived from both an indicator of techno-economic and environmental performance.

The scope chapter outlines that eco-enviro indicators can be derived and applied as needed, providing they are adequately explained within the study. Two potential approaches (applying the principles of eco-efficiency, calculating trade-offs) are also covered in this section and both require a similar basis for calculation. In both cases the prerequisite step is to calculate the TEA and LCA indicators selected.

A hierarchy of indicators, similar to that given in the TEA chapter, is shown below in Figure 9. Here, each arrow represents an additional calculation (further calculations are required to reach the lowest level, but are excluded from the diagram). Weighted scores are included, implying that weighting **may** be used if required in the formation of combined indicators – however this comes with the caveats already established (public assertions shall not be made using weighted results).

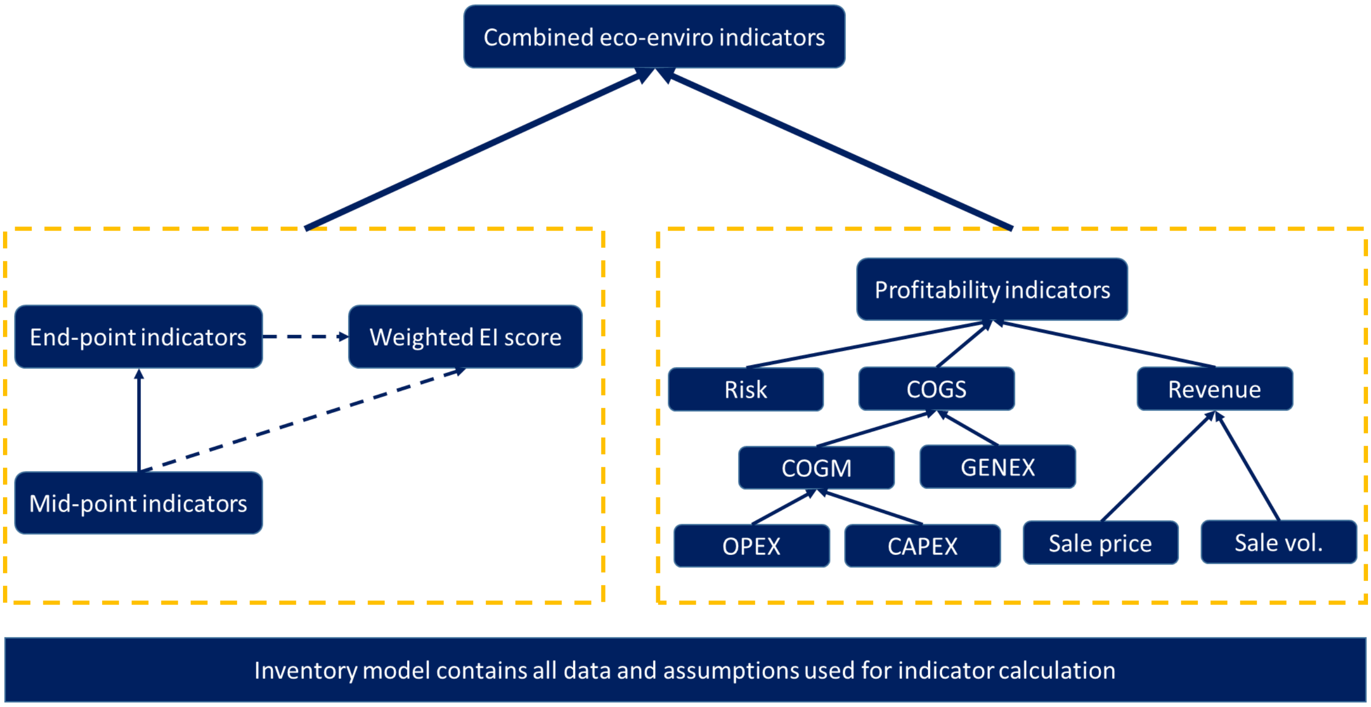

Figure 9 – Hierarchy of indicators

With regard to guidance provisions, very little additional guidance is deemed to be required; the TEA chapter outlines a number of general good practices (see section B.6.2.2 and B.6.2.3) for impact assessment in general.

The major potential pitfall at this stage relates primarily to incorrectly developing eco-enviro indicators without sufficient consideration for dimensions. Two challenges arise: First, there is a need to ensure that any effort to relate techno-economic and environmental performance is carried out on an equivalent basis. For this: Eco-enviro indicators **shall** be calculated using indicators that have a common basis for measurement. In most cases, this basis will be the functional unit itself, to ensure fair representation of the product system.

Second, there is a need to ensure that any set of derived indicators is sufficiently aligned with the goal in order to provide a reasonable conclusion. To some extent this is a communication task to be handled with the study commissioner, to ensure their needs are met. For CCU in particular, care **should** be taken to not equate global warming impact and environmental impact in general – if all combined eco-enviro indicators are based only on the former, this **should** be considered in the formation of any broader conclusions.

E.6.2.1 Provisions

Provisions E.9 – Impact Assessment	
Shall	1) TEA and LCA indicators for combined assessments **shall** be calculated within the bounds of the guidance already provided in earlier chapters 2) All CAPEX and OPEX calculations **shall** clearly state which system elements are considered within the bounds of each, ensuring that all of the product system is captured within the overall CAPEX and OPEX aggregations 3) To prevent misrepresentation, comparisons of CAPEX and OPEX **shall** only be carried out in situations where both the assessed and the comparison case use the same modelling approach 4) If used, combined 'eco-enviro' indicators **shall** be calculated using indicators that have a common basis for measurement
Should	1) Global warming impact and environmental impact **should** not be treated as interchangeable terms. If all combined eco-enviro indicators are based only on the former, this **should** be considered in the formation of any broader conclusions
May	1) Combined 'eco-enviro' indicators **may** be considered if required to achieve the intended study goal 2) The cost of purchasing other reference flows (if not modelled in detail) **may** be disaggregated from the detailed OPEX calculations 3) Weighting **may** be used if required in the formation of combined indicators, provided public assertions are not made using weighted results

E.7 Interpretation

General Introduction and Challenges

The interpretation phase of the study is multi-faceted: Providing the chance to 'close the feedback loop' of the iterative process (goal definition through impact assessment) and to evaluate the results of the study whilst deriving potential recommendations and conclusions. This iterative process can only be concluded when the goal has been achieved; if the goal cannot be achieved a refined goal and/or scope **shall** be adopted.

For integrated studies, the interpretation phase **should** explore the relationship between economic and environmental performance determined in the iterative phases. To ensure that the integrated goal is met, an integrated study **shall** ensure that at least one type of integration is employed from the type list given in section A.5.2: qualitative, discussion-based integration; combined indicator-based integration; and/or preference-based integration.

Sensitivity and uncertainty analyses can be applied in a manner similar to that used for TEA and LCA studies. When deployed, sensitivity and uncertainty analyses **should** be applied to both the economic and environmental aspects of the study – particularly if combined indicators are used within the study.

Conclusions drawn **shall** be based solely on the data quality, system boundaries, methodologies, and results. Recommendations are a subjective interpretation of the conclusions and thus **shall** be based exclusively on the conclusions.

E.7.1 Interpretation Overview

The interpretation phase of an integrated study is similar to that of standalone TEA and LCA; where the intention is to both 'close the feedback loop' of the iterative process and to evaluate the results of the study whilst deriving potential recommendations and conclusions. Given this similarity much of the same guidance remains applicable, a brief summary of this guidance is included in this chapter with some reference to additional provisions and concerns for integrated studies.

Interpretation is an ongoing process that is handled in parallel to the iterative cycle of the goal–scope–inventory–impact assessment, and is only finished when the goal has been sufficiently achieved. For integrated studies there is added complexity in that both the economic and environmental aspects of the goal must be satisfied. This is broadly an expansion of the phase, given that the key tasks in interpretation stay the same:

- Identify any significant problems within the study
- Evaluate the outputs of each phase to ensure completeness and consistency
- Determine conclusions, limitations, and recommendations

One key differentiator for integrated assessments in the interpretation phase is the ability to explore the relationship between economic and environmental performance. Exploring this relationship allows for the identification of potential trade-offs, either quantitatively through the use of indicators or qualitatively through general discussion. The interpretation phase **should** explore the relationship between economic and environmental performance determined in the iterative phases.

The analytical approaches used in single-dimension analysis (contribution, sensitivity, and uncertainty analyses) all remain applicable here, and are discussed in the next subchapter.

With regard to interpretation of indicators, if combined eco-enviro indicators are used these **shall** only be interpreted when the constituent TEA and LCA indicators are deemed to be of sufficient quality.

For CCU products there is often interest in determining whether a product system is ‘carbon neutral’ or ‘carbon negative,’ for which the approaches outlined in the LCA section **shall** be applied here also (see section C.7.1 for further details).

Conclusions drawn **shall** be based solely on the data quality, system boundaries, methodologies, and results. Recommendations are a subjective interpretation of the conclusions and thus **shall** be based exclusively on the conclusions.

With regard to integrated studies, Wunderlich et al. [9] analyzed a number of TEA and LCA studies for the chemical industry and highlighted a number of pitfalls during the development of their organizational framework that is captured in section A of these guidelines (see section A.5, specifically A.5.2). One such pitfall is the failure to adequately address the integrated goal; with this in mind an integrated study **shall** ensure that at least one type of integration is employed from the type list given in section A.5.2: qualitative, discussion-based integration; combined indicator-based integration; and/or preference-based integration.

E.7.2 Uncertainty Analysis & Sensitivity Analysis for Integrated Studies

A general definition for uncertainty analysis (UA) and sensitivity analysis (SA) is taken from the TEA guidelines:

- 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
- Sensitivity analysis (SA) examines 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 [26]

Additional reading on both analyses types can be found in parts B and C (B.7.2 and C.7.2 respectively).

In integrated assessments, determining uncertainty and sensitivity have increased dimensionality requirements with both economic and environmental aspects to consider. With this in mind, UA and SA **should** be conducted on inputs in both the economic and environmental dimensions, and a common approach (e.g. investigating sensitivity by varying a set percentage) **should** be applied across both for consistency reasons.

The suggested approach for application follows that outlined in part D (D.7.7.2 specifically if more details are required). First contribution analysis can be used to identify significant issues within the product system and which elements contribute most to them. This is followed by the handling of a sensitivity analysis to determine which inputs infer the most sensitivity and then an uncertainty analysis to investigate whether high uncertainty would also play a role in any conclusions drawn or recommendations provided.

An added advantage of integrated studies is that the sensitivity of inputs can be assessed in a broader range of impact indicators. Inputs that infer sensitivity in both key economic and environmental indicators **should** be discussed within the interpretation phase. An input that is shown to be sensitive in multiple dimensions **may** warrant investigation to determine if there is any correlated or causal relationship between these sensitivities, either as part of the study or as a recommendation for future work.

A CCU related example can be seen when considering the production of methanol. Methanol is sensitive in both economic and environmental impact categories to the hydrogen supply. A correlation can be drawn between the lower cost, higher global warming impact of SMR (without CCUS) derived hydrogen and the higher cost, lower global warming impact typically seen for electrolysis derived hydrogen.

Additionally, uncertainty and sensitivity analysis **may** be carried out on the combined eco-enviro indicators themselves. Multivariate analysis techniques such as principal component analysis (PCA) offer the chance to determine the covariance of the input variables to help identify correlations between them in a more structured manner than the one proposed above. Examples of the application of PCA to eco-efficiency type indicators can be found in literature [27][28].

E.7.2.1 Provisions

Provisions E.10 - Interpretation	
Shall	1) If combined eco-enviro indicators are used these **shall** only be interpreted when the constituent TEA and LCA indicators are deemed to be of sufficient quality 2) Determining whether a product system is carbon neutral or negative **shall** be handled in accordance to the guidance provided in C.7.1 3) Conclusions drawn **shall** be based solely on the data quality, system boundaries, methodologies, and results 4) Recommendations are a subjective interpretation of the conclusions and thus **shall** be based exclusively on the conclusions 5) An integrated study **shall** ensure that at least one type of integration is employed from the type list given in section A.5.2: qualitative, discussion-based integration; combined indicator-based integration; and/or preference-based integration
Should	1) The interpretation phase **should** explore the relationship between economic and environmental performance determined in the iterative phases 2) Uncertainty and sensitivity analysis **should** be conducted on inputs in both the economic and environmental dimensions, and a common approach (e.g. investigating sensitivity by varying a set percentage) **should** be applied across both for consistency reasons 3) Inputs that infer sensitivity in both key economic and environmental indicators **should** be discussed within the interpretation phase
May	1) An input that is shown to be sensitive in multiple dimensions **may** warrant investigation to determine if there is any correlated or causal relationship between these sensitivities 2) Uncertainty and sensitivity analysis **may** be carried out on the combined eco-enviro indicators

E.8 Interpretation: Multi-Criteria Decision Analysis

General Introduction and Challenges

NOTE: Multi-Criteria Decision Analysis is NOT a phase of LCA or TEA. The inclusion of MCDA here is as a purely optional, additional methodology that may help to meet the study goal or support the making of a decision in which the outputs of a combined assessment may be of value.

MCDA is an umbrella term that covers a range of methodologies that can be used to structure and ultimately resolve a range of problems that involve multiple and often conflicting criteria. Such methodologies can be applied to the assessment indicators of a TEA or LCA alone, but here the focus is on utilizing these methods in evaluating the outputs of integrated studies.

It is not uncommon to find in CCU that good performance of economic and environmental indicators is in competition, necessitating trade-offs between the economic viability of a technology and its associated environmental impact. Decisions in this trade-off space are also difficult, with a need for subjective input to determine what a user deems an acceptable increase in one criterion if that would mean decreased performance in another. MCDA provides users with a structured, repeatable approach to assist in decision making and the communication of preferences that feed into this.

MCDA **may** be used with integrated TEA and LCA studies, and may be of particular value where the study goal involves the need to make a decision from discrete options, or to optimize to a known set of objectives.

If used, the impacts of uncertainty and sensitivity on the results of the decisions analysis **should** be investigated.

E.8.1 Introduction to MCDA for Integrated Studies

The concept of utilizing multi-criteria decisions analysis (MCDA) was previously introduced briefly in the TEA guidelines, where it is discussed within the interpretation chapter. A brief introduction to the concept is covered there, and revisited within this section. A more detailed introduction to the concepts of MCDA can also be found in the relevant supporting worked example [29]. Additional resources on specific methodologies should be sought if required: The introduction here is brief, and the development of detailed guidance for the deployment of MCDA is beyond the scope of these guidelines.

MCDA **may** be used with integrated TEA and LCA studies, and may be of particular value where the study goal involves the need to make a decision from discrete options, or to optimize to a known set of objectives.

Multi-criteria approaches are common in existing integrated TEA and LCA studies where the goal involves decision making in some form (see section E.8.1.1 for some recent examples within CCU). Wunderlich et al. list MCDA as form of integration (and this is captured in part A of these guidelines) in which the constituent studies require a high degree of alignment if the method is to be used.

The advantages of applying MCDA approaches in these scenarios are self-evident: integrated assessment produces a collection of indicators that are impossible to compare in a purely objective manner. Decision making on a collection of indicators is therefore intrinsically biased, and it is here that MCDA can assist in both consistent decision making and communicating the underlying process.

It should be noted that the indicators typically found in LCA and TEA for CCU themselves also suffer from this same lack of direct comparability – and for this reason it is possible to apply MCDA within the interpretation phase of either method, without having to consider an integrated approach. So why should MCDA be given additional consideration specifically in this chapter?

There are two answers to that question: the aforementioned use of MCDA in integrated studies; and the application of TEA and LCA in CCU specifically. Most CCU technologies can be described as 'emerging' and thus TEA tends to focus on assessing how economically viable a technology/process is in its current state (or an anticipated future state) of technical performance in comparison with existing technologies that provide equivalent functionality. Whilst there is some scope for variation in what is considered 'economically viable,' most studies consider this to be a determination of whether a product can be delivered to market in a manner that is 'economically sustainable' – i.e., the cost of producing the product is at least equal to the market price of the comparable product, allowing for the producer to break even (examples of where this can be seen in calculations include [30][31][32]).

Thus, a focus on determining a minimum selling price or a production cost is common, and a comparison of these to typical market prices forms the basis of any conclusions made. These conclusions may include determining areas of focus or making other decisions and, in this sense, it can be seen that whilst multiple criteria can be assessed, decisions tend to be shaped predominantly by economic feasibility.

For LCA within CCU, a similar review shows a focus on reducing the fossil carbon intensity of product systems. This is generally reflected in a bias towards minimizing global warming, which is typically concurrent with a reduction in abiotic fossil depletion (note: in CCS operations a decoupling of this relationship can be seen). Such a focus for CCU is logical – a CCU technology that ultimately increases global warming fails to deliver on its core concepts of circularity and reducing fossil carbon dependency.

However, when considering integrating both TEA and LCA there are at least two competing quantitative criteria of undoubted interest yet which cannot be easily compared, namely economic performance and global warming impact. Obviously, considering only two factors would be somewhat simplistic, even if they are often deemed the most impactful. The use of MCDA allows for a broader spectrum of indicators to be factored in, and their relative importance to the decision maker can easily be compensated (and communicated) in the methodology chosen.

The choice of assessment criteria and MCDA method will likely depend on the study goal and the preferences of the practitioner and/or decision makers. Criteria **may** refer directly to specific indicators calculated in the prior phase, to composites or derivatives of these indicators, or additional data points collected specifically for use within the MCDA. If specific data are collected to augment the decision-making process, this **shall** be documented and reported with an explanation provided of its relevancy for inclusion. Care should also be taken to ensure that any additional data are sufficiently aligned with the scope of the study.

Given that not all calculated indicators need to be used in the MCDA process, the selection of criteria **shall** be recorded and explained in detail within the report, also stating why specific indicators were not selected for use.

Finally, uncertainty and sensitivity **should** be analyzed to investigate their potential impact on the final decision preference.

E.8.1.1 Additional Resources on MCDA Within CCU

Reviews and introductions to MCDA in general can be found readily. These include general overviews [33] and method specific reviews on methodologies and applications [34][35]. Additional resources can be found elsewhere - see the MCDA worked example and part B.7.4 of these guidelines for further references.

Additional resources on MCDA application within CCU can also be found. Recent application examples include: the selecting of emerging CCU products for short- to mid-term deployment [36], the application of MCDA for screening potential CCU products [37], using MCDA in a CCUS application [38], use of MCDA in decision making in related industries such as renewable energy [39], and application within supporting emission reduction technologies for the cement sector through CO_2 mineralization [40].

E.8.2 MCDA Methodologies for Integrated TEA and LCA Studies

MCDA methodologies can be divided into two categories: *attributional* and *objective* approaches. The category deployed will depend on the problem formulation.

E.8.2.1 Multi Attributional Decision Making

Multi-attributional decision making (MADM) methodologies see the user selecting a preferred option (or an order of preference) from a finite list of alternatives to be considered. The criteria for the assessment are 'attributes.' For each alternative to be assessed, each attribute **should** be assigned a value or range for fuzzy applications – in other words, missing data inputs are not preferred although some MCDA methodologies can handle this (see literature on handling uncertainty in MCDA [41][42]).

Beyond this, few restrictions are placed on the data types utilized: Categorical (e.g., a classification), discrete (e.g., a specific price), or continuous data (e.g., a price range) can be used. Data types within an attribute **should** be consistent for ease of comparison, and any deviation from this **shall** be explained in the relevant report section.

For CCU-focused integrated studies the set of alternatives to choose from will vary from study to study and goal to goal:

- A study focused on assessing the best use of a constrained resource could compare competing technologies
- A study focused on technology deployment could compare competing locations and associated properties (e.g. carbon intensity of electricity, cost of electricity)

- A study focused on hotspot identification could compare potential research scenarios to minimize the impact of one or more identified hotspots

The amount of effort required to generate an increasing number of alternatives will likely depend on what an alternative consists of (e.g., generating a deployment scenario for one technology is likely easier than adding a whole new technology to a study).

There are numerous common methodologies that can be considered for deployment, all of which can be categorized in various different manners (see the associated worked example for more details). Table 4 provides an overview of common methods and a selection of software/tools available for their implementation; the entries are organized by their ability to be applied to specific problem types. Neither list (methods or software) is exhaustive, and is mainly included to provide an introduction for readers.

No recommendation will be made for a specific methodology within these guidelines. To do this would be unnecessarily prescriptive, and risks steering practitioners away from using methodologies (and software) that they may have access to. It should be noted however that some methodologies are easier to apply than others, particularly if the calculations are to be done manually (e.g., the AHP family).

As a brief summary, problem classifications have been adopted from [43]:

- **Choice problem**: This selects one single alternative as the best or can reduce a group of options to “all good options”
- **Ranking problem**: The alternatives are ordered from best to worst; these can be scores, comparisons, etc.
- **Sorting problem**: The alternatives are sorted into categories and decisions can be made on these classifications (e.g., preferred alternatives in scenario X, preferred alternatives in scenario Y, and rejected alternatives)
- **Description problem**: The goal of the study is to help describe the alternatives and the consequences of these
- **Elimination problem**: Similar to the sorting problem, but with only two classes defined, namely ‘accepted’ and ‘rejected’
- **Design problem**: The goal of the study is to create a new alternative to meet the needs of the decision maker (essentially a bridge to multi objective decision making approaches)

Table 4 – Types of MADM identified for use in each problem type, and selected software options for these, adapted from [43]

Problem	MCDA method	MCDA software/tool	Output
Choice	AHP, ANP, MAUT/UTA, MACBETH,PROMETHEE,ELECTRE (I, II, II), TOPSIS, hybrid methods	Smart Picker Pro, Electre III-IV, Right choice, MakeItRational, M-MACBETH, Win4DEAP	Single score
Ranking	AHP, ANP, MAUT/UTA, MACBETH,PROMETHEE,ELECTRE (I, II, II), TOPSIS, DEA, Hybrid methods	Smart Picker Pro, Electre III-IV, Right choice, MakeItRational, M-MACBETH, Win4DEAP	Rank
Sorting	AHPSort, UTADIS, FlowSort, Electre-Tri	Smart Picker Pro, Pro Electre Tri	Classification

E.8.2.1 Multi-Objective Decision Making

Multi-objective decision making (MODM) sees the user optimizing a solution for a problem given multiple, typically competing, objectives to optimize towards. Unlike attributional approaches, the set of alternatives that can be selected from is not pre-determined or finite, but one in which a very large number of (or infinite) solutions can be determined from.

For CCU technologies these objectives in their simplest form may typically take the form of 'minimize production costs,' 'minimize GHG emissions,' and 'minimize other environmental impacts.' These objectives are represented mathematically by objective functions that can be optimized simultaneously to reach a most preferred solution. Indicators and values from an integrated study can be used in the formulation of these objective functions.

In combined assessment, objectives from both the economic and environmental aspects of the study **shall** be used.

The scientific literature includes many approaches to solving MODM [44]. Among the most popular are both 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) [45].

E.8.2.2 Provisions

Provisions E.11 – Interpretation: Multi-Criteria Decision Analysis	
Shall	1) If specific data are collected to augment the decision-making process, this **shall** be documented and reported with an explanation provided of its relevancy for inclusion 2) The selection of criteria **shall** be recorded and explained in detail within the report, also stating why specific indicators were not selected for use 3) For MODM applications, objectives from both the economic and environmental aspects of the study **shall** be used
Should	1) Uncertainty and sensitivity **should** be analyzed to investigate their potential impact on the final decision preference Provision 2) For MADM applications: - For each alternative to be assessed, each attribute **should** be assigned a value or range for fuzzy applications - Data types within an attribute **should** be consistent for ease of comparison, and any deviation from this **shall** be explained in the relevant report section
May	1) MCDA **may** be used with integrated TEA and LCA studies 2) Criteria **may** refer directly to specific indicators calculated in the prior phase, to composites or derivatives of these indicators, or additional data points collected specifically for use within the MCDA

E.9 Reporting

General Introduction and Challenges

For life cycle assessment, ISO 14044 recommends that '*the results and conclusions of the LCA shall be completely and accurately reported without bias to the intended audience*'. This recommendation **shall** be applied to the reporting of integrated studies, with the obvious caveat that the inclusion of a decision-making methodology such as MCDA will introduce bias to any potential conclusions or recommendations outlined. In studies that apply an MCDA method, both the unbiased indicators (from the impact assessment phase) and the resultant MCDA outputs **shall** be reported clearly and separately to allow for communication both of the study results and the further decision analysis.

E.9.1 Reporting Overview

The final phase of the study is the production of a report in which 'the results and conclusions of the LCA shall be completely and accurately reported without bias to the intended audience' as stated in ISO 14044.

A key aspect of reporting effectively is that of transparency; all limitations and assumptions need to be clearly communicated with reference to how these impact the results and conclusions of the study. With this in mind there is a clear need to demarcate the boundary between objective analysis and impact assessment, and subjective decision making that takes place based on the results of this.

Therefore, the following guidance is outlined:

- The recommendations of ISO 14044 to report results and conclusions completely and accurately **shall** be followed, with all limitations and assumptions clearly stated and discussed with reference to how they impact the study conclusions
- When decision-making approaches are used, such as MCDA, these **shall** be clearly communicated separately from the impact assessment results

In general, the guiding principles outlined for both reporting LCA in general (with the ISO 14- series standards and ILCD handbook) and reporting TEA and LCA for CCU specifically (Chapters B and C) are applicable here. As with the LCA and TEA chapters, a checklist is provided that **may** be used as a guide for reporting.

E.9.1.1 Provisions

Provisions E.12 - Reporting	
Shall	1) The recommendations of ISO 14044 to report results and conclusions completely and accurately **shall** be followed **2)** When decision-making approaches are used, such as MCDA, these **shall** be clearly communicated separately from the impact assessment results
Should	
May	1) The checklist provided **may** be used as a guide for reporting

E.9.2 Checklists for Integrated Reporting

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 unambiguously the research question(s)
- ❑ State the classification of the assessed CCU technology

Scope of the Study

- ❑ State functional unit clearly and unambiguously according to guideline; report changes resulting from solving multi-functionality
- ❑ State the approach taken to economic modelling within the product system (system-wide or limited perspective)
- ❑ State system boundaries according to guideline
- ❑ State relevant issues, including data quality and assumptions
- ❑ State technology readiness level (TRL) of processes and sub-processes
- ❑ Report production or storage capacity
- ❑ Report geographical and temporal scope
- ❑ State software system (and version) and data library (and version) used for LCA modelling
- ❑ State selected TEA and combined eco-enviro indicators (if used)
- ❑ State type of review and provide additional information about reviewers

Inventory and Impact Assessment

- ❑ State main results of life cycle inventory and life cycle impact assessment
- ❑ State key assumptions, relevant parameters, and their data quality for TEA assessment
- ❑ State main results of TEA impact assessment
- ❑ If results are reported on a relative basis, report basis
- ❑ Describe uncertainty and sensitivity analysis and report results separately

Interpretation

- ❑ State any conclusions, recommendation, and limitations
- ❑ If used, ensure MCDA results are reported separately from impact assessment results

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

Scope of the Study:

- ❑ State functional unit clearly and unambiguously according to guideline; report changes resulting from solving multi-functionality
- ❑ State the approach taken to economic modelling within the product system (system-wide or limited perspective)
- ❑ State performance characteristics, any omission of additional function in comparison, and how performance is measured (might apply for products with different chemical structure and/or composition to their conventional counterparts)
- ❑ State system boundaries according to guideline, and cut-off criteria including a system boundaries flow chart
- ❑ State omitted life cycle stages and processes (might apply for products with different chemical structure and composition to their conventional counterparts)
- ❑ State relevant issues, including data quality and assumptions
- ❑ State method(s) to solve multi-functionality
- ❑ State life cycle impact assessment methods
- ❑ State data quality needs and how energy and material inputs and outputs are quantified
- ❑ State software system (and version) and data library (and version) used
- ❑ State selected TEA and combined eco-enviro indicators (if used)
- ❑ State type of review and provide additional information about reviewers

Inventory Analysis

- ❑ Include flow diagram of assessed process system(s)
- ❑ State types and sources of required data and information
- ❑ State calculation procedures and any limitations to these
- ❑ State all assumptions made

- ❑ 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_2, hydrogen, electricity, minerals, fossil feedstocks, or catalysts
- ❑ State any confidentiality issues
- ❑ Describe sensitivity analysis for refining system boundaries
- ❑ Include calculated full LCI results (if this does not contravene confidentiality agreements)
- ❑ Document technological and economic parameters, where possible based on the functional unit and reference flow
- ❑ State data representativeness and appropriateness of LCI data
- ❑ State results obtained from scenario analysis (including scenarios) and threshold values, if any
- ❑ Report CO_2 capture cost; otherwise, if not available, include statement
- ❑ Document data independently for each system element

Impact Assessment / Calculation of Indicators

- ❑ Include results of life cycle impact assessment
- ❑ For TEA and eco-enviro indicators: state calculation procedures, including potential additional assumptions and estimates utilized
- ❑ For TEA and eco-enviro indicators: present equations for each indicator applied; for uncommon methods, describe motivation
- ❑ State coverage of impact categories – e.g., report if any LCA impact categories are not used (e.g., in carbon footprinting)
- ❑ If results are reported on a relative basis, report basis
- ❑ State if delayed emissions occur and include emission time profile if needed
- ❑ If applied, state discounting method and discounted results

Interpretation

- ❑ Ensure the specific integrated goal/research question(s) is(are) addressed sufficiently
- ❑ Include and describe the results
- ❑ Negative emission in cradle-to-gate studies shall not be interpreted as CO_2 sinks if 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 uncertainty and sensitivity analysis and report results separately
- ❑ Include completeness check
- ❑ Include consistency check
- ❑ State assumptions and limitation associated with the interpretation of results
- ❑ Include conclusions
- ❑ Include recommendations, if any
- ❑ If used, ensure MCDA results are reported separately from impact assessment results

E.10 References

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PART F
Social LCA for CCU

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Content Part F

F.1 Introduction

One challenge of modern times is how to foster active and meaningful public engagement with issues and decisions of relevance to society. Reducing human impact on the climate requires profound changes in our habits, along with systemic changes in how we produce and use energy. A precondition for implementing these fundamental changes is to take into account their potential impacts on all social dimensions, and not only on the aforementioned economic and environmental spheres. For example, as most carbon capture and utilization (CCU) technologies require high inputs of renewable energy, they may have substantially different socio-economic impacts between regions that have readily available renewable resources versus those that don't. Additionally, it is essential to avoid the risk of industrial lock-in that fails to cover the societal targets of sustainability. In this context, Social Life Cycle Assessments (S-LCA) provide an affective and structured methodology to incorporate social elements within the framework of sustainability evaluation.

While the guidance on TEA and LCA for CO_2 utilization already presented in these guidelines elaborate on the methodological framework for assessing the environmental, economic, and technical performance of CO_2 utilization technologies, with the further development of CO_2 utilization technologies and their forthcoming access to the market, questions regarding their social impacts are emerging. To integrate all the elements necessary for comprehensive evaluation and reporting of a product or service's sustainability character (Murphy, 2012), this chapter introduces the social dimension as the missing assessment pillar. The term Social Impact Assessment (SIA) refers to methods that aim to evaluate the socio-economic performance of a product or service. In this context, Social Life Cycle Assessment (S-LCA) has recently emerged as one of the best methodological frameworks for assessing these socio-economic impacts using a life cycle perspective. This methodology is still at an early stage of development, although robust guidelines have been already published (UNEP, 2009) and updated (UNEP, 2020). Even though the following sections incorporate the latest advancements in S-LCA frameworks, for the aforementioned reasons, the application guidelines presented herein are rather general, and case-specific applications for CCU are outlined only occasionally.

The following chapter provides an overview on the status of S-LCA and the present limits and potentials for applying this tool to CCU technologies. Moreover, a preliminary discussion is provided on future research strands needed to best shape and adapt S-LCA practices to CO_2 utilization technologies and ensure compatibility with other sustainability criteria. Finally, it is worth noting that the following chapters do not provide guidance on how to conduct S-LCA for CCU, but rather highlight pitfalls and opportunities that should be investigated via future empirical studies into CCU.

F.2 Emergence of S-LCA

S-LCA has appeared within the last decade in the field of Sustainability Science (Iofrida et al., 2018), which considers the three major environmental, economic, and social spheres of sustainability (Murphy, 2012). This tool, for evaluating the social and socio-economic performances of products, emerged as the broad concept of sustainability took center stage in the transformation of societies toward sustainable futures (Klöpffer, 2003). The development of S-LCA finds its conceptual background in Life Cycle Thinking (as does LCA), and seeks to investigate both foreseeable and unexpected social challenges (i.e., risks and impacts) of technologies or processes[1]. The importance of

[1] https://www.lifecycleinitiative.org/starting-life-cycle-thinking/what-is-life-cycle-thinking/

S-LCA is nowadays recognized, for example by the European Union[2], in all areas where social challenges are expected. The first guidelines on how to conduct S-LCA were published as a result of an emerging discussion on the topic (UNEP, 2009). These guidelines, which were subsequently updated in 2020[3], "provide a map, a skeleton and a flashlight for stakeholders engaging in the assessment of socio-economic impacts of products life cycle." Following the publication of the UNEP Guidelines and the Methodological Sheets for Social Life Cycle Assessment[4] (Benoît et al., 2013), a multitude of peer-reviewed articles applying S-LCA have been published (see reviews by Huertas-Valdivia et al., 2020; Macombe et al., 2018; Arcese et al., 2018), highlighting a growing interest among scientists, policymakers, and industrial actors. The high resonance of the UNEP Guidelines in the policy arena is substantiated by the publication of the 'Social Life Cycle Assessment, State of the Art and Challenges for Supporting Product Policies' by the European Commission's Joint Research Centre (JRC, 2015), which presents the state-of-the-art of S-LCA and provides some examples of its application. Beyond UNEP, social issues are at the forefront of global sustainability endeavors in their relevance to 14 of the 17 Sustainable Development Goals (the only SDGs not directly related to social aspects being SDGs 9, 14, and 15) (UNEP, 2020).

Tokede and Traverso (2020) have screened all S-LCA case studies published since the preparation of the first version of the UNEP Guidelines, identifying 58 studies, with more than 50% published in the *International Journal of Life Cycle Assessment*. While the number of S-LCAs is growing (see Figure 1), it is notable that the overall number of publications is still very low compared with the multitude of articles published each year on LCA, even taking into consideration that only a fraction of those studies analyze CO_2 utilization technologies.

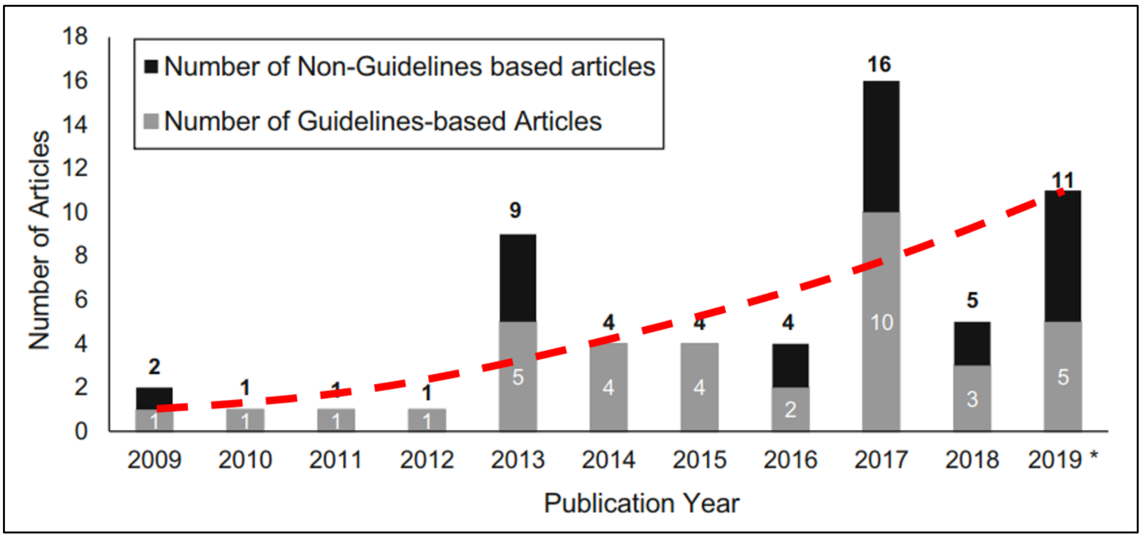

Figure 1. Adapted from Tokede and Traverso, 2020. Total number of S-LCA studies by publication year (with overall number at the top), and trend line. #

[2] The European Commission highlighted the importance of monitoring and ensuring social welfare, with the publication of the "Social Portrait of Europe" (EC, 1991) and more recently with "The Social Situation in Europe" (EC, 2015b).

[3] The most recent version of the S-LCA UNEP Guidelines (UNEP, 2020) updated the previous version from 2009, and builds upon collective revisions by the UNEP steering committee.

[4] This document suggests impact categories, inventory indicators, and data sources.

F.3 When and why to perform Social-LCA for CCU

S-LCA provides an effective and structured methodology for incorporating social elements into the framework of technology sustainability assessment. The following sections discuss aspects and conditions that must be taken into consideration when deciding whether or not an S-LCA must be conducted, and that may have relevant implications when assessing CCU.

F.3.1 Closing the sustainability gap

As previously mentioned, S-LCA studies are not performed as frequently as LCA or TEA studies to date. As a general note, social and socio-economic aspects are no less important than environmental or economic considerations when assessing the overall sustainability character of a product or service. For this reason, the authors of these guidelines believe that S-LCA shall be performed complementary to LCA and TEA. For CCU, industrial settings and conditions leading to best social and socio-economic performances may be implemented in future CCU business plans, thereby avoiding belated and costly retrofitting of infrastructures and value chains. When comparing different industrial options, social performances are strictly dependent on how much these value chain options differ (e.g., for some CCU concepts, different actors might be involved in the value creation than for the conventional value chain), or which locations or regions are involved in the industrial processes (e.g., the implementation of CCU processes with high hydrogen demand might lead to importing blue or green hydrogen from developing regions). Therefore, a previous assessment of the differences among several production methods (and to which portions of the value chain these differences apply) is a good indicator of the extent of the expected social impact changes, and should guide practitioners or decision makers to decide when to perform or commission a S-LCA study in addition to their TEA or LCA. We recommend basing such decisions on whether there are significant changes among the actors in the value chain or the locations of value creation, as those will lead to the largest differences in S-LCA. (see provisions, below).

Provisions D 4.2 – When to perform an S-LCA	
Shall	A S-LCA shall be performed when comparing two different systems or scenarios with entirely different value chains that are transnational.
Should	A S-LCA should be performed when assessing CCU technology that will have a multiregional value chain that is expected to differ from that in the base case.
May	A S-LCA may be performed when assessing CCU technology that has a similar value chain to the base case and will be deployed in the same region.

F.3.2 International character of CCU value chains

The S-LCA should focus on both the specific industrial process under consideration, and the entire related supply chain (i.e., from upstream until the end of life). This approach is advisable from an ethical but also from a practical perspective, as a given technology or industrial process can impact societal dimensions at each phase, until, for example, disposal of the product. In fact, social issues can affect both upstream and downstream parts of the value chain (e.g., involving wholesalers or logistic services), in turn presenting social risks for the production processes under consideration. Specifically, for the case of CCU, carbon dioxide, hydrogen, and energy inputs may be supplied by different sources and regions, thereby necessitating an in-depth assessment of social import externalities. In particular, concepts that require large volumes of hydrogen will often involve major transnational or transregional considerations, since production may be limited to a few regions (e.g., hydrogen is foreseen to be produced in renewable-rich countries or via imported natural gas). When it comes to renewable energy requirements, wind and solar resources are particularly abundant in the Global South, which is particularly vulnerable to negative social repercussions due to political or economic situations, such that the impacts experienced in a certain region may not appear in others (i.e., site-specific). Therefore, S-LCA is a potent tool to take socio-economic contexts into consideration and provide results that apply specifically to the areas of interest. Such cases highlight the importance of carefully evaluating broader system boundaries in S-LCA for CCU, and discuss the implications of different system boundaries in S-LCA, LCA and TEA (see sections B.4.3.2 and C.4.2) for the same CCU technology.

Another reason for assessing the socio-economic impacts of CCU deployment in the Global South is the potential that these technologies have for countries that have abundant renewable energy resources such as solar energy. While the option to deploy CCU technologies for decentralized energy production may offer opportunities for domestic energy supply, in the future it may be possible to trade energy carriers globally. Here, early assessment of the potential impacts of CCU will be necessary in order to align future CCU development pathways in poor regions with the aims of the SDGs.

F.3.3 CCU at early stage of maturity

As CCU is still at an early developmental stage, policy makers can take the opportunity to design deployment regulations that protect and promote ethical standards beyond production and commercialization. Thus, identifying potentially negative social impacts can pose serious risks to the implementation of a proposed CCU product or service. Conversely, late socio-economic assessment of a product or technology delays the identification of relevant risks. Therefore, it is recommended to investigate the likelihood and extent of such risks before a new product or service supply chain is established, in order to address these aspects at an early stage and prepare mitigation measures where applicable. Even considering that most CCU technologies are still at an early stage of development, the evaluation of potential negative impacts and risks at these stages may already be possible (see chapter on early technology LCA). Therefore, decision makers should give serious consideration to this option. Through the early identification of impacts, appropriate modifications to the implementation pathways of CCU technologies could be proposed to both industrial players and political actors. The avoidance of downsides for individuals or social categories will particularly benefit local administrators, with important return-on-investment in the form of political support. Styring et al. (2021), for example, warn about the risks of leaving behind less advantaged social groups, such as when transitioning from fossil-based to more costly electric vehicles. Early S-LCA may well characterize such impacts and evaluate the magnitude and reality of such risks.

Differently, the assessment of possible social impacts is also recommended at later stages of development, if earlier assessment was not possible. In this case, the identification and evaluation of social issues may also foresee future potential adversities and enable decision makers to respond in a timely manner. Accordingly, unknown social issues and indirect relationships across established supply chains may still be flagged.

F.3.4 Highlighting positive impacts

The most recent UNEP Guidelines emphasize that impact categories and sub-categories relevant for S-LCA have the potential to negatively or positively impact the stakeholders engaged with the product or service, underlining the need to improve performance rather than only highlight concerns. McCord et al. (2021) underline that both positive and negative impacts can be expected of CCU technologies, so that the assessment framework must be tailored towards the identification of both. Therefore, in contrast to environmental LCA that reports on the likelihood and extent of environmental challenges, S-LCA has the advantage of also identifying and quantifying potential positive social impacts (Norris, 2006). As the results are highly valuable for governments and decision making, expanding the information deliverable by S-LCA, by providing assessment on potential benefits in specific areas and for specific groups of stakeholders, is of particular importance. Moreover, assigning positive social impacts to a technology or service brings additional incentives around engaging with a given business, beyond merely economic or environmental benefits. The 2020 UNEP Guidelines identify three different types of positive impacts: 1) Positive social performance going beyond business as usual; 2) Positive social impact through presence (product or company existence), and 3) Positive social impact through product utility. In order to thoroughly evaluate negative as well as positive social repercussions, a shared agreement on specific indicators is needed, although insufficient progress has been made in this regard. From a survey conducted by Di Cesare et al. (2018), only 26% of all articles analyzed debates on the positive aspects of the case studies investigated. According to the authors, the reasons behind this delay are several and relate to the epistemological questions around the discipline of sustainability (Bond et al., 2011; Seager et al., 2004), the late implementation of innovative key approaches such as transdisciplinarity (Sala et al., 2013), and the ambiguity of positive repercussions (e.g., a positive impact for a certain category may imply negative effects on another; EC, 2015c). New CCU projects could spur employment and may therefore represent a valuable option, particularly in areas affected by low employment. Moreover, CCU projects may support areas undergoing decarbonization, by offering alternative job opportunities, or promoting safe and healthy living conditions by curtailing emissions of atmospheric pollutants. Therefore, any potential social benefits of CCU should also be identified in order to fully inform decision makers and citizens, which may also help mitigate opposition and therefore stimulate market adoption.

F.3.5 S-LCA, policy making, and citizens

Analysis of all the three pillars of sustainability (social, environmental, and economic) provides relevant information for political decisions. Policy makers must ensure that each product or service best complies with both international and regional socio-economic standards, and must make use of specific skills and instruments to guide them in comparing existing technological options. For an informed and fact-based decision-making process, a good understanding of all positive and negative social externalities is also important. Such information often does not exist, or knowledge is limited to macro-economic studies rather than to specific products or producers. For LCA and especially S-LCA, there is no predeterminable relationship between the characteristics of a product or technological processes and its potential externalities (Lehmann et al., 2013); consequently, each value chain must be analyzed individually. This requirement is much more relevant for CCU given the lack of references like close technology options. Specifically for these technologies, market regulators and policy makers must be aware of this caveat when only limited information is available on social performance. Citizens also have a social obligation to act responsibly when purchasing products and services. To make informed decisions, they need to be aware of the risks and externalities associated with products, as communicated by governments or local institutions, or via alternative channels. It is therefore clear that social performance data must be made available to policy makers as well as to the general public after being investigated, and that closer attention should be given to CCU technologies due to their early developmental status. As the JRC (2015) states: "policy makers need to know where (social) externalities (are likely to) occur and how significant they are and the same is true for citizens." An effective top-down information exchange can play an important role in particular circumstances where such information is not easily distributed to societies, such as where the regulatory frameworks that are in place do not demand thorough investigation of social impacts.

F.3.6 The role of industry

The increasing pressure on the corporate sector to follow more sustainable development pathways led to the concept of Corporate Social Responsibility (CSR) or business to Society (B2S) (McWilliams and Siegel, 2001). S-LCA can provide an analysis of the social performance of a product or service, thereby highlighting potential consequences of business practices. The transformation of value chains to address negative social impacts is only possible if industries and entrepreneurs are aware of the implications of their products or activities. Such improvements can directly affect all stakeholders at each stage of the value chain. CSR intends to ensure social compliance not merely with international legal frameworks, but also with common ethical standards beyond corporate interests (McWilliams et al., 2006). To bring about real change, this self-regulatory social-protection mechanism should expand to other actors in the value chain also via influence of the main business actors and beyond, to organization connected through contractual relationships. Cooperation with NGOs and public institutions represents the best approach to comprehensively tackling social issues, and collectively identifying hotspots of impacts throughout the value chain. CCU technologies are very different in terms of their processes, final products, infrastructures, and local impacts. Consequently, it is not possible to define a “one-size-fits-all” strategy to facilitate the ”spread” of ethical practices beyond the CCU firm, but industry partners and local authorities can identify and develop solutions applicable to their specific case study with the support of S-LCA practitioners.

F.4 How to perform a S-LCA

S-LCA is the result of combining the systematic approach of environmental LCA with theory and methods grounded in social sciences (JRC, 2015). Although a methodological S-LCA framework has been proposed by the SETAC Guidelines, a lively scientific discussion is underway among experts, aiming at harmonizing approaches. Uncertainties surrounding the several proposed methods relate in particular to the different approaches suggested for each specific scope, and to the lack of experience and publications in the field. More specifically, Lofrida et al. (2018) differentiated these existing issues as relating to the object of the assessment, sources of impacts, assessment methods (a current status or cause–effect relationships), and the supposed application of features from other LCA methods.

S-LCA can be conducted the following two different approaches: focusing on the impact of a product (or service), or else on the impact of the main stakeholder (i.e., the producing organization). In the first approach, the main goal is to assess what social repercussions are to be expected when a product is manufactured in a specific manner. In the second approach, often referred to as Social-Organizational LCA (SO-LCA), a company or organization is at the core of the analysis, and the goal is to assess its social-economic performance by focusing on all its activities, and on relationships with its stakeholders. In most cases, the implementation of a CCU technology will mainly require S-LCA to assess the social performance of the product delivered.

S-LCA can be adapted to the goal that the practitioner wants to pursue. When the method is applied to products or organizations, S-LCA is geared toward identifying the potential social repercussions of a product or service, but it can also evaluate existing social impacts. While the former seeks to understand which social effects may be triggered by the activities of an organization based on one or more indicators, the latter analyzes existing causal relationships between the company's activities and human well-being. In other words, “actual social impacts “are the changes that affect stakeholders as a result of an activity, based on observed data” (UNEP, 2020, p. 25).

F.4.1 Phases of S-LCA

The methodology applied when conducting a S-LCA (and SO-LCA as well; see paragraph E.4) follows the Life Cycle Thinking approach and is in large part based on the ISO standards 14040 and 14044 relative to environmental LCA. Therefore, the four main phases of S-LCA follow those of environmental LCA and TEA (namely: Goal and scope definition; Inventory; Impact assessment; and Interpretation) in an iterative manner, meaning that the assessment can be repeated to incorporate new or improved data, or to shape the assessment toward specific case studies (Figure 2).

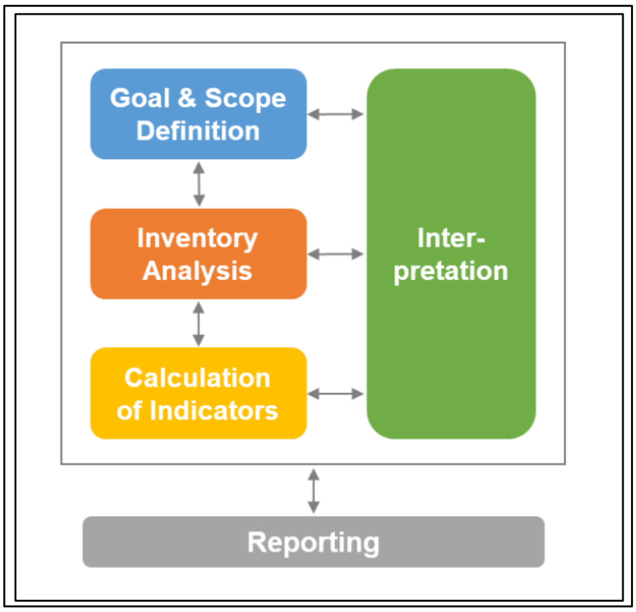

Figure 2: The four iterative phases of S-LCA (JRC, 2015; Benoît Norris, 2012).

F.4.2 Research question and goal definition

S-LCA for CCU can complement LCA or TEA in investigating additional impacts related to the implementation of a particular CCU technology. Definition and importance of the research question and the resulting goals were presented previously in the LCA and TEA chapters (see section C.3). Following the same approach, the research question and goal definition for S-LCA shall be aligned with those posed for the LCA or TEA studies. A S-LCA can be performed for different reasons, ranging from assessing the overall social sustainability character of a product or service, or a focus on specific social aspects of particular interest (e.g., fair working conditions). Other research questions could be related to identifying social hotspots along the value chain, or comparing different technological options. For S-LCA, close collaboration, between the decision makers commissioning the study and S-LCA practitioners, is also highly recommended at this stage. To provide examples of the research question for a S-LCA, we can take as reference those that have been presented for TEA or LCA (see Chapter C 3.1 and B 3.2.2.1) and adapt them to socio-economic fields. The LCA research question for LCA "Is a CCU-based product or service environmentally beneficial compared to the same product or service derived from fossil carbon sources?"; when aligned to S-LCA, this might become: "Does a certain CCU-based product present social benefits or disbenefits when compared to the same product derived from fossil carbon sources?" Another common research question is: "Where are the environmental hot spots for technology improvement, to reduce environmental impacts in the life cycle of a CCU product/process?" which, transferred to S-LCA, could be: "Where are the social hotspots for technology improvement to reduce social impacts in the life cycle of a CCU product/process?"

Similarly, the S-LCA research question shall also be defined following that posed for the TEA study, namely: "Is the CCU product economically viable in a future scenario?" which for S-LCA becomes: "Is the CCU product compatible with social standards in a future scenario?"). Table I provides an overview of some of the discussed research questions for LCA and TEA (see Chapter C 3.1 and B 3.2.2.1) and suggestions for potential S-LCA research questions. In addition to research questions where an economic or environmental counterpart can easily be outlined, others can be framed focusing solely on social aspects. Such research questions would address specific social impact categories, such as working conditions for a certain stakeholder, changes in the job market, etc.

Table I: Potential S-LCA research questions for CCU

Type of study	Original research question	Potential research question for S-LCA
LCA	Is a CCU-based product or service environmentally beneficial compared to the same product or service derived from fossil carbon sources?	Is a CCU-based product or service socially beneficial compared to the same product or service derived from fossil carbon sources?
	Where are the environmental hotspots for technology improvement, to reduce environmental impacts in the life cycle of a CCU product/process?	Where are the social hotspots for technology improvement, to reduce social impacts in the life cycle of a CCU product/process?
	What is the environmentally preferred CCU technology to make best use of a scarce resource, e.g., renewable energy?	What is the socially preferred CCU technology?
	What are the environmental footprints of products or services used as the basis for customer decisions (product declaration)?	What are the social impacts of products or services used as the basis for customer decisions on a pre-defined reference scale (product declaration)?
TEA	What are the major cost and value drivers?	What are the major drivers for improvements in social performance?
	What aspects need to be worked on (next)?	What aspects need to be worked on (next) from the S-LCA perspective?
	How does the current state of development rank amongst alternatives?	How does the current state of development rank amongst alternatives from a S-LCA perspective?
	Is the CCU product economically viable in a future scenario?	Does the CCU product promote social benefits in a future scenario?
	How does investment in a CCU product deployment / demonstration project / full-scale plant compare to alternatives?	How does investment in a CCU product deployment / demonstration project / full-scale plant compare to alternatives from a S-LCA perspective?
	What are the current states, favorable conditions, best practices, and necessary actions for regional CCU value chains?	What are the current states, favorable conditions, best practices, and necessary actions for regional CCU value chain alternatives from a S-LCA perspective?
	What regulatory clarification and support (type, timing, and budgets) is required for specific CCU products or services?	What regulatory clarification and support (type, timing, and budgets) is required for specific CCU products or services to be most socially beneficial?

F.4.2.1 Provisions

Provisions D 4.3 – Goal definition	
Shall	The goal and research question shall be aligned with the underlying LCA or TEA study and specified towards the S-LCA needs.
Should	-

May	In case further questions on social impacts are of interest to the practitioner / the commissioner of the study, a secondary goal and research question may be added which is only assessed in the S-LCA.

F.4.3 Scope definition

The scope of a study (TEA, LCA, or S-LCA) defines the object under investigation and the methodological framework applied to the analysis (for more information, see sections B.4 and C.4). The choices around the scope definition for a S-LCA depend on the research question and goal of the study. If a TEA or LCA for the same product or service already exists and the main goal for the S-LCA is to integrate economic and environmental data with social impacts, then the scope shall be aligned with that adopted in the LCA or TEA study. This includes and mainly pertains to applying the same functional units (e.g., tonnes of CCU product produced), reference flow (e.g., 1 tonne of CCU product produced), and unit operations (e.g., CO_2 capture, hydrogen production, product synthesis, product use, product disposal). If an additional secondary research question exists that cannot be aligned with the underlying LCA or TEA study, we recommend following the UNEP Guidelines to frame the scope definition that best fit the research question.

As a second step during the scope definition process, stakeholder-specific impact subcategories and indicators are chosen (note: in LCA for environmental impacts, stakeholder specification is not necessary, which differs from S-LCA). The stakeholder groups which might be impacted by a CCU product or service must be at the focus of the assessment. The UNEP Guidelines identified six main stakeholder groups that should be taken into consideration in a S-LCA: Workers; Local communities; Society, Consumers, Children; and Value chain actors. Their selection depends on the goal and scope of the study, the intended use, the value chain, etc., and must be reported transparently in S-LCA studies. Based on the stakeholders selected for the study and the life cycles pf products/services, impact categories and subcategories are defined, with each of these measured by performance indicators. Impact categories commonly reported in studies include: human rights, working conditions, cultural heritage, governance, education, fair salaries, human health, and socio-economic repercussions. The stakeholder groups and impact categories can also be selected by taking into consideration other international activities engaged in monitoring and managing social issues, such as the 2030 UN Agenda and its 17 Sustainable Development Goals[5]. Clear connections can be drawn between S-LCA utilization and compliance with the SDGs (see section F.2). In a similar fashion, the UNEP Guidelines also provide guidance on appropriate selection from the vast number of indicators used in S-LCA. These choices will determine the social aspects that will be investigated in the study and define the areas of pertinence of the results. Broadly speaking, indicators must be selected based on goal, scope, data availability, specific contexts, and the stakeholders under focus (Dale et al., 2013). A detailed overview of S-LCA indicators and impact categories is presented in the Methodological Sheets for Social Life Cycle Assessment, where guidance is provided on their selection and utilization. Examples of relationships among stakeholder groups, impact categories, and indicators are presented in Table II. For more comprehensive guidelines on how to choose stakeholder groups, impact categories, and indicators in S-LCA studies, we refer the reader to the UNEP Guidelines, which shall be used by the practitioner.

Table II. Example stakeholder groups, impact categories/subcategories and indicators in S-LCA (from Benoît et al., 2013).

Stakeholders	Impact categories/subcategory	Indicators

[5] https://sdgs.un.org/2030agenda

(1) Workers	Health and safety	• Quality or quantity of information/signs on product health and safety (-> For new CCU products, accurate labelling may be valuable) • Number of consumer complaints • …
	Fair salary	• Minimum wage by country (-> This parameter could be relevant for increasing public acceptance of new CCU products, and accelerating market penetration) • Lowest-paid worker compared to the minimum wage • …
(2) Consumers	Privacy	• Country ranking related to regulations on data sharing • Number of consumer complaints related to breaches of privacy or loss of data within the last year • …
	Transparency	• Consumer complaints regarding transparency (-> loss of trust in reported CO_2 savings may compromise quick market penetration of CCU products) • Presence of a law or norm regarding transparency • …
(3) Local communities	Delocalization and migration	• Number of individuals who resettle that can be attributed to organization (-> CCU plants may be located in areas where communities are losing jobs, e.g., coal-based areas in Germany, former oil-rich areas in the US) • International migrants as a percentage of population • …
	Community engagement	• Transparency of government policymaking • Public trust in politicians (->The way politicians promote new technologies or products should be centered on transparency and loyalty) • …
(4) Society	Contribution to economic development	• Economic situation of the country/region (GDP, economic growth, unemployment, etc.) • Relevance of the considered sector for the (local) economy • …
	Corruption	• Risk of corruption in the country and/or sub-region • Risk of corruption in the sector (->These aspects have particular importance when countries with poor legal standards are engaged in the value chain, such as in the case of hydrogen production as a new energy carrier) • …
(5) Children	Child labor	• Percentage of children working by country and sector • Absence of working children under the legal age of 15 years
(6) Other value chain actors	Fair competition	• Membership that behaves in an anti-competitive way (-> Competition may be an interesting focus of research, once new products made via CO_2 utilization are in competition with conventional products) • Documented statement to prevent engaging in anti-competitive behavior

		• …
	Supplier relationships	• Sufficient lead time • Absence of coercive communication with suppliers • …

F.4.3.1 Further reading

A detailed description of the scope definition for S-LCA is found in the UNEP Guidelines (2020).

Provisions D 4.4 – Scope definition	
Shall	1) The functional unit, reference flow, and boundaries of the assessment shall be aligned with the scope of the underlying LCA or TEA. 2) In case a secondary goal and research question for the S-LCA are defined but cannot be aligned with the primary scope, the UNEP Guidelines shall be followed to define the secondary scope. 3) The stakeholder groups affected by the implementation of the CCU technology as well as the subcategories and indicators shall be selected in accordance with the UNEP Guidelines; neglection of a stakeholder group shall be reported and justified.
Should	-
May	-

F.4.4 Inventory and Impact assessment

Based on the scope definition, data inventories must be identified that provide information about all the parameters needed for the impact assessment. S-LCA also requires data from large databases that are accepted by the practitioner's community, and that are used for computation and to obtain results. Currently, the main 'hotspot' databases available for compiling S-LCAs are the Social Hotspot Database (Benoît-Norris et al., 2013) and the Product Social Impact Life Cycle Assessment (PSILCA) database (Ciroth and Eisfeldt, 2016). Yet, S-LCA relies on a multitude of datasets that either involve particularly time-consuming searches and analysis, or else simply do not yet exist. Gaps may be even more relevant for CCU technologies due to their generally low TRL and absence on a large scale.

F.4.4.1 Further reading

A detailed description of the Inventory and Impact assessment in the UNEP Guidelines (2020).

F.4.4.2 Provisions

Provisions D 4.4 – Inventory and Impact assessment	
Shall	The inventory and impact assessment shall be performed following the UNEP Guidelines for S-LCA.
Should	-

May	-

F.4.5 Interpretation and reporting

Interpretations of S-LCA follow the same principles as for LCA and TEA described in chapter C 7 and chapter B 7, which shall also be followed by the practitioner. As the S-LCA should be performed in addition to an LCA and/or TEA, the use of multicriteria decision analysis (MCDA) approaches is recommended in order to derive meaningful decisions based on LCA, TEA, and S-LCA. This requires that all studies are well aligned, to allow comparison. Additionally, MCDA approaches can also be used in S-LCA for weighing between the different indicators used in the S-LCA alone.

Provisions D 4.4 – Inventory and Impact assessment	
Shall	The interpretation shall follow the principles described for LCA and TEA in this chapter.
Should	-
May	Multicriteria decision analysis may be considered to evaluate different results within S-LCA or when comparing with results from LCA or TEA.

F.5 CCU in the social-LCA literature

At present, CO_2 utilization technologies remain largely absent from the S-LCA literature. Some S-LCA studies on CCU were recently published in peer-reviewed journals, mainly discussing impact categories, indicators, and the application of different methodologies. Pieri et al. (2018) presented a detailed description of the CCU value chain, observing that at the time of publication no social impact assessment of CO_2 utilization technologies existed, and remarking on the importance of taking into account the social sustainability dimension in future works. Proposals have also been made to analyze the broad sustainability character of CO_2 utilization technologies by assessing their compliance with the international sustainability targets defined in the SDGs, including assessment of potential negative effects (Almanza and Corona, 2020; Olfe-Kräutlein, 2019). A recent survey among experts in the fields of CO_2 utilization and S-LCA (Rafiaani et al., 2019) points uncertainties in the process of selecting social aspects, and in developing a system of impact categories based on the interests of different stakeholder groups: As an example, Table III shows subcategory rankings following MCDA analysis, as derived from Rafianni et al. (2019).

Table III. Ranking of the impact categories for each stakeholder group. From Rafiaani et al., 2019.

Stakeholder	Impact Category/Indicator
Consumers	1. End of life responsibility 2. Transparency 3. Feedback mechanism 4. Consumer privacy
Workers	1. Fair salary 2. Health and safety 3. Equal opportunities/discrimination

	4. Working hours 5. Social benefits/social security 6. Freedom of association and collective bargaining
Local community	1. Safe and healthy living conditions 2. Secure living conditions 3. Local employment 4. Community engagement 5. Access to material resources 6. Access to immaterial resources

These results summarize expert perceptions on which indicators are most important for assessing CCU, and provide a reference point for decision processes in future studies. Nevertheless, great uncertainty remains concerning the quality of the methodological frameworks chosen: the same authors reported that most of the experts engaged in the questionnaire where not particularly familiar with CCU technologies, thereby adding an element of inaccuracy that itself is difficult to assess. In addition, the study does not provide enough insights concerning the array of social impacts that may be expected from any CCU technology, an outcome that should be central to future CCU-focused S-LCAs.

McCord et al. (2021) developed a first S-LCA methodological framework, tailored to CCU technologies, which is equally applicable to early or high levels of development. The authors adapted the method suggested by the UNEP Guidelines to create a “screening type” of assessment framework complementing and exploring the trade-offs between techno-economic (TEA), environmental (LCA), and social (S-LCA) impact assessments. The presented framework has multiple applications: it allows comparison of deployment scenarios, of different CCU technologies, or comparison of different routes to product creation. The framework does not incorporate MCDA methods to rank indicators, although the authors suggest utilizing MCDA as a decision-making tool based on the aims or priorities delineated by the study commissioner. Moreover, they emphasize the inclusion of data relating to supplies of raw materials and their sources, as well as on renewable energy availability, as a key indicator for CCU and especially for Power-to-X technology, where high volumes of renewable hydrogen are required. This brief review of the development of S-LCA as an assessment method and its importance for CO_2 utilization technologies shows a slow but constant development. In the coming years, a refinement of S-LCA frameworks for CCU can be expected, as a growing number of technologies will achieve maturity and hence attract significant political debate on if and how their market implementation will contribute to sustainability goals.

F.6 Ensuring integration of TEA, LCA, and S-LCA

S-LCA is a potent tool to assess socio-economic impacts. A further step towards completing the sustainability assessment of a CCU product or service is to integrate these results with data on economic and environmental performances. In order to achieve this, S-LCA must be conducted in alignment with LCA and TEA methodologies, to allow integration of outputs under different conditions, and to balance the trade-offs among the social, environmental, technical, and economic dimensions. At the beginning of this Guidelines document, we described different methods for TEA and LCA integration, the associated challenges, and how this can provide added value for thoroughly evaluating CCU technologies. Different integration methods can be applied according to the conditions of each individual case (e.g., ex-ante, when techno-economic and environmental analyses are performed jointly in a single study; or ex-post, when linking the results of independent TEA and a

LCA studies), and the methodology for economic and environmental integration presented in Part E can be considered the most advanced form yet developed for CCU. Similarly, Wunderlich et al. (2021) reviewed methods for TEA and LCA integration, focusing on their respective limits and challenges, and suggesting solutions to specific cases. Having introduced S-LCA under the perspective of analyzing CCU technologies, the next step is to suggest how to implement the social dimension within the integration exercise, so to enable a comprehensive and complete sustainability assessment. As S-LCA is a new area of study, no provisions in this direction have been published to date, and neither is that the scope of the present chapter. Nevertheless, we emphasize that TEA, LCA, and S-LCA practitioners must work jointly and exchange knowledge on potential challenges and solutions in order to facilitate complete integration of the various approaches. This is particularly arduous for ex-ante analysis such as combined indicator-based integration, as here practitioners must develop combined indicators that effectively address the single dimensions of sustainability of CCU technologies, while at the same time expressing their mutual relationships (i.e., trade-offs). In this context, McCord et al. (2021) argue that assessment phases must be aligned whenever feasible (such as goal and scope definition, inventory compilation, etc.), and common inventory databases are recommended. The difficulty of the integration effort in addition to the individual complexities of techno-economic, environmental, and social analysis, make this task particularly burdensome. Adding S-LCA to the equation increases even further the complexity of the integration exercise, requiring future conceptual research and case-study investigations to develop and refine novel approaches in sustainability assessment. Moreover, the low maturity of most CCU technologies confers greater uncertainty to databases, adding various challenges and pitfalls to the achievement of successful integration.

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