



Techno-Economic Assessment Guidelines for CO₂ Utilization

Arno W. Zimmermann¹, Johannes Wunderlich¹, Leonard Müller², Georg A. Buchner¹, Annika Marxen¹, Stavros Michailos³, Katy Armstrong⁴, Henriette Naims⁵, Stephen McCord⁴, Peter Styring⁴, Volker Sick⁶ and Reinhard Schomäcker^{1*}

¹ Institute of Chemistry, Technische Universität Berlin, Berlin, Germany, ² Institute of Technical Thermodynamics, RWTH Aachen University, Aachen, Germany, ³ Energy 2050, The University of Sheffield, Sheffield, United Kingdom, ⁴ UK Centre for Carbon Dioxide Utilization (CDUUK), The University of Sheffield, Sheffield, United Kingdom, ⁵ CO₂ Utilisation Strategies and Society, Institute for Advanced Sustainability Studies (IASS), Potsdam, Germany, ⁶ The Global CO₂ Initiative, The University of Michigan, Ann Arbor, MI, United States

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*Correspondence:

Reinhard Schomäcker
schomaecker@tu-berlin.de

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Carbon Capture and Utilization (CCU) is an emerging technology field that can replace fossil carbon value chains, and that has a significant potential to achieve emissions mitigation or even “negative emissions”—however in many cases with challenging technology feasibility and economic viability. Further challenges arise in the decision making for CCU technology research, development, and deployment, in particular when allocating funding or time resources. No generally accepted techno-economic assessment (TEA) standard has evolved, and assessment studies often result in “apples vs. oranges” comparisons, a lack of transparency and a lack of comparability to other studies. A detailed guideline for systematic techno-economic (TEA) and life cycle assessment (LCA) for CCU technologies was developed; this paper shows a summarized version of the TEA guideline, which includes distinct and prioritized (shall and should) rules and which allows conducting TEA in parallel to LCA. The TEA guideline was developed in a co-operative and creative approach with roughly 50 international experts and is based on a systematic literature review as well as on existing best practices from TEA and LCA from the areas of industry, academia, and policy. To the best of our knowledge, this guideline is the first TEA framework with a focus on CCU technologies and the first that is designed to be conducted in parallel to LCA due to aligned vocabulary and assessment steps, systematically including technology maturity. Therefore, this work extends current literature, improving the design, implementation, and reporting approaches of TEA studies for CCU technologies. Overall, the application of this TEA guideline aims at improved comparability of TEA studies, leading to improved decision making and more efficient allocation of funds and time resources for the research, development, and deployment of CCU technologies.

Keywords: CO₂ utilization, CCU, carbon capture and utilization, techno-economic assessment, TEA, standardization, harmonization, life cycle assessment

INTRODUCTION

Reports by the Intergovernmental Panel on Climate Change (IPCC) and the US National Academies emphasize that meeting the global temperature goals of 1.5°C or even 2°C above pre-industrial levels will require the removal of carbon dioxide (CO₂) from the atmosphere (IPCC, 2018; National Academies of Sciences Engineering and Medicine, 2019). Carbon Capture and

Utilization (CCU) is an emerging technology field that can replace fossil carbon value chains with significant potential in emissions mitigation or even negative emissions (Mikkelsen et al., 2010; Artz et al., 2018; Kätelhön et al., 2019; Tanzer and Ramirez, 2019). CCU includes a variety of technologies that separate the greenhouse gas CO₂ from point sources or ambient air and consume CO₂ to make products or services, aiming to provide economic, environmental, and social benefits. CCU products include concrete (e.g., Lafarge, Carboncure), carbonate aggregates (e.g., Carbon8, MCI), fuels (e.g., Sunfire, SkyNRG), polymers (e.g., Covestro, Novomer, Econic), methanol (e.g., CRI) or carbon monoxide (e.g., Opus12) (CO₂ Sciences and The Global CO₂ Initiative, 2016; Zimmermann et al., 2017; Bushuyev et al., 2018). Even though CO₂ is an abundant resource in the atmosphere, its economic capture and cost-effective use still require substantial research and development efforts. To advance further development of CCU requires allocation of funds and time resources primarily to economically promising technologies. It is therefore paramount to assess the economic viability of a process upfront using a detailed techno-economic assessment (TEA) in addition to an environmental assessment that is based on life cycle assessment (LCA). TEA is a methodology framework to analyze the technical and economic performance of a process, product or service and “includes studies on the economic impact of research, development, demonstration, and deployment of technologies” (SETIS ERKC, 2016), quantifying the cost of manufacturing and market opportunities.

For the related field carbon capture and storage, a set of international standards (ISO 27912–ISO 27919) has been developed that clarify the scoping and evaluation of CO₂ capture systems (see ISO, 2016a). For CCU, TEA is reported to be commonly used in industrial companies following internal standards—however usually remains unpublished. Published CCU-related TEAs, such as government reports or academic papers, do not yet follow consistent approaches (Zimmermann and Schomäcker, 2017). In contrast to LCA, the number of publications is by orders of magnitude smaller for TEA, and overarching methodological standards are lacking. Most academic TEAs in CCU follow chemical engineering text books such as Peters et al. (2003), Sinnott and Towler (2009), and Turton et al. (2012). In recent years, CCU-relevant TEA-only approaches for example by Sugiyama (2007), Otto et al. (2015), and TEA-LCA-integrated approaches for example by Azapagic et al. (2016) and Thomassen et al. (2019) have been suggested. While providing great practices, the available approaches remain currently too generic, leaving a significant number of methodological choices open, or lack sector-specific guidance for CCU. The current discussion in scientific conferences, industry reports, and academic literature points out that comparing the economic viability or technological feasibility of the various CCU approaches, either of individual technologies or a system of technologies, is challenging and that the number of apples vs. oranges comparisons is high (Pérez-Fortes et al., 2014a; Naims et al., 2015; Roh et al., 2016; Yuan et al., 2016; Zimmermann and Schomäcker, 2017). The significant challenges in TEA for CCU development are the

lack of transparency in assumptions and intermediate results as well as the lack of a generally accepted TEA standard; all of which make assessments and comparisons of CCU technologies difficult.

To address these challenges, thereby increase comparability and put decision making to advance CCU technologies on a rigorous and transparent basis, the first of a kind guideline for standardized TEA for CCU technologies was developed; the work presented here is a summary of this detailed guideline document (Zimmermann et al., 2018). The TEA guideline was developed based on an extensive literature analysis and in a co-operative and creative approach, weighing the various opinions and perspectives present in the field and striving for a consensus. The guideline further provides systematic, step by step guidance on how to produce sound comparisons and how to create and provide transparency, comparability, and reliability of TEA studies for CCU technologies. The TEA guideline was developed in parallel with a guideline for Life Cycle Assessment (LCA) in a one-year project by the partners RWTH Aachen, The University of Sheffield, IASS Potsdam and TU Berlin. Besides the detailed guidelines and this work, several additional publications are available: An overview of both guidelines (Armstrong et al., 2019), a summary LCA guideline (Müller et al., submitted), three worked examples for methanol, e-fuels and mineral aggregates (Michailos et al., 2018; McCord et al., 2019; Zimmermann et al., 2019).

APPROACH

The TEA Guidelines were developed in seven phases, literature analysis, workshop 1, creation of draft, workshop 2, revision of draft and expert review before they were published in an extended report, see **Figure 1**.

For the first phase of the TEA guideline development, literature analysis, a prior study that analyzed 29 papers (Zimmermann and Schomäcker, 2017) was extended following a similar approach; Literature was identified systematically through keyword search covering CO₂ utilization and techno-economic assessment in the Web of Knowledge search engine. As in the prior study, a narrow and a broad search were carried out on September 6th, 2017 and resulted in a list of 219 peer-reviewed journal articles (“papers”) [for search terms see **Appendix**, for further description of literature selection (see Zimmermann and Schomäcker, 2017)]. Besides the 29 papers from the prior study, further 34 new papers, which focused on both CCU technologies and applied techno-economic assessment, were identified. Additional six relevant papers and 11 non-peer-reviewed publications (“reports”) that fulfilled the criteria but did not show up in the search results were added. Overall, 69 papers and 11 reports (see **Table A1**) formed the basis for analysis. Furthermore, relevant procedures and rules of standard literature were included (Peters et al., 2003; ISO 14044, 2006; Sinnott and Towler, 2009; EC-JRC, 2010; Turton et al., 2012). The literature analysis resulted in a systematic overview of assessment approaches, economic, technical and environmental assumptions, methods, and indicators applied.

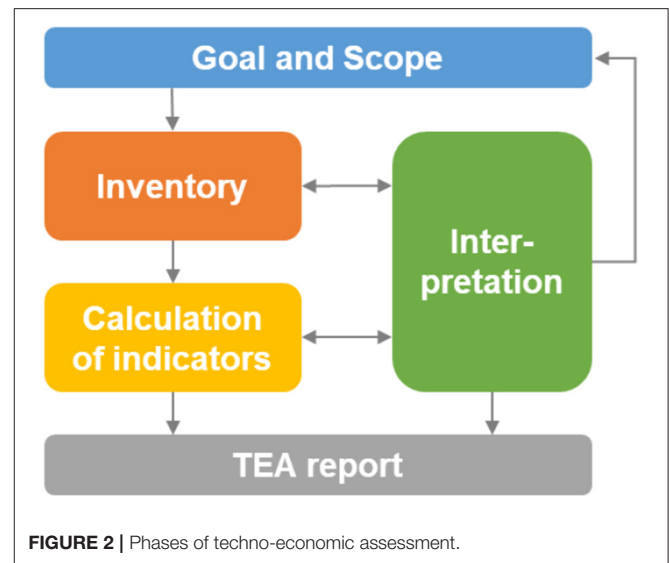


A list of 30 key issues for further discussion in co-creation workshop 1 was derived (see **Figure A1**). The relevant LCA phases and procedures of ISO 14044 and the ILCD handbook were adapted to TEA.

The second phase of the TEA Guidelines development was preparing, conducting, and evaluating workshop 1, a two half-day, in-person discussion meeting, hosted in November 2017 at IASS Potsdam. Four semi-structured discussion sessions were held on 30 key issues, one for each assessment phase, resulting in specific guidance for each of the key issues. The discussion group consisted of 5 project members and 10 external participants, which were invited based on their publications and presentations on techno-economic assessment in CO₂ utilization. The group of 10 external participants represented a diverse set of backgrounds (40% industry, 40% academia, 20% policy).

The third phase was the drafting of the detailed guidelines, an iterative and interactive process, including all co-authors of this publication. The first draft was based on the literature overview, literature best practices, and guidance of workshop 1 and follow-up discussions on the 30 key issues.

The fourth phase was preparing, conducting, and evaluating workshop 2, a full day in-person discussion meeting hosted on April 10th, 2018, at TU Berlin. The session design used three groups, rotating through topical sessions on goal and scope, inventory, interpretation and reporting, presenting feedback, and discussing change requests independent of each other. Based on the documentation and recordings, 266 individual change requests were identified. Besides the 15 members of the project team, 34 external participants attended. External participants



were invited as in workshop 1 based on prior work, representing a diverse set of backgrounds (26% industry, 38% academia, 35% policy).

The fifth phase was the revision of the detailed guideline draft, during which the 187 most urgent change requests were implemented. The remaining requests were left for the following version due to time constraints, but are currently under consideration in a follow-on project.

The sixth phase comprised of a written review from four leading academic researchers (“peer-review”), which was implemented in the revision of the draft. Finally, the detailed guideline document was published in the depository of the University of Michigan (Zimmermann et al., 2018) and launched at the ICCDU 2018 conference in August for a scientific audience as well as at the EIT house in Brussels in October 2018 for a policymaker and industry audience (IASS, 2018).

TEA GUIDELINES

Overview

This article presents the summary of the TEA Guidelines, including all required and recommended guideline rules, which are printed in bold:

- **Shall** rules, the minimum requirements to achieve a standardized assessment, and
- **Should** rules, the recommended requirements to produce an assessment of greater depth;
- Please note that the “may” rules are not covered in this article, but only in the detailed guideline document.

This work transfers and applies many concepts from ISO 14044 (ISO 14044, 2006) and the ILCD handbook (EC-JRC, 2010) to TEA. Following LCA, TEA is subdivided into the phases: goal and scope, inventory, calculation of indicators, interpretation, and reporting (see **Figure 2**); due to its importance reporting is counted as an own phase of the assessment. In the goal

phase, practitioners define the goal for the overall study. In the scope phase, experts define what aspects to include and how to conduct the comparison. In the inventory phase, they collect all relevant data. In the calculation phase, experts specify the calculation procedure and produce the results. In the interpretation phase, practitioners evaluate the quality, consistency, and robustness of outcomes; while they carry out some aspects of interpretation throughout the study, they produce conclusions and recommendations only at the end. As TEA is an iterative process, practitioners will likely go back in loops, specifying and improving the assessment in each round. Finally, all phases and their outcomes are summarized in a TEA report (see Figure 2).

Goal

In the first phase, the goal of the study is defined, including the main questions, the context, the intended use, the limitations, and the audience of the analysis. The goal determines all other parts of the TEA study. While practitioners define an initial goal at the beginning of the work, they can refine or adapt it during the study—but with caution.

Perspectives and Principles of Assessment Goals

Prior studies and the here conducted analysis of CCU literature show that comparisons between TEA studies are often challenging (Zimmermann and Schomäcker, 2017), especially when comparing technologies of varying disciplines, markets, and technology maturities. First and foremost, all assessments need to be based on process concepts that are technologically plausible; for example, proposed concepts do not violate the laws of thermodynamics. Before the assessment, a “sanity check,” for example, checking kinetics as well as mass and energy balances, needs to be conducted by practitioners also synonymously described here as “experts.” As research, development, and deployment of CCU products involve a range of stakeholders, TEAs for CCU are typically conducted from different perspectives—in this report three different perspectives as specified: R&D, corporate and market (see Table 1). Each perspective targets a different audience and poses its specific questions, relevant for defining the assessment goal. When comparing product applications (*e.g., is it more profitable to use methanol as a chemical or as a fuel? Is it more land-efficient to use algae for food or fuel?*), the assessment needs to be carried out first by each application individually before a comparison can be carried out.

In summary and following the principles of LCA, goals of TEAs **shall** state clearly and unambiguously:

- The study context, especially comparison to what, location, time horizon, scale and 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*)

TABLE 1 | Common TEA perspectives.

Common perspectives	Description
R&D perspective	Assessment of specific project(s) in research or development; either identification of significant barriers and drivers (hot-spots) for a single project or comparison of various projects
Corporate perspective	Analysis of projects in development and deployment; assessment of investment alternatives and comparison to existing processes; use of detailed process data is common
Market perspective	Analysis of new concepts and their transformation of value chains; focus on the effects of new policies, the best use of resources or the best way of obtaining a specific utility

- Commissioners and authors of the study (*e.g., funding organization, university, company, individual*)
- Limitations in the usability from assumptions or methods (*e.g., time, location or specific use cases of the products*).

Assessment Scenarios

As TEA studies are supporting decision making with long-term implications, especially for CCU products that often require substantial investments, scenario analysis can be a useful approach to investigate the impact of different core assumptions. Practitioners can define TEA scenarios either in the initial goal phase or when having reached the interpretation phase where experts identify key data for improvement and refine the study goal in another iteration (also see iterative approach in sections Data Quality and Uncertainty and Sensitivity Analysis). If scenario analysis is applied, all scenarios used for analysis **shall** be distinct and physically as well as economically plausible. Scenarios used **should** alter factors accounting for dynamic changes (*e.g., analysis of various competing technology developments or consequences of large-scale technology adoptions, analysis of different potential states in future markets and regulation or societal acceptance*). The base case scenario **shall** serve as a baseline for analysis extending current trends in terms of technology performance, sales prices, and volumes as well as policies and acceptance. Scenarios **shall** be developed in interaction with the stakeholders of the study to ensure they remain relevant to the audience. Scenario assumptions and data **should** be provided at open access to facilitate future work. The analysis and reporting of uncertainty for each scenario are essential and are further described in interpretation (see section Interpretation). If practitioners integrate TEA and LCA, they **shall** use the same set of scenarios. The LCA guidelines offer four scenarios (status quo, low decarbonized, high decarbonized, full decarbonized), which can serve as a helpful starting point for scenario definition (see LCA guidelines, Annex 10.1). For further reading on scenario analysis see Liu et al. (2008), Mahmoud et al. (2009), Amer et al. (2013).

Scope

Building on the goal, practitioners describe in the assessment scope what aspects of a product they will assess and how they

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

CCU class	CO ₂ -based fuels	CO ₂ -based chemical products	CO ₂ -based material products	CO ₂ -avoidance
Product application	Fuels for efficient and clean transportation	Methanol for chemical production	Polyols for flexible foams Waste treatment for industrial ashes	Lowering CO ₂ emissions of another process (e.g., cement or steel)
Market segment	Fuels with low NO _x /soot emissions or heavy-duty vehicles	Chemicals with a low carbon footprint	High-quality flexible foams for mattresses Low-quality aggregates for low-cost concrete	Large-scale CO ₂ avoidance for steel plants Small-scale CO ₂ avoidance for biogas plants

will compare it to competing solutions. Significant activities in the scope phase are identifying the intended product application, the subject of analysis (product system) and in what dimension it is compared to other systems (functional unit), in what quantity it is compared to other systems (reference flow), further specifying the system (system elements), defining what is included and excluded from the assessment (system boundaries), selecting systems for comparison (benchmark systems), understanding how far the technologies are from market-entry (technology maturity) and what parameters and measures are used (criteria and indicators). From the scope, practitioners can derive the requirements for the following phases inventory, calculation, and reporting (ISO 14044, 2006; EC-JRC, 2010).

Product Applications and Functional Units

CCU product applications

In general, the product application **shall** be defined according to the study goal and documented clearly in the report. Potentially, CCU products can provide applications other than similar, conventional products (e.g., *carbonation of mineral slags is waste treatment but also creates aggregates for cement*). The definition of product applications depends on how many applications exist. For products with a small number of applications, practitioners **should** define one relevant application (e.g., *fuels for transportation, polyols for foams*). For products with a large number of applications or where the application cannot be specified, the product itself **should** serve as the application (e.g., *methanol, or carbonate aggregates*) and the expert **should** include a detailed description of the product (e.g., *molecular structure and properties*). For cases of multiple applications, a key question is how many can be carried out at the same time. If multiple applications can be carried out in parallel, practitioners **should** define a relevant “application-mix” (e.g., *for multiple ash sources for CO₂ mineralization*). If only one of multiple applications can be carried out at a time, selecting only one application is sufficient (e.g., *polyols for flexible or rigid foams, energy storage for household-scale or grid-scale*).

The product applications **should** be defined specific to the market segment as it is recommended to compare products with equal performance. Comparing products with different performances is possible but requires a good understanding of price-performance correlations (e.g., *market segments: low*

carbon footprint, commodities, and specialties). In corporate-perspective TEAs, practitioners **should** include a description of at least one customer group and their needs. They can classify customer needs as essential, desirable, and useful (Cussler and Moggridge, 2011). Fulfilling all essential user needs is obligatory for customer acceptance. Fulfilling a desirable user needs can provide a competitive advantage. **Table 2** lists examples of CCU product applications and market segments.

Functional units and reference flows

The functional unit is the dimension of how practitioners compare the reference system to a benchmark (e.g., *mass or distance*). The functional unit **shall** be defined according to the study goal and documented clearly in the report. The functional unit definition depends on product properties and the number of applications. For products with the same chemical structure, composition, or characteristics as benchmark products (“substitutes”), experts **shall** define the functional unit on a mass or energy basis. For products with a structure or characteristics different to benchmark products (“non-substitutes”), practitioners **shall** derive the functional unit from the product performance (e.g., *performance of new power storage vs. existing solutions*). The reference flow is the quantity of comparison (e.g., *1 kg, 1 MJ, 100 km*), typically over a period (e.g., *20 years*). 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, softcore, 180 cm width, 10-year durability*) (EC-JRC, 2010). If the TEA study is conducted together with an LCA, the functional unit **shall** be consistent for both studies. **Table 3** lists examples.

Product Systems

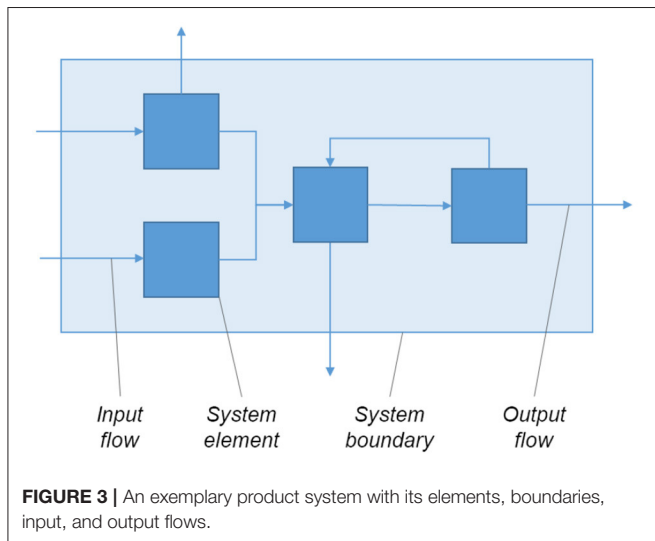
Deriving a CCU product system and its elements

The “system boundary” defines the limits of the assessed product system and describes which system elements belong to it. Material flows and energy flows crossing the system boundary are referred to as “input flows” and “output flows” (see **Figure 3**).

When defining system elements, choosing an appropriate level of detail is crucial; Practitioners **shall** use process units as a basis for system elements (e.g., *electrolysis, CO₂ capture, methanol synthesis*). The assessment **should** not only be carried out for the product system overall, but each system element individually,

TABLE 3 | Examples of CCU substitutes, the basis of comparison, functional units and reference flows.

CCU class/ Properties	Substitutes				Non-substitutes
	Chemical products	Material products	Fuels	Energy storage systems	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 the performance of new to existing solutions
Reference flow	e.g., 1 t methanol, 1.6 Mt/a plant output over 20 a	e.g., 1 t concrete, 50 kt/a plant output over 20 a	e.g., 1 MJ of H ₂ , 2.5 Mt/a diesel over 20 a	e.g., storing 1 MJ of electricity, 80 MWh battery	e.g., 1 t, 1 MJ, the output of conventional plant over 20 a

**FIGURE 3** | An exemplary product system with its elements, boundaries, input, and output flows.

meaning that each system element **should** serve as the accounting unit for inventory, calculation, interpretation, and reporting. General guidance on defining the scope for product systems that include carbon capture is provided by the standards ISO 27912 and ISO 27919 (ISO, 2016a, 2018).

Deriving CCU product system boundaries

Overall, the system boundaries **shall** be consistent with the TEA goal and perspective. Practitioners can derive TEA system boundaries from two points of views: the perspective of the study and product properties. TEAs with an R&D or corporate perspective typically focus on product development and draw the system boundaries around the activities of a company (gate-to-gate). This approach resembles the cradle-to-gate approach in LCA as economic “impacts” of resource extraction are represented by input prices. TEAs with a market perspective can draw the system boundaries around a whole value chain involving multiple organizations, spanning from processing to the use phase and disposal. Such TEA gate-to-grave system boundaries are especially relevant for policy audiences.

Furthermore, TEA system boundaries need to be consistent with product properties. For substitutes, the use and disposal

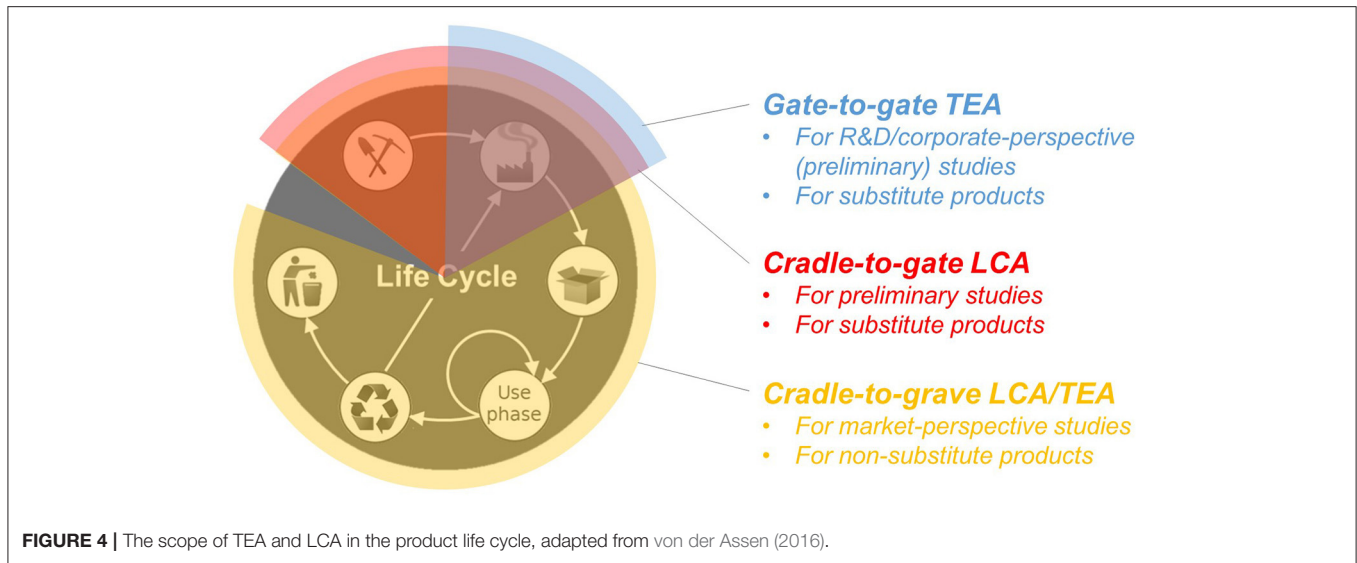
phases are likely to be the same as for benchmark products; a gate-to-gate approach is therefore sufficient. For non-substitutes, the indicator values could significantly change when including the use and disposal phases, due to a different structure and properties. This change **should** either be addressed by including price-performance correlations in gate-to-gate assessments which help to include rational decision making of users, or by extending the system boundaries to cradle-to-grave to include impacts from the whole life cycle (also see LCA Guideline, chapter C.4.2.1). If the intention is to integrate economic and environmental assessment, practitioners **shall** derive the system boundaries from the LCA Guidelines; also see **Figure 4** for different boundary possibilities.

The approach of Life Cycle Costing (LCC) can be helpful when extending the boundaries to cradle-to-grave (Swarr et al., 2011a; Sell et al., 2014; ISO, 2017). However, the high number and wide variety of LCC approaches lead to reduced comparability of the studies. Recent discussions of integrating LCC and LCA exist, which could be helpful when addressing an integrated techno-economic-environmental assessment with cradle-to-grave boundaries (see Swarr et al., 2011b; ISO, 2017; Miah et al., 2017; Dong et al., 2018).

Including or excluding CCU upstream processes in system boundaries

Common questions are whether to include or exclude CO₂ capture, separation and transport processes, hydrogen or electricity production. Any exclusion does not mean that the study does not account for the upstream economic impacts, but that practitioners replace process-specific technical and economic data with average or generic data. Therefore, such exclusion cannot result in zero cost input flows, as it is unlikely that suppliers provide CO₂ or H₂ or electricity without charge.

The decision **shall** be made for each process individually to serve the assessment goal, data availability, data requirements, and the audience. In the case of an independent TEA, experts shall include any upstream process that lies in the focus of the assessment goal, that is required for linking other system elements, or that significantly contributes to the uncertainty of the results. If practitioners conduct TEA and LCA studies in parallel, CO₂ capture, separation, and transportation **shall** be included in system boundaries (see LCA Guidelines chapter



4.2); other upstream processes **shall** follow the LCA principles. Following the iterative approach (see section Data Quality), it might be that an upstream process is excluded at first and added later when it becomes apparent that they significantly contribute to uncertainty. If this is the case, but practitioners exclude upstream processes nevertheless, they **shall** provide a reason.

Multiproduct systems

Product systems can have multiple raw materials or multiple products (also called multifunctionality). However, comparing systems with different products is challenging. For systems with multiple products, practitioners **should** take into account relationships and dependencies between products. When the system produces multiple products, such as coupled products, at the same time (dependent products), experts need to include all dependent products in the assessment (e.g., *coupled products of water electrolysis—both, hydrogen and oxygen, need to be included*). How to address multiproduct systems in TEA depends on the perspective of the study and whether the practitioners integrate TEA and LCA studies. If LCA and TEA studies are integrated, experts **shall** apply the same method for solving multiproduct systems. However, setting the system boundaries and creating the inventory can be challenging (see LCA Guidelines, chapter 4.3). If practitioners do not integrate TEA and LCA studies, their approach can follow any principle that ensures meaningful results. TEAs for multiproduct systems typically calculate indicators for all products combined without separating the indicator value for the particular products (e.g., *calculating profits for a whole plant, including all products it makes*). Another approach is allocation, where experts allocate a share of the result to each product following a key. One particular allocation approach is economic allocation, where, for example, the overall profit can be allocated to each product by the revenue that this product generates. However, an economic allocation is challenging in case of highly uncertain prices and therefore practitioners need to apply it carefully.

Presentation of a product system

Product systems, their elements, and boundaries **shall** be presented in a graphical scheme (see Figure 3), such as an extended block flow diagram. The required specifications for all input flows **shall** be described, including mass flows and their composition, energy flows, and their type of carrier, temperature, and pressure.

Benchmark Product Systems

The term “benchmark” is used for other products or services providing the same application. Benchmark product systems can have similar or different technologies compared to the reference product systems (e.g., *thermochemical, electrochemical, biochemical or photochemical pathways*) and belong either to existing technology regimes (e.g., *CCU methanol compared to conventional methanol*) or to new ones (e.g., *transport by CCU fuel vehicles vs. battery electric vehicles*). Essential for identifying and selecting relevant benchmarks is a good understanding of the product application (see section Product Applications and Functional Units). Benchmarks **shall** be selected and stated according to application and assessment goal. Customer needs **should** be used to identify where the product might have a competitive advantage (Cussler and Moggridge, 2011; Saavedra, 2016). Practitioners **shall** select the currently most common or “best in class” products as benchmark products; one or multiple products can be selected (e.g., *comparing a CCU material to three materials available on the market*). Besides, they **should** additionally include benchmark products that might be relevant in the future in the assessment (e.g., *extending the prior comparison by two promising future material concepts*).

Assessment Indicators

In the following “criterion” is referred to as a parameter in decision making (e.g., *profitability*), “indicator” as a representative measure for a criterion (e.g., *net present value*) and “method” as the way of generating an indicator (e.g., *an equation for net present value*). Practitioners derive the

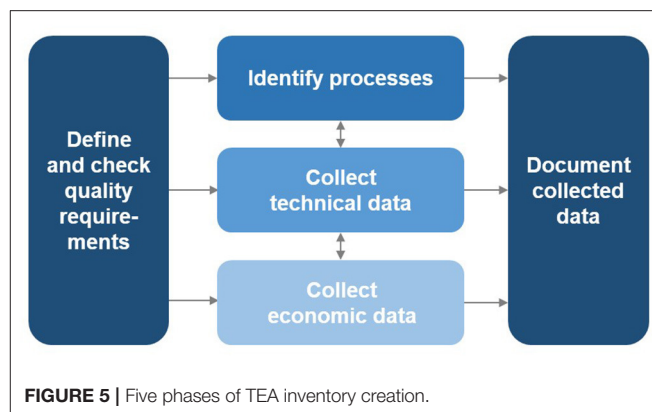
TABLE 4 | List of example criteria and indicators.

Area	Criterion	Indicator examples
Technical	Energy demand	Heat demand, cooling demand, electricity demand, primary energy demand
	Energy efficiency	Lower heating value efficiency, higher heating value efficiency, energy/exergy efficiency, CO ₂ capture penalty
	Mass demand	Mass demand of individual inputs, mass of CO ₂ converted
	Mass efficiency	Atom economy, yield, percentage of CO ₂ converted
Economic	Processing effort	Operational expenditure (OpEx)
	Investment effort	Capital expenditure (CapEx)
	Product margin	Market-derived margin for a product, company-internal margin
	Product volume	Market volume for a product, company-internal demand
	Resource availability	Market volume for feedstocks, company-internal availability of resources, number of suppliers
	Profitability	Profit, net present value, internal rate of return
	Profit/cost per functional unit	Cost per kg benchmark product equivalent, cost per km, cost per MJ stored
Techno-economic	Technology maturity	Technology Readiness Level (TRL) regarding market introduction (Horizon2020 definition), company internal maturity rating

choice of criteria, indicators, and methods from the assessment goal and technology maturity, which needs to be defined before the assessment (Buchner et al., 2018, 2019). A lack of indicator standardization was demonstrated for CCU TEAs: A high number of indicators is currently used to evaluate one criterion, and different methods are applied to derive one indicator, representing a significant obstacle for comparison (Zimmermann and Schomäcker, 2017). **Table 4** shows examples of criteria and indicators.

Many TEAs use the indicators technology readiness levels (TRL), operational expenditure (OpEx), and capital expenditure (CapEx); however, the used definitions and calculation methods vary widely. The detailed guidelines cover definitions and methodological approaches of TRL, OpEx, and CapEx (for CapEx and OpEx see section Economic Indicators, for TRL see detailed guideline section A). Indicators and methods can be selected from the list presented above, or from the pool of indicators used in similar TEA studies or chemical engineering textbooks:

- General TEA indicators and methods for the chemical industry can be found here (Peters et al., 2003; Sinnott and Towler, 2009; Turton et al., 2012)
- Specific indicators for the assessment of early-stage technologies are discussed here (Sugiyama et al., 2008; Patel et al., 2012; Kabatek and Zoelle, 2014; Otto et al., 2015; Buchner et al., 2018)



- Specific indicators for the assessment of product systems including carbon capture are provided in the standards ISO 27912 and ISO 27919 (ISO, 2016a, 2018).

The selected indicators **shall** be compliant with the assessment goal (e.g., *select cost and revenue indicators for a corporate-perspective TEA*) and accessible for the intended audience (e.g., *detailed indicators for researchers, aggregated indicators for politicians*). As the goals for CCU TEAs relate to techno-economic questions, indicators from both fields **should** be selected. The selected indicators and methods **shall** be compliant with technology maturity, which indicates whether data is available and whether estimation methods can be used (e.g., *approximated or measured energy demand for OpEx*). With increasing maturity, the level of technical detail increases and the understanding of products, costs, and markets improve; overall data becomes more reliable and representative and estimation methods increase in quality. Depending on the maturity simpler or more complex indicators can be chosen (e.g., *simpler static relative profit vs. more complex dynamic net present value*).

Inventory

After the goal and scope phase, the inventory phase follows next. The general approach to establish the inventory model covers five interlinked phases: defining requirements for data quality, identifying relevant technical processes, collecting technical and economic data as well as documenting the collected data (see **Figure 5**). In this paper, data is described according to its type (process-specific, industry-average, or generic) and according to its sources (primary or secondary).

Data Quality

First, practitioners **shall** define quality requirements for each data point—according to the assessment goal and scope (e.g., *for methanol production—primary, process-specific data for the system elements of reaction and distillation, and secondary, average data for all other system elements*). Second, data quality **shall** be checked and documented during data collection. The aim is to substantially reduce time and effort by first collecting high-quality data sets only when these contribute sensitively to the TEA result and second increasing data quality step by step until it matches the requirements (iterative approach). The iterative

approach reduces effort by helping to identify and increase the quality of significant data points only. Sensitivity analysis and uncertainty analysis help to characterize each parameter during the inventory model creation (see section Uncertainty and Sensitivity Analysis).

In each iteration, practitioners **should** choose types and sources of data according to the quality requirements. In the first iteration, low data quality can be the starting point. In the second and following iterations, experts need to raise the quality requirements and collection effort where necessary (*e.g., input price data from an open internet platform in the first iteration, from a commercial price database in the second iteration, and from a market study in the third iteration*). If practitioners cannot improve data quality to a satisfactory level, they might not be able to answer the questions posed in the goal. Thus, they **should** either adjust goal and scope according to data availability or discontinue the study. In general, with increasing maturity of the assessed process, more process-specific and primary data **should** be used, as this data increasingly represents the projected process at the deployment stage. However, experts **should** use generic or average data from secondary sources, where sufficiently representative.

Practitioners **should** aim at collecting data available at the corresponding technology maturity: The technology maturity of a product system gives an indication, whether specific data points can be collected directly at high quality or need to be estimated. For CCU, where many early-stage technologies are under development, and for which relevant, high-quality economic data is not available, data estimation is particularly important. Based on the available data from the present technology maturity, the projected plant (TRL 9) is estimated. Practitioners **shall** state any problems with the acquisition of confidential data clearly.

Collecting Data

Overall, data collection **shall** follow data requirements, selected methods and indicators, and the defined assessment goal. As TEA aims to guide the improvement of the overall product system, but also of individual elements, the collection and documentation of data for each identified system element become necessary. The level of detail **shall** follow the identified processes based on the system elements.

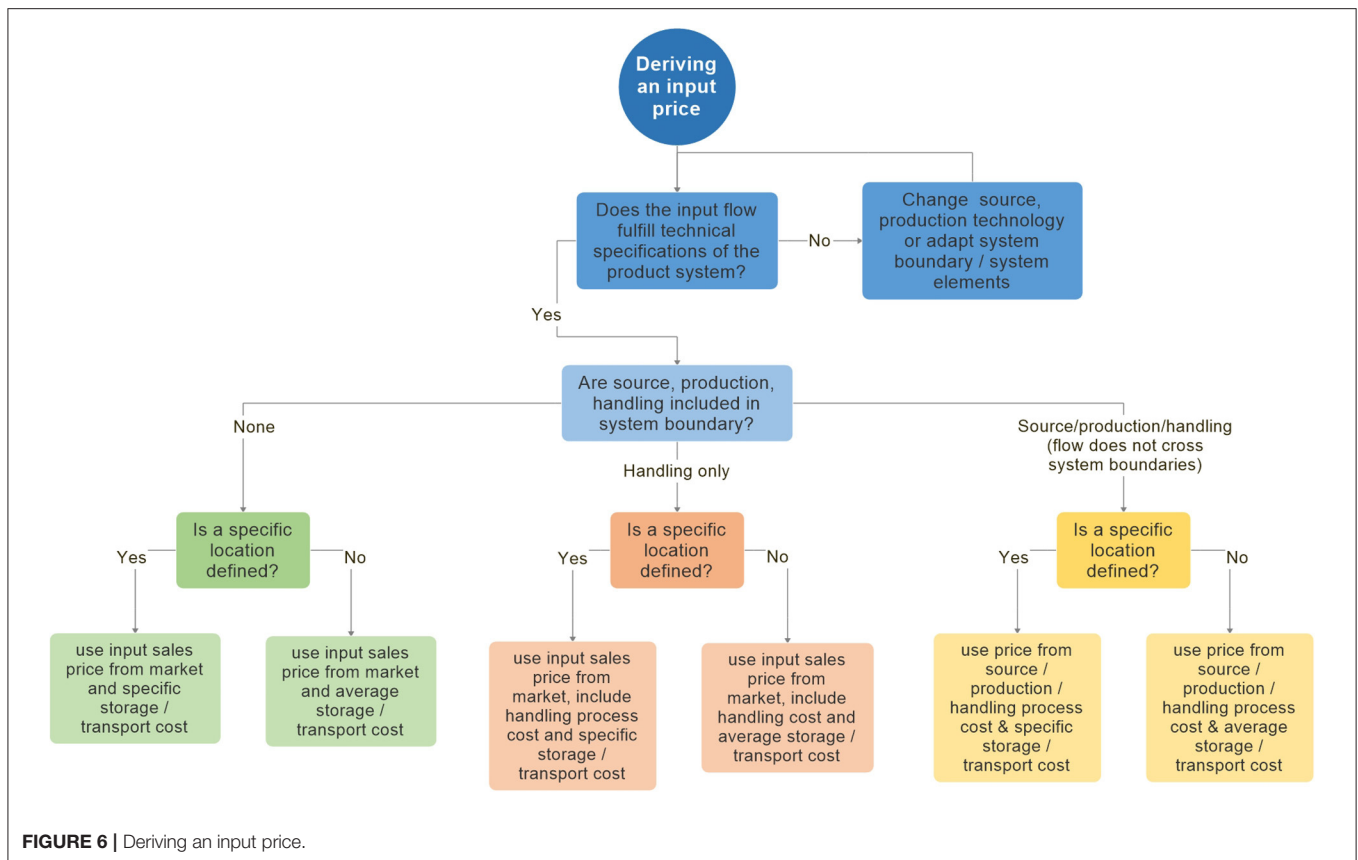
Technical data comprises energy and material flows, process conditions, and equipment specifications, among others; practitioners obtain technical data primarily from process design. Economic data comprises of costs of equipment, prices of inputs and outputs as well as market information. Similar to technical data, economic data can be obtained from a variety of sources (*e.g., quotes, databases, experts, literature*) but in contrast validity is much more limited to the scenario (*e.g., location of quote*) and values can vary significantly between sources (*e.g., internal company prices vs. market prices*). When collecting data from different sources, practitioners **should** carry out harmonization, which means keeping uniformity and aligning assumptions (*e.g., adapting data to the same year, continuous use of lower heating value*). Where possible, technical and economic data **shall** be related to the functional unit and reference flow.

For analyzing the economic criteria, practitioners require data on cost, sales prices, and market volumes. In many cases, the cost of a plant is not available but needs to be estimated (see section Economic Indicators). For deriving the sales price of substitutes, a value-based approach is recommended; a cost-plus pricing approach can serve as an approximation. For the sales price of non-substitutes, a price-performance approach can be used. The market volume for substitutes can be derived from the market volume of benchmark products; estimating the market volume for non-substitutes can be challenging.

Practitioners **shall** describe the temporal and regional context of the study (*e.g., value chain characteristics*) as well as their related limitations and risks, and justify context-specific assumptions and parameters. If prices or market volumes are estimated based on similar studies, a reasonable overlap between temporal and geographical conditions is required, so limitations are not underestimated. For example, governmental regulations might strongly vary between locations and impact the feasibility of the product system (*e.g., subsidies on feedstock, taxes, environmental regulations*).

For economic data in the inventory model, input prices play a crucial role. It is, therefore, necessary to derive prices for input flows that cross the system boundaries. In some cases, it might be of additional interest to derive a price of a flow between system elements (*e.g., the internal production cost of 1 kg of hydrogen via electrolysis as a basis for comparison to other production alternatives*). Deriving an input price, in general, depends on three major factors: technical specifications, assessment boundaries, and location. First, the technical specifications of the input flow need to match the requirements by the product system, such as in quantity, quality, and development over time. If the input flow does not meet these requirements, practitioners need to change the input 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 need to define whether or not the source, production, or additional handling steps, such as purification, compression or heating, of a flow are included or excluded by the assessment boundaries. In the example, experts need to account for the added purification step in the assessment. Please note that if they include the 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, instead it flows between system elements; however, deriving a price for such flow can be of interest. Third, if practitioners define a specific location of the input source, the specific cost for transportation and storage can be used, otherwise applying average cost is sufficient. In the example, the production could be in the same industrial park, and experts could include simple transportation cost by pipeline.

Practitioners **should** also adapt the quality of price data and the number of sources to technology maturity. In early research and development stages, market-average price data **should** be used; typically, few secondary sources are sufficient. In development stages, experts **should** include market-average price data that is date and location specific; typically, secondary



sources are still sufficient, but multiple sources need to be included. In deployment, practitioners **should** use process-specific data and primary sources. The detailed guidelines provide a further description.

If the technology maturity is low, experts have to include learning curves and improvements for the system elements, for both reference product systems as well as the benchmark systems; The cost reduction from building the first of a kind (FOAK) and nth of a kind (NOAK) plant needs to be taken into account (Rubin, 2014, 2016; van der Spek et al., 2017a,b)

Deriving a CO₂ Price

Deriving a CO₂ price depends on technical specifications, system boundaries, and location (see **Figure 6**). First, the technical specifications of flue gas source, CO₂ capture, and utilization need to be consistent. Key factors are, for example, CO₂ concentration or quantity. Furthermore, practitioners need to clarify whether the product system uses the CO₂-containing flue gas directly or requires an additional purification step. Some CCU processes require concentrated and therefore typically more expensive CO₂-containing flows, while others operate with less concentrated and therefore also typically less expensive ones as the purification step can be left out. If the specifications of the CO₂-containing flow do not meet the requirements of the product system (*e.g., too high impurities or too low CO₂ concentration*), practitioners can change the source or production technology or adapt the system boundaries or system elements, such as separation processes to the assessment. While experts

should consider a source or supply with the lowest technically required concentration of CO₂, they cannot only base the choice of emission source on the lowest price. Source and capture processes need to be critically reviewed, as these might cause higher environmental burdens compared to alternatives, requiring a proper LCA. A practice-relevant overview of flue gas qualities is provided in the standard ISO 27912 (ISO, 2016a).

Second, deriving a CO₂ price is dependent on the system boundaries, meaning whether practitioners include or exclude CO₂ source, capture, and compression from the assessment. The CO₂ price **shall** be related to the assessment scope, especially to emission source and CO₂ capture technology. When experts include CO₂ capture in the system boundaries, the base case CO₂ price **shall** represent the cost of capture and compression; the CO₂ price **shall** be calculated based on the full process providing the CO₂ stream. Including handling steps such as CO₂ purification or compression in the assessment, also requires to include handling cost based on the process. When practitioners exclude CO₂ capture, they **should** derive the base case CO₂ price from a market price, which they can collect from a supplier quote.

Third, deriving a CO₂ price is dependent on whether a specific location has been defined or not, meaning that assessments with a specified location require data of local CO₂ sources, while others can be sufficiently assessed with regionally average data. If the assessment goal and scope define a particular location, a location-specific CO₂ price **shall** be derived. When the practitioners exclude the CO₂ capture from the system boundaries, a location-average price is sufficient, but the distance

between the source and the utilization plant **should** be also considered. The CO₂ price **shall** be estimated considering transport. Detailed guidance on pipeline transport of CO₂ can be found in the standard ISO 27913 (ISO, 2016b).

One typical pitfall when deriving a CO₂ price from literature is mixing up the cost of CO₂ captured, and the cost of CO₂ avoided. “Cost of CO₂ captured” relates all processing cost of CO₂ capture to the amount for CO₂ available for utilization; practitioners **shall** report the cost of CO₂ captured or otherwise include a statement. In contrast, “cost of CO₂ avoided” (or “CO₂ abatement cost”) relates all processing cost of capture and production to the amount of CO₂ emissions avoided; “CO₂ avoided” means the difference in CO₂ emissions between the product system and the benchmark system. To calculate the quantity of CO₂ avoided, life cycle assessment is required, underlining the active link between TEA and LCA.

In the inventory model and the TEA report, the key technological and economic assumptions for deriving a CO₂ price **shall** be documented, such as:

- Technologies: capture, compression, transport and storage concepts, CO₂ concentrations, flow rates, flow conditions
- Prices: process-specific or average, cost of CO₂ capture
- Limitations: regional restrictions, reference year and applied transformation factors.

When deriving the CO₂ price from literature, the reported values range from 5 USD/tCO₂ to 180 USD/tCO₂ (Metz et al., 2005; Zero Emission Platform, 2011; Lackner et al., 2012; Wilcox, 2012; de Coninck and Benson, 2014; Smit et al., 2014; Naims, 2016; Leeson et al., 2017), while the EU Prodcom database reports an EU-28 market average value of 78 EUR/tCO₂ (70 USD/tCO₂) for 2016 (Eurostat, 2018). Any selected cost data or cost ranges from literature **shall** be checked and harmonized to ensure the use of adequate assumptions, such as same units, same base year, appropriate scales, matching technology maturity and consistent boundary conditions.

This work refrains from recommending the use of regulatory adjustments or cost lowering mechanisms regarding the estimation of CO₂ prices in the base case. Although specific examples of such mechanisms exist (e.g., *emission trading schemes or carbon taxes*), significant regional differences and future political decisions add to high underlying complexity. Including these mechanisms in the base case, would decrease comparability between TEAs, which is, therefore, not recommended. Instead, practitioners **may** consider the use of regulatory adjustments for additional scenarios to the base case.

Other Key CCU Inputs

Besides CO₂, there are many more crucial inputs for CCU technologies, such as hydrogen, electricity, and mineral inputs, which are discussed in the following section. The detailed guidelines provide guidance on further inputs.

Hydrogen as an input

Hydrogen generation can have both substantial economic and environmental impacts for many CCU studies. Deriving a

hydrogen price is, like any price, dependent on the three significant factors: technical specifications, system boundaries, and location (see **Figure 6**).

First, the technical specifications of hydrogen production need to be consistent with its consumption, which can be hydrogen concentration in the output stream, output quantity, or process durability. If not already completed in the maturity assessment, practitioners **shall** document the maturity of the underlying hydrogen production technology and discuss their current and future viability. Experts **shall** include a mature hydrogen production (TRL 9) as system element in the base case; future and low carbon footprint technologies **should** be included as scenarios (see Häussinger et al., 2011 and IHS Markit, 2015). When selecting the hydrogen production process, practitioners **should** favor “green” hydrogen generation and need to consider environmental trade-offs. If the specifications or the hydrogen-containing flow do not meet the requirements of the product system (e.g., *too many impurities or too low process durability*), practitioners can change the production technology (e.g., *from alkaline electrolysis to PEM electrolysis*), adapt the system boundaries or change the system elements (e.g., *adding the separation of impurities*).

Second, deriving a hydrogen price is dependent on the system boundaries, whether practitioners include or exclude hydrogen production from the assessment. If hydrogen production turns out to be a significant cost driver, data requirements are high, and therefore, experts **should** include hydrogen production in the system boundaries. If the hydrogen production is included, the hydrogen price **shall** be calculated based on the full process cost. If hydrogen production is excluded, practitioners **shall** use the input sales price from the market. Including system elements for handling (e.g., *purification or compression*) in the assessment, also requires to add process based costs for these handling elements.

Third, deriving a hydrogen price is dependent on the location. If a specific location has been defined (e.g., *onsite production or delivery from within the industrial park*) the storage and transport cost **shall** be included relating to this location. If a specific location has not been defined in greater detail (e.g., *delivery by road from the Netherlands or shipping from Saudi Arabia*) cost of transport and storage **shall** be included, but it is sufficient to use average cost. For hydrogen prices (also see Hart et al., 2015; IEA, 2015). In general, the hydrogen price **shall** represent the cost of production or a market price; hydrogen generation and compression **shall** both be represented in the price. All parameters, especially energy sources and prices, **shall** be clearly documented.

For transparency, hydrogen generation **should** be described systematically and in detail. Typical pitfalls when deriving hydrogen prices are:

- Assuming an optimistic future hydrogen production technology or a larger than currently feasible production scale in the base case scenario
- Selecting an inexpensive but environmentally impactful hydrogen production technology and omitting an analysis of the environmental trade-offs

- Assuming intermittent electricity input, but omitting technologic or economic trade-offs (e.g., *OpEx vs. CapEx at different utilization rates, start-stop mechanisms*).

Electricity as an input

Depending on the type of CCU technology, the consumption of electricity might contribute significantly to the economic performance or to the environmental impacts of the product system. Electricity production from renewable resources is of particular interest as it allows for a strong reduction of environmental impacts. Deriving the price for electricity is, as any input price, dependent on the three factors technology specifications, system boundaries, and location (see **Figure 6**). First, the technical specifications of electricity production need to match the requirements of the product system, especially in terms of availability over time and quantity. For example, in the case of intermittent electricity production, either the consuming system elements can handle intermittency, or an additional system element for electricity storage is required. The final choices of electricity production and potential storage technologies need to be clearly documented. Furthermore, a regional electricity grid mix **should** be included either in the base case or a scenario as this increases comparability. Second, deriving the electricity price is dependent on the system boundaries, meaning whether electricity production is included or excluded from the assessment. If electricity production is included, its price **shall** be calculated based on full process cost. If electricity production is excluded from assessment boundaries, the price **shall** be based on a market sales price, such as a spot price. There is extensive literature on electricity pricing, for example from Eurostat's Energy database and the US Energy Information Administration (see EIA U.S. Energy Information Administration, 2020; Eurostat Energy Database). Free or negative electricity prices can be assumed in additional scenarios but **should not** be included in the base case. Third, deriving the electricity price is dependent on the location of electricity production. If the location is defined, specific transportation cost can be included, otherwise using average transportation cost is sufficient.

Typical pitfalls when deriving electricity prices are:

- Excluding a scenario with grid mix electricity
- Assuming free or negative electricity prices in the base case scenario.

Minerals as inputs

Carbonation of minerals, as a CO₂ utilization concept, generally works either with mined minerals (e.g., *olivine, serpentine*), mineral wastes (e.g., *fly ash and steel slags*), or using CO₂ for concrete curing (see Pan, 2015). Deriving prices for mineral inputs follows, as any input price, the three factors technical specifications, system boundaries, and location (see **Figure 6**). First, the technical specifications of the mineral input need to match the requirements of the process; mineral conformation and impurities vary from site to site and might require an adaption of the product system and its elements. Therefore, the quality of raw material from the mining or waste site **should** be considered. In the case of treating waste, potential existing

regulatory mechanisms rewarding waste treatment **should** also be considered. Second, deriving a price for mineral inputs depends on the system boundaries, especially whether and which steps for mining, transportation, handling/pre-reaction, and post-reaction are included in the assessment. For example, in many processes grinding and milling of the raw material is necessary to obtain the required particle size. Any system elements that are included within the system boundary **should** be assessed and documented clearly; prices need to be based on full process cost. For all excluded system elements, using market or regulatory prices is sufficient, but might be challenging to retrieve due to the strong regional variety and low transparency of these markets. Third, deriving the price of mineral inputs is dependent on the location. If the location is defined, specific transportation such as from the mine to the processing facility or from the processing facility to the construction site can be included, otherwise using average transportation cost is sufficient. In addition to the base case, scenarios with varying transport distances and energy sources **should** be included in the assessment.

Documentation of Data Collection

The documentation of inventory data represents the backbone of any assessment—strong documentation helps to assess effectively, troubleshoot quickly, and communicate efficiently. In the beginning, it is recommended to create a model or template with separate sections for an assessment summary, assumptions (separately for base case and scenarios, for technical and economic assumptions), flow data (separated by system elements), calculation of indicators and sensitivity, detailed individual calculations and finally references. Using such a template helps to document data while it is being collected and run several iterations for improving data quality. Technical and economic data **should** be documented based on system elements and based on the functional unit and reference flow while ensuring that the model can adapt if the reference flow is changed. Data uncertainty and potential regional or temporal context such as present in regional prices, currency exchange rates, or market sizes **shall** be included in the documentation. The comparability between assessment studies strongly depends on the units used for reporting results. Parameters **shall** be documented in SI-Units within the metric system, due to their broad acceptance and clear definitions. In the case that non-SI-units are used, a clear documentation and unit definition **shall** be provided. In addition, a conventional flow diagram consisting of system elements, mass, and energy flows **may** be extended by relevant TEA data, to visualize technical and economic parameters efficiently (“TEA flow sheet”). Errors in the inventory model often become apparent during documentation. TEA flow diagrams help to identify errors in mass and energy balances. Furthermore, the thermodynamic limitations of conversions need to be checked thoroughly. For the TEA report, economic data **should** be displayed in a separate list.

Calculation

Following the selection of indicators and the collection of data, calculation methods are selected, and the calculations

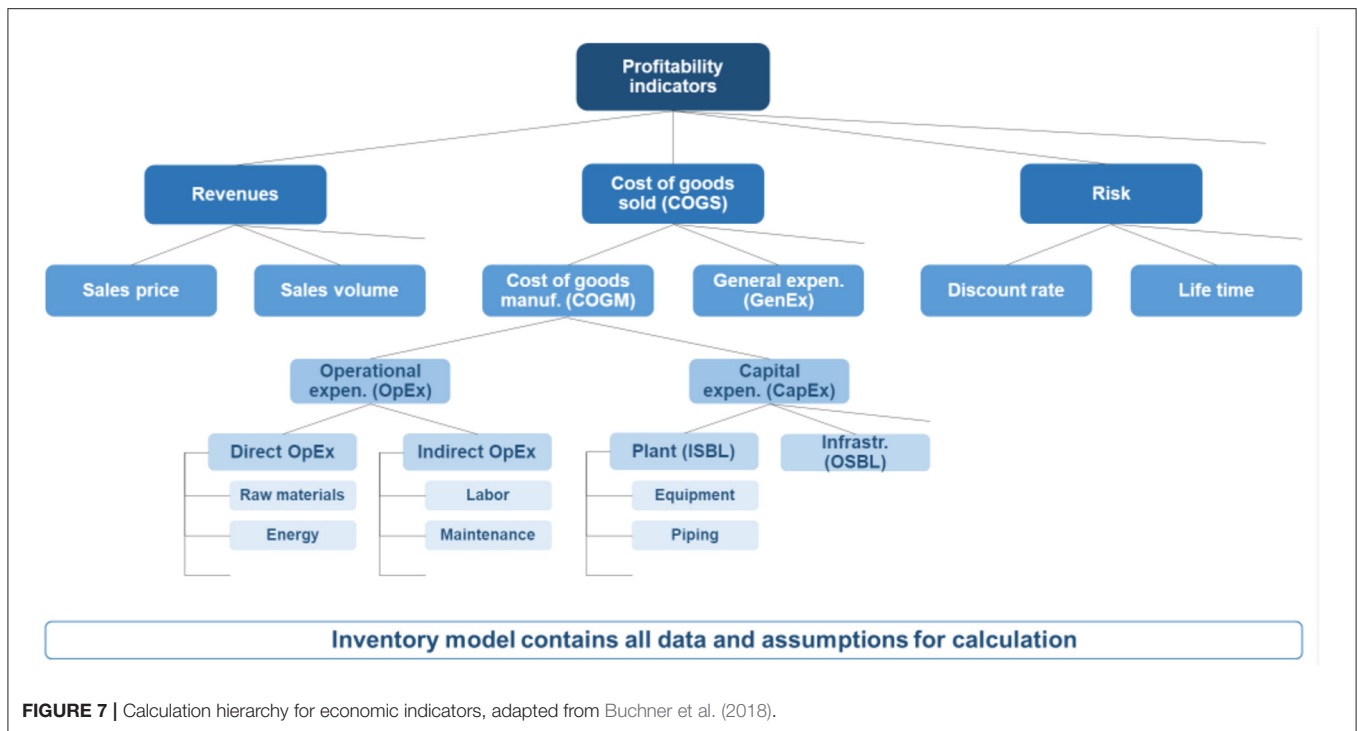


FIGURE 7 | Calculation hierarchy for economic indicators, adapted from Buchner et al. (2018).

conducted in the calculation phase. The results or model outputs serve as a basis for the interpretation. In this chapter, best practices for calculation are discussed first, followed by a more detailed description of economic indicators and approaches for normalization and weighting.

Best Practices

Indicator calculation best practices build on the inventory model: practitioners **shall** organize indicator calculation separately from inventory (in a different file or sheet) but link to it allowing indicators to update following changes of the inventory. Calculation **shall** be organized transparently listing all indicators and equations, relevant inputs and results for system elements individually as well as for the product system overall in SI-units or including a unit definition. Results **should** be organized separately (in a different file or sheet) from the calculation. If any data gaps remain, practitioners **shall** document them. Existing literature offers frameworks (Dysert, 2003; Lagace, 2006; Cheali et al., 2015; Buchner et al., 2018) and detailed descriptions of calculation methods (Peters et al., 2003; Sinnott and Towler, 2009; Turton et al., 2012).

Economic Indicators

Commonly used economic indicators are the investment cost indicator “capital expenditure” (CapEx), the processing cost indicator “operational expenditure” (OpEx) and profitability indicators, which are discussed below. CapEx and OpEx generate the cost of goods manufactured (COGM); addition of general expenditure (GenEx) results in the cost of goods sold (COGS). Profitability indicators can be calculated from COGS considering revenues and risk, as shown in **Figure 7**.

Capital expenditure

Capital expenditure (CapEx) is a key indicator serving the investment criterion in a techno-economic assessment. CapEx can either be interpreted directly or can be used for calculating further indicators such as COGM, COGS or profitability indicators, see **Figure 7**. CapEx comprises the initial investment for “designing, constructing, installing [and commissioning] a plant and the associated modifications needed to prepare the plant site” (Sinnott and Towler, 2009); working capital bound in the operation is often also included. CapEx includes investment for the core plant, “inside battery limits” (ISBL), and investment for connection and infrastructure, “outside battery limits” (OSBL). For orientation in selecting adequate methods, **Table 5** provides an overview of typical CapEx estimation methods clustered by maturity phases and AACE International estimate classes (Christensen and Dysert, 2005).

Calculating CapEx for CCU technologies is challenging as projects can vary widely in technologies making the choice of calculation method difficult. Furthermore, CCU projects are often in the research and development phase lacking detailed data and leading to significant uncertainty in CapEx estimates. Practitioners **shall** select CapEx calculation methods that comply with the goal and scope of the study. They **should** select CapEx methods that are as precise possible but only as precise as available data permits following the iterative approach; this means first using rough estimation, second identifying the key parameters and third selecting more accurate methods. CapEx methods common in literature **should** be selected, or otherwise, the use of uncommon methods **shall** be explained. A challenge for CCU technologies is that CapEx methods are typically based on company experience with fossil resource-based processes and

TABLE 5 | Overview of typical capital expenditure calculation methods.

Phases AAE estimate classes	Research 5 and 4	Development 4 and 3	Deployment 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")

emphasize individual technology parameters differently, leading to under- or overestimation. Therefore, multiple methods **should** be selected, helping to understand the uncertainty in the specific estimation case. For many CCU technologies, the practitioners can choose whether a component belongs inside or outside battery limits—experts **should**, therefore, state ISBL and OSBL components. For early to mid-maturity, OSBL cost **should** be calculated as a factor of ISBL cost. If high-quality data of similar plants or equipment is available, cost transformation **should** be applied; as the cost of each component scales differently, the scaling exponent needs to be defined for each component individually. At mid to high technology maturity, experts **should** analyze how the cost of the main components scale. Once a site is selected, OSBL **should** be estimated independent of ISBL and before building the plant; then all CapEx items **should** be estimated independently; extrapolation via factors needs to be avoided. Building on the inventory documentation, the practitioners **shall** state all additional assumptions, requirements, adjacent estimates used. The detailed guideline document discusses further optional CapEx calculation options, such as forced detail, learning curves and contingency and lowering of accuracy demands. A comprehensive CapEx estimation framework compliant with these TEA Guidelines is described in Buchner et al. (2018).

Operational expenditure

Operational expenditure (OpEx) is a key indicator serving the processing criterion in techno-economic assessment and can either be interpreted directly or used for calculating further indicators such as COGM, COGS and profitability indicators, see **Figure 7**. OpEx comprises all cost for production, including both variable (direct) cost such as raw materials or utilities and fixed (indirect) cost such as labor cost and maintenance. For orientation in selecting adequate methods, **Table 6** provides an overview of typical OpEx estimation approaches clustered by maturity phases.

The practitioners **shall** select methods that comply with the goal and scope of the study; factors for calculation, especially for fixed OpEx, **should** be carefully adapted to the defined scenarios. As for CapEx, experts **should** select OpEx methods that are as precise as possible but only as precise as available

TABLE 6 | Overview of typical operational expenditure calculation approaches.

Phase	Research	Development	Deployment
Raw 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 and other variable OpEx	Based on stoichiometry, 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

data permits following the iterative approach; the selected OpEx methods need to be suited to the technology maturity. OpEx methods common in literature **should** be selected, or otherwise, the use of uncommon methods **shall** be explained. In early research and development, experts **should** consider data from similar plants for energy, utility, and other variable OpEx as well as for fixed OpEx. In late research and development, as soon as fixed capital investment is available, factored estimation for fixed OpEx **should** be used. In deployment, before plant commissioning, all cost items **should** be calculated in detail for fixed OpEx. Building on the inventory documentation and as for CapEx, the practitioners **shall** state institution-specific assumptions, requirements, adjacent estimates.

Profitability indicators

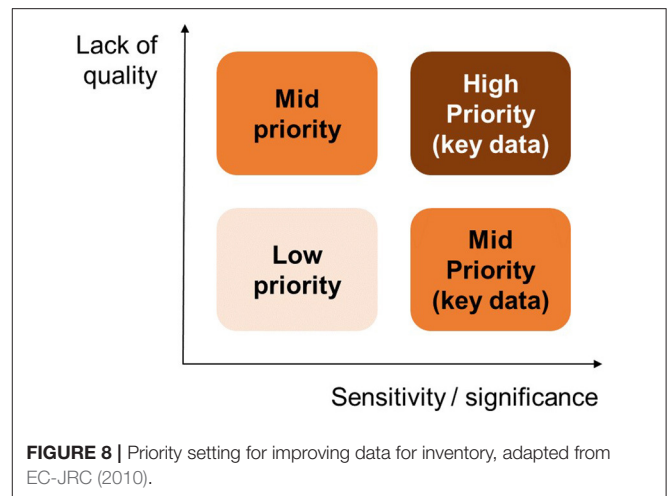
Profitability indicators such as profit, net present value or internal rate of return serve the profitability criterion in techno-economic assessment, comprising of revenues, costs such as CapEx and OpEx and risk. Profitability indicators measure if, how much, and when money can be earned in comparison to an alternative investment (Ward, 2001).

As discussed for OpEx and CapEx, the practitioners need to select profitability indicators and methods that comply with the study's goal and scope that are precise and reasonable following the iterative approach and common in literature. As various calculation approaches exist even for the same profitability indicator, experts **shall** present equations and motivations for each indicator. Furthermore, the selected profitability indicators and methods need to be suited to the technology maturity; this work provides some additional guidance in the following: In the research phase, practitioners **shall** perform qualitative evaluation if a quantitative evaluation is not (yet) possible. When a mass balance is at hand, the **shall** calculate quantitative profitability indicators. Also, experts **should** normalize the profit calculated in

order to facilitate concept comparison. In the development and deployment phase and when the addressable market volume is derived, practitioners **shall** calculate an absolute profit measure. Only following an advanced scenario description, experts **shall** introduce dynamic indicators; if dynamic indicators are required, the practitioners **shall** calculate the net present value. In dynamic calculations, quantifying the risk and selecting an adequate discount rate with a suitable risk profile poses a significant challenge. Rather than taking an average capital market interest rate, experts need to select an interest rate representing an investment with the same risk profile. Many companies use their weighted average cost of capital (WACC) if the project's risk profile is similar to that of the company. The practitioners **shall** consider if a company's WACC applies to the project and adapt the WACC to the project's characteristics or obtain a discount rate from other models. The selected discount rate **should** represent the same risk profile as the product system. In the later development stages, different interest rates **should** be accounted for as the rates depend on the life span of the financing instrument. In the deployment phase, experts **shall** perform detailed economic simulations which consider the project's financial structure and **should** replace cost items with actual cash flows as soon as they are realized. For further information, see the detailed guideline document and Buchner et al. (2018).

Normalization and Weighting

As CCU technologies cover a broad range of chemistry fields (e.g., *thermochemical, biochemical, electrochemical, photochemical*) and include projects at varying technology maturity, normalization and weighting of results might be useful but has to be conducted carefully. Especially for CCU products with diverse technologies and markets, various trade-offs between different indicators and criteria exist (e.g., *OpEx vs. CapEx, market price vs. market volume*). Normalization and weighting are optional approaches for further processing of previously calculated indicators to facilitate interpretation and decision-making. Normalization is the comparison of different indicators by eliminating the units of measurement so that relations are depicted instead of absolute values. Normalization can be used for the comparison of different TEAs, to show relations within a single TEA or enable the combined presentation of indicators. Weighting is assigning quantitative weights to (normalized) indicators. Weighting also includes aggregating, which means adding up weighted indicators. Practitioners have to normalize indicators with different dimensions (preferably to dimensionless indicators) before they can aggregate them. While indicators that have the same dimension and are based on the same assumptions do not require prior normalization. Nevertheless, this work recommends normalization in order to create a common basis and scale. However, if practitioners or the audience only consider the results, both normalization and weighting can lead to a loss of information. Normalization and weighting schemes are specific to technologies and projects; they include subjective choices and have to be carried out with great caution.



Interpretation

Interpretation is conducted in parallel to all TEA phases checking quality, consistency, completeness, and reliability of the inventory data (model inputs) and associated intermediate or final results (model outputs) in relation to goal and scope of the study. Key activities during the interpretation phase are conducting uncertainty and sensitivity assessments, interpreting results, and producing a multicriteria decision analysis, all of which are discussed below. The outcomes of the interpretation phase are conclusions and limitations which serve as a basis for decisions and recommendations for future research, development, and deployment.

Uncertainty and Sensitivity Analysis

Practitioners **shall** provide conclusions, limitations, and a basis for recommendations in the report—which actively build on the analysis of uncertainty and sensitivity. This work recommends the following procedure to analyze the uncertainty and sensitivity of calculated indicators:

1. Characterization of uncertainty
2. Uncertainty analysis
3. Sensitivity analysis
4. Improving data quality iteratively.

First, the practitioners need to characterize uncertainty. Uncertainties can occur in the categories: input, model, and context. Input data uncertainty may result from errors of measurement, from probability distributions of variables, or from estimations with low accuracy. Model structure and process uncertainty may result from limitations of how well the model reflects the observed system. Context uncertainty may result from methodological choices in the goal and scope phase (Saltelli, 2002; EC-JRC, 2010; Igos et al., 2019).

Second, practitioners conduct uncertainty analysis, relating uncertainties from model input, the model itself, or the context on the model outputs. Uncertainty analysis thereby becomes a quality test by considering all sources of uncertainty and validating whether the model output supports the underlying

decision process. Input data uncertainty is typically analyzed quantitatively through intervals (ranges with upper, mid and lower bounds), variance, probability distributions, possibility distributions, or fuzzy intervals (Saltelli et al., 2000; Igos et al., 2019). If data is available to derive probability distributions, using probabilistic methods is recommended. 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. A comprehensive uncertainty propagation method is Monte-Carlo-Analysis. Probability distribution approaches require a good knowledge of the probability distribution functions of the variables—this is often not the case at early technology maturity. Especially in early maturity, qualitative methods can be helpful, for example, degree of confidence approaches such as the pedigree matrix (Fernández-Dacosta et al., 2017). Practitioners can analyze model structure uncertainty by validating the model outputs with measured data or data from similar systems. Context uncertainty can be analyzed by identifying different scenarios and comparing the results or comparing model results with real observations. Scenarios are first defined in the goal phase but might be adapted, or further scenarios might be added when reaching the interpretation phase, after identifying key variables that have a significant influence on the model output (e.g., *different energy mixes and their respective prices or different system boundaries and associated costs and prices*). Scenario analysis goes beyond considering the parameters' known uncertainty ranges but instead considers possible future events on a broader scope. Overall, uncertainty analysis **shall** be conducted. Practitioners **shall** select and analyze one or more output variables or indicators and identify output uncertainty.

Third, practitioners conduct a sensitivity analysis, studying how sensitive the model output is to variations of one or more model inputs. Sensitivity analysis is complementary to uncertainty analysis—it reveals how the uncertainty of the output is constructed and discloses critical input variables that can contribute most to the uncertainty (Saltelli et al., 2000). This work discusses two kinds below: local and global sensitivity analysis. Local sensitivity analysis often also called 'one at a time' method, describes a variation of one input variable around a base value keeping all other input variables fixed. One kind of local sensitivity analysis is threshold analysis, where the smallest or highest value of an input variable is studied that is sufficient to cause a recognizable alteration in the model results that would change the decision. Global sensitivity analysis describes the investigation of how the variation in the model output can be attributed to variations of all input variables. Global sensitivity analysis should be applied to analyze the effects on the output of both individual inputs and interactions between the input variables. Practitioners **shall** conduct sensitivity analysis and identify key variables. For quick screening purposes or at early technology maturity, practitioners **should** conduct a local sensitivity analysis and a threshold analysis for critical variables; a discussion of hotspots, for example, in process design can also be helpful. It is recommended to focus interpretation at early technology maturity on informing about next steps

in R&D, rather than on recommending whether to continue or cancel a technology development. If the goal is to cover the whole parameter space, a global sensitivity analysis **should** be conducted.

Fourth, practitioners aim at improving input data iteratively by identifying key variables from the results of uncertainty and sensitivity analysis. Experts then prioritize data according to (lack of) quality and sensitivity. High priority should be placed on data with both a significant lack of data quality and high sensitivity (see **Figure 8**). If practitioners cannot improve data quality, an overall high uncertainty of results can remain; this needs to be documented (Lagace, 2006). Experts **should** focus on the improvement of data with substantial contribution and sensitivity on the overall result.

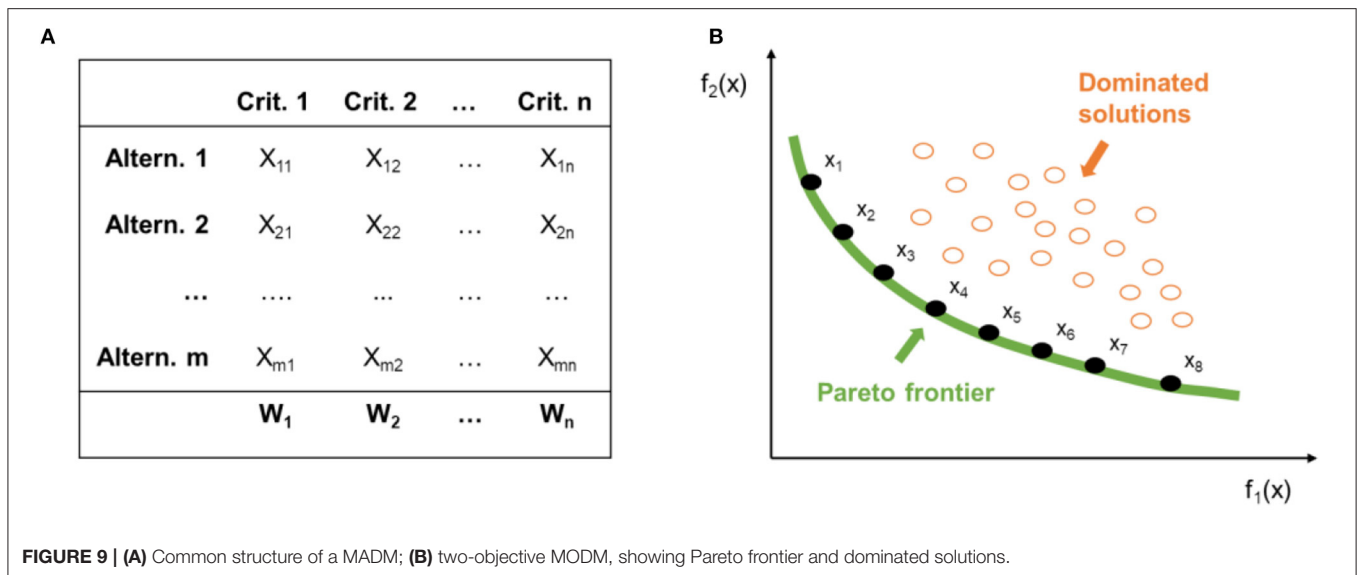
Interpretation of Indicators

To address the assessment goal, in particular its central questions and tasks, the criteria selected in the study need to receive an indication, meaning a positive, negative, or indifferent evaluation. Practitioners derive such an indication for each criterion from the interpretation of the corresponding indicators. Indicators, in particular the ones without an inherent comparison, shall be interpreted by comparing the indicator value of the product system in focus to one or multiple benchmark values. Some indicators (e.g., *internal rate of return, net present value*) already include a comparison and provide an evaluation within the calculation; such comparative indicators can be additionally set into relation with further alternatives if required by the assessment goal. If the practitioners use the indicator "internal rate of return" (IRR), interpretation of IRR **shall** be only conducted together with an absolute profitability indicator without an inherent comparison, such as profit. Overall, the interpretation of any indicators **shall** be made in compliance with their definition, especially according to limitations. Furthermore, indicators **shall** be interpreted according to the specifications set in goal and scope. For example, if the goal defines a threshold value, the difference of calculated and threshold value is to be evaluated. Finally, interpretation **shall** be conducted independently from a subsequent decision making step.

Practitioners **should** interpret uncertainty ranges of indicators if different alternatives exist. The interpretation of uncertainty ranges of multiple alternatives strongly depends on the practitioners' risk preferences, meaning if the expert is risk seeking or risk averse. Risk preferences may be documented and accounted for as a separate parameter in multicriteria decision analysis. Alternatively, a threshold value within the uncertainty range can be defined under (or above) which the expected values are accounted for with a defined factor.

Multicriteria Decision Analysis

Following uncertainty and sensitivity analysis, and the interpretation of indicators, practitioners usually identify a spectrum of criteria relevant for decision making; this whole spectrum **should** be presented to decision makers. If the goal



defines more than one objective and requires to study trade-offs between different targets, multicriteria decision-making (MCDA) can be a helpful approach. MCDA is a method for supporting decisions that involve multiple dimensions, such as economic, social, and environmental criteria, and allows to evaluate trade-offs systematically (Wang et al., 2009). Two categories exist: Multiple Attribute Decision Making (MADM), a ranking approach with finite solutions, and Multiple Objective Decision Making (MODM), a design approach with infinite solutions.

MADM allows studying a discrete decision space and a predetermined set of alternatives. MADM methods use normalization and weighting in order to rank alternatives according to preferences. If applied, MADM **shall** include a wide range of technical and economic criteria, also see **Figure 9**, left.

In contrast, MODM allows studying a continuous decision space providing a group of solutions called the “Pareto optimal set.” MODM may be used to identify and display all trade-offs among the investigated indicators. If MODM is applied, conflicting concepts **shall** be analyzed which means that achieving the optimum for one objective requires some compromise on one or several other objectives, also see **Figure 9** (Hwang and Yoon, 1981; Triantaphyllou et al., 1998; Kahraman, 2008). MADM and MODM can also be applied to analyze trade-offs between LCA and TEA results, which is especially relevant if practitioners integrate both studies.

Reporting

The relevant approaches and results of all prior phases are documented in the TEA report, where practitioners present their findings to an audience. Good reporting practice is vital, as the TEA can only be of value if the audience understands it. A good practice is a TEA report that presents the work comprehensively, clearly and related to the goal of the study, thereby addressing the needs of the audience; a TEA report needs to be more than a mere presentation of indicator values. The requirements of the

audiences vary, and thus, the corresponding reporting style and content can take numerous forms.

Audiences

The different TEA perspectives, R&D, corporate, and market perspective (see section Perspectives and Principles of Assessment Goals), target different audience groups. R&D experts and funding agencies are a typical audience for R&D perspective TEAs. R&D experts demand detailed technical information and the use of specific terminology; they use TEA reports for technical feedback and planning the next steps in R&D. Funding agencies and political analysts require intermediate level technical information and, also, a summarized description of social and economic benefits. Funding agencies and political analysts use TEA reports for funding decision making and communication to governmental or public stakeholders. Company managers or investors are the typical audiences for corporate perspective TEAs. They require a summary and a detailed report, including detailed economic indicators and also technical indicators at an intermediate level; it is recommended to introduce technical terminology. Managers and investors use TEA reports for funding decision making and project management. Policy audiences, i.e., lawmakers, associations, or NGOs, as well as journalists, are the general audiences of market perspective TEAs. This group demands information on broader economic, societal, and environmental impacts—creating a need for the integration of TEA, LCA, and social impact assessment. Policy audiences require a summary and a main report and use TEA reports for designing policy creating long term opportunities or barriers for the technology. Journalists typically demand summarized reports in an easy to understand language; journalists use TEA reports to inform the public and shape opinions, overall influencing acceptance or resistance of the public. In general, TEA reports need to be tailored to the audience’s requirements. Any report **shall** use clear language to avoid misinterpretations, particularly in

summaries and **should** take into account the terminology and language commonly known for the audience.

Reporting Styles

The report may take numerous styles (*e.g., scientific article, investor pitch, media briefing*); the perspective and target audience set the outline for the reporting style. In general, reports **should** include a summary in written form (such as an executive summary) and a technical summary in table form (see detailed guideline document, TEA section, Table 16 Annex). Such technical table summary enables the reader to access the data used in the assessment easily. The results **should** be presented for the overall system, as well as for individual system elements. Such presentation allows the audience to understand the impact of individual system elements and identify where technology advances would create the most significant benefits. Finally, the report **should** list the names and backgrounds of the practitioners that carried out the study and include a description of whether and how a review was conducted.

Content

Once practitioners have identified the report audience and style, they can select the relevant content. Overall, the TEA report **shall** cover all phases of the study: goal, scope, inventory, assessment, and interpretation. In particular, the report **shall** present all assumptions, data, methods, results, recommendations, and limitations transparently and as detailed as possible given the audience and style of the report. Furthermore, data sources and references need to be stated to guarantee reproducibility and traceability. If experts seek compliance with the TEA Guidelines version 1, they **shall** use the provided reporting checklist. Practitioners need to take great care when preparing the content of reports that aim to prepare major decisions, may they be for policy or investment. To avoid misinterpretation, uncertainty and sensitivity of results need to be reported, in particular, all critical variables and their effects on the model result (Igos et al., 2019).

TEA reports for CCU technologies often face challenges in enabling the reader to understand the terminology and to make sense of the assumptions and context of results. First, the terminology can be unknown to the audience and easily confused as it is often the case for “amount of CO₂ used” and “amount of CO₂ avoided”; practitioners need to ensure that the report terminology is well defined and easy to understand for the audience to improve understanding. Second, switching assumptions or including new scenarios can lead to a drastic change of study results, such as switching from a continuous CO₂ policy scenario to a policy change or from stable electricity supply to intermittent supply; to improve understanding, experts could present the changes in results clearly and discuss the limitations of the chosen assumptions. Third, audiences often struggle to understand the context of the results including input and output flows, such as the often large energy requirements or the market size compared to the production capacity; to improve understanding, practitioners could provide comparisons

with existing real-world examples such as the number of wind turbines.

DISCUSSION

This work presents a systematic and holistic approach of how to conduct techno-economic assessments for carbon capture and utilization technologies. The work summarizes the current state of the art, building on a broad literature review, institutional reports and the feedback of more than 50 experts from industry, academia and policy that was collected through a series of workshops and resulted in a detailed TEA and LCA Guidelines document (Zimmermann et al., 2018) that enables transparent and comparable assessments.

The TEA guidelines define a robust framework that has received global attention since its release in 2018. The guidelines represent the summary of the current discussion. However, some concepts are still subject to change; the authors see the guideline as a living document and invite all users to contribute to updating the document. As next steps, five aspects should be addressed: First, to build on the acceptance of the first version of the detailed guidelines document (Zimmermann et al., 2018) it could be used to inform the development of an ISO standard. Second, the goal and scope of both TEA and LCA assessments remain different, assessments are currently not aligned, and thus, results have to be interpreted individually for each assessment. Stronger alignment between both TEA and LCA would be beneficial, in fact, crucial, in particular, for the identification of trade-offs between environmental and economic indicators. Third, in many cases CCU technologies promise to reduce environmental impacts and achieve costs competitiveness. This evaluation can, however, be challenging for early-stage technologies because the availability of quantitative and scalable data is low at these stages. For this reason, further methods to assess the potential for technologies with low maturity are needed. Fourth, the technical terminology, length, and reporting complexity of TEA and LCA reports have been identified to be a significant challenge for policy audiences that aim to derive policies. Therefore, guidance on how to commission and understand TEA and LCA results for policy audiences as well as detailed guidance for practitioners on how to produce TEA and LCA reports for a particular target audience must be subject to future research. Fifth and finally, these TEA guidelines were designed for carbon capture and utilization technologies, which include a variety of technologies, including thermochemistry, electrochemistry, photochemistry, and many more. Fundamentally, the applicability of these guidelines for TEAs outside of CCU is expected but will have to be demonstrated.

CONCLUSION

The principal goal of this work was to develop unifying guidelines on how to conduct as well as report rigorously and transparently techno-economic assessments (TEA) for carbon capture and utilization (CCU) processes. To meet this

need, a harmonized TEA assessment guideline for CCU was developed in an international effort as presented in this paper. The work includes approaches for improved comparisons, such as guidance on technology maturity, on defining system boundaries or on identifying benchmark systems. This work further provides guidance for increasing transparency and comparability, such as guidance on the interpretation of uncertainty and sensitivity as well as best practices for reporting. To the best of our knowledge, this guideline is the first TEA framework with a focus on CCU technologies and the first that is designed to be conducted in parallel to LCA due to aligned vocabulary and assessment steps. A combined and broadly reviewed detailed guidelines document that also includes detailed guidance for life cycle assessment (LCA) was made publicly available (Zimmermann et al., 2018) and has found broad dissemination. In the process of developing and disseminating the guidelines document, the authors identified additional needs and opportunities. Subjects for future work are further harmonization with related efforts and eventually the development of a global standard, extended alignment or even integration of TEA and LCA providing detailed guidelines, further guidance on early maturity technologies and on addressing policy audiences as well as the application of this TEA framework on technologies beyond CCU. This work, therefore, extends the LCA CCU framework, the detailed TEA and LCA Guidelines and the worked examples, current literature, improving the design, implementation, and reporting of TEA studies. Overall, the application of this TEA guideline is expected to lead to improved transparency and decision making for the development of climate mitigating, negative emission CCU technologies.

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AUTHOR CONTRIBUTIONS

AZ, JW, LM, GB, AM, SMi, KA, HN, SMc, PS, VS, and RS were involved in the conception and the revision of the article. AZ carried out the writing, and summarizing the detailed guideline document, which is composed of contributions of all authors. All authors approved the final version of the article and agreed to be accountable for what it contains.

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SUPPLEMENTARY MATERIAL

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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