

A MULTIPERIOD MODEL FOR PORTFOLIO OPTIMIZATION OF CARBON CAPTURE AND UTILIZATION

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Abstract

Deployment of carbon capture and utilization (CCU) requires strategic decisions, such as the selection of emission sources and CCU technologies, and tactical decisions, such as the determination of the extent of capture and utilization at each planning period, as they depend on time-varying factors like source characteristics, capture targets, and products demands. Previous works have developed portfolio optimization models that can assist only some of these decisions. This paper introduces a comprehensive multiperiod optimization model, deterministic mixed-integer nonlinear programming (MINLP) model, for CCU planning by 1) selecting the emission sources and capture technologies, 2) implementing capture facilities for the sources, determining capture extent at each period and allowing capacity expansions for these facilities to account for variations in sources and capture requirements over time, and 3) selecting the utilization technologies and determining the utilization extent based on product demand at each planning period. The nonlinearities in the cost models make the model intractable for large-size problems with multiple CCU technologies for longer planning horizons. The developed two-step iterative solution approach first relaxes the MINLP using piecewise linear relaxation to a mixed-integer linear programming (MILP) model, which is solved to obtain a lower bound. The MILP solution is used to generate binary cuts and as an initial guess to solve the MINLP model and obtain an upper bound. The steps are employed iteratively with an increasing number of segments to generate tight bounds. The approach solved a problem with 10 emission sources for 10 year planning period to 0.015 % gap in 139000 seconds.

Keywords

Multiperiod optimization, Mixed-integer nonlinear programming, Carbon capture and utilization.

Introduction

Increasing global energy demand and greenhouse gas (GHG) emissions are significant and conflicting challenges. These challenges motivated industries to consider carbon capture as an emission mitigation option. Carbon capture is cost-intensive and depends on factors like emission source characteristics, capture technology used, and the decision to utilize or sequester carbon (Hasan et al., 2014).

Portfolio optimization models have been developed in previous studies to minimize the overall cost of carbon capture, utilization, and sequestration (CCUS) by selecting emission sources, capture technologies, utilization technologies, and storage sites (Hasan et al., 2014; Zhang et al., 2018; Roh et al., 2019). However, steady-state conditions have been assumed over the planning period in

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these works, i.e., the decision variables were not allowed to change over the planning horizon. This assumption can result in large penalties due to over- or under-estimating capture facility capacities, as the emission rates can vary over time. For example, for an emission source with a production increase in the later stages of the planning horizon, adding an expansion to the capture facility might cost less than building a large capture facility *a priori*. Such decisions can also impact the selection of capture technologies. Furthermore, the carbon reduction target and the demand for utilization products might vary over time.

Some previous works have developed multiperiod models for CCUS planning. Han et al. (2012) developed a model to account for the variations in emission rates and capture target. Duarte et al. (2022) have extended the work to consider selecting capture technologies but considered only carbon utilization by enhanced oil recovery and studied the time-varying factors associated with it. These models do not allow capture facility capacity expansions or consider the variation in product demands over time.

In this paper, a CCU portfolio optimization model that accounts for the changes in the emission sources, carbon reduction targets, and utilization product demands over the planning period is introduced. The MINLP model selects the emission sources, capture and utilization technologies, and allows expansions to the capture facilities under the time-varying environment to minimize carbon capture and utilization costs. However, it becomes intractable for problems with many capture and utilization technologies and longer planning horizons. A two-step approach that relaxes the nonlinear terms is developed to solve it.

Problem Statement

The main goal is to develop an optimization-based framework that assists the deployment of CCU by determining strategic and tactical decisions: (i) selection of emission sources and capture technologies to capture carbon, (ii) determination of the extent of capture based on the emission reduction target, (iii) addition of capacity expansions to the capture facilities, if necessary, over time, (iv) selection of utilization technologies that can utilize the captured carbon and generate revenue, and (v) consideration of the variations in the emission source characteristics, product prices, emission targets, and demand over the planning horizon.

For the given yearly CO₂ reduction targets or utilization product demands, the objective is to minimize the net cost of the CCU network. The net cost is the difference between the cost of carbon capture and utilization and the revenue from selling the utilization products over the given period.

Superstructure Representation

The multiperiod portfolio optimization framework has been developed to (i) integrate the emission sources, carbon capture technologies, and carbon utilization technologies under a single network, (ii) account for the variations in the

emission characteristics, emission reduction targets, and product prices over the planning horizon, and (iii) allow for capacity expansions for the capture facilities.

The superstructure in Figure 1 illustrates the CCU network. It consists of a set of carbon emission sources (S_i) from which carbon is captured using one of the capture technologies (CT_j) in the capture facilities (C_{ij}). Necessary expansions (E_{nt}) are added to the capture facilities over time (t). One or more utilization technologies (UT_k) convert captured carbon to products and by-products (P_k).

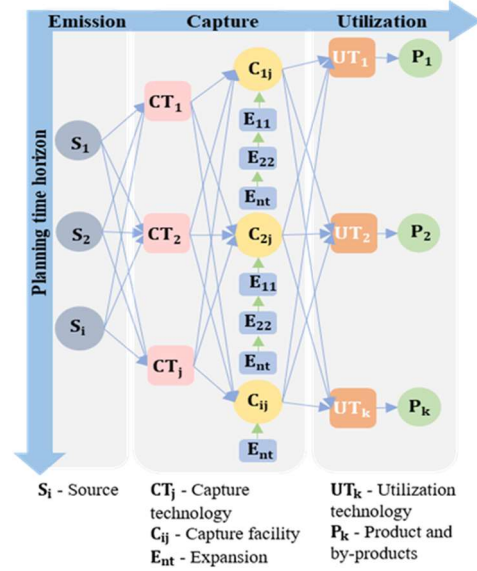


Figure 1. Superstructure representation of the CCU network

Multiperiod Optimization Model Formulation

The objective is to minimize the net cost of the CCU network over the planning horizon. The net cost is the difference between the total cost of carbon capture and utilization and the total revenue from utilization product sales (Eq. 1). The cost of carbon capture involves the cost of dehydration, capture, and compression. A capture facility is assumed to be constructed near every source carbon is captured from. The transportation costs are set to zero.

$$\begin{aligned}
 \text{Min } (TC - TR) &= \sum_{i,t} DC_{i,t} + \sum_{i,j,t,n} (CIC_{i,j,t,n} + COC_{i,j,t,n}) \\
 &+ \sum_{k,t} (UIC_{k,t} + UOC_{k,t}) - \sum_{k,t} UR_{k,t} \\
 &\forall i \in I, j \in J, k \in K, t \in T, n \in N \quad (1)
 \end{aligned}$$

The sets $i \in I, j \in J, k \in K, t \in T$, and $n \in N$ represent carbon emission sources, capture technologies, utilization technologies, planning period, and capture facilities. For a capture facility, $n = 1$ represents the initial capacity, and $n > 1$ represents the expansions. The variable TC is the

total cost of dehydration, capture, compression, and utilization, and TR is the total revenue from the utilization products. The variable $DC_{i,t}$ is the cost of dehydration of saturated flue gas from source i at time t . The variables $CIC_{i,j,t,n}$ and $COC_{i,j,t,n}$ correspond to the investment and operating costs of capture facility/expansion n of source i using capture technology j at time t . These costs include the cost of compression. The variables $UIC_{k,t}$ and $UOC_{k,t}$ are the investment and operating costs of utilization technology k at time t , and $UR_{k,t}$ is the revenue from the sales of utilization products of technology k at time t .

Binary Variables

Two binary variables, $y_{i,j,t,n}$ and $y'_{k,t}$, are defined in Eqs. (2) and (3) to represent the selection of capture technology for emission source i and utilization technology for the captured carbon for time t .

$$y_{i,j,t,n} = \begin{cases} 1, & \text{if CO}_2 \text{ is captured from source } i \text{ in} \\ & \text{facility } n \text{ by tech } j \text{ during time } t \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

$$y'_{k,t} = \begin{cases} 1, & \text{if captured CO}_2 \text{ is utilized by tech } k \\ & \text{during time } t \\ 0, & \text{otherwise} \end{cases} \quad (3)$$

Parameters

The parameters of the model are for: **(1)** Emission sources ($i \in I$): The carbon composition (X_i) and the flue gas flow rate ($F_{i,t}$) of the emission sources at the planning period t are given. **(2)** Capture technologies ($j \in J$): The cost models (Hasan et al., 2014) estimate the investment and operating costs using technology-specific parameters (α_j , β_j , γ_j , m_j , n_j , α'_j , β'_j , γ'_j , m'_j , and n'_j). Each technology has a lower (XL_j) and an upper carbon composition (XH_j) bound for CO₂ capture with at least 90% recovery and purity. **(3)** Utilization technologies ($k \in K$): The parameters R_k and U_k denote the amounts of (i) raw materials and utilities and (ii) captured carbon required to produce one ton of the utilization product by technology k . The parameters $CR_{k,t}$ and $CP_{k,t}$ are the cost of one ton of raw materials and utilities and the selling price of one ton of products at time t . The demand for each product at time t is $D_{k,t}$.

Disjunctive Constraints

If a capture facility n for source i that uses capture technology j is included in the network at time t , i.e., $y_{i,j,t,n} = 1$, flue gas of carbon composition X_i and flow rate $F_{i,t}$ is treated by the capture facility of capacity $c_{i,j,t,n}$. The capacity should be greater than the amount of feed treated at the time, $f_{i,j,t,n}$. The investment cost ($CIC_{i,j,t,n}$) is a function of X_i and $c_{i,j,t,n}$ while the operating cost ($COC_{i,j,t,n}$) is a function of X_i and $f_{i,j,t,n}$. If the capture facility is not included in the network, $y_{i,j,t,n} = 0$, these

variables take a value of zero. The corresponding disjunction is given in Eq. (4) and is reformulated using Big-M. The selection of sources and technologies depends on the binary variable $y_{i,j,t,n}$, while the extent of capture depends on the variables $c_{i,j,t,n}$ and $f_{i,j,t,n}$.

$$\left[\begin{array}{l} y_{i,j,t,n} = 1 \\ \sum_{n \in N} f_{i,j,t,n} \leq F_{i,t} \\ c_{i,j,t,n} \geq f_{i,j,t,n} \\ CIC_{i,j,t,n} = f(X_i, c_{i,j,t,n}) \\ COC_{i,j,t,n} = f(X_i, f_{i,j,t,n}) \end{array} \right] \vee \left[\begin{array}{l} y_{i,j,t,n} = 0 \\ f_{i,j,t,n} = 0 \\ c_{i,j,t,n} = 0 \\ CIC_{i,j,t,n} = 0 \\ COC_{i,j,t,n} = 0 \end{array} \right] \quad \forall i \in I, j \in J, t \in T, n \in N \quad (4)$$

The disjunctive model for the utilization technologies follows a similar logic. The variable $z_{k,t}$ is the amount of utilization product produced by technology k at time t . It is computed from the amount of carbon utilized by the technology k ($cc'_{k,t}$) at time t and the amount required to produce one ton of the utilization product (U_k). Its investment cost ($UIC_{k,t}$), operating cost ($UOC_{k,t}$) and revenue ($UR_{k,t}$) are functions of $z_{k,t}$. The selection of utilization technologies is implemented by binary variable $y'_{k,t}$, and the disjunction is given in Eq. (5).

$$\left[\begin{array}{l} y'_{k,t} = 1 \\ z_{k,t} = U_k cc'_{k,t} \\ UIC_{k,t} = f(z_{k,t}) \\ UOC_{k,t} = CR_{k,t} R_k z_{k,t} \\ TAR_{k,t} = CP_{k,t} z_{k,t} \end{array} \right] \vee \left[\begin{array}{l} y'_{k,t} = 0 \\ z_{k,t} = 0 \\ UIC_{k,t} = 0 \\ UOC_{k,t} = 0 \\ TAR_{k,t} = 0 \end{array} \right] \quad \forall k \in K, t \in T \quad (5)$$

Other Constraints

The model ensures carbon is captured from source i by at most one technology and by the same technology in the subsequent periods using the constraints in Eqs. (6) and (7). CO₂ recovery and purity of at least 90% is achievable from source i using capture technology j only if the feed CO₂ composition is in the range, $XL_j \leq X_i \leq XU_j$ (Eq. (8)).

$$\sum_{j \in J} y_{i,j,t,n} \leq 1 \quad \forall i \in I, t \in T, n \in N \quad (6)$$

$$y_{i,j,t,n} \geq y_{i,j,t-1,n} \quad \forall i \in I, j \in J, t \in T, n \in N \quad (7)$$

$$(XH_j - X_i)(X_i - XL_j)y_{i,j,t,n} \geq 0 \quad \forall i \in I, j \in J, t \in T, n \in N \quad (8)$$

The capacity of an implemented expansion should not change over time, which is enforced using big-M constraints in Eqs. (9) and (10). Equation (11) ensures the implementation of n^{th} expansion only after implementing $n - 1^{\text{th}}$ expansion. It also enforces the implementation of at most one expansion per source at a given time.

$$-M(1 - y_{i,j,t,n}) + c_{i,j,t+1,n} \leq c_{i,j,t,n} \quad \forall i \in I, j \in J, t \in T, n \in N \quad (9)$$

$$c_{i,j,t,n} \leq c_{i,j,t+1,n} + M(1 - y_{i,j,t,n}) \quad \forall i \in I, j \in J, t \in T, n \in N \quad (10)$$

$$\sum_0^t y_{i,j,t,n} \leq \sum_0^{t-1} y_{i,j,t,n-1} \quad \forall i \in I, j \in J, n \in N \quad (11)$$

The amount of carbon captured is a function of the feed gas composition and amount treated. The total carbon captured (cc_t) by all capture facilities from all sources at planning period t is computed using Eq. (12), and it should meet the CO₂ reduction target of that period. A 50% reduction target is modeled in Eq. (13) as an example. The amount of captured carbon utilized by the utilization technologies ($cc'_{k,t}$) cannot exceed the total amount captured (cc_t), per Eq. (14). Similarly, the amount of product produced by utilization technology k ($z_{k,t}$) should not exceed the annual product demand ($D_{k,t}$) (Eq. (15)).

$$cc_t = \sum_{i \in I} \sum_{j \in J} \sum_{n \in N} f(X_i, f_{i,j,t,n}) \quad \forall t \in T \quad (12)$$

$$cc_t \geq 0.5 \sum_{i \in I} f(X_i, F_{i,t}) \quad \forall t \in T \quad (13)$$

$$\sum_{k \in K} cc'_{k,t} \leq cc_t \quad \forall t \in T \quad (14)$$

$$z_{k,t} \leq D_{k,t} \quad \forall k \in K, t \in T \quad (15)$$

Implementation of Cost-Model Functions

The cost of dehydration is \$10.22 per ton of CO₂ in saturated flue gas (Hasan et al., 2014). The investment and operating costs depend on the feed composition (X_i) and flow rate ($F_{i,t}$) in the models developed by Hasan et al. (2014). The variable $F_{i,t}$ is replaced with capacity ($c_{i,j,t,n}$) and treated flow rate ($f_{i,j,t,n}$) to estimate the investment and operating costs in Eqs. (16) and (17) to account for the changes in emission rates over time.

$$CIC_{i,j,t,n} = \alpha_j + (\beta_j X_i^{n_j} + \gamma_j) c_{i,j,t,n}^{m_j} \quad \forall i \in I, j \in J, t \in T, n \in N \quad (16)$$

$$COC_{i,j,t,n} = \alpha'_j + (\beta'_j X_i^{n'_j} + \gamma'_j) f_{i,j,t,n}^{m'_j} \quad \forall i \in I, j \in J, t \in T, n \in N \quad (17)$$

Solution Approach for the Developed MINLP model

Equations (1) to (17) yield a multiperiod deterministic MINLP model that captures the changes in carbon emission, capture targets, and product demands over the planning horizon. However, it is computationally expensive to solve and becomes intractable quickly as the number of sources, technologies, and planning period increase.

The developed two-step approach (Figure 2) uses piecewise linear relaxation to obtain a relaxed MILP model, which provides a lower bound for the MINLP. The MILP solution is used to generate binary variable cuts for the MINLP and initialize local MINLP solvers. The solution of the MINLP with the cuts provides an upper bound. The optimality gap is tightened by iteratively partitioning the nonlinear functions into more segments in the MILP relaxation.

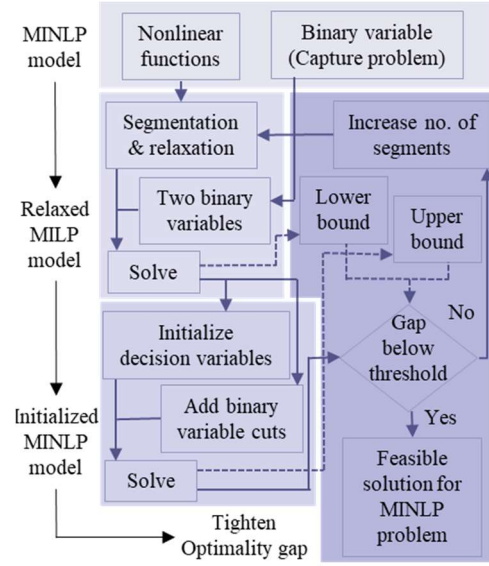


Figure 2. The two-step solution approach. Solid lines represent the approach sequence and dashed lines information flow.

Approach to Generate the MILP Relaxation

The nonlinear terms in the MINLP model are in Eqs. (16) and (17), and they are of the form $\psi = f(\phi^\omega)$ where ω is a constant such that $0 < \omega < 1$. A piecewise linear relaxation technique (Polisetty and Gatzke, 2005; Fahmi and Cremaschi, 2015) was used to obtain a relaxed MILP model. The nonlinear functions are segmented, and each segment is relaxed by building two tangent lines at the breakpoints of each segment (over-estimators) and a straight line connecting the function evaluations at the bounds (under-estimator).

For the MILP relaxation, the nonlinear functions of the form $\psi = f(\phi^\omega)$ with $\phi_L \leq \phi \leq \phi_U$ are divided into N_p segments. The length of each segment is a by Eq. (18) when the segments are partitioned equally. Each segment is represented as $v_{np} = f(x_{np})$, where $\phi = \sum_{np=1}^{N_p} x_{np}$ and $\psi = \sum_{np=1}^{N_p} v_{np}$. A binary variable b_{np} is introduced to represent the selection of the segment np (Eq. 19). The binary variable is also used to enforce selecting only one segment (Eq. (20)) and activate the bounds of each segment by Eq. (21). Equation (22) uses a disjunctive model to implement the under- and over-estimators of each segment.

Using MILP Relaxation in MINLP to Obtain a Lower Bound

The nonlinear cost functions in Eqs. (16) and (17) are relaxed by partitioning them into L and L_1 segments. The binary decision variable $y_{i,j,t,n}$ for carbon capture in the MINLP problem is replaced with two new binary variables (Eqs. 23 and 24) that account for selecting the partitioned segments for the two relaxed cost functions (investment and operating cost models), as given in Eqs. (18) and (19). Two

disjunctive models are developed to define the under and upper estimators for the two cost functions based on the formulation given in Eq. (22). The resulting MILP model is solved to obtain a lower bound for the MINLP model.

$$a = \frac{\phi_U - \phi_L}{Np} \quad (18)$$

$$b_{np} = \begin{cases} 1, & \text{if segment } np \text{ is selected} \\ 0, & \text{if otherwise} \end{cases} \quad (19)$$

$$\sum_{np=1}^{Np} b_{np} = 1 \quad (20)$$

$$\phi_L + a(np-1)b_{np} \leq x_{np} \leq \phi_L + a(np)b_{np} \quad np \in Np \quad (21)$$

$$\left[\begin{array}{l} \mathbf{b}_{np} = \mathbf{1} \\ v_{np} \leq \left. \frac{\partial f(x_{np})}{\partial x_{np}} \right|_{\phi_L + a(np-1)} (x_{np} - \phi_L - a(np-1)) + f(\phi_L + a(np-1)) \\ v_{np} \leq \left. \frac{\partial f(x_{np})}{\partial x_{np}} \right|_{\phi_L + a(np)} (x_{np} - \phi_L - a(np)) + f(\phi_L + a(np)) \\ v_{np} \geq \frac{f(\phi_L + a(np)) - f(\phi_L + a(np-1))}{(\phi_L + a(np)) - (\phi_L + a(np-1))} \\ (x_{np} - \phi_L - a(np-1)) + f(\phi_L + a(np-1)) \end{array} \right] \quad (22)$$

$$\forall \left[\begin{array}{l} \mathbf{b}_{np} = \mathbf{0} \\ -\infty \leq x_{np} \leq \infty \\ -\infty \leq v_{np} \leq \infty \end{array} \right] \quad \forall np \in Np$$

$$g_{i,j,t,n,l} = \begin{cases} 1, & \text{if segment } l \text{ is selected} \\ 0, & \text{if otherwise} \end{cases} \quad (23)$$

$$h_{i,j,t,n,l1} = \begin{cases} 1, & \text{if segment } l1 \text{ is selected} \\ 0, & \text{if otherwise} \end{cases} \quad (24)$$

Solving the MINLP Model to Obtain an Upper Bound

The MILP solution of $g_{i,j,t,n,l}$ is used to add binary decision variable cuts to the decision variable for carbon capture of the MINLP problem ($y_{i,j,t,n}$) as given in Eq. (25). The MILP solution is also used to initialize the capacity ($c_{i,j,t,n}$) and flow rate ($f_{i,j,t,n}$) variables of carbon capture and decision variable $y'_{k,t}$, and product amount variable, $z_{k,t}$, of carbon utilization for local solvers. The solution of the initialized MINLP problem with binary cuts provides an upper bound for the original MINLP problem.

$$y_{i,j,t,n} \leq \sum_{l \in L} g_{i,j,t,n,l} \quad \forall i \in I, t \in T, n \in N \quad (25)$$

Results and Discussion

The emission sources data from Hasan et al. (2014) and the capture technologies and utilization technologies from Hasan et al. (2014) and Roh et al. (2019) are used to construct model parameters. All costs are converted to 2019. The optimization models are formulated in Python V3.8.6 using PYOMO V6.4.1. The MILP models are solved

using CPLEX V20.10, and the initialized MINLP models are solved using DICOPT V2 through GAMS V24.8.5, all on an Intel Xeon Gold 6248R 3 GHz processor with 32 cores and utilizing a maximum of 100 GB RAM.

The test problem contains 10 emission sources (CO₂ composition ranging from 4-47%), four capture technologies, and four utilization techniques. The planning period is 10 years, discretized into 10 equal time periods. The impact of changes in annual emissions and biannual increase in capture targets by 10% (from 30% to 70%) over the planning horizon is studied using the MINLP model.

The approach solved the problem to a 0.015% optimality gap. The solution is summarized in Figure 3. The MILP relaxation required ten linear segments to achieve this optimality gap. For the capacity variable, the maximum value of the incoming feed gas flow rate from each source over the planning horizon was used ($\max(F_{i,t}) \forall i \in I$) as the Big-M value. For the flow rate variable, the incoming flow rate from each source at each period was used ($F_{i,t}$). In the MILP relaxation, the maximum value of these variables was bounded with these factors to obtain tighter under- and over-estimators.

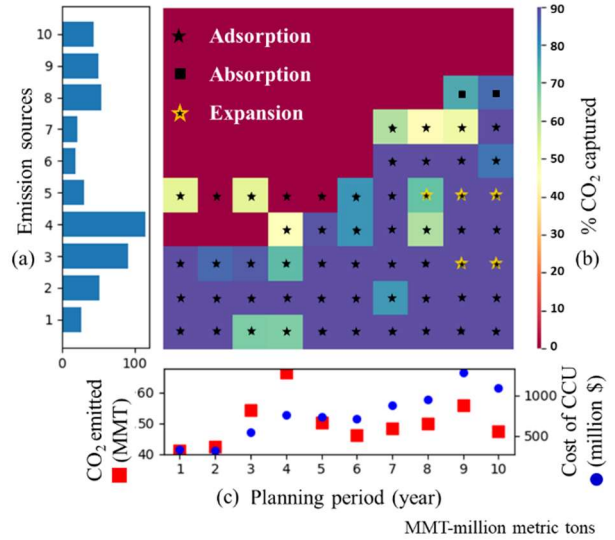


Figure 3. (a) Yearly total CO₂ emissions by sources, (b) Fraction of CO₂ captured yearly from each source, and (c) Total CO₂ emitted and CCU cost over the planning horizon

Sources 1-6 with CO₂ composition of over 10% are preferred for capture over other sources (Figure 3 (b)). Adsorption was preferred for sources with high CO₂ composition and emission. Alternatively, absorption was preferred for the 8th source due to its low CO₂ composition and emission. The first expansion to a capture facility was implemented in the 8th planning period owing to the higher capture target (60%). One more expansion was added to source 3 in the 9th year to meet the 70% annual capture target. The total annual CCU costs over the planning

periods are plotted in Figure 3(c). The cost trend follows the emission trend and increases with the increase in capture targets. The trend suggests that the total CCU cost is affected by the annual operating costs of carbon capture. The total cost was highest during the 9th and 10th years owing to the highest capture target (70%), which required implementing a capture facility at Source 8 using absorption and expanding the facility at Source 3. Four considered utilization technologies produce methanol, acetic acid, dimethyl ether (DME), and formic acid. Though formic acid and DME have a higher unit price, methanol and acetic acid production were preferred owing to their higher demand.

The upper and lower bounds generated by the solution approach and the solution time as a function of the number of linear segments in MILP relaxation are given in Figure 4. The relative gap has improved from 4% to 0.015% as the number of segments is increased from one to 10. A drastic increase in solution time was observed for eight segments yielding a relative gap of 0.023% compared to the seven segments case, which gives a 0.23% gap.

The upper and lower bounds generated by the approach at different computational times are compared with the ones by BARON V22.3.21 in Figure 5. BARON yielded a solution with a relative gap of 5% in over 8000 s, while the solution approach required 150 s to obtain the same gap using one linear segment in the MILP relaxation. Local solvers such as DICOPT solved the MINLP problem in over 250 s, but the optimal solution was 3% larger than the upper bound generated by the solution approach in 150 s.

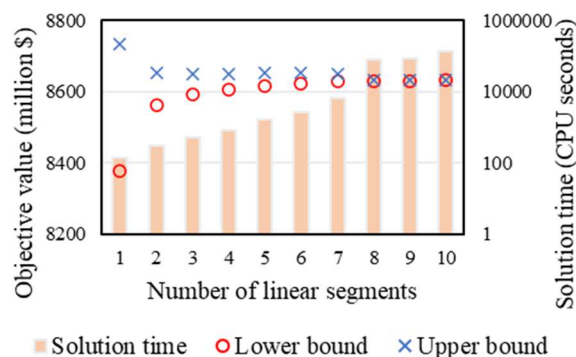


Figure 4. Bounds and the solution time for the number of linear segments in MILP relaxation.

Conclusions and Future Directions

This paper developed a multi-period portfolio optimization model to minimize the net cost of CCU in a time-varying environment. It also developed an approach to solving the MINLP model efficiently. The case study results revealed that the solution approach could generate upper and lower bounds with less than 5 % relative gap within 150 s for large instances and yield relative gaps as small as 0.015%. This work will be extended to include

transportation costs and CO₂ storage options, study the effect of uncertain emission source characteristics, annual CO₂ reduction target, and utilization product prices and demands, and analyze the effect of technology readiness level (TRL) on the project portfolio.

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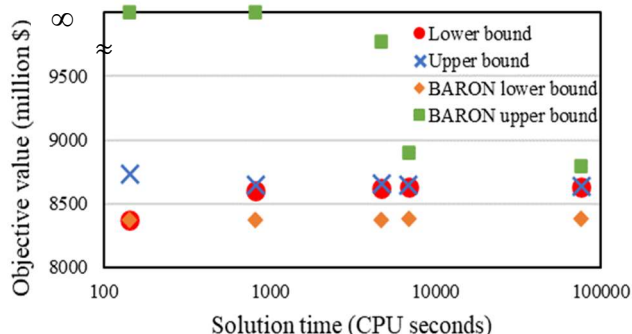


Figure 5. Bounds generated by the solution approach and BARON

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