An Exploration of Direct Air Carbon Capture Design and Deployment

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Princeton University

I hereby declare that this Independent Work report represents my own work in accordance with University regulations.

Vinay Konuru

Attestation

I attest that no humans or animals were used for this project and that this project is compliant with IACUC and IRB policies.

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Abstract: Direct air carbon capture has been identified by both governments and researchers as a critical technology to achieving net-zero emissions targets. However, development of this technology is still in its nascency and its impact on energy systems is not well understood. I am conducting an exploration of this technology to gain a better understanding on how it can be improved and effectively deployed from an engineering standpoint and what its impact on emissions will be from a system modeling perspective. This involves building a small, pilot DAC unit capable of capturing 500 kilograms of CO_2 per year and simulating the impact of larger DAC units on system-wide emissions using macro-energy systems modeling. This research will provide insight into the policy and technical challenges of building and deploying large scale DAC plants and provide recommendations for overcoming these challenges.

Acknowledgements

Thank you to Professor Kelsey Hatzell, Professor Jesse Jenkins, and Dr. Aniruddh Mohan for your guidance and support on this project. Thank you to my brother Jeevesh Konuru for offering engineering guidance. And finally, thank you to Director Ijeoma Nwagwu and the High Meadows Sustainability Fund for their generous funding and supporting this research.

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Introduction

Direct air carbon capture has been an active discussion in climate change and energy systems discussions this year. Climate modelers have shown the need for the large-scale deployment of this technology to achieve net-zero emissions in our energy systems. The IEA reported earlier this year that we need a global DAC capacity of about 900MT to achieve net-zero under current transition pathways. Access to this technology can be used to help decarbonize hard-to-abate industries like aviation and cattle in the short term, while providing a means to help control atmospheric carbon levels in the long term. To incentivize investment and learning in this space, the federal government's Inflation Reduction Act offered large tax credits for investment into DAC technology. Several companies have been bolstered by these credits and have begun building large scale DAC plants. Critics of DAC technology argue that its deployment will delay progress towards decarbonization by inefficiently using limited supplies of renewable energy that could be otherwise used for more pressing sectors like hydrogen production. This discussion on the proper implementation of DAC and incentives raises several interesting and critical questions: Does direct air carbon capture as is currently being incentivized actually reduce overall systems emissions? Are current implementations of DAC technology moving in the right direction in terms of reducing cost and improving efficiency? And how should policies and incentives be structured to ensure that DAC technology is used effectively from an energy systems perspective? In this research, I'm studying DAC from both a plant and systems perspective by building a pilot DAC system and simulating the impact of such systems on a macro-energy systems model. This multi-faceted approach will allow me to consider how we can reduce the costs and improve the efficiency of individual DAC plants, while also optimizing how we can control their impact on our overall energy systems emissions.

To effectively communicate my work this semester, this report will be divided into two sections that encompass my work on this project this semester: a macro-energy system modeling section and a system design section.

Macro Energy Systems DAC Model

Macro-energy systems models represent energy systems from the perspective of a central planner, optimizing the design and deployment of energy generating and consuming resources to meet a set of economic and social objectives. For example, macro-energy systems models are often used in modeling the optimal mix of generation technologies to meet clean energy standards at the lowest cost by considering the tradeoffs in cost and efficiency of various available technologies. Such tools are useful in understanding the interactions between different variables and their impact on overall system characteristics. These models are most often represented as multi-integer linear programming (MILP) problems and solved using optimization solvers such as Gurobi.

I am building on the GenX energy systems model developed by Professor Jesse Jenkins to research the impact of direct air carbon capture on system-wide emissions on the Texas electric grid. This has required learning the GenX codebase, designing a linear programming problem to represent the constraints of DAC technology, translating this problem formulation into code, and running simulations on model grid systems. In the following sections, I will briefly describe the work and challenges I encountered in implementing this system as well as discuss the results of my simulations.

MILP Problem Formulation

To implement a technology in a macro-energy systems model, I need to develop a set of constraints and objectives that define the operation of this resource within the context of the larger energy system. In the case of DAC, the objective is to minimize the cost of building sufficient capacity to meet an emissions capture requirement. Because DAC technology is not profitable under current policy incentives, this emissions capture requirement is required to force the system to build DAC capacity. The constraints in this system include the ramping limit to turn the DAC system higher or lower, the heat and power requirements to operate the DAC plant, and the limits of the heat exchanger within the plant. To make sure the DAC plant operates within the constraints of the larger energy system, I also needed to design additional power-balancing constraints to ensure that the power drawn by the system was less than power produced by generators on any given time step of the simulation.

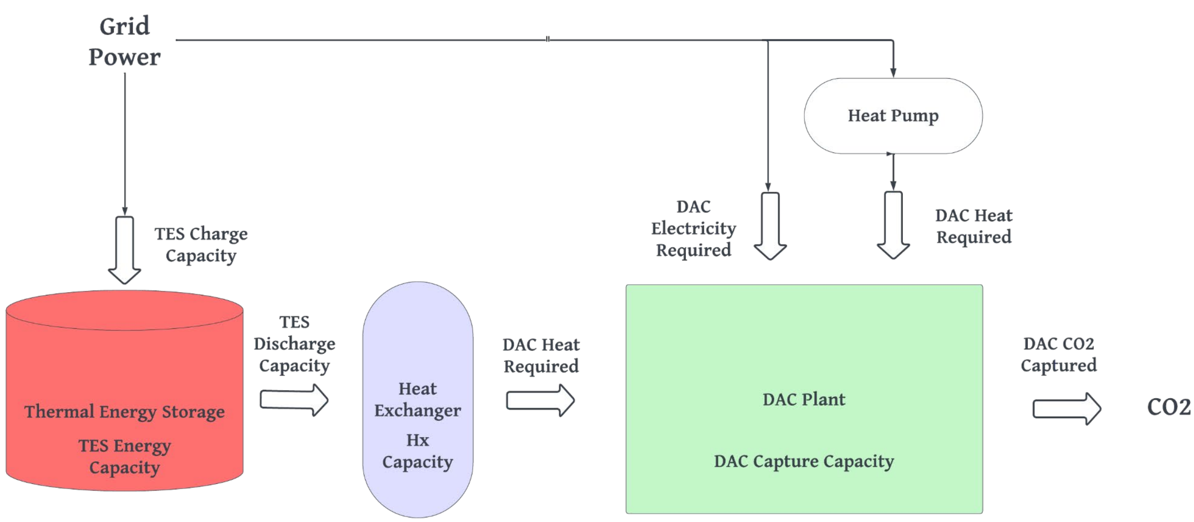

Diagram of operation of DAC+TES system to improve the DACs plant's ability to take advantage of low-cost, renewable electricity.

As will be shown in the results of these simulations, DAC plants were not able to effectively take advantage of available renewable energy resources because of their slow ramping limits. This caused their overall costs and CO2 removal efficiency to increase because they needed to rely on high-cost, high-carbon electricity when renewable energy resources were not available. To overcome this, I also designed a linear program to co-locate thermal energy storage (TES) systems with DAC units to explore the impact this storage could have on the operational costs and efficiency of the plant. This involved adding state of charge constraints, as well as limits to the max charging and discharging rates for these systems. The complete problem formulation for this DAC+TES system is included in the appendix.

Data Acquisition

To run these simulations, I needed data of a realistic US grid system as well as values for the operational requirements and limits of DAC and TES technologies. To represent the grid, I am using an open-source dataset of the Texas ERCOT grid system, which includes the grid's current distribution of generating resources, the intermittency of renewable generators, and the transmission constraints between different regions of the state. To represent the limits and energy requirements of DAC systems, I am using values derived by ASPEN simulations of DAC plants from the past work of Dr. Aniruddh Mohan and Hongxi Luo in Princeton's ZERO Lab. And to represent TES plants, I am using values drawn from previous modeling work exploring the costs of this technology[1]. The data used is available in the GitHub Repository in the Appendix.

Results

DAC without Thermal Storage

As described, I first simulated a DAC plant connected directly to the electric grid for both its heat and power needs. I represented the DAC heating power demand using a heat pump with a COP of 2. I enforced an annual capture capacity of 1 MT of CO2. The results from this simulation shown below illustrate how the DAC plant's inability to ramp forces it to continue steady operations even during periods of high-cost power.

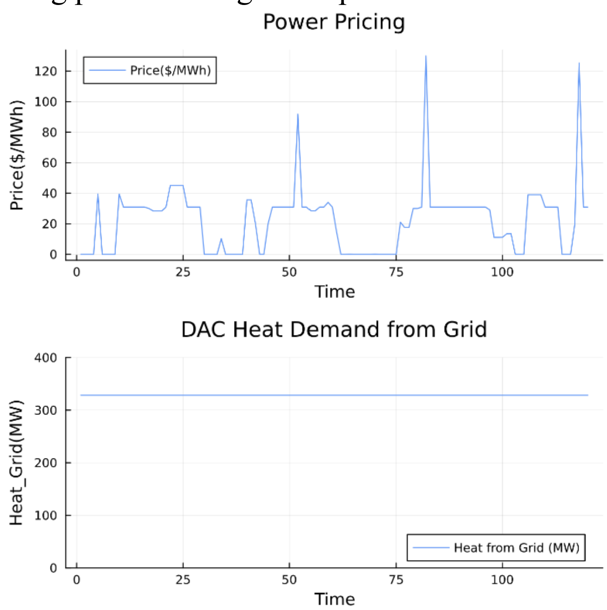

Figure 1 DAC plant has no flexibility to avoid high-cost electricity periods, increasing the operational costs of the system

In addition, the operation of this DAC plant released 400kT of CO2, meaning that the net emissions reductions of the DAC plant were only about 600 kilotons - a 60% plant efficiency in terms of CO2 removal.

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[1] [1] Stack, Daniel C., et al. 'Performance of Firebrick Resistance-Heated Energy Storage for Industrial Heat Applications and Round-Trip Electricity Storage'. *Applied Energy*, vol. 242, 2019, pp. 782–796, https://doi.org10.1016/j.apenergy.2019.03.100.

DAC with Thermal Energy Storage

Next, I added the TES module to the simulation. I modeled the TES unit like a battery, incorporating wrapping within subperiods for state of charge (SOC) constraints and a gradual self-discharge of 5% per day. The TES generates heat using grid power, stores it, and then discharges the heat to its respective co-located DAC plant through a heat exchanger. This new system took much greater advantage of low-cost power by using the ramping capabilities of the TES unit. The optimal sized TES for each DAC plant was a 14.5-hour battery shown below.

Energy Capacity (MWh)	Charge Capacity (MW)	Discharge Capacity (MW)
32396.3	2232.7	468.4

The simulation results show how the TES unit often charges during periods when low-cost power is available and discharges at a continuous rate, allowing the DAC plant to meet its heating needs at a lower cost and with fewer operational emissions.

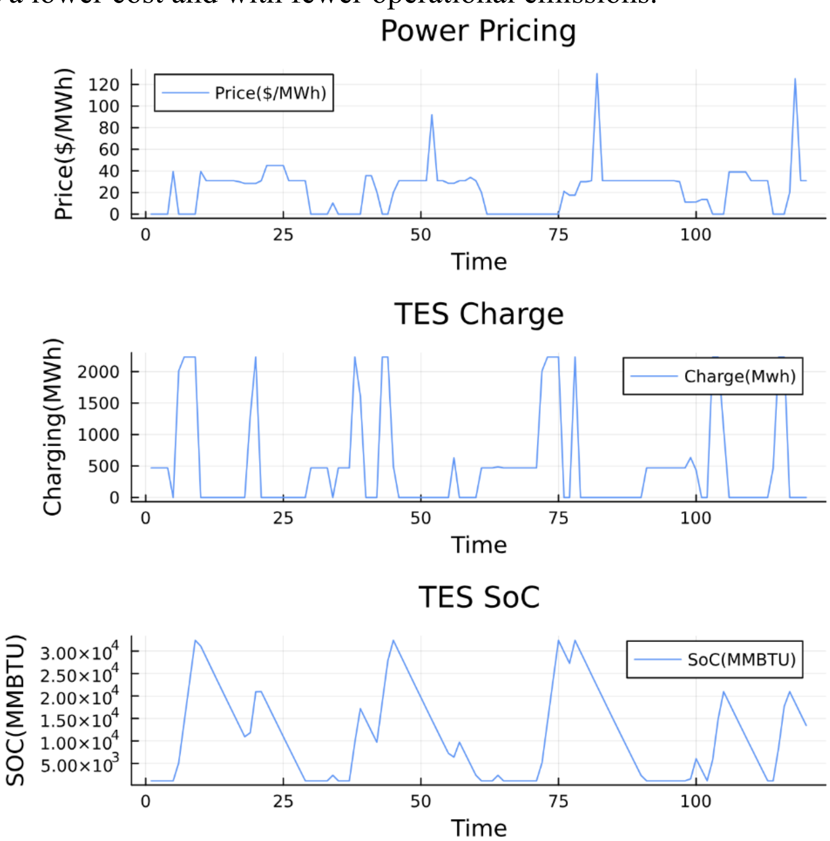


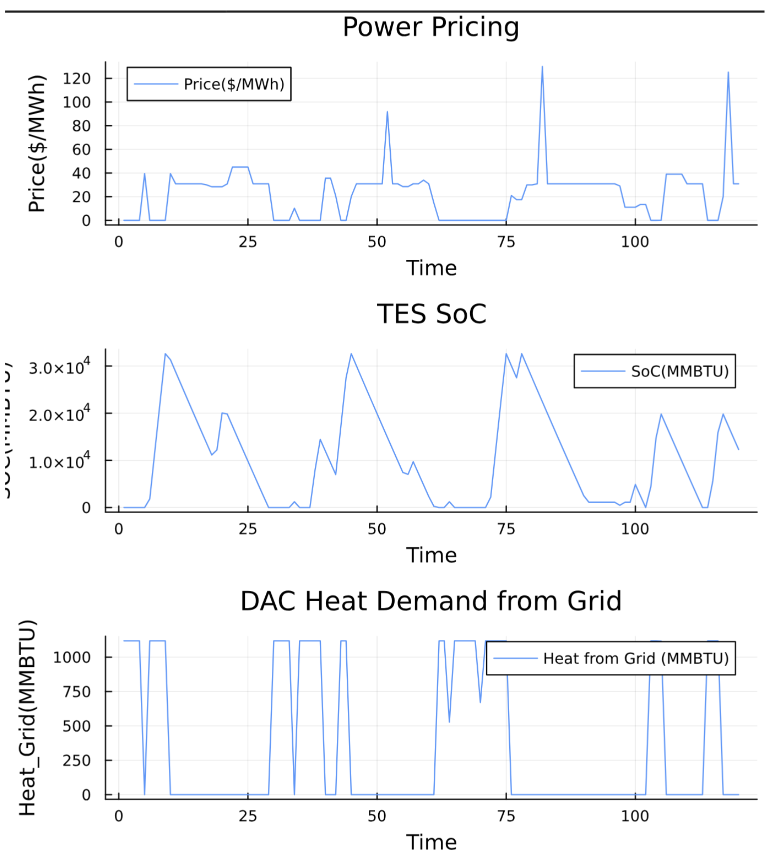
Figure 2 TES charges during periods of low-cost power (Plots 1 and 2) and discharges gradually to the DAC (Plot 3). During periods where there is no charge in the TES, it charges and discharges at equal rates to supply heat directly to the DAC.

In this case, the total operational emissions of the DAC plant were actually negative because the electricity demand of TES unit drove the construction of more renewable generation in the system. This meant that even though the DAC plant was built to only capture 1MT of CO_2, the system's overall emissions reduced by about 1.5MT.

DAC with TES and Grid-Power

It's not always optimal to supply the full heating needs of the DAC from only the TES unit. The DAC unit could generate heat from grid power directly during periods when low-cost power is available at a higher efficiency than drawing from the TES because it could avoid the discharge inefficiencies of the TES. This could also allow the TES unit to lower its charging capacity because it could charge without discharging when low-cost power is available, thus lowering overall system costs. To represent this, I allowed the DAC model to choose whether to draw heat from the grid or the TES unit at any given time, requiring that the two sources of heat together met the heating demand of the DAC facility. The result of the simulation is shown below.

Energy Capacity (MWh)	Charge Capacity (MW)	Discharge Capacity (MW)
32617.1	1987.7	468.4



The results generally align with the previously stated intuition. The TES unit maintains its energy and discharge capacity but lowers its charging capacity because the DAC plant can now also generate heat from the grid. The DAC plant seems to supply all of its heating needs either directly from the grid or from the TES, rarely combining sources. It prefers drawing from the grid when electricity prices or low and when the TES is out of stored power, reflecting the increased efficiency in avoiding the TES.

This ability to pull from both the electric grid and the TES to source power further improves plant efficiency and reduces costs. In this case, the 1MT DAC plant reduced system emissions by 1.6MT.

Analysis of DAC Plant Implementations

Comparing these three systems side-by-side reveals insight into a discrepancy between how DAC technology is currently priced versus its costs to the actual energy system.

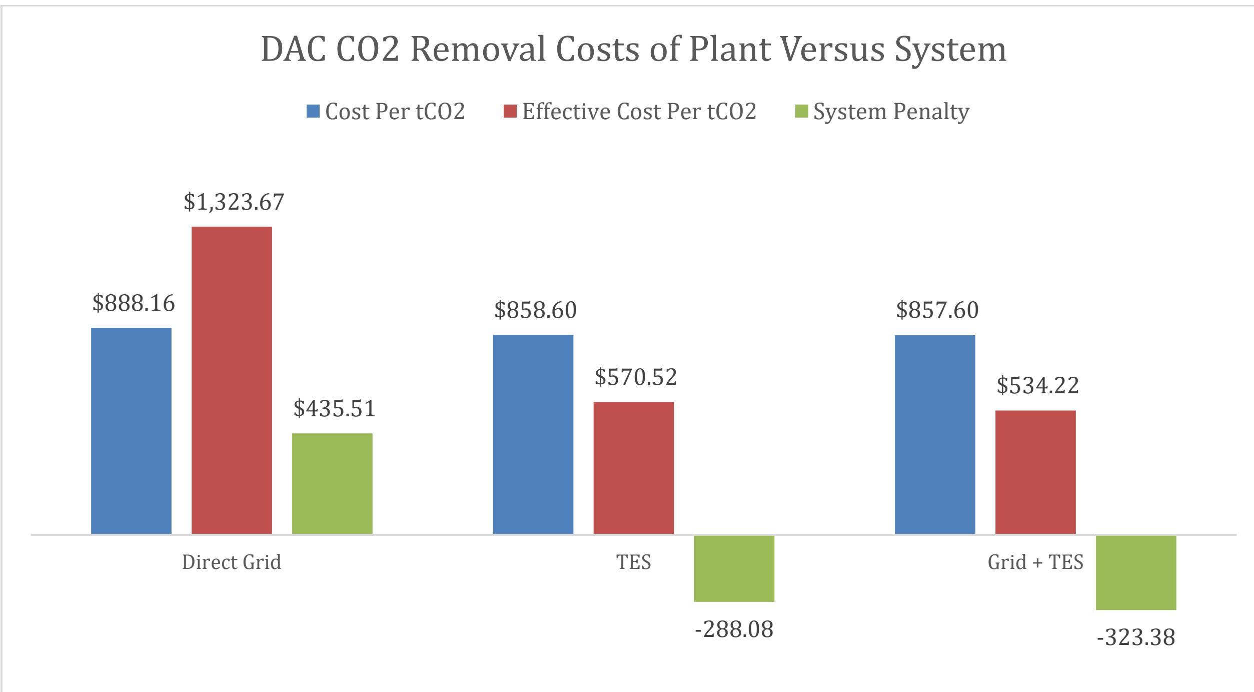


Figure 3 The cost of per ton of CO2 removal compared across three DAC plant implementations, demonstrating the large difference in costs when considering system-wide emissions reductions rather than individual plant reductions

These three DAC plant implementations all remove 1MT of CO_2 per year through their operation, resulting in their costs being relatively similar. Though because of the differences between how these different DAC systems are connected to the grid, the amount of CO_2 they each removed from the energy system is vastly different. As we've seen, the DAC system directly connected to the grid only reduced emissions by 600kT, while the systems with TES reduced emissions by over 1.5MT. By calculating the cost of CO_2 removal in terms of their impact on system-wide emissions reductions, we can see a significant deviation in the cost of these systems. As the system penalty shows, the difference between the cost per ton of CO_2 removal at the plant level versus at the system level be large. This demonstrates a need for policies to incentivize the construction of DAC plants that maximize system-wide emissions reductions rather than simply measuring the CO_2 captured at the plant. This is challenging because calculating the impact of an individual DAC plant on overall energy systems emissions is only possible in the context of a planning problem. But by using these modeling tools, we can identify effective designs for DAC plants and build policy that incentivizes the construction of such DAC technology.

Overall, this modeling work has shown that DAC systems can vary greatly in their efficiency of truly reducing emissions. Therefore, these projects need to be regulated in how and where they are built to maximize their emissions reduction potential. In addition, carbon credit markets need to implement means of incorporating this emissions reduction efficiency of DAC plants to avoid misrepresenting the degree of carbon removed from the atmosphere. Without proactive policy measures, DAC could become a net-harm to emissions reductions goals of our energy systems.

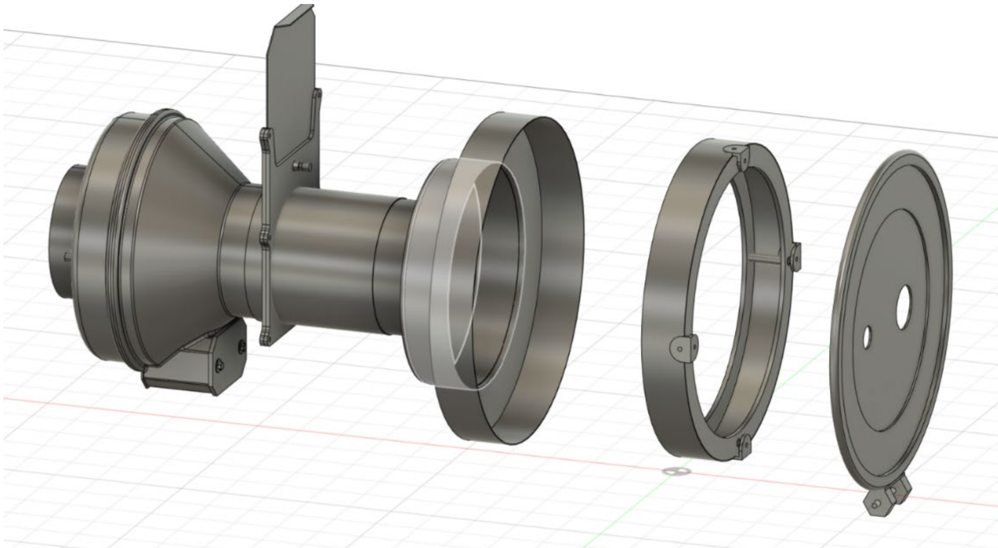
Next Steps

Because the optimal usage of energy storage charging and discharging decisions is based on opportunity cost, I plan to modify the presented problem formulation to incorporate uncertainty to improve the realism of the optimization. Next, I plan to model the impact of requiring that DAC plants only source their input power from newly built renewable generators to reduce the impact that DAC technology will have on decarbonizing other technologies. Comparing these system costs with our current simulations will give a more realistic understanding of the opportunity costs of investing in DAC relative to other technologies on the overall energy system.

DAC System Design

In addition to the work modeling macro-energy systems, I've been continuing to make progress on building a pilot DAC system. This semester, I've focused on creating a CAD model of my system, synthesizing and then testing my sorbent, and integrating the resistive heating system into my packed bed design.

CAD Design



I implemented the above CAD design of the DAC system to help with more easily sizing components and iterating on the architecture of the system. It has also helped with more effectively communicating challenges I'm facing when seeking guidance. I am currently implementing the desorption system in CAD to help with sizing the compressor and storage tank and to ensure the steel drum can handle the associated pressure requirements.

Sorbent Synthesis

Last semester, I planned to use a silica gel sorbent impregnated with PEI to capture CO2. However, I identified a flaw in my calculations earlier this semester that required recalculating the static pressure required to push air through my sorbent bed. This led to me realizing that the silica gel sorbent I planned to use would require me to generate higher static pressures than my fan could produce. Rather than changing the fan, I decided to choose a sorbent with a larger pellet diameter to reduce the pressure requirements of the system. After conducting a literature review on the tradeoffs of different sorbents, I decided to switch to using Zeolite 13X impregnated with PEI.

Figure 4 Setup for synthesizing sorbent(top) and seven gram sample of Zeolite 13X impregnated with PEI(bottom)

Drawing from examples in literature on the synthesis of this sorbent, I produced small batches of the chemical for testing as shown above.

Figure 5 Test bed for measuring CO2 adsorption capacity of sorbent sample (left) and CO2 desorption setup(right).

I then created a test bed to measure the adsorption rate and capacity of the chemical by conducting a breakthrough analysis of the sorbent[2]. Using a LI-COR 850 Gas analyzer, I pumped ambient air through a jar at a low flow rate and measured the CO2 concentration in the effluent gas over several hours. To calculate the amount of CO2 absorbed by the sorbent, I subtracted this CO2 concentration from the concentration of CO2 in the lab's ambient air and integrated this over the testing period. To reuse the sorbent and repeat this breakthrough analysis, I set up a CO2 desorption station to regenerate the sorbent. The setup shown above heats up the sorbent to between 90-100°C in a water bath using a hot plate, while running nitrogen gas through the jar. This heat allows the PEI to release the CO2, while the nitrogen gas pushes the CO2 out the jar

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[2] Analysis of adsorbents for direct air capture of carbon dioxide using breakthrough analysis. https://www.micromeritics.com/downloads/Appnotes/DAC-App-Note.pdf

and prevents the sorbent from reacting with the air around it. I gathered data over several trials using the adsorption and desorption setup to produce the results shown below.

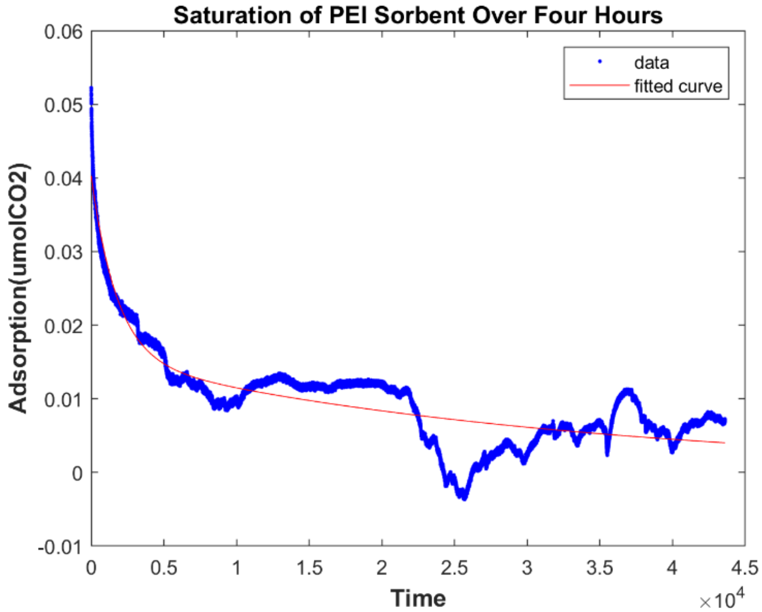

Figure 6 CO2 adsorption rate of sorbent over 4.5 hours using the LI-COR 850 Gas Analyzer

Integrating the fitted curve shown above, I found that the capacity of my Zeolite sorbent was about 0.05 mmol of CO2 per gram of sorbent. This was approximately 20% of the capacity of the sorbents I found in literature. I plan on testing with different ratios of PEI to zeolite pellets in future trials to improve this capacity before synthesizing a larger sorbent batch.

Resistive Heating Setup

To consistently regenerate the sorbent and release the CO2 in my machine, I need to build a reliable heating system that can evenly heat all the sorbent to 100C without burning any of it at 200C. I am designing my heating system for the DAC machine using high resistivity Kanthal wire. By controlling the current delivered to this wire, I can change its temperature. Though, evenly distributing the heat from this wire across the whole packed bed has been a challenge.

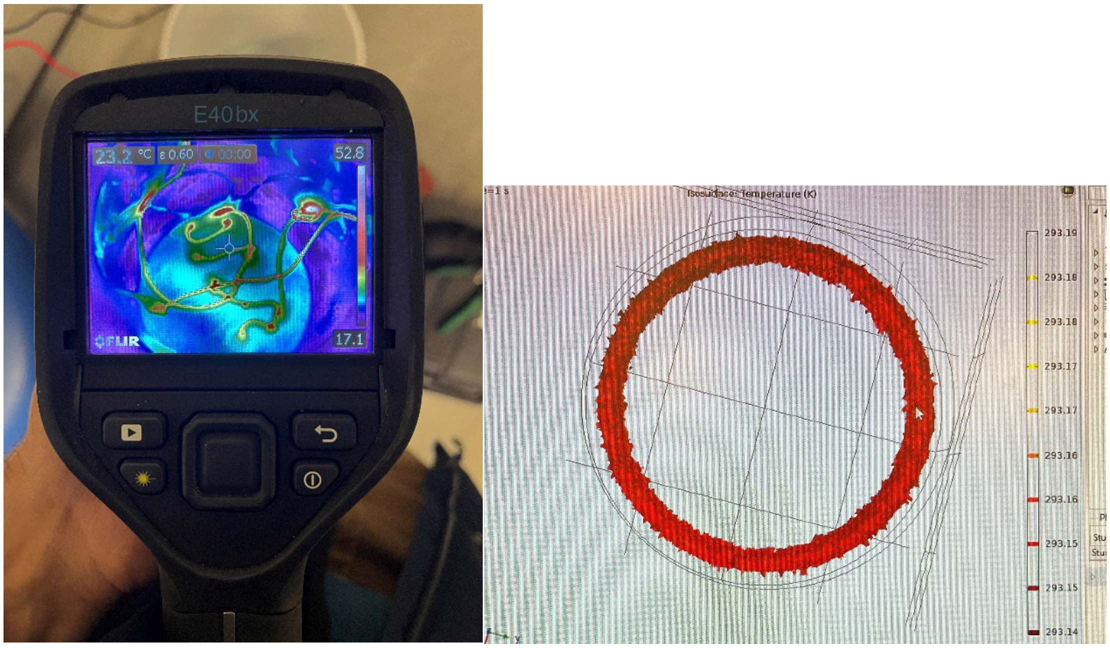

Figure 7 Kanthal wire under thermal camera (left) and COMSOL simulation of resistive heating system in packed bed (right)

Kanthal wires dissipate heat poorly because of their small cross-sectional area. This is demonstrated in the thermal camera monitor above where the wire is shown to hot while the air around it is still cool. This is an issue because it means that the resistive heating setup that I planned to build will not be able evenly heat the chemical bed. I simulated the initial toroidal design for the resistive heating system in COMSOL, revealing how this issue will prevent the sorbent in the center of the packed bed from being regenerated.

Rather than covering more of the packed bed with this Kanthal wire, which risks burning the sorbent, I am planning to instead sandwich the resistive wires between layers of thin, meshed fabric and place these layers inside the packed bed. This will help distribute the heat radiating from the Kanthal wires more evenly through the bulk of the sorbent bed without needing to risk burning the sorbent.

Next Steps

My next steps for completing this DAC system will be 1) redesigning the resistive heating system using the meshed fabric layers, 2) procuring a pump and gas tank for the desorption system and 3) installing pressure and temperatures sensors within and around the packed bed inside the steel drum. Once these steps are complete, I will be able to turn the system on and begin testing its operation.

Conclusion

I'm excited about the progress I've made this semester. I believe taking this multi-faceted approach to understanding DAC has helped me build a firmer grasp on the fundamental tradeoffs of this technology at both a plant scale and an energy systems level perspective. I am looking forward to continuing my work on this project over Winter Break and sharing my completed study in my thesis.

Appendix

A1. GitHub Repository: https://github.com/vinaykonuru/GenX

A2. Problem Formulation

Y = set of all TES, T = set of all time samples

TES Variables:

$$vS\_TES[y \; in \; Y, t \; in \; T] \; \geq \; 0$$
$$vCHARGE\_TES[y \; in \; Y, t \; in \; T] \; \geq \; 0$$
$$vDISCHARGE\_TES[y \; in \; Y, t \; in \; T] \; \geq \; 0$$
$$vCAP\_CHARGE\_TES[y \; in \; Y] \; \geq \; 0$$
$$vCAP\_DISCHARGE\_TES[y \; in \; Y] \; \geq \; 0$$
$$vCAP\_ENERGY\_TES[y \; in \; Y] \; \geq \; 0$$

DAC Variables:

$$vCAP\_DAC[y \; in \; Y] \; \geq \; 0$$
$$vCO2\_DAC[y \; in \; Y, t \; in \; T] \; \geq \; 0$$
$$vHx\_DAC[y \; in \; Y, t \; in \; T] \; \geq \; 0$$
$$vDAC\_elec\_heat[y \; in \; Y, t \; in \; T] \; \geq \; 0$$

TES Constraints:

$$vS\_TES[y \; in \; Y, t \; in \; INTERIOR\_SUBPERIODS] = vS\_TES[y, t-1] + \frac{vCHARGE\_TES[y,t]}{Eff\_up} + \frac{vDISCHARGE\_TES[y,t]}{Eff\_down} + \frac{vS\_TES[y,t-1]}{Self\_discharge}$$

$$vS\_TES[y, t \; in \; START\_SUBPERIODS] = vS\_TES[y, t \; + hours\_per\_period - 1] + \frac{vCHARGE\_TES[y,t]}{Eff\_up} + \frac{vDISCHARGE\_TES[y,t]}{Eff\_down} + \frac{vS\_TES[y, t + hours\_per\_period - 1]}{Self\_discharge}$$

$$vCHARGE\_TES[y,t] \; \leq vCAP\_CHARGE\_TES[y], y \in Y, t \in T$$
$$vDISCHARGE\_TES[y,t] \; \leq vCAP\_DISCHARGE\_TES[y], y \in Y, t \in T$$
$$vS\_TES[y,t] \; \leq \; vCAP\_ENERGY\_TES[y], y \in Y, t \in T$$

$$Total\_Power\_Balance \mathrel{+}= \sum_{y \in Y, t \in T} vCHARGE\_TES[y,t]$$

$$\text{Total\_Cost} \mathrel{+}= \sum_{y \in \text{Y}} \text{vCAP\_CHARGE\_TES[y]} * \text{Cost\_per\_MW} + \text{vCAP\_DISCHARGE\_TES[y]} * \text{COST\_PER\_MMBTU} + \text{vCAP\_ENERGY\_TES[y]} * \text{Cost\_per\_MWh}$$

DAC Constraints:

$$\sum_{t \in T,} vCO2\_DAC[y,t] \le vCAP\_DAC[y], y \in Y$$

$$\sum_{y \in Y, t \in T,} vCO2\_DAC[y,t] \le ANNUAL\_CO2\_REQUIREMENT$$

$$eDAC\_Heat\_Requirement[y,t] = vCO2\_DAC[y,t] * MMBTU\_per\_ton\_CO2, y \in Y, t \in T$$

$$eDAC\_Power\_Requirement[y,t] = vCO2\_DAC[y,t] * MWh\_per\_ton\_CO2, y \in Y, t \in T$$

$$vDISCHARGE\_TES[y,t] + vDAC\_elec\_heat[y,t] * MMBTU\_per\_MW = eDAC\_Heat\_Requirement[y,t]$$

$$eDAC\_Heat\_Requirement[y,t] \le vHx\_DAC[y], y \in Y, t \in T$$

$$Total\_Power\_Balance \mathrel{+}= \sum_{y \in Y, t \in T} eDAC\_Power\_Requirement[y,t]$$

$$\text{Total\_Cost} \mathrel{+}= \sum_{y \in \text{Y}} \text{vCAP\_DAC[y]} * \text{Cost\_per\_ton\_CO2} + \text{v\_Hx\_DAC[y]} * \text{Cost\_per\_MMBTU}$$