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Optimal Planning and Design of CO₂ Capture and Utilization Systems with Social Discount Rates

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With the drastic consequences of climate change, such as increased global temperatures and rising sea levels, becoming more prevalent, the importance of reducing greenhouse gas emissions is heightened. One of the primary steps necessary to address this global environmental issue is to achieve net-zero emissions by adopting technologies that capture and sequester greenhouse gases. CO2 capture and utilization (CCU) stands out as one of the feasible strategies in mitigating and combatting climate change. This is because its characteristic of reusing and turning captured CO₂ into valuable products addresses the economic drawbacks of CO₂ capture and storage (CCS). This economic benefit incentivizes CO₂ capture. To efficiently capture and utilize CO₂ from power plant sources, decision support tools are necessary for the optimal planning and design of CCU systems. In this work, a linear programming (LP) model for matching CO₂ sources and utilization facilities in a CCU system is developed, considering CO₂ discounting, purity requirements, and material balance constraints. Purity or quality stipulations are necessary in the field of CCU since utilization facilities set purity standards before captured CO₂ can be used in their processes. CO₂ discounting, on the other hand, is included to quantitatively consider the effective CO₂ emissions resulting from the delay made by various CCU industries or technologies. While CCU does not reduce the total amount of emissions like CCS, delaying the release of CO2 into the atmosphere is considered more beneficial than its direct emission. CCU can also be integrated with CCS so that more flexible systems with a wider array of options to achieve net-zero emissions can be generated. The developed model is then applied to a realistic CCU system case study to generate insights into the use of the model and its results. Using a conservative social discount rate of 5% on a CCU system with eight CO₂ sources and four utilization facilities, an objective value of 2,639.70 monetary units and a CO₂ discounting equivalent to 1.01 years were obtained from the model.

1. Introduction

The world currently faces a climate crisis as the increase in greenhouse gases (GHGs) in the atmosphere has pushed global temperatures up by 0.18 °C per decade in the last 40 y (Lindsey and Dahlman, 2021). The increase in global temperature can lead to rising sea levels and climate change; affecting the way the environment provides ecosystem services. The goal to act against climate change has been identified as one of the top priorities for sustainable development through the United Nations (UN) Sustainable Development Goals (SDGs). With this objective of mitigating climate change, three general strategies are primarily researched (Fawzy et al., 2020): (a) managing the solar and terrestrial radiation of the earth by radiative forcing techniques in geoengineering; (b) reducing the usage of fossil fuels and other non-renewable sources of energy, and; (c) adopting technologies that capture and sequester GHGs to reduce their levels in the atmosphere. It is important to consider that no single technology or solution can address the climate change problem. Each of these solutions contributes to mitigating its effect.

This study focuses on the third approach, specifically carbon dioxide (CO₂) capture and utilization (CCU). The technology involves capturing CO₂ from point sources, transporting it, and converting it into valuable products (Ghiat and Al-Ansari, 2021). This technology stems from carbon dioxide capture and storage (CCS) where CO₂ from capture-retrofitted power plants is sequestered to prevent them from being released into the atmosphere (Jana and De, 2020). CCS involves permanently storing CO₂ underground, preventing it from entering the

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atmosphere. On the other hand, CCU involves converting CO₂ into valuable products. It would provide an additional source of income and, consequently, an incentive for capturing CO₂ (Hasan et al., 2015). CCU supplies a needed advantage for carbon capture to become a feasible and popular method of combatting climate change, especially with the costs attached to the capture technologies.

While CCU addresses the economic drawbacks of CCS, it has disadvantages that are not found in simply storing GHGs. Companies usually require a certain purity or concentration standard for captured CO_2 to be accepted as feed material for their manufacturing plants (Mikulčić et al., 2019). This requirement is expected to come up in the food and beverage industry, pharmaceuticals industry, and other industries that chemically convert CO_2 into a valuable product (Silk, 2018). Besides this, CCU will also not keep the captured CO_2 from reaching the atmosphere; it will only delay the emission of the gas as the products of the recycled CO_2 can still discharge the said greenhouse gas at the end of its use (Hepburn et al., 2019). While this seems to invalidate the use of CCU, delaying is still better than the direct emission of CO_2 since it slows down the build-up of this greenhouse gas in the atmosphere, and there is a way to quantify the benefits it provides. One approach to maximize the benefit of emissions delaying is to use the concept of social discount rates.

Social discount rates (SDRs) are an economic term in cost-benefit analyses used to quantify how fast the cost of releasing CO₂ decreases per unit time (Roberts, 2016). This concept is frequently used in climate change mitigation since it calculates the present value of a future cost, such as the future effect of current GHG emissions and resource consumption (Shepherd et al., 2020). CO₂ accumulates in the atmosphere as it is released so delaying its emission is still preferable to its direct emission (Aresta et al., 2018). Due to the compounding nature of SDR in CO₂ emissions cost, a reasonably high discount rate encourages longer delays in CO₂ emissions, encouraging CO₂ utilization involving products with longer lifetimes.

To efficiently capture and utilize CO₂ from power plant sources, decision support tools are developed to aid in the planning and optimization of CCU systems (Rudin et al. 2017). Process systems engineering techniques, specifically pinch analysis and mathematical programming, are the primary approaches used in optimizing CCU and CCS systems (Tapia et al., 2018). Noteworthy mathematical programming model examples in the field of carbon capture are mentioned in this study. First is a source-sink matching model that minimizes the total costs of a CCUS supply chain in the United Kingdom by Leonzio et al. (2020). Second is a scalable infrastructure model for CCS, also known as SimCCS application, that minimizes the total costs of a CCUS system considering pipeline geolocation and uncertainty analysis by Middleton et al. (2020). Third is a model that optimizes the costs of a CCUS case in Germany (Leonzio et al., 2019). Fourth is a model for strategic planning of the economic impacts and environmental implications of a CCUS supply chain by Zhang et al. (2019). Last is the optimal source-sink matching model in CCS systems with injection rate, time, and capacity constraints by Tan et al. (2012). The last four enumerated works are mixed integer linear programming (MILP) models, which are a type of programming that limits selected variables to integers (Dua and Pistikopoulos, 2000) and is especially useful due to its flexibility and simpleness (Éles et al., 2020).

Based on a Scopus-indexed literature search as of March 2022, there are no papers that involve modelling and optimization of CCU, CCS, or CCUS systems considering CO₂ discounting with SDRs. Most of the papers that tackle this topic focus on evaluating the value and trend of the acceptable social discount rate of CO₂ for political and economic review (Moore, 2019) and observing the effect of different values of SDRs for a certain CO₂-emitting system (Shen et al., 2021). With this research gap on the modelling of CO₂ discounting, the need for a decision support tool that considers the discounting of CO₂ when utilized should be addressed to provide better insights for planning CCU systems. There is also insufficient work on considering the purity or concentration constraints when matching CO₂ sources with utilization plants in CCU systems. Mohd Nawi (2016) developed a pinch analysis technique for matching CO₂ sources with utilization plants but focusing on maximizing CO₂ utilization for minimum storage only.

To optimize the effective CO_2 emissions considering the delay made by CCU technologies in this model, the social discount rate is considered. The purity requirement of the utilization plants is also a novel constraint included in the model. This linear programming (LP) model determines which plants or CO_2 sources require a capture technology retrofit, which CO_2 utilization facilities to match with the power plant, and how much CO_2 must flow from each CO_2 source to each utilization facility. These considerations are important in planning which optimal CO_2 network must be developed so that delay-discounted CO_2 emissions are at a minimum. The remaining parts of the paper is arranged as follows. The next section, which is Section 2, provides the formal problem statement, discussing the nature of the CCU system to be optimized. Section 3 provides the discussion of the optimization model while Section 4 presents the case study and, lastly, Section 5 provides the conclusions and future work.

2. Problem statement

The CCU system consists of m capture-retrofitted power plants or CO₂ sources, and there are n CO₂ utilization facilities. Each ith source (i = 1, 2, 3, ..., m) generates captured CO₂ at a rate of G_i t gas/y and operates for an unlimited amount of time. It generates captured CO₂ with a constant concentration or purity of C_i t CO₂/t gas. Each jth utilization facility (j = 1, 2, 3, ..., n) has a minimum CO₂ flow rate demand (or lower bound) of D_{i}^{L} t gas/y and a maximum CO₂ flow rate limit (or upper bound) of D_i^U t gas/y. The minimum flow rate demand signifies the requirement of the utilization plant at normal operation while the maximum flow rate is based on the plant's maximum operating capacity. It is also characterized by a minimum CO₂ concentration standard of Cmin., t CO₂/t gas. The captured CO₂ leading to each facility is mixed before the CO₂ concentration is compared to its standard. All sources and utilization facilities are available at the same time and operating in steady state. Although these sources and facilities do not end at the same time, the optimal network is assumed to span when all of them are available and operating. It is assumed that each utilization facility produces CO₂-based products that have t_i y of lifetime. The cost of emitting CO₂ decreases by a constant factor of DF every y where DF < 1. Considering the temporal aspects assumed previously, the present time used in discounting the delay in CO₂ emission is based on the time when the emissions are produced, not the beginning of the planning horizon. The model should determine the CO₂ flow rates between the sources and utilization facilities that will minimize the cost of discounted CO₂ emissions.

3. Optimization model

The objective function of the model is to minimize the total cost of emitting CO_2 , as shown in Eq(1), in arbitrary monetary units.

$$\min \sum_{i} (\sum_{i} F_{ii} (DF)^{t_{j}} + F_{i.\text{atm}})$$
(1)

where F_{ij} is the flow rate of CO₂ coming from the ith source going to the jth facility in t gas/y and $F_{i,atm}$ is the CO₂ flow rate from source *i* that is emitted to the atmosphere in t gas/y. Since the cost of CO₂ decreases by a factor of *DF* per y, this social discount factor is raised to the time that each utilization facility delays the release of CO₂. The term $F_{ij}(DF)^{t_j}$ is equivalent to the delayed emission of the CO₂ utilized in facility *j* when the product generated in *j* has an operating life of t_j y. The delay or utilization time is taken as a compounding factor for the CO₂ flow rate. It must be noted that in the model, the SDR is converted into the discounting factor, *DF*, using Eq(2) on the basis of calculating a future value with compounding interest or discount rate.

$$DF = \frac{1}{1 + SDR} \tag{2}$$

For the constraints, the first is that the total flow rate to sink *j* must be between the range of flow rate demands from D_i^L to D_i^U , and this is shown in Eq(3) and Eq(4).

$$\sum_{i} F_{ij} \ge D_{i}^{L} \qquad \qquad \forall j \tag{3}$$

$$\sum_{i} F_{ij} \le D_i^U \qquad \qquad \forall j \tag{4}$$

Second, the total flow rates exiting a certain source must be equal to the generation rate of that source. But if the demand of all utilization facilities is less than the supply, the model will become infeasible. The remaining CO_2 from each source must then be allocated by the model to a dummy sink, as shown in Eq(5). The CO_2 that enters this dummy sink is not utilized, but is emitted, which means the CO_2 generated is emitted right away and not discounted.

$$\sum_{i} F_{i,i} + F_{i,\text{atm}} = G_i \qquad \qquad \forall i \tag{5}$$

With this modification of the source balance constraint, all CO₂ leaving a source will be accounted for by the objective function even those immediately emitted since they will not be multiplied by the discount factor and will not lower in cost.

The purity requirements for each utilization facility must be met as the final constraint and are bounded by a minimum CO₂ concentration, $C_{\min,j}$ in t CO₂/t gas, as shown in Eq(6).

$$\sum_{i} C_{i} F_{ij} \ge C_{min,j} \sum_{i} F_{ij} \qquad \forall j$$
(6)

where C_i is the CO₂ concentration of the captured CO₂ from source *i* in t CO₂/t gas. The term $C_i F_{ij}$ is the amount of pure CO₂ from source *i* to facility *j* in t CO₂/y. It must be greater than or equal to the minimum pure CO₂ flow

rate given by the term $C_{\min,j}$. The total flow rate that enters a utilization facility is equal to $\sum_i F_{ij}$ which is used in Eq(5) to obtain the CO₂ purity requirement.

It can be observed from the equations that all are linear equations which makes the model an LP model. Even though there is an exponential term in the objective function and a factor of concentration in the purity constraint, these factors are parameters or constants and only F_{ij} are variables. The model is to optimize the objective function given by Eq(1) subject to the constraints in Eq(3) to Eq(6). It is a modified transportation model in which the costs are the delayed CO₂ emissions from utilization. The model is implemented using the software Lingo in a PC with 3.00 GHz of processor and 24 GB of RAM using a case study in the following section. Computational time is negligible.

4. Case study

To give a better understanding of the model and how it is deployed, realistic data were investigated in this paper. Eight CO₂ sources with their corresponding industries, captured CO₂ flow rates, and CO₂ stream concentrations were adapted from the study of Mohd Nawi et al. (2016). Four utilization facilities with purity standards and demand limitations were also acquired from their case study. Other parameters, such as the social discount factor, minimum demands, and utilization time of each facility, were assumed. Table 1 and Table 2 show the data obtained from Mohd Nawi et al. (2016) and the parameters for each source and sink. The purity constraint of the first utilization facility, U1, was altered from 0.99 to 0.90 since achieving a concentration of 0.99 is impossible if all the CO₂ concentrations from the sources are lower than 0.99. A conservative average SDR of 5 % was chosen for the system, as suggested by the calculations of Moore (2019). A total of 43 to 561.6 t/y of CO₂ needs to be allocated to all utilization facilities, which consist of a beverage plant, enhanced oil recovery facility, methanol production, and microalgae plant.

Source Name	Industry	CO ₂ Gas Amount, G _i (t gas/y)	CO ₂ Purity, C _i (t CO ₂ /t gas)
S1	Cement	138.8	0.90
S2	Refineries/chemical	608.5	0.70
S3	Power (coal based)	1174.3	0.85
S4	Power (natural gas based)	101.5	0.88
S5	Agricultural	69.9	0.65
S6	Petrochemical	615.4	0.80
S7	Gas processing	36.5	0.90
S8	Iron and steel (corex)	27.9	0.95

Table 1: Parameters of captured CO₂ sources for the case study

Table 2: Parameters	of CO ₂ utilization	facilities for the	case study
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Facility Name	Industry	D _j ^U (t/y)	D _j ^L (t/y)	C _{min,j} (t CO ₂ /t gas)	t _j (y)
U1	Beverage plant	50.0	4	0.90	1
U2	Enhanced oil recovery	208.3	16	0.80	10
U3	Methanol production	83.3	6	0.50	3
U4	Microalgae production	220.0	17	0.10	4

Solving the model yields 40 variables and 24 constraints. The optimal solution is visualized in Figure 1. The objective value or the minimum cost of emitting CO₂ was reported to be 2,639.70 in monetary units, and this is the global optimum of the linear programming system as determined by Lingo. All the CO₂ from S2 and S6 are emitted to the atmosphere, accounting for 44.14 % of the total supply available and 55.35 % of the total emissions. The total discounted CO₂ emissions generated is 561.59 t/y which is 20.25 % of the total 2,772.8 t/y of CO₂ supply. The total discounted emission means that by utilizing the CO₂ captured from the industries considered, the delay or discounting in CO₂ emissions for the whole CCU system is equivalent to 1.01 y in this case. This was calculated by equating the objective value to the product of the total CO₂ supply and the discounting term, $(DF)^t$, then solving for the time. This short delay is due to the small demand for CO₂ in the utilization facilities. The maximum demand of each utilization facility was met by the CO₂ supply from the various sources, where the demand of the whole CCU system is only 20 % of the total supply. The result can also be interpreted as S2 and S6 no longer requiring a capture retrofit since no more utilization facilities can handle their supply. On the other hand, all the CO₂ from S7 are sent to U4 while S1, S3, S5, and S8 branch their CO₂ supply to two utilization facilities, some of which emit a portion of their CO₂ directly to the atmosphere.

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Figure 1: Results of the model using Lingo for the case study with CO₂ flow rates in t/y.

Besides the objective value and value of the variables, sensitivity analysis is also provided by Lingo. The dual prices for all sources were reported to be -1, which means that any one unit increase in the exiting CO_2 flow rates of the sources will increase or worsen the objective value by one monetary unit. This indicates that any increase in the captured CO_2 generation rate will only be sent to the DUMMY sink, i.e. released immediately to the atmosphere.

The utilization facilities have dual prices of 0.047, 0.386, 0.136, and 0.177 for the maximum entering CO₂ flow rates to U1, U2, U3, and U4. It is noticeable that U2 has the highest positive dual price which means that it will decrease or improve the objective value the most per one unit increase in maximum CO₂ flow rate. This is because U2 has the highest delay time, equal to 10 y. The same can be said about U1 having the lowest dual price since it has the lowest delay time of 1 y. Meanwhile, the dual price is zero for the minimum entering CO2 flow rates, D_i^L , to U1, U2, U3, and U4, but they have a surplus of 46.00, 192.30, 77.30, and 203.0 t/y. This states that increasing or decreasing the minimum flow rates will not affect the objective value, and they can increase by an amount equal to the surplus before the objective value changes. This is expected since the objective of the model, which is minimizing the cost of emitting CO₂, signifies that utilization facilities must be fully used. This is equivalent to feeding them the maximum demand that they can handle; the minimum demand can be ignored. On the other hand, the reported surplus of D_L^i to the DUMMY sink is 2,211.20 t/y. In comparison, this is equal to the difference between the total CO₂ supply and the total demand, which highlights the fact that the full maximum demand of each utilization facility is met. The analysis of this case study implies that in planning CCU systems, the demand for CO₂ must be greater than or equal to the supply to maximize CO₂ discounting. With the lack of present large-scale industries or technologies that use CO₂ as a raw material, further research on converting captured CO₂ into valuable products is necessary.

5. Conclusions

A decision support tool that minimizes the cost of emitting CO_2 in a CCU system by considering captured CO_2 generation rate, market demand and limitations, purity or concentration standards, and social discount rates was formulated. This linear programming model was then tested on a case study using realistic CCU system data obtained from past literatures. Other parameters, such as utilization time and minimum CO_2 demand of utilization facilities, were assigned. A sensitivity analysis was made on the results of the model, which emphasized the need for CO_2 utilization since the maximum CO_2 demand of each available utilization facility was selected by the model to minimize the cost of CO_2 emission. It is recommended for future studies and further decision support tools to evaluate the social discount factor more accurately since different countries have different SDRs and vary the model to account for SDRs that are a function of time. CCS can also be integrated into the CCU system so that both utilization facilities and CO_2 sinks are the options for the CO_2 destination after capture.

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