Optimization-based framework for techno-economic and environmental assessment of CO2 capture, utilization, and storage strategies

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Abstract

Carbon capture, utilization, and storage (CCUS) is one of the promising and effective solutions addressing climate change and energy security in the near-term. Since the CCUS technologies have different technological constraints for CO2 sequestration, it is essential to apply a unified evaluation framework to assess and analyze various CCUS technologies in perspective of CO2 disposal. In this study, we aim to assess and analyze the CCUS technologies in specific problems of maximizing net present value (NPV) and CO2-eq reduction considering various constraints. This study developed an optimization-based framework to analyze and assess the CCUS technologies regarding technical, economic, and environmental performance. To achieve this goal, we developed a superstructure involving a series of technologies (e.g., CO2 capture, transportation, CO2 conversion, and separation) to storage and utilize captured CO2. We then estimated the technical and economic parameters (i.e., mass flow, energy flow, sizing data and costing data) based on the literature and the process model by developed Aspen Plus. The optimization models were developed to identify the optimal CCUS strategies with different criteria: NPV, and CO2-eq reduction. With scenario-based analysis, this study also determined that the priority of various CCUS technologies considering critical constraints such as the cost and CO2-eq inventory of H2 according to the resource of H2 and utility. This paper offers actionable policy guidance with NPV and CO2-eq reduction for high carbon-footprint nations considering the CCUS strategy.

**Keywords**: CO2 utilization and storage, optimization-based assessment, techno–economic analysis, life cycle assessment.

* 1. Introduction

The increasing challenge of climate change has amplified the significance of carbon capture, utilization, and storage (CCUS) technology (Naims & Eppinger, 2022). Given the increasing global temperatures and the growing urgency of environmental issues, CCUS has become an essential technology in combating these challenges (Abanades et al., 2017). The importance of this technology is emphasized by global efforts aimed at reducing CO2 emissions and shifting towards environmentally sustainable energy alternatives. Despite the recognized importance of CCUS, its global implementation remains limited, with less than 1% of the projected CO2 captured (Mac Dowell et al., 2017). This is primarily attributed to the slow pace of CCUS implementation, compounded by issues such as high costs, regulatory obstacles, and technological limitations. The significant disparity between the projected CO2 captured and actual CCUS implementation highlights the need for more efforts and strategic planning in the field of CCUS. Carbon capture utilization for energy (CCU4E) technologies have demonstrated significant promise among the several CCUS technologies, particularly in the generation of energy products (Hepburn et al., 2019). In our previous study, we conducted a techno-economic assessment of CCU4E technologies comparing their viability and competitiveness with conventional energy sources (Do et al., 2022). However, for successful implementation of CCU4E technologies, it is essential to not only assess their techno-economic viability but also to clearly identify and understand the actual constraints and potential of CCU4E technologies. This involves a detailed understanding of market information (e.g., market size, market price) and global information (e.g., renewable energy potential and hydrogen availability). In this study, we developed an optimization-based assessment framework for planning CCU4E technologies from technical and environmental perspectives. This framework aims to offer a strategic approach to planning CCU4E implementation, considering a practical constraint that impact its feasibility and effectiveness. By integrating technical, economic, and environmental analyses, we identified optimal pathways for CO2 utilization in energy production, balancing the goals of sustainability, economic viability, and environmental protection.

* 1. Methodology

Figure 1 presents our methodological approach for assessing CCU4E. We developed a CCU4E superstructure which includes a variety of technologies for converting captured CO2 into valuable energy products as shown in Figure 2. We developed process models for 20 CCU4E pathways. The mass and energy balance were obtained from developed process model. Sizing and costing data were also estimated. We obtained chemical market information (i.e., product prices and market sizes) and global information (i.e., renewable energy potential and hydrogen availability (Hepburn et al., 2019). We developed an optimization model considering various constraints such as technical, market, and global information. To analyze the capability of optimization model, we developed different scenarios considering different resource type. By analyzing different scenarios, we could provide practical insights for CCU4E implementation, contributing to efforts in combating global climate change. Our methodology also encompasses a long-term perspective, extending our planning and analysis horizon up to the year 2050. This extended timeframe allows for a more comprehensive assessment of the evolving landscape of CO2 utilization and the changing dynamics of energy production.



**Figure 1.** Methodology for the assessment of CO2 utilization strategy for energy products



**Figure 2.** Superstructure of CO2 utilization for energy products

* 1. Optimization model

In this study, we developed an optimization model using mixed integer linear programming (MILP) to identify the optimal CO2 utilization strategies. This model is composed of a comprehensive set of data, including technology-specific, market, and global information. Our strategy for CO2 utilization encompasses various pathways for producing multiple energy products. Each pathway begins with feedstocks like CO2 and hydrogen and involves a sequence of conversion and separation technologies to produce one or more target fuels. In this study, we developed two objective functions. The first, defined in Eq. (1), aims at maximizing NPV. The NPV is calculated by considering the total revenue (TRE) and the total costs (TCO) associated with the CO2 utilization processes, along with depreciation (dp), the discount rate (d), and tax considerations (TAX). The total revenue is derived from the combined profits of selling energy products and by-products and includes the salvage value of facilities at the end of their life cycle. On the other hand, total costs encompass the investment required for facility establishment, operational expenditures, and variable costs like feedstock and utility expenses. In the optimization model, our second objective function is focused on maximizing CO2-eq reduction, which is crucial for assessing the environmental impact of the CO2 utilization strategies. This evaluation is conducted through two key parameters: the CO2 inventory of products (CP) and net CO2 equivalent emissions (NCE). The CP is a measure of the total CO2 emissions associated with each produced fuel or by-product. It reflects the environmental footprint of producing these energy products considering all emissions from the point of CO2 capture to the final product output. On the other hand, the NCE refer to the balance of CO2 emissions and reductions throughout the entire process of CO2 utilization.

|  |  |
| --- | --- |
|  | (1) |
|  | (2) |

The optimization model was constrained by the demand satisfaction and feed availability as expressed in Eqs. (3) – (5).

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | | (3) |
|  |  | (4) | |
|  |  | | (5) |

where  is the production of product and by-product in country during time,is the potential market size of product in country during time, the consumption of feedstock in country during time, is the amount of CO2 captured in country during time , is the amount of hydrogenin country during time .

* 1. Case study

In this study, we consider CO2 captured from the flue gas of a 500 MW coal-powered electric utility, amounting to approximately 3.1 million tons of CO2 annually. The detailed process modeling was conducted using Aspen Plus V.11, and the comprehensive specifics of each process can be found in Do et al. (2022). This reference elaborates on mass and energy flow, as well as sizing and costing data for all processes, which were crucial inputs for our model's analysis and development. Several organizations have projected the availability of CO2 captured in the future. Based on these predictions, there will be a reduction of 20 Gt of CO2 emissions in the announced pledges scenario (APS) in 2050, compared to stated policies scenario (STEPS). This reduction can be attributed to advancements in CO2 capture technologies, improved energy efficiency in industries, and a significant shift towards renewable energy sources. By 2020, under the APS, it's anticipated that there will be a cumulative capture of 42 Mt of CO2. Driven by technological advancements and policy implementations, this amount is expected to see a substantial rise, reaching an estimated 4300 Mt/y by 2050. The economics of CO2 utilization, particularly for liquid fuel production, are intricately tied to the costs of CO2 capture. It's noteworthy that almost half (47%) of the expenses of a CO2-EOR project are attributed to CO2 capture.For example, costs in the power and heat sector can range from 62 to 163 $/ton. Such fluctuations in costs highlight the uncertainties in gauging the availability of low-cost CO2 for future capture. Given the range of CO2 prices and the inherent uncertainties in predicting low-cost CO2 availability, we assumed that only about 30% of the total CO2 captured by 2050 in the APS scenario will be available at a cost-effective rate of 35 $/ton. To estimate hydrogen availability, we utilized forecasts for low-carbon hydrogen production up to 2050, as provided by Wood Mackenzie. Based on these projections, we assumed that the availability of green hydrogen to be equivalent to the hydrogen production from electrolysis, while black hydrogen availability was assumed to correspond with the production from fossil with CCS.

* 1. Results and discussion

Our study primarily aimed to identify optimal CCU4E strategies that maximized NPV and CO2-eq reduction. To achieve this goal, we developed two different scenarios considering different combinations of utility and hydrogen types. Note that black utility refers to conventional utility sources from the grid, while green utility denotes renewable electricity and heat sources. For considering hydrogen types, black hydrogen refers to natural gas-based hydrogen with a CO2 capture process, which is one of the most widely used. Green hydrogen refers to the hydrogen from electrolysis which is one of the most ecofriendly hydrogens. By analyzing the most widely used and ecofriendly hydrogen through cost and environmental optimization, we could identify the optimal strategy in terms of financial viability and CO2-eq reduction for CCUS technologies. In P1 and C1 scenarios, the CCUS technologies only utilizes black hydrogen and black utility. On the other hand, in P2 and C2 scenarios, the CCUS technologies only utilizes green hydrogen and green utility. It is identified that the P1 scenario, utilizing black hydrogen and utility, was found to be the most financially viable option among the scenarios, with the lowest financial loss at -174 MM$/y. On the other hand, the P1 scenario also resulted in the least CO2-eq reduction among all scenarios, achieving only 472 Mt/y. This is because the P1 scenario relies on black utility and hydrogen which are more cost-effective but result in comparatively lower CO2-eq reductions. Within the P1 scenario, the optimal strategy included producing a range of fuels through specific processes. The optimal strategy in the P1 scenario involved the production of MeOH via direct hydrogenation, the synthesis of DME from MeOH, the creation of olefin through the MTO process, and the conversion of MTG.



**Figure 2.** Optimal CO2 utilization strategies for energy products in different scenarios.

In the P2 scenario, where green hydrogen and utility were implemented, a significant shift in fuel production strategy was observed compared to the P1 scenario. For example, while the P1 scenario involved the production of FT fuel, Olefin, MeOH, and DME, the P2 scenario shifted to producing FT fuel, Olefin, DME, and Gasoline. This is because the adoption of green hydrogen and utility in the P2 scenario led to higher costs, influencing the shift in fuel production strategy. In the P2 scenario, we observed significant shifts in both NPV and CO2-eq reduction compared to the P1 scenario. For instance, the NPV in the P2 scenario decreased to -421 MM$/y, compared to -174 MM$/y in the P1 scenario, representing a relative decrease of about 142%. On the other hand, the CO2-eq reduction markedly increased to 1469 Mt/y, up from 472 Mt/y in the P1 scenario, representing a substantial increment of approximately 211%. With these results, we have identified a clear trade-off between economic costs and environmental benefits in CO2 utilization strategies. In the C1 and C2 scenarios, which prioritized maximizing CO2-eq reduction, the optimal strategy only consists of the production of olefin and gasoline, due to the CO2-eq inventory of olefin and gasoline. With these results, we identified that focusing on fuels with a high CO2-eq inventory can lead to significant environmental improvements. When focusing solely on the CO2-eq inventory of products, there is an inherent trade-off in terms of economic implications. For example, while the P1 scenario resulted in a financial loss of -174 MM$/y, the C1 scenario results at higher financial loss of -212 MM$/y. From our analysis, we identify that CCU4E strategies present a complex interplay between economic costs and environmental benefits. These findings highlight the necessity of carefully considering both economic and environmental factors in CO2 utilization strategies.

* 1. Conclusions

In this study, we developed an optimization-based framework for the systematic analysis and evaluation of CO2 utilization strategies considering economics and environmental impacts. This framework integrates a range of conversion and separation technologies for various fuel production. Then, we developed optimization model with objective functions considering various constraints. With the optimization model, we explored different scenarios with black and green hydrogen and utility sources. It was identified that the P1 scenario, employing black hydrogen and utility, emerged as the most financially sustainable option, incurring the least financial loss. However, the P1 scenario also achieved the lowest CO2-eq reduction, indicating a trade-off between economic feasibility and environmental impact. The P2 scenario, with green hydrogen and utility, demonstrated a notable shift towards increased CO2-eq reduction but at a higher economic cost. The results highlight the significance of resource selection and objective function in the planning of CCU4E strategy for the financial viability and CO2-eq reduction potential. Our study contributes to the understanding of sustainable CO2 utilization, offering guidance for policymakers and companies in developing strategies that balance environmental impact with economic feasibility.

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