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Economic Feasibility Studies for Carbon Capture and Utilisation Technologies: A Tutorial Review

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Abstract

Carbon Capture and Utilization (CCU) involves the capture and use of CO₂ as a resource to create valuable products. The economic viability of CCU technologies is crucial for its implementation in real life. The competitiveness of various CCU technologies has been investigated frequently resulting in a variety of economic feasibility studies and economic indicators. This study performs a tutorial review, in which practical guidance is given on the implementation of TEAs for chemical CCU technologies. The tutorial review will critically examine the economic feasibility studies that have been performed in this field and will advise how these studies can be improved in the future. A thorough review of the literature set is performed, in which we evaluate the quality of the economic feasibility studies in the literature set by comparing these studies to the guidelines from Zimmermann et al. (2020). The five phases of an exhaustive TEA are (I) goal and scope, (II) data inventory, (III) calculation of indicators, (IV) interpretation, and (V) writing the report. We evaluate the implementation of these five phases in the economic feasibility studies in the literature set. The tutorial review shows that economic feasibility studies for chemical CCU technologies can and should be improved in various manners. Phase I and II are often skipped or incomplete. Phase III, the calculation of assessment indicators, shows diversity in the indicator base which hampers comparability across CCU technologies of the technical and economic criteria that are key for the feasibility. Phase IV, the interpretation of results, is often missing in the literature set or lacks thorough uncertainty and sensitivity analyses. These findings suggest that future economic feasibility studies should be made in a more standardized way to improve both the quality and comparability of economic feasibility studies. This tutorial review has raised important questions about the management of uncertainty and flexibility in economic feasibility studies. The integration of Real Options Analysis (ROA) within the TEA is proposed to analyse the investment decision in CCU technologies in a dynamic setting.

Introduction

In 2018, annual global anthropogenic CO₂ emissions exceeded 36 billion tons (Ritchie and Roser 2017). Although the share of renewable energy has increased drastically in the last decade, our reliance on fossil fuels will continue to exist in the short and medium-term. To stay below the '+2°C' target, it will not suffice to reduce energy consumption, impose carbon taxes and increase energy efficiency (Greenfish 2019). CO₂ emissions from power plants and heavy industry must be reduced significantly to achieve the climate objectives (European Commission 2019). Moreover, the depletion of resources by consuming resources faster than they can be replenished is becoming an increasingly important issue for the present and future generations (Vijay Kumar et al. 2020). Hence, Carbon Capture and Utilization (CCU) technologies are acknowledged as a crucial component of the decarbonization strategy. CCU can lower the concentration of CO₂ in the atmosphere in two ways: (i) by decreasing CO₂ emissions at the source itself and (ii) by increasing the efficiency of industrial processes and replacing the conventional fossil-based raw materials (Aresta and Dibenedetto 2007; Baena-Moreno et al. 2019). CCU technologies can provide substitutes for fossil resources, hence slowing down the depletion of fossil resources.

Although the terms are often confounded, Carbon Capture and Storage (CCS) and CCU are two distinct concepts. CCS technologies capture CO₂ emissions from large point sources and inject the captured CO₂ into geological formations for long-term storage underground (Leonzio et al. 2019). Contrary to CCS, CCU does not store the CO₂ permanently underground but utilizes it as a raw material to produce other goods or services. Thus, CCU can add additional revenue streams to the reduction of CO₂ emissions.

The International Energy Agency (IEA) distinguishes two main CCU pathways: (i) the direct use or non-conversion of CO₂, in which the CO₂-molecule is not chemically altered, and (ii) the indirect use or conversion of CO₂ into fuels, chemicals, or building materials. Table 1 provides the breakdown of CCU into the two pathways (indirect and direct use) and their major applications. Examples of products are given for each application. Commercial CCU applications today mostly involve the direct use of CO₂, e.g. the use of CO₂ for production of food and beverages, in greenhouses, or CO₂-enhanced oil recovery (EOR). In 2015, the largest user of CO₂ was the fertilizer industry, where around 130 Mt CO₂ per year was directly used to produce urea. The second-largest user was the oil industry, with an annual consumption of 70–80 Mt of CO₂ for EOR. The use of CO₂ for the production of fuels, chemicals or building materials was in 2015 still negligible (around 4% of global CO₂ consumption). However, in recent years, the conversion route has attracted more and more interest, driven by national and international climate mitigation objectives, the rise of (cheap) renewable energy and the quest for energy security (IEA 2019).

Table 1
Classification of CCU pathways, based on Fig. 2 from the *Putting CO₂ to use*-report from the IEA (IEA 2019)

| Pathways | Applications | Examples |
|-----------------|---------------------|--|
| Direct use | Yield boosting | <i>Greenhouses, algae, fertilizer/urea</i> |
| | Solvent | <i>EOR</i> |
| | Heat transfer fluid | <i>Refrigeration</i> |
| | Other | <i>Food and beverages, medical uses, welding</i> |
| Indirect use | Fuels | <i>Methane, methanol, gasoline/diesel</i> |
| | Chemicals | <i>Chemical intermediates, polymers</i> |
| | Building materials | <i>Cement, concrete</i> |

For the indirect use of CO₂, three main technology routes can be identified: the biological, mineralization or chemical route (Chauvy et al. 2019). Figure 1 presents a schematic overview of the different CCU routes. Biological routes employ the natural ability of micro-organisms to capture and convert CO₂ into chemicals or fuels (National Academies of Science Engineering and Medicine 2019). One example is the use of green algae to convert the CO₂ into other organic compounds. Mineralization, or carbonation, is a natural process where CO₂ reacts with calcium- or magnesium-containing minerals to produce valuable

construction materials (CO₂ Value Europe). In chemical routes, the CO₂ is used as a reactant or feedstock for the synthesis of commodity chemicals and fuels (National Academies of Science Engineering and Medicine 2019).

The sparked interest in CCU technologies also generated a large body of research in recent years. A crucial aspect is the techno-economic feasibility of the technology for its implementation on a commercial scale. Techno-economic assessment (TEA) is a methodology framework to assess both the technical and economic performance of a novel process, to quantify the cost of manufacturing and to evaluate market opportunities (Zimmermann et al. 2020). Despite the importance of the TEA, no generally accepted methodologies are practised yet and thus, the comparability and readability of techno-economic assessments of novel CCU technologies remain low (Zimmermann et al. 2020). To introduce more transparent and comparable TEAs, Zimmermann et al. (2020) developed guidelines for TEAs, particularly for CCU technologies. Guidance is given on the formal structure that the TEA should follow, starting with the definition of the goal and scope of the TEA, followed by the inventory, the calculation of indicators, the interpretation, and the writing of the report to finish the TEA. We will evaluate whether the five phases, identified by Zimmermann et al. (2020), are carried out or not in economic feasibility studies for CCU technologies.

According to Sick et al. (2019), TEA is a very useful methodology to assess the feasibility of CCU technologies. However, a TEA is also very flexible in its application; results may vary significantly, depending on the defined system boundaries and assumptions. The variety of indicators makes it also difficult to compare results. Therefore, Sick et al. (2019) expressed the need for a harmonized framework for TEAs for CCU technologies. Naims (2020) also expressed the need for TEAs of novel CO₂-based products. In sum, TEAs are an important instrument in the development of novel CCU technologies. However, because of its flexibility, the quality of the TEAs may differ significantly between different studies. Several researchers have expressed their concerns on the comparability of the results of different TEAs before (Zimmermann and Schomäcker 2017; Sick et al. 2019) Therefore, it is important to be able to assess the quality of a TEA or an economic feasibility study in general, before concluding whether or not the CCU technology is economically viable based on that particular study. This paper will attempt to evaluate the quality of the performed assessments in a literature set of economic feasibility studies.

Centi et al. (2020) also observed the need for a critical reflection on the evaluation of CO₂ economics. Their critical analysis reveals a large variability in the estimated cost of methanol and methane production, beyond the commonly assumed 30% variation in costs in preliminary techno-economic assessments. Stemming from the variety in methodologies, parameters and boundary limits, different conclusions can be drawn on the techno-economic feasibility of a CCU technology, even if the assessment is based on the same data. The need for a proper contextualization of results is acknowledged, in terms of the context of the study (time, location, method and data) and in the context of the proper CO₂ value chain. The lack of homogeneity in terms of costs for raw materials, methodologies and system boundaries is recognised, however, these different aspects of the economic evaluations are not analysed in more detail. In other words, Centi et al. (2020) observed large variations in the results but

did not further analyse what differences in economic assessments produced that variability. The current paper fills this gap by analysing the methodological choices made in economic evaluations for CCU technologies and how these choices can explain the observed divergence in the results.

This study performs a tutorial review, in which practical guidance is given on the implementation of TEAs for chemical CCU technologies. The tutorial review will critically examine the economic feasibility studies that have been performed in this field and will advise how these studies can be improved in the future. A thorough review of the literature set is performed, in which we evaluate the quality of the economic feasibility studies in the literature set by comparing these studies to the guidelines from Zimmermann et al. (2020). A detailed and critical analysis of these studies with respect to the implemented methods has not been done before.

The scope of this paper is limited to the indirect use of CO₂, and more specifically to the chemical CO₂ utilization route. The direct use of CO₂ is excluded because these technologies are already available on a commercial scale today. Economic assessments for technologies in the market are more clear-cut and thus, an extensive review of these methods is not needed. Moreover, the IEA (2019) observed an increased interest in the indirect use pathway in recent years, resulting in a growing body of literature. Within the conversion route, we choose to focus on chemical CO₂ utilization technologies. A literature set arranging the relevant economic assessments for chemical CO₂ utilization technologies is established. This literature set will serve as the starting point for our analysis.

Four main objectives are set for this paper. First, we aim to evaluate the quality of the economic feasibility studies by comparing the studies in the literature set to the TEA-guidelines of Zimmermann et al. (2020). Second, we will map the differences in the methodological choices and assumptions that may produce variation in results. Thirdly, the techno-economic feasibility of various chemical CCU technologies for methanol synthesis are compared, to identify the existing barriers and drivers for the commercialization of methanol-producing CCU technologies. Fourthly, additions to the TEA-framework of Zimmermann et al. (2020) are proposed to further improve the quality of the TEA.

This tutorial review aims to contribute to the growing area of research on CCU by exploring to what extent economic feasibility studies differ, in what aspects they differ and how these studies can be improved further. Hence, this tutorial review can help CCU researchers to rethink and critically reflect on their economic feasibility studies. The tutorial review provides a basis to evaluate the quality of a TEA, which can be helpful to assess whether or not the results of the TEA are credible or not. For unexperienced CCU researchers, this tutorial review can provide a good starting point to understand how to perform decent economic assessments.

The paper is organized as follows. The next section is devoted to the Method of this tutorial review. The selection of the literature set and the TEA-guidelines from Zimmerman et al. (2020) are explained in more detail. Three important methodological choices – assessment indicators, system boundaries and the cost of CO₂ – are also clarified further here. This is then followed by the Results section. The attributes of the

literature set are discussed, including the type of CCU products that are investigated and the type of methods that are used to evaluate the economic feasibility. Afterwards, we discuss how the studies in the literature set correspond to the TEA-guidelines from Zimmermann et al. (2020). This is followed by a more detailed revision of four important methodological choices, one per phase: the chosen system boundaries (I – Goal and Scope), the assumed cost of CO₂ (II – Data Inventory), the selected assessment indicators (III – Calculation of Indicators) and the presence or absence of uncertainty and sensitivity analysis (IV – Interpretation). The economic feasibility studies of methanol synthesis processes are discussed in more detail afterwards. Finally, the Results section ends with three possible additions to the TEA-guidelines from Zimmermann et al. (2020). In the Discussion, the observed shortcomings in the literature set are listed. The paper ends with concluding remarks on TEAs for CCU technologies and some recommendations on how to move forward in this research area.

Method

A systematic literature search was conducted to establish a comprehensive literature set. Three consecutive search queries were performed in the online databases Web of Science Core Collection (Web of knowledge 2021) and Scopus (Scopus 2021), in January 2021. The first search included variations on 'techno-economic' and 'analysis', combined with different synonyms and spelling methods of 'Carbon Capture and Utilization'. A secondary search focussed on the chemical transformation CCU technologies, by including terms related to 'chemical transformation'. The third search included the term 'raw material', because of the use of CO₂ as raw material or input. The searches in Web of Science and Scopus resulted in a total of 69 unique results. This was further reduced to 24 papers, by excluding the papers that didn't fit the scope of this review. Finally, 3 relevant articles, which were already known to the authors, were added manually to the literature set, bringing the total up to 27 papers. The full literature set is shown in Table A.2. in the Appendix 'Literature set'. This literature set is the starting point for this in-depth tutorial review: the literature set will be analysed thoroughly (i) to appraise the quality of the techno-economic feasibility studies, (ii) to map the differences in the methodological choices and assumptions that may produce variation in results and, (iii) to propose further additions or improvements that can be made to the TEA-guidelines from Zimmerman et al. (2020).

Techno-economic assessment (TEA)

Techno-economic assessment (TEA) is a methodology framework with different understandings and different applications circulating in literature. The European Commission describes the TEA as a cost-benefit comparison that can be used for multiple tasks, including the evaluation of techno-economic feasibility of a project, the investigation of cash flows over the lifetime of a project and the comparison of the economic feasibility of different technologies providing the same service (Lauer 2008). Following Van Dael et al. (2015), the TEA framework should help to make choices during the development of the technology or process. This TEA framework consists of four steps (Van Dael et al. 2015): (i) a market study, (ii) the technological backbone, including Process Flow Diagram (PFD) and mass and energy

balances (M&EB), (iii) the economic evaluation, and (iv) the sensitivity assessment. Thomassen et al. (2019) advocated the implementation of a prospective techno-economic and environmental assessment framework, that integrates both the techno-economic feasibility and the environmental impacts into one assessment. The most recent guidelines for TEAs for CCU, were published by Zimmermann et al. (2020). They propose the division of TEA in five phases: (i) setting the goal and scope, (ii) building the data inventory, (iii) calculating the indicators, (iv) interpreting results, and (v) writing the TEA-report. Their framework was based on a comprehensive literature review and multiple workshops with leading CCU-researchers, resulting in a TEA framework for CCU technologies that is broadly supported by the CCU community. For this reason, these guidelines are used in this study as a benchmark, to which the techno-economic feasibility studies for chemical CCU technologies are compared. Figure 2 presents these five phases of the TEA framework by Zimmermann et al. (2020).

A high-quality TEA should start with defining *the goal and scope* of the study. This includes describing the reasons for carrying out the TEA, which questions it should address, defining the system boundaries and choosing the assessment indicators. Setting the scope also includes the definition of the benchmark system, to which the product's performance can be compared. The chosen benchmark system is often the best-in-class or the market leader.

This is followed by the creation of a *data inventory* for the TEA. The Block Flow Diagram (BFD) or PFD depicts how the process design looks like, from an engineering perspective. The M&EB describe the flows in the system and are used as input to calculate the selected assessment indicators. Besides the technical data, economic data must be gathered as well. A market study is performed to examine the competitive environment for the novel CCU technology. Data on product prices, utility prices and the price of CO₂ are collected in the data inventory.

The third phase is the *calculation of the assessment indicators*. These can be technical, economic and/or environmental indicators, depending on the scope of the TEA.

The *interpretation*-phase is a crucial step for high-quality TEAs. In this phase, both the uncertainty and sensitivity of the results of the TEA should be assessed. Uncertainty analysis quantifies the level of uncertainty that is associated with the results, caused by uncertainty in the data or propagation of errors in the data. Sensitivity analysis, on the other hand, identifies the sources of uncertainties in the input variables that are responsible for the uncertainty in the model output. The interpretation of the results is thus very important, as it helps to understand the impact of your results and helps to reveal what should be improved to the technology, process or product in order to become competitive.

Finally, all findings should be written in a formal *report*.

Naturally, TEAs are not only performed in the CCU research field. The structure as described above can be applied to other research fields, where the techno-economic feasibility of technologies needs to be assessed. Some parts of the TEA methodology that will be described in this tutorial review are, however, specific to CCU technologies. The chosen system boundaries are specific for the CO₂ value chain. The

cost of CO₂ is an important element in the data inventory that must be considered for the CCU technologies. In general, the majority of CCU technologies are still at early stage of development (IEA 2019), which also needs to be taken into account in the TEA. This is discussed further in the tutorial review.

In this tutorial review, we will assess whether and how these phases are present in the techno-economic feasibility studies in the literature set. Of course, not all studies in the literature set perform a TEA. Other economic assessment methods are practised as well to assess the economic feasibility. Economic assessment methods can show a large variety of quality, ranging from 'back-on-the-envelope' calculations to well-structured and detailed assessment methods. Life Cycle Costing (LCC) is a well-structured method that assembles all costs over the entire lifetime of a product. More specifically, LCC aggregates all costs that the producer of a product will incur over the product's lifespan (Accounting Tools). The TEA differs from the LCC in its integration of the economic assessment, where both costs and revenues are estimated, and the technical assessment (Zimmermann et al. 2018). Other types of economic assessment methods are e.g. business models and cost-benefit analyses (CBA). In a CBA, other societal costs and benefits can be added to the analysis, while technical parameters are less important compared to a TEA.

Since the TEA framework offers such a complete methodology to assess the techno-economic feasibility, by integrating costs, revenues and technical parameters, all economic assessments in the literature are contrasted with the five phases of a TEA, as depicted by Zimmermann et al. (2020).

Four methodological choices are analysed in more detail. Firstly, the chosen system boundaries will be critically reviewed. Secondly, the various costs or prices of CO₂ that are assumed in the literature set will be summarized and evaluated. Thirdly, the calculated assessment indicators, with focus on the economic indicators, in the literature set will be listed and compared. Finally, the implementation of the interpretation-phase in the literature set. will be evaluated.

System boundaries

System boundaries are defined by the researchers and determine which stages of the CO₂ value chain are included or excluded from the economic analysis. To this end, a simplified CO₂ value chain and its possible system boundaries are presented in Fig. 3. The value chain of the conversion of CO₂ into fuels or chemicals involves the following stages: the capture of CO₂, the actual conversion of CO₂ into the final product, the production of low-carbon energy to drive the (energy-intensive) transformation process, the transport of energy and materials for the conversion process and the delivery of the final product to the customer (Jarvis and Samsatli 2018). When system boundaries are drawn around the CCU plant itself, a gate-to-gate approach is applied. As indicated in Fig. 3, this includes the conversion of CO₂ into the valuable product but excludes the CO₂ capture and the transport of the final product. In other words, the economic assessment covers the processes between the front and the end gate of the CCU plant. Adding the CO₂ capture process gives the cradle-to-gate system from a manufacturer's perspective. When

transport and distribution of the final product are included as well, a retailer's perspective is adopted. The cradle-to-grave approach includes the entire value chain, from resource extraction to end-of-life treatment (Carbon Trust; Zimmermann et al. 2018). Hence, the choice of system boundaries defines which economic impacts are included or excluded from the analysis. Besides, the chosen boundaries also affect how the price of CO₂ is incorporated in the economic assessment.

The cost of CO₂

In a CCU plant, the CO₂ is treated as a valuable resource and converted into a commercial end-product. However, the cost of CO₂ can be incorporated into the economic assessment in various manners. The presumed CO₂ price level is often related to the chosen system boundaries and affects the outcomes of the economic indicators. Various assumptions are possible. The observed approaches in the literature set are discussed in more detail in the Results-section.

Assessment indicators

Zimmermann et al. (2020) already observed a lack of a common indicator basis in TEAs for CCU technologies, which hampers comparison between different TEAs and technologies. We will list the observed economic indicators per category, analyse which indicators are the most common, and evaluate the chosen assessment indicators.

Technical indicators are criteria to assess the technical performance of the process or technology. Energy efficiency or energy demand and the conversion rate of CO₂ are common technical indicators for CCU technologies.

Economic indicators are metrics or evaluation criteria used by researchers to assess the economic feasibility of the CCU technology under investigation. A distinction can be made between cost-oriented indicators and profit-oriented indicators. Cost-oriented indicators solely comprise relevant costs of the CCU technology. Capital Expenditures (CAPEX) and Operational Expenditures (OPEX) are typical examples of cost-oriented indicators. Another cost-oriented indicator is the Levelized Cost of Product (LCOP), which is a measure for the unit selling price that is required for the CCU technology to earn a certain return on investment (ROI) (Fernandez-Dacosta et al. 2017). The LCOP is often practised as an economic indicator in an LCC analysis. Profit-oriented indicators, on the other hand, integrate both costs and revenues of the CCU plant. The Net Present Value (NPV) is a well-known example of a profit-oriented indicator. NPV is the present value of the difference between all revenues and costs over a certain period (Investopedia). In other words, the NPV gives today's value of a future stream of cash flows. The NPV is commonly used as an indicator in the economic evaluation of a TEA.

Environmental indicators are indicators to evaluate the environmental impact of the process or technology. Examples are the net amount of CO₂ used, CO₂ emissions, or depletion of fossil fuels.

The calculated values of all assessment indicators are highly dependent on the assumptions that are made during the economic assessment.

Uncertainty and sensitivity analyses

Uncertainty and sensitivity analyses are the key instruments in the interpretation-phase to review the reliability of data and to put the results in perspective. Uncertainty and sensitivity analysis are, although related, two distinct types of analyses to explore the uncertainty in a model.

Uncertainty analysis (UA) characterizes the output distribution and aims to define and quantify the level of uncertainty in the model output (Saltelli et al. 2019).

Sensitivity analysis (SA), on the other hand, identifies the sources of uncertainties in the input variables that are responsible for the uncertainty in the model output. In other words, SA studies how the uncertainty in the model output can be apportioned to the sources of uncertainty in the model inputs (Saltelli 2002). While UA helps to estimate the level of uncertainty that is present, SA serves to allocate the uncertainty in the model output to the input variables. Ideally, the UA precedes the SA: one cannot apportion the uncertainty to input variables (= SA) without first estimating it (= UA) (Saltelli et al. 2019).

Both UA and SA have their role in the interpretation-phase of the TEA. Saltelli et al. (2019) listed several best practices for UA and SA; we summarize the most important recommendations here. Firstly, *global* exploration of the input variables is preferred over local or one-at-a-time (OAT) analysis, both for SA and UA. Global analyses investigate the variation of multiple variables simultaneously, whereas local analyses look at the variation in input variables one-at-a-time. Monte Carlo is the most common technique for global analyses, wherein repeated random sampling is performed to get a probability distribution for the output. Secondly, UA and SA should be performed *together* in general. Thirdly, the UA and SA should focus on a *question* that is originally addressed by the model. How CCU researchers deal with UA and SA in their economic feasibility studies, is discussed in the Results-section.

Results

Two important attributes of the literature set are surveyed first: the product categories that were analysed and the type of economic assessment methods that were used in the literature set. The tutorial review contrasts the studies in the literature set with the TEA-structure from Zimmermann et al. (2020), followed by a detailed analysis of four methodological choices. The synthesis of methanol via chemical CCU technologies is reviewed to identify barriers preventing commercialization of this technology. Finally, enhancements to the TEA-structure from Zimmermann et al. (2020) are proposed.

Attributes of the literature set

The literature set consists of 27 papers, covering various types of chemical CCU technologies and products. The indirect use CCU pathway transforms the low-value resource CO₂ into higher-value

products, at a sufficiently large scale. In general, three product categories are discerned: CO₂-derived chemicals, CO₂-derived fuels and CO₂-derived building materials (IEA 2019). CO₂-derived chemicals include a wide variety of chemicals or intermediates, such as urea, syngas or formic acid. CO₂-derived fuels can be liquid hydrocarbon fuels, syngas, methanol or methane. CO₂-derived building materials are typically produced through mineralization processes, hence this product category was not observed in our literature set. Figure 4 presents the breakdown of the literature set according to the product category. Methanol, methane and hydrogen can serve both as a chemical and a fuel. Therefore, separate categories were created for these products. As shown in Figure 4, methanol (16 studies) is the most prevalent product in the literature set, followed by CO₂-based chemicals (11) and fuels (5). Figure 5 presents a more detailed breakdown of the CO₂-based chemicals and fuels: a diverse range of products is observed.

Table 2 summarizes the labelled economic assessment methods that were observed in the literature set. Naturally, techno-economic analysis or assessment is the most common label used by the researchers in the literature set: 12 papers claim to perform a techno-economic analysis or assessment. Six studies combine the techno-economic assessment with an evaluation of the environmental impacts. Two studies design a business model, one study limits the assessment to LCC, and the remaining six papers use a variety of methods. In the next section, we will analyse how the studies in the literature set accord to the TEA structure proposed by Zimmermann et al. (2020).

Table 2: Labelled economic assessment methods in the literature set

| Labeled method | # of studies |
|---|---------------------|
| Business model | 2 |
| LCC | 1 |
| Market simulation model | 1 |
| Multi-objective Mixed Integer Linear Program (moMILP) | 1 |
| Multi-scale analysis | 1 |
| Process and economic analysis | 1 |
| Technical and economic feasibility | 1 |
| Technical and economical evaluation | 1 |
| Techno-economic analysis/assessment | 12 |
| Techno-economic and climate impact analysis | 1 |
| Techno-economic and environmental assessment/evaluation | 4 |
| Techno-economic and life cycle assessment | 1 |
| Total | 27 |

Compliance with TEA structure

The studies in the literature set were read thoroughly and compared to the guidelines from Zimmermann et al. (2020). For the first phase, we assessed if the system boundaries were explicitly defined or not and whether a benchmark system or product was selected. The creation of the data inventory was assessed by checking whether a technical inventory (PFD and M&EB) and market study were present or not. For the third phase, we observed which type of indicators were selected: technical (TECH), economic (ECON) or environmental (ENV). Fourthly, the implementation of the interpretation-phase was evaluated by examining if a sensitivity analysis (one-at-a-time or combined) or a Monte Carlo simulation was performed, or not. Naturally, the final step, the writing of the report, was performed for all studies.

Table 3 shows to what extent the economic feasibility studies in the literature accord with the guidelines from Zimmermann et al. (2020). A colour code – green, orange and red – is used to indicate whether or not these steps were implemented in the study. A green block indicates that this step is fully present, an orange block indicates that the step is only half-completed and a red one implies that the step is missing in the study. More specifically, the orange colour for the system boundaries indicates that the system boundaries were not defined explicitly in the paper. For the technical inventory, an orange block implies that either the PFD or M&EB was absent in the study. An ‘orange’ market study means that the market study is rather limited (e.g. only one forecast for future market). For the indicators, the green block implies that at least one of this type of indicator is present; it does not say anything about the quality of the selected indicator. In the interpretation-phase, either sensitivity analysis (SA) OAT, SA combined or a Monte Carlo simulation is performed in the literature set. The final step, the writing of the report, is left out of Table 3 as this is performed for all studies.

It can be seen from the colour codes in Table 3 that the majority of the studies in the literature set lacked several important phases. A market study was missing in 15 papers and only half-completed in 9 papers of the literature set, the system boundaries were not explicitly defined in 16 papers and the technical backbone was also missing or incomplete in 9 papers. The interpretation-phase was skipped in 10 studies, although this step is crucial to interpret the results of the assessment correctly. Pérez-Fortes et al. (2016b, a) incorporated all five phases in their studies for methanol and formic acid synthesis, resulting in decent economic feasibility studies. The quality of their assessment could only have been improved by performing a more detailed Interpretation-phase, to account more for the uncertainty in the data.

The TEA framework from Zimmermann et al. (2020) aimed to harmonize TEA methodologies in the CCU research area. However, as shown in this tutorial review, this framework is far from being implemented in practice. Most studies in the literature fail to do multiple phases of the proposed TEA-structure by Zimmermann et al (2020). This demonstrates that significant efforts will be needed to harmonize TEAs in CCU research.

It is also apparent from Table 3 that the economic feasibility studies differ significantly in their applied methodologies to assess the economic feasibility of a CCU technology. Except for two studies of Pérez-

Fortes et al. (2016b, a) and two studies of Godini et al. (2020b) and Yang et al. (2021), all studies differ in the implementation of one or multiple phases. The methodological differences in the literature set, highlighted in Table 3, can give rise to diverging quality of the economic feasibility studies

Table 3: Presence of the five TEA-phases of Zimmerman et al. (2020) in the literature set, indicated by color codes.

| I - Goal and Scope | | II - Data Inventory | | III - Calculation of Indicators | | | IV - Interpretation | | | References |
|--------------------|------------------|---------------------|--------------|---------------------------------|-------|-----|---------------------|-------------|---------------|---|
| System boundaries | Benchmark system | Technical inventory | Market study | TECH | ECON | ENV | SA OAT | SA combined | MC simulation | |
| Green | Green | Red | Green | Red | Green | Red | | | | (Horschig et al. 2019) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Hoppe et al. 2018) |
| Green | Green | Red | Green | Red | Green | Red | | | | (González-Aparicio et al. 2017) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Putra et al. 2017) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Deng and Adams II 2020) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Jens et al. 2019a) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Kuenen et al. 2016) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Lainez-Aguirre et al. 2017) |
| Green | Green | Red | Green | Red | Green | Red | | | | (John et al. 2021) |
| Green | Green | Red | Green | Red | Green | Red | | | | (Pérez-Fortes et al. 2014) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Zhang et al. 2017) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Godini et al. 2020b; Yang et al. 2021) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Kim et al. 2018a) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Gonzalez-Aparicio et al. 2018) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Zhang et al. 2019) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Zhang et al. 2015b) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Dimitriou et al. 2015) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Yusuf et al. 2019) |
| Green | Green | Red | Green | Red | Green | Red | Green | | | (Kim and Han 2020b) |
| Green | Green | Red | Green | Red | Green | Red | Green | Green | | (Bellotti et al. 2019) |
| Green | Green | Red | Green | Red | Green | Red | Green | Green | | (Chiuta et al. 2016) |
| Green | Green | Red | Green | Red | Green | Red | Green | Green | Green | (Lee et al. 2020) |
| Green | Green | Red | Green | Red | Green | Red | Green | Green | | (Fernandez-Dacosta et al. 2017) |
| Green | Green | Red | Green | Red | Green | Red | Green | Green | | (Szima and Cormos 2018) |
| Green | Green | Red | Green | Red | Green | Red | Green | Green | | (Pérez-Fortes et al. 2016b, a) |

Goal and Scope: system boundaries

The system boundaries of the analysis determine which phases of the CCU process are included or excluded from the economic evaluation. Interestingly, 18 out of 27 papers analysed economic feasibility from gate-to-gate. Thus, the great majority of papers draws the boundaries around the CCU plant itself. The carbon capture process is not analysed or simulated in detail. The remaining nine papers set the boundaries from cradle-to-gate, from a manufacturer’s perspective (Dimitriou et al. 2015; Lainez-Aguirre et al. 2017; Putra et al. 2017; Fernandez-Dacosta et al. 2017; Hoppe et al. 2018; Jens et al. 2019b; Bellotti et al. 2019; John et al. 2021; Yang et al. 2021). These papers included the capture of CO₂ within their system boundaries but did not specify the costs related to the transport and distribution of the end-product and the end-of-life treatment of the product. Figure 6 (a) presents the breakdown of the literature set based on the chosen system boundaries.

Data Inventory: the cost of CO₂

How the system boundaries are defined, also affects how the cost of CO₂ is incorporated in the economic assessment. In CCU processes, the CO₂ is a feedstock which is converted into a valuable product. The cost of CO₂ is addressed in various manners in the literature set. The studies with system boundaries set from cradle-to-gate include the carbon capture in their detailed analysis. Figure 6 (b) shows how many gate-to-gate studies do account for the costs of carbon capture, by including average costs based on literature or data from industry. Six gate-to-gate studies consider the costs of carbon capture in some way, the remaining 12 neglect the costs related to carbon capture. The treatment of the cost of CO₂ can be subdivided further. Table 4 summarizes five different approaches to the cost of CO₂ which were observed in the literature set.

In the first approach, zero costs are assumed for CO₂: the price of CO₂ as a raw material is zero, there are no costs of capture and a carbon tax or credit is absent as well. Hence, CO₂ is assumed available for free as a waste product from other existing plants in this scenario.

The second approach treats CO₂ as a greenhouse gas (GHG): a carbon tax or credit scheme is included in these papers. Despite the assumed presence of a carbon tax penalty or credit, the CO₂ which is fed into the CCU plant is still seen as a flue gas which can be 'purchased' at zero cost. Capture costs are not taken into account either. The carbon tax or credit scheme that is adopted is typically favourable for the CCU plant. The implemented carbon tax imposes a penalty on the conventional CO₂ emitting plant and increases its costs, relative to the CCU plant. Taking it one step further, the tax savings made by a CO₂-emitting plant due to the CCU plant, could be passed on to the CCU plant. In the most extreme case, the CCU plant is eligible for carbon credits due to its emission savings (Chiuta et al. 2016). These carbon credits are rewarded to plants whose emissions are below the specified cap in the EU Emission Trading System (ETS) and can then be sold again on the carbon market. Consequently, the CCU plant becomes relatively cheaper compared to the reference plant in the presence of any carbon tax or credit scheme as described above. The four papers in Approach 2 adopt a cap-and-trade system that is equal or very similar to the EU ETS. However, CCU currently does not fall within the legal scope of the EU ETS. Transfers of CO₂ are currently only allowed under very specific conditions, being that the "the transfer of inherent CO₂ should only be to other EU-ETS installations and the transfer of pure CO₂ should only occur for the purposes of storage in a geological storage site" (European Commission 2012). Thus, the CO₂ emissions consumed by a CCU plant do not represent emissions savings according to the ETS. Nevertheless, carbon tax savings and even carbon credits are commonly assumed benefits in economic evaluations of CCU technologies.

In the third approach, the CO₂ is considered to be a raw material for the CCU plant, which is readily available at the gate of the plant. However, the price of CO₂ can vary from negative to positive, where negative prices mean that the CCU plant receives revenue for using the CO₂. These references all perform

a sensitivity analysis, to investigate the effect of the CO₂ price fluctuations on the economic feasibility. These references estimate the CO₂ price level based on the existence of a carbon market; thus, a carbon tax/credit scheme is present once again.

Table 4: Five different approaches for incorporating the cost of CO₂ in the economic assessment were observed. Three characteristics distinguish the pricing schemes: whether or not the CO₂ is treated as a raw material (with a cost), whether or not the cost of capture is included and whether or not a carbon tax/credit scheme is adopted.

| Approach | Pricing schemes | | | References |
|--|-----------------|------------------------|--------------------------|---|
| | <i>RM price</i> | <i>Cost of capture</i> | <i>Carbon tax/credit</i> | |
| 1. Zero costs | - | - | - | (Pérez-Fortes et al. 2014; Kuenen et al. 2016; Horschig et al. 2019; Godini et al. 2020a; Yang et al. 2021) |
| 2. CO ₂ as GHG | - | - | P | (Zhang et al. 2015a, 2017; Chiuta et al. 2016; Szima and Cormos 2018; Kim and Han 2020a) |
| 3. CO ₂ as RM | P | - | P | (Pérez-Fortes et al. 2016b; Kim et al. 2018b; Gonzalez-Aparicio et al. 2018; Zhang et al. 2019) |
| 4. Fixed capture costs | P | P | - | (Pérez-Fortes et al. 2016a; González-Aparicio et al. 2017; Lee et al. 2020; Deng and Adams II 2020) |
| 5. Cradle-to-gate | - | P | - | (Dimitriou et al. 2015; Putra et al. 2017; Jens et al. 2019b; Yusuf et al. 2019) |
| | | | P | (Lainez-Aguirre et al. 2017; Hoppe et al. 2018; John et al. 2021) |
| <i>RM, Raw Material; GHG, Greenhouse Gas</i> | | | | |

The fourth approach includes a fixed cost for the capture of CO₂ in the price. A surplus is added to the price of CO₂ because it needs to be captured first. The process of capturing CO₂ is not modelled in these references. Instead, the price of captured CO₂ is based on average or generic data that is available in the literature.

Finally, the fifth approach includes the cost of carbon capture by including the capture unit in its analysis. Whilst other references draw their boundaries around the CCU plant and exclude the capture unit from the modelling, these references model the capture unit carefully and calculate all costs associated with it (investment costs, operating costs, etc.). In other words, a cradle-to-gate approach is adopted by these papers. Although these papers all include the costs associated with the capture unit in their economic analysis, the price of CO₂ as a raw material is assumed to be zero in these papers. CO₂ is considered to be a flue gas from an emitting plant which is also part of their system; thus, the CO₂ source is within the

boundaries of the analysis. In other words, the CO₂ itself is free of charge, but it is the capturing of the CO₂ which is costly. Four of these papers do not consider the presence of a carbon tax or credit, while the two remaining papers do include a carbon tax/credit scheme in their analysis. One paper is excluded from Table 4 because it doesn't fit one of these five approaches. Fernandez-Dacosta et al. (Fernandez-Dacosta et al. 2017) perform a break-even analysis, which results in the minimum price of CO₂ that would make the CCU plant more profitable than the conventional plant. In this paper, the price of CO₂ is a result of the economic analysis, not an input.

Table 4 highlights the differences between the five approaches. However, estimated values for the cost of CO₂ vary greatly within one approach as well. Figure 7 (a) presents the ranges of assumed carbon taxes and credits in Approach 2. Chiuta et al. (Chiuta et al. 2016) presume that a carbon credit can be granted to a CCU plant as well, as shown by the negative number in Figure 7 (a).

Figure 7 (b) presents the prices of CO₂ that were observed in Approach 3. Once again, large differences between these papers can be observed. A very high negative price of 400 €/ton CO₂ is assumed in Pérez-Fortes et al. (2016b), implying a significant carbon revenue for the CCU plant. Other papers make more modest estimates, up to 100 €/ton CO₂. For comparison, the carbon prices on the European Emission Allowances market fluctuated around 25 €/ton CO₂ at the beginning of 2020 (Ember 2021). At the beginning of 2018, the carbon price was only about 8 euros per tonne of CO₂. Assuming that the carbon price would rise from 25 euros to 100 or even 400 euros per tonne CO₂ soon seems overly optimistic. In reality, carbon prices remain to date relatively low and their evolution will be prone to policy changes.

Two preliminary conclusions can be drawn from Figures 7 (a) and 7 (b). Firstly, a large range of assumed prices of CO₂ is observed in the literature set. Secondly, researchers tend to be overly optimistic about the future levels of the carbon price, while CO₂ emissions treated in CCU processes are not yet considered as emission savings in the current EU ETS framework.

Figure 7: (a) The assumed ranges for carbon taxes and/or credits observed in Approach 2, in euro per ton CO₂ (b) The assumed prices for CO₂ as raw material observed in Approach 3, in euro per ton CO₂

Calculation of Indicators: the selection of assessment indicators

Table 5 lists all economic indicators used in the literature set, split up into cost-oriented and profit-oriented indicators. In total, 18 different economic indicators were found over 27 papers. First, some general reflections on the use of economic indicators are expressed. This is then followed by a closer look at the cost-oriented and the profit-oriented indicators respectively.

Firstly, a diverse set of indicators is observed in the literature set. Interestingly, the majority of the indicators only appears once or twice in the literature set. The NPV (9), (Total) Product(ion) Cost ((T)PC – 8) and (Discounted) Payback Period ((D)PBP – 7) are the only indicators used repeatedly in more than

five different papers. This variety of indicators makes it difficult to compare the economic feasibility of various CCU technologies. Sick et al. (Sick et al. 2020) already raised this issue and reported the need for a harmonized TEA toolkit. A second observation from Table 5 is the prevalence of cost-oriented indicators. Cost-oriented indicators are used if the revenues of the CCU plant are not known yet or very uncertain. The market prices of the end-products, produced in the CCU plant, are very uncertain in many cases (Dimitriou et al. 2015). However, cost-based indicators can never be used on a stand-alone basis to assess the economic feasibility. Cost-based indicators can compare the cost efficiency of the CCU-based process to the conventional production process. However, the revenues of the CCU process are equally important to assess the economic feasibility. Finally, the majority of papers in the literature set combines several economic indicators to assess the economic feasibility of the CCU plant. For example, NPV, Internal Rate of Return (IRR) and (D)PBP are often used jointly (Zhang et al. 2015b, 2017).

Table 5: List of economic indicators, subdivided into cost-oriented and profit-oriented indicators

| Economic indicators | # of uses | References |
|-----------------------------------|------------------|---|
| <i>Cost-oriented indicators</i> | | |
| CAPEX | 3 | (Pérez-Fortes et al. 2014; Fernandez-Dacosta et al. 2017; Yusuf et al. 2019) |
| CoE | 2 | (Bellotti et al. 2019; Yusuf et al. 2019) |
| LCOP | 2 | (Chiuta et al. 2016; Fernandez-Dacosta et al. 2017) |
| OPEX | 2 | (Fernandez-Dacosta et al. 2017; Yusuf et al. 2019) |
| TAC | 1 | (Putra et al. 2017) |
| T(F)CI | 4 | (Dimitriou et al. 2015; Zhang et al. 2015a, 2019; Deng and Adams II 2020) |
| Total cost | 1 | (John et al. 2021) |
| (T)PC | 8 | (Dimitriou et al. 2015; Zhang et al. 2015a, 2019; Kuenen et al. 2016; Kim et al. 2018a; Hoppe et al. 2018; Lee et al. 2020; Deng and Adams II 2020) |
| Utility costs | 1 | (Jens et al. 2019c) |
| <i>Profit-oriented indicators</i> | | |
| (D)PBP | 7 | (Zhang et al. 2015a, 2017; González-Aparicio et al. 2017; Fernandez-Dacosta et al. 2017; Kim et al. 2018a; Godini et al. 2020b; Deng and Adams II 2020) |
| IRR | 3 | (Zhang et al. 2017; González-Aparicio et al. 2017; Bellotti et al. 2019) |
| Market uptake (# plants) | 1 | (Horschig et al. 2019) |
| MSP | 2 | (Jens et al. 2019a; Kim and Han 2020b) |
| NPV | 9 | (Zhang et al. 2015a, 2017; Pérez-Fortes et al. 2016c, a; Lainez-Aguirre et al. 2017; Kim et al. 2018a; Szima and Cormos 2018; Deng and Adams II 2020; Yang et al. 2021) |
| Profit | 2 | (González-Aparicio et al. 2017; Gonzalez-Aparicio et al. 2018) |
| PVR | 1 | (Kim et al. 2018a) |
| Sales | 2 | (Kuenen et al. 2016; Putra et al. 2017) |
| TPR | 1 | (Zhang et al. 2019) |

Cost-oriented indicators are used in 15 studies in the literature set and used on a stand-alone basis (without profit-oriented indicators) in 6 studies. The (T)PC, CAPEX and Total (Fixed) Capital Investment

T(F)CI are the most frequent cost-oriented indicators. OPEX, LCOP and Cost of Electricity (CoE) are all practised twice. CAPEX and OPEX are usually computed in an intermediate stage to calculate the final indicator, such as the NPV. In this literature set, several papers selected CAPEX and/or OPEX as final indicators to assess the economic performance. As explained before, the use of cost-oriented indicators alone to assess the economic feasibility is rather problematic, as these indicators do not take into account whether the CCU process generates sufficient revenues to be economically feasible or not. Nevertheless, the level of CAPEX can have an impact on the economic feasibility of the CCU technology, e.g. in Zhang et al. (Zhang et al. 2017) and Hoppe et al. (2018) the CAPEX is mentioned as a decisive factor for the economic feasibility. Hence, the CAPEX should be estimated as correctly as possible. Due to the complex composition of the CAPEX, measuring it accurately is a challenging task. Various computation methods exist, making it difficult for readers to interpret the results. Therefore, researchers should always be transparent on how the CAPEX was estimated and what was included or excluded from their calculations. The cost estimation methodology described in Towler and Sinnott (2013) provides a clear procedure to estimate the CAPEX. The CAPEX is split into the Fixed Capital Investment (FCI) and Working Capital. The FCI is further split into the inside battery limits (ISBL) investment, the outside battery limits (OSBL) investment, the engineering and construction costs and the contingency charges.

The LCOP can be calculated in various ways as well. The term 'LCOP' is used twice in the literature set and it is computed differently in the two papers. Chiuta et al. (Chiuta et al. 2016) define LCOP as the total annual costs of a system divided by the throughput of the product. In Fernández-Dacosta et al. (Fernandez-Dacosta et al. 2017), the LCOP incorporates all positive and negative cash flows of the project levelized over the project lifetime and divided by the levelized amount of the product that is generated in that period. This adds proof to the statement that standardization in economic evaluations for CCU technologies is still lacking, as different formulas are used, even for the same indicator.

Profit-oriented indicators integrate both costs and revenues in one indicator, providing a more complete picture of the economic feasibility of a CCU technology than the cost-oriented indicators. The NPV and (D)PBP are the most frequently used profit-oriented indicators, with mentions in 9 and 7 papers respectively. The NPV is used in one-third of the literature set, which makes it a very popular economic indicator. Although the use of NPV is very common in economic assessments, the use of NPV also has some drawbacks. Assumptions need to be made about the discount rate, the projected returns and the investment costs (Investopedia). Moreover, under the presence of uncertainty, the use of NPV can lead to suboptimal decisions when the investment is irreversible and/or possible to delay, according to Real Options theory (Dixit and Pindyck 1994). The PBP indicates how long it takes before the investment is repaid, but fails to account for the time value of money (Investopedia). The DPBP discounts future cash flows, and thus recognizes the time value of money. The (D)PBP gives a clear indication of how long it will take to earn back the initial investment. However, the (D)PBP remains limited to the amount of time needed to repay the initial investments. It does not consider the cost or revenue streams thereafter.

In sum, the economic assessment indicators currently lack standardization, both in the choice of indicators and the formulas used to calculate them. In the literature set, the NPV is the most popular and

complete indicator to assess the economic feasibility. However, the use of this indicator also has its limitations, which should be recognised by the researchers who use it as a criterium. To include more flexibility in the investment decisions and to account for the uncertainties in the assessment, additional analyses should be performed.

Interpretation: uncertainty and sensitivity analysis

Following the guidelines from Zimmermann et al. (2020), the fourth phase of a TEA should be the correct interpretation of the results. Interpretation should be done to check the consistency, reliability and quality of the data inventory and the related results. Uncertainty and sensitivity analyses are the key instruments to review the reliability of data and to put the results in perspective. Uncertainty and sensitivity analysis are, although related, two distinct types of analyses to explore the uncertainty in a model.

Figure 8 shows how the interpretation-phase was fulfilled in the literature set. Fourteen papers performed a local SA, where the value of one input variable at a time is varied to investigate the impact on the results. Chiuta et al. (2016) implemented a local sensitivity analysis to investigate the impact of various input variables separately, but they also analysed the combined effect in a future outlook. Lee et al. (2020) performed a Monte Carlo simulation to identify the cumulative probability of the H₂ production cost. Here, the Monte Carlo technique is used as UA: the level of uncertainty is quantified by estimating the cumulative probability of the production cost. Eight studies didn't implement any type of uncertainty or sensitivity analysis. Fernandez-Dacosta et al. (2017) performed a pedigree analysis to qualitatively identify the uncertainties and executed a SA to identify the uncertainties quantitatively. Two studies performed scenario analysis to investigate how results change under different scenarios (Hoppe et al. 2018; Horschig et al. 2019).

Figure 8 shows the absence of UA in the literature set in general and the lack of combining both UA and SA in the economic feasibility studies. In the literature set, local SA is clearly the preferred instrument in the interpretation-phase. A local SA is sufficient for a quick screen on the most important input variables. However, if one aims to explore the entire input variable space, global SA should be performed. The observations from this literature set show a lack of education in UA and SA, as most CCU researchers limit the interpretation to a local SA.

Methanol synthesis via CCU technologies

Based on the studies in the literature set, methanol is the most prevalent chemical CCU-based product. Olah (2013) identified methanol as a 'feasible and economic substitute for oil', thus launching the so-called 'methanol economy'. Methanol is commonly used as a raw material in the production process of chemical products, to substitute the use of oil in manufacturing. Methanol can also be used as an energy carrier, both as a transportation fuel and as an intermediate energy storage medium. Global methanol production surpassed 80 million tonnes in 2018 (Carbon Recycling International 2021). Thus, the

potential market volumes for methanol are larger than those for products that only serve as chemicals. Consequently, the potential CO₂ emissions reduction of CCU-based methanol production can be significant.

However, the economic feasibility of the various methanol synthesis CCU technologies still shows divergent patterns. Table 6 lists the calculated NPVs for 6 economic feasibility studies in the literature set. The estimated NPVs range from negative to highly positive. This observed dispersion in NPV can be explained by the variety in CCU technologies, plant location and methodological choices or assumptions that were made.

Table 6: NPV for methanol synthesis via various CCU technologies. NPV estimates in US \$ are converted to euro with 1 US \$ = € 0.85.

| References | NPV (min; max) (M€) |
|------------------------------|---------------------|
| Pérez-Fortes et al. (2016c) | - 1,036.20 |
| Lainez-Aguirre et al. (2017) | - 1,148.60 |
| Zhang et al. (2017) | 410.90; 729.98 |
| Szima and Cormos (2018) | - 295.75 |
| Deng and Adams II (2020) | - 48.45; 79.05 |
| Yang et al. (2021) | 58.70; 109.50 |

Table 7: market-based and technical factors that should be improved (i.e. lowered in the case of costs, increased in the case of prices of products) to become economically feasible. Direction of improvement indicates whether this factor should increase or reduce to become economically feasible.

| <i>Market-based factor</i> | <i>Direction of improvement</i> | <i>Reference</i> |
|---|---------------------------------|---|
| MeOH price | Increase | (Pérez-Fortes et al. 2016b; Lainez-Aguirre et al. 2017; Zhang et al. 2017; Gonzalez-Aparicio et al. 2018) |
| CAPEX | Reduce | (Zhang et al. 2017; Hoppe et al. 2018; Bellotti et al. 2019) |
| NG price | Reduce | (Zhang et al. 2017) |
| Carbon tax | Increase | (Zhang et al. 2017; Kim and Han 2020b) |
| Electricity cost | Reduce | (Szima and Cormos 2018; Hoppe et al. 2018; Bellotti et al. 2019) |
| CO ₂ price | Reduce (negative) | (Pérez-Fortes et al. 2016b) |
| H ₂ price | Reduce | (Pérez-Fortes et al. 2016b; John et al. 2021) |
| O ₂ price | Increase | (Bellotti et al. 2019) |
| Cost of CO ₂ capture | Reduce | (Bellotti et al. 2019) |
| Discount rate | Reduce | (Kim and Han 2020b) |
| Carbon tax | Increase | (Kim and Han 2020b) |
| <i>Technical factor</i> | <i>Direction of improvement</i> | <i>Reference</i> |
| Plant scale | Increase | (Zhang et al. 2017) |
| Energy efficiency | Increase | (Lainez-Aguirre et al. 2017) |
| Electricity consumption | Reduce | (Szima and Cormos 2018) |
| Local electricity grid carbon intensity | Reduce | (Deng and Adams II 2020) |
| Electricity consumption | Reduce | (Kim and Han 2020b) |

The methodological decisions made in the studies in Table 6, were already summarized in Table 3. As can be seen from Table 3, the studies presented in Table 6 made different methodological choices: the cost of CO₂ was treated differently, the system boundaries included different stages of the CCU value chain and various types of sensitivity analyses were performed. It can also be seen that most of the methanol synthesis CCU technologies are not yet economically feasible at the moment. However, most of these studies identified some of the barriers that need to be removed to make the CCU process economically competitive with its benchmark. The market-based and technical factors that were identified by the studies as the most important aspects preventing commercialization are summarized in

Table 7, per study. The price of methanol should increase to make the CCU processes economically feasible. From Table 7, we can also again observe the various approaches to the cost of CO₂ that are practiced in economic feasibility studies for CCU technologies. Carbon taxes should increase, while the price of CO₂ and the cost of CO₂ capture should go down to improve the economic feasibility. The current level of the carbon tax remains too low to make the utilization of CO₂ profitable. Prices of raw materials (H₂, O₂ and natural gas) should decrease to make the CCU technologies competitive. The cost of electricity and electricity consumption is mentioned in the majority of the studies as a barrier; the energy efficiency of the CCU process should improve or the cost of electricity should decrease to become competitive.

Extending the TEA methodology

The guidelines written by Zimmermann et al. (2020) provide a standard for CCU researchers to perform TEAs. Their framework can hopefully lead to more harmonization in future CCU research. To date, the diversity in methods, indicators and assumptions remains considerable. The TEA structure proposed by Zimmermann et al. (2020) could also be extended to further improve the feasibility study of novel CCU technologies.

One possible enhancement to the TEA is the integration with an environmental assessment. Thomassen et al. (2019) propose a new integrated Environmental and Techno-Economic Assessment (ETEA) framework. Wunderlich et al. (2021) more recently also recommended the integration of the TEA with the Life Cycle Analysis (LCA) to assess the potential of sustainable chemical technologies. Reporting results of TEA and LCA separately may result in conflicting conclusions, which complicates decision-making. The integration of both techno-economic and environmental assessments is highly relevant to society today. Novel technologies need to have lower environmental impacts than their conventional counterparts to have a positive impact. However, unless these technologies can compete with the conventional equivalent, green technologies will never be adopted. Therefore, both the environmental and economic performance should be examined from the start to optimize the novel technology.

The TEA methodology could also be further refined by integrating the Technology Readiness Level (TRL) in the TEA framework. Buchner et al. (2018) proposed a TEA framework for the chemical industry, based on the TRL of the studied technology. This framework can also be very useful for CCU technologies. CCU technologies are often still low-mature technologies, which asks for particular assessment indicators. The framework of Buchner et al. (2018) proposes the use of 'static' indicators, which do not account for time dependence, for technologies with TRL 1-4. Surprisingly, only two studies in the literature set explicitly stated the TRL of the technology under investigation (Pérez-Fortes et al. 2016b, a). The lack of integration of the TRL in economic feasibility studies is worrying, as the level of maturity can have impact on the assessment. Future research should address how assessment indicators for CCU technologies should be adapted for low TRL technologies.

The TEA methodology can also be extended by including flexibility in the investment decision. In classic economic analysis, an investment decision is a now-or-never decision: invest now, or never. However, the decision to invest or not can be much more flexible in practice. The investor has the option to invest now or to wait for more information in the future. Moreover, various technology options could be available to choose from. This flexibility in the investment decision is shown in Figure 9. The investor can invest immediately in Year 1, or wait year after year for more information. The investor can invest in a chosen technology after 1 or 2 years of waiting or start with one technology and scale-up later with the other technology. Figure 9 presents this continuum of possible decision paths for the investor. By introducing this flexibility in the investment decision, a value is granted to waiting. Once an investment is made, the other option ('waiting') is lost: an opportunity cost is incurred. The value of this lost option, or the value of waiting, should be calculated and incorporated in the economic assessment (Dixit and Pindyck 1994).

The NPV is the difference between the estimated positive and negative cash flows over the plant lifetime, converted to the present value by a discount rate that reflects the risk profile and conditions in the capital market. This methodology, which is used frequently in economic assessments, completely neglects the value of waiting for more information. The level of the discount rate that is used in NPV calculations must also be chosen and it should reflect the risk profile of the investment at a particular point in time. However, the risk profile of the investment can change over time, while the discount rate is kept constant. Over time, the technology is developed further and technical or market uncertainties can be reduced. To integrate this evolution, one could work with a dynamic discount rate that is adapted to the adjusted risk profile. However, this does not soften the 'now-or-never decision that is imposed by the NPV methodology. The NPV criterium simply states that one should invest whenever the NPV is positive and this decision must be made at one particular moment. However, in a real-life market, the estimated cash flows will change due to uncertainties, competition and changed market conditions. Therefore, flexibility can be very valuable for management to alter its strategy, as new information becomes available and uncertainty about future cash flows and market conditions is resolved (Trigeorgis 1993). To incorporate more managerial flexibility in the economic analysis, the TEA could be extended with a Real Options Analysis (ROA). ROA is a financial valuation technique, used to estimate the opportunity cost of the option that is lost. According to the Real Options Theory, one should only invest when the NPV of the project or technology is greater than the value of the lost option (Dixit and Pindyck 1994). This theory also allows us to build a decision tree for a project, which allows for different investment decisions at different points in time, depending on the evolution of the investigated technology or project. The Real Options Theory has already been applied to CO₂-EOR projects, to account for this value of information. Compennolle et al. (2017) for instance investigated the impact of oil and CO₂ price uncertainties on the investment decisions for a CO₂-EOR value chain and show that market price uncertainty typically postpones investment at both the CO₂ capture unit and the EOR plant. Zhang et al. (2021) also raised the issue that traditional methods are no longer capable of dealing with the technological, market and policy uncertainties of low-TRL CCU technologies. They propose a Real Options model that includes different types of uncertainties and aim to investigate the impact of policy incentives on CCUS technologies in China. Applying this model to the European context would be very valuable for the development of CCU in

the EU. Moreover, not only the effect of policy incentives, but also the effect of technological or market uncertainties should be analysed in more detail.

Efforts should be made to extend the application of ROA to novel CCU technologies. Not only can this help to introduce flexibility in the investment decision, but also account for the various technological and/or price uncertainties which can have an impact on the optimal timing of the investment in CCU technologies. Various types of technical uncertainty can prevail, for example, uncertainty on the energy and conversion efficiencies. Low-maturity technologies, in particular, can have a high level of technical uncertainty. Market or price uncertainties concern the market variations which can be difficult to predict, e.g. the CO₂ price, product prices, etc. The carbon tax can be an important driver for the profitability of the CCU technology, while raw material and product prices can be serious barriers, as discussed before. ROA can be a convenient tool to incorporate these types of uncertainty in the assessment fittingly. For example, the evolution of the CO₂ price can be modelled by a Geometric Brownian Motion (GBM), which is a stochastic process that can be used to model the evolution of uncertain variables.

The interpretation-phase alone, as described by Zimmermann et al. (2020), is not sufficient to analyse the investment decision in CCU technologies in a realistic marketplace. Because of the generally low TRL of CCU technologies, better methods to deal with the high level of uncertainty in economic assessments should be recommended. The guidelines from Zimmermann et al. (2020) should be adapted to include more managerial flexibility in their economic assessment. ROA offers a method that is already implemented in other research fields to account properly for more flexibility.

Discussion

The guidelines from Zimmermann et al. (2020) give guidance on the implementation of TEAs for CCU technologies or projects. In this study, we contrasted previous economic feasibility studies to their framework. As shown in this tutorial review, their framework is far from being implemented in practice. This tutorial review has revealed several shortcomings in the economic feasibility studies for CCU technologies that were performed previously.

Firstly, the system boundaries were not defined explicitly in 16 papers from the literature set and the majority of these studies was limited to a gate-to-gate assessment. The ideal economic feasibility study includes the entire value chain (cradle-to-gate or even cradle-to-grave). However, gate-to-gate boundaries can be satisfactory, if this fits with the goal of the study and if it is well-argued. Secondly, the utilized CO₂ was treated in various manners in the literature set: as a free of charge resource, as a revenue stream thanks to avoided carbon tax payments or as a raw material with a (capture) cost. We urge to be careful with the integration of avoided carbon tax payments as a revenue stream since CCU is to date not included in the EU ETS legislative framework. Zimmermann et al. (2020) also do not advise to include legislative frameworks or cost lowering mechanisms for the estimation of CO₂ prices, because of regional differences and uncertainty due to future political decisions. CCU researchers should acknowledge that capturing CO₂ always comes at a cost: including zero costs for the CO₂ as a resource is not realistic. Even

when the boundaries are set gate-to-gate, the CO₂ cost should be derived from market prices (Zimmermann et al. 2020). Thirdly, the observed set of assessment indicators in the literature set is diverse. Together with Zimmermann et al. (2020) and Sick et al. (2020), we advocate for a more harmonized indicator base. Using the same indicator set, with the same underlying formulas, would increase transparency, readability and comparability of (techno-)economic feasibility studies for CCU technologies. Finally, the interpretation of results should be elaborated more in economic feasibility studies. Local SA was the preferred instrument in the literature set. Global SA, where the value of multiple parameters is varied simultaneously would be a better method to cover all input variables (Saltelli et al. 2019). In the literature set, either UA or SA was performed in isolation, while UA and SA should be run in tandem ideally. The shortcomings in the literature set concerning UA and SA show that there is still some room for progress here in the CCU research field.

Chemical CCU technologies are generally technologies at low TRL, dealing with high levels of uncertainty. The correct treatment of uncertainty is thus crucial in economic feasibility studies. Because of the low TRL and the various types of uncertainties in the development phase, it is also important to introduce flexibility in the decision-making process. The interpretation-phase alone, as suggested by Zimmermann et al. (2020), is insufficient to account for the different types of uncertainty in the CCU project and does not allow to incorporate more managerial flexibility in the decision whether or not and when to invest in a CCU project. Therefore, we propose the inclusion of ROA to include more managerial flexibility in the investment decision.

Besides the introduction of ROA, we also suggested basing the TEA framework on the TRL of the investigated CCU technology. The existing framework of Buchner et al. (2018) recommends the use of static indicators for TRL 1-4. However, static indicators do not account for time dependence and usually only consider one period. This is in contrast with the suggestions of ROA to include more dynamic analysis and more flexibility in the economic assessment of CCU technologies. We observe a precarious balance between adapting the indicators to the limited data availability by simplifying the assessment indicators, on the one hand, and incorporating the uncertainties and flexibility in the analysis by modelling the uncertainties in the model by complex processes, on the other hand. It is a choice between either using the data you have to its best extent, without fully acknowledging the impact of uncertainties or future developments, or modelling the uncertainties in the model by rather complex processes to account for managerial flexibility. Future research should focus on trying to find the right balance between these two approaches, which both have strengths and weaknesses, for the economic assessment of CCU technologies.

Conclusion

This study set out to evaluate the quality of economic feasibility studies for chemical CCU technologies, to detect differences in methodological choices and assumptions in these studies and to identify current barriers and drivers for the commercialization of CO₂-based methanol synthesis. The guidelines formulated by Zimmermann et al. (2020) are used as the benchmark for TEAs for CCU technologies. This

tutorial review has shown the variation in the applied methods for economic feasibility assessments. The TEA was the most commonly used method to assess the economic viability of chemical CCU technologies. However, when these studies were contrasted to the guidelines from Zimmermann et al. (2020), we exposed that different phases of a high-quality TEA were lacking in the majority of studies in the literature set. The system boundaries were often not defined explicitly (I – Goal and Scope) and the market study was often not performed as well (II – Data Inventory). The Interpretation-phase was skipped in several studies or carried out in an unsatisfactory manner. The synthesis of methanol via chemical CCU technologies was reviewed in more detail. The economic feasibility of the different technologies diverged, due to different technologies, locations, and methodological assumptions. In general, most of the CCU-based methanol production processes were not yet competitive, compared to their conventional counterpart. The most prevalent barriers that were identified in the literature set for the commercialization of CCU-based methanol synthesis are the price of methanol, the cost of electricity and electricity consumption. To further enhance the TEA guidelines from Zimmermann et al. (2020), we recommend to integrate an environmental assessment or LCA with the TEA, to adapt the assessment to the TRL of the technology and to implement ROA in the TEA. The implementation of Real Options Theory (Dixit and Pindyck 1994) is necessary to allow more flexibility in the investment decision. The NPV criterium, which was the most common economic assessment indicator in the literature set, only allows now-or-never decisions. If we aim to integrate various types of uncertainties in the assessment and the way these uncertainties can diminish or increase over time, economic feasibility studies should extend their assessment beyond the estimation of the NPV. Further work is needed to investigate how ROA can be integrated into the TEA structure as proposed by Zimmermann et al. (2020).

Abbreviations

| | | | |
|--------|--|------|--------------------------------|
| CAPEX | Capital Expenditures | | |
| CBA | Cost-Benefit Analysis | NG | Natural Gas |
| CCU | Carbon Capture and Utilization | NPV | Net Present Value |
| CoE | Cost of Electricity | OPEX | Operational Expenditures |
| DPBP | Discounted Payback Period | PBP | Payback Period |
| EOR | Enhanced Oil Recovery | PFD | Process Flow Diagram |
| ETEA | Environmental and Techno-Economic Assessment | RM | Raw Material |
| EU ETS | EU Emission Trading System | ROA | Real Options Analysis |
| GHG | Greenhouse gas | ROI | Return on Investment |
| IRR | Internal Rate of Return | SA | Sensitivity Analysis |
| LCA | Life Cycle Analysis | TEA | Techno-Economic Assessment |
| LCC | Life Cycle Costing | TFCI | Total Fixed Capital Investment |
| LCOP | Levelized Cost of Product | TPC | Total Production Cost |
| M&EB | Mass & Energy Balances | TRL | Technology Readiness Level |
| moMILP | multi-objective Mixed Integer Linear Program | UA | Uncertainty Analysis |

Declarations

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Conflicts of interest

The authors declare that there are no conflicts of interests.

Availability of data and material

All data can be found in the literature set, shown in Table A.2.

Code availability

Not applicable.

Author's contributions

Not applicable.

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