FUTURE OF CO_2 MANAGEMENT SYSTEMS: DESIGN AND OPERATIONS

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Abstract

Over the past ten years, many scenarios for deploying carbon capture and storage (CCS) have changed from application to baseload (primarily coal) power plants to broader application to natural gas and industrial systems with power generating applications likely requiring greater flexibility to ramp operations in response to market dispatch. Moving forward, CCS systems have the opportunity to be designed for much higher capture rates to help achieve U.S. climate goals, including decarbonization of the electricity sector by 2035 and economy-wide decarbonization by 2050. This paper highlights recent new computational approaches for the optimal design and operation of CO_2 capture systems under highly variable operation by considering dispatch under different market scenarios. It further highlights advances in optimizing systems for high rates of capture, by altering both design and operating conditions. Finally, it summarizes initial analysis of incorporating polishing steps to further reduce CO_2 emissions from a flue gas source.

Keywords

Carbon capture, multi-scale model, optimization

Introduction

U.S. research efforts on carbon capture and storage (CCS) began in the early 1990's with a focus on application to large, baseload coal-fired power plants with very high capacity factors under the premise that it was most important to reduce emissions from large point sources. Research focused on improving efficiency as a way to reduce overall costs. A target of 90% capture was adopted as the sweet spot, above which parasitic power losses to run the capture and compression system would be too large to be economically justifiable. These design and operating parameters drove the majority of research and development through the 2010's.

More recently, there have been dramatic changes in the energy landscape. A significant number of coal-fired power plants have retired in the face of economic competition from natural gas combined cycle plants, which were more efficient and less costly. In addition, the cost of renewable generation has dropped significantly, further transforming the energy mix in many markets. Today, most fossil power plants operate in a load following mode, ramping up and down to balance the demand not met by renewable generators. Thus, the concept of baseload fossil generation is no longer the context in which CCS systems are likely to be deployed in many countries.

Furthermore, significant goals to achieve net zero carbon emissions in the power sector by 2035 and a net zero economy by 2050 have caused the 90% capture target to be revisited. Recent publications (Du, 2021; Schmitt, 2022) have suggested that capture rates of 95-99% are economically and technically viable. For example, Mitsubishi

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(2021) indicates that its new KS-21 solvent achieved a sustained capture rate of 99.8% at Norway's Test Centre Mongstad.

Finally, CCS for applications beyond power is becoming increasingly important as industry seeks to reduce its emissions more broadly. Many industries such as steel, cement, and chemicals contribute significant CO_2 emissions (US DOE, 2022). CCS can be an effective approach to mitigate many of these emissions (Hughes, 2022).

The development, scale-up, and deployment of CCS to a more diverse range of applications and operating conditions will require new approaches to modeling and optimization that reflect the changing design and operating conditions emerging during the current energy transition. This paper highlights three recent capabilities that are being used to support the design and operation of carbon capture systems of the future.

Design of Flexible Capture Systems

With fossil power plants increasingly needing to ramp up from and down to their minimum operating loads as they are dispatched to meet demand, the overall capacity factor of the plant decreases, increasing their levelized cost of electricity. The low capacity factors result in the fixed costs (such as capital, operations, and maintenance) being amortized over fewer hours. This effect will likely be even more pronounced in a decarbonized grid with very high variable renewable energy (VRE) penetration (Mills et al., 2020). Implementing CCS under these conditions is challenging because it is difficult to justify the additional capital for a system that is rarely used.

Instead of a traditional techno-economic analysis approach that assumes a constant value for the product (in this case electricity), a fixed design for the capture system, and an overall capacity factor, a dynamic approach is needed that can capture the time varying value of the electricity produced. The design of the system can then be determined by maximizing the net present value of the overall system as it will be operated within the context of a particular generator that will be dispatched within a specific electrical grid.

The price of electricity within an electric grid varies based on time and location and is referred to as a locational marginal price (LMP). These are typically determined by an energy market in which generators bid into an hourly day ahead and a "real time" (actually 5 to 15 minutes) market that manages mismatches between forecast and actual demand. These LMPs commonly vary from \$0/MWh to over \$100/MWh. Recent prices in Europe have been even higher.

Predicting LMPs is dependent on the mix and location of generators within a specific grid and requires a production cost model. While historical LMP signals can be obtained from publicly available resources, having a production cost model is helpful to assess the impact of a particular generation mix on LMP signals. The price signals (historical or predicted) can then be used in a "price-taker" approach to inform design decisions. While not accounting for how the generator under consideration will affect the overall supply and demand of the market, it adequately captures the variability of LMPs to enable a reasonable estimate of the economics of a new design. Gao et al. (2021) discuss a more rigorous, multiscale framework that explicitly models the complex interactions between an energy system's bidding, scheduling, and control decisions and the energy market's clearing and settlement processes.

Gooty et al. (2022) use the price-taker approach to incorporate market signals for the optimal design of a temperature swing adsorption (TSA) based carbon capture system to retrofit a natural gas combined cycle (NGCC) under several scenarios. They formulate a two-stage, stochastic, multi-period optimization problem in IDAES® (Lee et al., 2021). The formulation considers binary design decisions on whether to build a capture system for a given market and operating binary decisions to allow for plant and/or capture system shutdown. Continuous decision variables include the design (capture percentage, maximum capacity) and operating variables (operating capture rate, flue gas flow rate). To make the resulting Mixed Integer Nonlinear Programming (MINLP) problem tractable, reduced-order models constructed from rigorous first-principles models were used to represent the NGCC, the capture system, and the compression train system.

Results indicate the optimal solution is highly dependent on region, the spread in LMPs, and carbon price. LMP datasets for different regions from Cohen and Durvasulu (2021) and Jenkins et al. (2021) were used in conjunction with representative carbon prices. At a carbon price of \$100/tonne, only regions with a low frequency of near zero LMPs, resulted in a preference to build the capture system. Increasing the carbon price to \$150/tonne resulted in the capture system being built in more regions. In most cases, adding the capture system resulted in a higher capacity factor. The optimal size and capture rate varied depending on market and carbon price. In some cases, building a smaller capture system had a higher NPV than building the capture system with the largest capacity and highest capture rate. The work demonstrates the necessity of optimizing the design and operating conditions of flexible CCS systems in the context of the electricity market.

High CO_2 Capture Rates

With increasingly rigorous emissions reduction targets, the cost optimal CO_2 capture rate is being reconsidered from the historical 90%. Rigorous optimization of point source CO_2 capture systems with 95% capture rates or even higher is needed to explore the design space and determine optimal design and operating conditions. In addition, given the low driving force of the flue gas exiting the scrubber, there is potentially greater uncertainty in such systems, requiring rigorous uncertainty quantification and model validation to help ensure that these systems can reliably maintain high capture rates in the face of process variability. With a sufficiently high capture rate, net negative emissions at the process level are possible (i.e., the flue gas leaving the stack has lower CO_2 concentrations than inlet air into the combustor).

Morgan et al. (2015, 2017, 2018, 2021) and Soares Chinen et al. (2018) have developed highly accurate, predictive models of CO_2 capture systems that have been validated at multiple scales under a variety of operating conditions and capture levels. Recently, these validated models were used to determine the optimal cost of avoided CO_2 (COAC) for an NGCC system with MEA based CO_2 capture for different capture rates ranging from 90% to 99.5%

The analysis was conducted using the Framework for Optimization and Quantification of Uncertainty, and Surrogates (FOQUS) (Eslick et al., 2014), which enables derivative free optimization of external models. In this case, the models included detailed, custom, costing models and a model of the CO_2 capture system in the commercial Aspen Plus® process simulator. The analysis optimized levelized cost of electricity (LCOE) (as defined by James et al., 2019) of a 650 MWe-scale greenfield NGCC power plant integrated with an MEA capture system, over a range of CO_2 capture levels. Decision variables include absorber and stripper column packing heights and diameter, the CO_2 loading of the lean solvent into the absorber, and the temperature of the CO_2-rich solvent at the exit of the lean/rich heat exchanger.

The lean CO_2 loading dictates the steam requirement for solvent regeneration, which is provided from the IP/LP crossover of the NGCC. The exit temperature of the rich solvent from the lean/rich heat exchanger dictates the area of that heat exchanger. The constraints include bounds on the decision variables, equality constraints on material and energy balances, and the target CO_2 capture rate. Inequality constraints prevent flooding in the absorber and stripper. Absorption temperature is fixed at 40°C for all cases except at the highest level of CO_2 capture (99.8%), which used 30°C to reduce the negative impact of increasing CO_2 capture on LCOE.

Figure 1 shows the results of the optimization in terms of COAC, which is relatively flat until 98% capture. At that point costs begin to rise exponentially due to the reduced driving force caused by the low CO_2 partial pressure. Past 99.1%, (to the right of the vertical dotted line) the CO_2 concentration leaving the stack is less than the CO_2 concentration in the air. In this region, the incremental COAC rises rapidly, from approximately \$460/tonne for capture from 99% - 99.5% to \$1,160/tonne for 99.5 - 99.8%.

While the optimization provides insight on the cost and performance of high capture rates from point source processes, they also indicate how to optimally operate them. While optimal lean loadings of 0.2 [mol CO_2/mol MEA] for MEA systems have been established for 90% capture targets (Gjernes et al., 2017; Du et al., 2021), the results shown in Figure 2 indicate a benefit from lowering lean loading as the capture rates increase. This increases the working capacity of the solvent, reducing solvent circulation rates to achieve higher residence times and helps counteract the reduced driving force caused by the decreasing final partial pressure of CO_2 exiting the absorber. While this slows the rate of increase in specific reboiler duty (SRD) and absorber height required to counteract the reduced driving force, these cost drivers still begin to increase exponentially beyond capture rates of 98-99%. These preliminary results require further examination to determine impacts of uncertainty and process non-idealities to better inform low-risk, high-capture process designs.

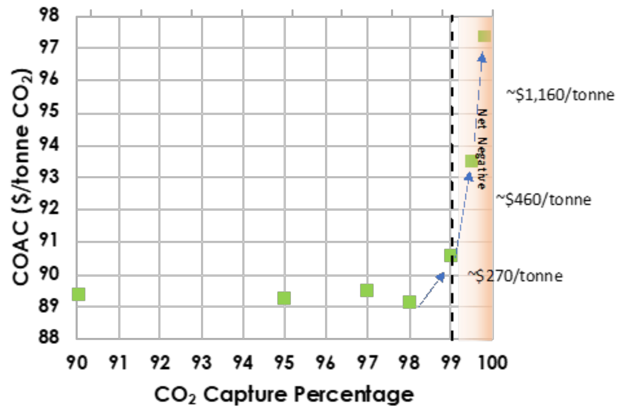

Figure 1. Optimized Cost of Avoided CO_2 (COAC) as a function of increasing capture rates. Incremental costs are given for the cost to capture between 98% to 99%, 99% to 99.5% and 99.5% to 99.8%.

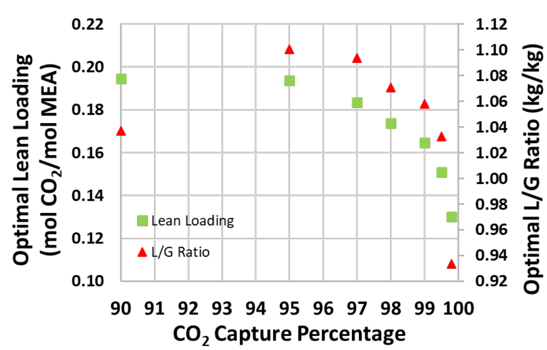

Figure 2. Optimal lean loading and L/G ratio of the absorber for each capture rate. Both lean loading and L/G decrease as capture rates increase, allowing for higher solvent working capacity and higher liquid residence time.

Higher Capture Rates via a Polishing Step

The previous section showed that the incremental costs when going from a capture rate of 90% to 98% for an MEA-based post combustion capture system are minimal. However, the COAC increases exponentially as the capture rate is increased to a level that will achieve net-zero or net-negative emissions at the plant level (as shown in Figure 1). One option to further reduce emissions at the plant level is to employ a polishing step after the primary CO_2 capture system where the exhaust gas is injected to a system that is specifically designed for capturing CO_2 from streams with very low CO_2 concentrations, potentially leveraging materials designed for direct air capture.

Modeling and optimization of such combined systems (primary + polishing) is required to determine the optimal integration and design that yields the lowest overall cost. A preliminary optimization framework to evaluate potential strategies was implemented using IDAES® (Lee et al., 2021). The framework employed a second-generation solvent-based CO_2 capture system (primary system) in combination with a sorbent-based CO_2 polishing system. A surrogate model of the primary CO_2 capture system was also developed to predict capital and operating costs as a function of capture rate and flue gas flow rate. The sorbent-based temperature swing adsorption (TSA) process was modeled using a simple, 0D, equilibrium-based model described by Joss et al. (2015) that predicts cycle times and key performance indicators such as productivity, regeneration energy required, etc., as a function of design and operating variables. The models of the primary system and TSA polishing system were integrated with a first principles NGCC model. Design and operating variables of the TSA were optimized while minimizing the combined cost of capture for a fixed capture system design at a specific capture rate.

Two cases were analyzed: (i) a polishing step integrated with the NGCC for steam and power, (ii) a polishing step that imports power from the grid and steam from an electric boiler. All cases were compared for three different capture rates within the primary system: 90%, 95%, and 97%. Figure 3 shows the costs for all cases normalized with

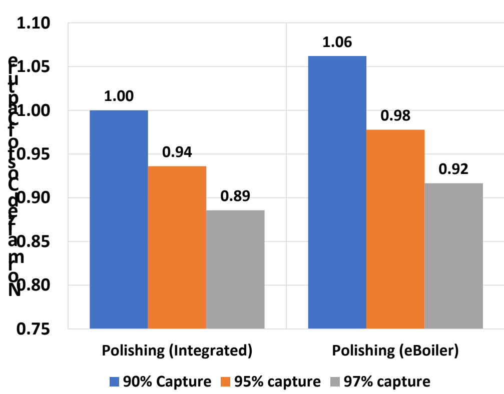

Figure 3: Normalized costs for achieving net negative emissions at the plant level by adding a polishing system to a primary CO_2 capture system with different capture rates.

the cost for 90% primary capture + integrated polishing step as a baseline for similar net-negative levels.

Based on same assumptions for cost and performance across these cases, two key insights emerge. First pushing the capture percentage to 97% in the primary capture system is the least cost option when compared to lower capture rates of 90% and 95%. This can be attributed to the almost flat incremental cost of capture from 90% to 98% that was also observed in the previous section. Second, integration with the NGCC for steam and power results in synergistic advantages compared to purchasing an electric boiler (that leads to additional capital) and electricity from the grid (that could lead to additional associated emissions depending on the generator mix).

Conclusions

This paper has introduced three future scenarios for CO_2 management systems: highly flexible systems, significantly higher capture rates, and coupling CO_2 capture with polishing systems. All of these have the potential to advance U.S. decarbonization goals; however, they require advanced process systems engineering insights to understand their potential by exploring broad design and operating spaces. These may include multi-scale linkage with electricity markets to understand dynamic operating conditions. They may also include pushing operating conditions into regions traditionally considered cost prohibitive and infeasible. Finally, they may include coupling traditional capture technology with new innovations. In all cases optimization frameworks will play a key role in determining the best combinations and the most cost-effective way to operate such systems to achieve net-zero goals.

Acknowledgments

This work was conducted with support from the U.S. Department of Energy's Office of Fossil Energy and Carbon Management through the Simulation-Based Engineering, Carbon Capture, and Solid Oxide Fuel Cell Programs as well as ARPA-E Flexible Carbon Capture and Storage (FLECCS) Program.

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