Modeling System-Wide Emissions Impact from Deploying Direct-Air Carbon Capture Plants with Thermal Energy Storage

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

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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 (DAC) has been identified by both governments and researchers as a critical technology to achieving net-zero emissions targets. DAC deployment has begun to increase in recent years, bolstered by the Inflation Reduction Act and demand from hard-to-abate sectors. Though, the impact of large-scale DAC deployment on our electricity systems is not well understood. One major challenge for DAC plants is the lack of operational flexibility as a high capital cost asset with slow ramping rates. Combined with DAC's high heat requirements, this makes it challenging for DAC plants to utilize intermittent renewables to power their operations. In this research, we examined how solid-sorbent DAC plants fitted with different configurations of thermal energy storage (TES) systems could better take advantage of renewable resources. We also explored how such DAC with TES compared with plants that used heat pumps, analyzing their costs of carbon reductions from both the plant and electricity system perspective. To do this, we modified the GenX electricity sector capacity expansion model with custom modules to incorporate direct air capture, thermal energy storage, and heat pumps. We found that DAC plants with TES can increase their emission reductions by over 75% at the electricity system level compared with heat pump based systems, but that their cost of capture increases by $75/tCO2 at the plant level. We also found that further cost reductions in the cost of TES down to $20/kWh will only reduce the costs to the DAC plant by $15/tCO2. This study provides a deeper understanding of the relevant tradeoffs of using TES within DAC plants and the impact of various DAC configurations on electricity system emissions.

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Chapter 1

Introduction

Chapter 1.1 Background and Overview

Negative emissions technologies (NETs) are an important element to reaching net-zero emissions targets. The 2023 IPCC report [1] found that such technologies would be required to meet net-zero by 2050 pathways to decarbonize hard-to-abate sectors in the near term and to better manage emissions and avoid a 2°C global warming scenario in the long term. Tax credits from the IRA [2] and demand from large technology and aviation companies [3] have bolstered implementation of such NET systems in recent years. Though, for these technologies to make a positive impact on the energy transition, we need to be intentional in how they are deployed to ensure they're truly reducing system wide emissions.

Currently, the most economically feasible NET is called direct-air carbon capture (DAC). DAC has grown in popularity both in climate discussions and within the startup space over the last few years because of it's potential to experience steep learning curves and its ability to accurately verify CO_2 removals – an important consideration when developing carbon credit economies. To incentivize investment and learning in this space, the federal government's Inflation Reduction Act (IRA) has offered large tax credits for investment into DAC technology. Several companies have taken advantage of these credits and have begun building large scale DAC plants, including Occidental Carbon's Stratos [4], a 0.5 $MtCO_2$ per year liquid sorbent plant powered by natural gas, and Heirloom's pilot plant, a 1$kTCO_2$ per year solid sorbent plant powered by electricity. As we begin to see the growth in the development of this technology, now is a critical moment to model and understand the implications and consequences of scaling DAC on the stability and emissions of our electricity system.

Two major challenges for DAC facilities are their significant heat requirements and their inflexibility as a high capital cost asset with slow startup and ramping rates. These factors make it difficult for DAC plants to utilize intermittent renewable resources to power their operations. Instead, to provide base load power, DAC plants currently rely on carbon-based energy sources such as natural gas and grid electricity, reducing the plant's net emissions reductions by between 20-50% [5] through their operational emissions. These challenges have led critics to conclude that DAC technology is simply too inefficient and costly to ever achieve the scale needed to meet decarbonization goals. Others argue that the deployment of DAC will simply delay progress towards decarbonization by inefficiently diverting capital and attention that could otherwise fund other critical, growing sectors such clean hydrogen and biofuel production.

One solution to this challenge is collocating DAC plants with thermal energy storage (TES) systems. TES has been gaining increased attention in recent years given its potential to decarbonize high-heat industrial operations. Its costs have also been lowering as our understanding of thermal materials [6] and modeling of heat flow has improved. These costs are expected to continue to drop with the recent inclusion of TES within the guidelines of the 45X Advanced Manufacturing tax credit [7, 8]. By charging the TES using low-cost, clean power when it is available and continuously discharging clean heat to the DAC, this DAC + TES system could operate continuously with lower operational emissions. Though, there are many implementation challenges and tradeoffs to this type of setup, including the high capital costs of constructing TES, the lower efficiency of heat storage relative to heat pumps, and the complexity of planning TES charging and discharging decisions within the constraints of DAC plant operations.

This discussion on the larger impacts of DAC on electricity sector emissions, the effectiveness of incentive structures driving DAC innovation, and the carbon removal potential of DAC + TES systems raises several interesting and critical questions:

- How would the incorporation of technologies like thermal energy storage (TES) into DAC plants change the economics and carbon removal efficiency of DAC operations?
- How should policies and incentives be structured to ensure that the impact of DAC plant operations on electricity system emissions are minimized?

To answer these questions, we will model various solid-sorbent DAC plant implementations, comparing the plant level and system level benefits of collocating with TES relative to using direct-grid powered heat pumps. We will then study the cost and emissions reductions of these DAC implementations from both a plant and system perspective using macro-energy systems modeling techniques. This dual perspective approach– considering the costs to both the private DAC owner and the overall energy system - will allow us to consider how we can reduce the costs and improve the efficiency of individual DAC plants, while also optimizing their impact on reducing overall energy system emissions. Our results will allow us to consider different policy recommendations for future DAC tax credit incentives and support DAC developers in planning plant designs that have positive system level effects at the lowest cost.

Chapter 1.2 Literature Review

The majority of current research in DAC focuses on building techno-economic models to develop estimates for the cost of CO_2 capture across various design decisions [9, 10]. The most explored design consideration is the type of sorbent used for CO_2 capture. Liquid sorbents like potassium hydroxide can achieve greater capture rates but require higher temperatures to release the CO_2 after it's been absorbed. Solid sorbents like Zeolites have lower capture rates but require lower temperatures for CO_2 regeneration [11]. Beyond the sorbent, the high energy requirements to operate DAC plants regardless of sorbent type make other factors like the method for procuring heat and power equally important for determining cost of CO_2 capture and impacts on the larger energy system [12]. For example, McQueen et. al found that the costs of CO_2 capture via DAC could vary by up to \$300/tCO_2 depending on whether the DAC plant uses gas or collocated renewable electricity as its energy source. The broad range of system design configurations for sourcing heat and power in literature, including nuclear, geothermal, natural gas, and solar powered plants [13, 14], demonstrate the complexity of the decision space for this problem. Though, across nearly all of these methods for sourcing heat and power, energy storage plays a critical yet under-emphasized role in lowering operational emissions and improving the utilization of intermittent renewables. Our study will help fill this gap by providing insight into how thermal energy storage can fit into these existing DAC models.

In Sievert et al. [15], the authors projected the cost of DAC by examining component level experience rates. They found that combining individual learning curves of components into a larger probabilistic model provided more nuance into how the cost of capture might be expected to fall with respect to specific design choices and learning scenarios. For example, certain components in solid sorbent DAC like compressors have shallower experience curves because they've already reached technological maturity, while other components like the sorbent itself can experience steep experience curves as we scale up chemical and manufacturing supply chains. With this more conservative estimate, Sievert found the cost of DAC would fall to \$341/tCO_2 (\$226-\$544) for liquid sorbent and \$374/tCO_2 (\$81-\$579) for solid sorbent plants if these technologies were to reach gigaton scale deployment. These estimates were reported to be about a 300% reduction from DAC costs estimates today and about ten times higher than cost estimates from single component experience curve projections. These broad cost ranges within and between these DAC cost models reflect the significant uncertainty about the future cost of DAC technologies and the need for further modeling and design work to support investment into DAC development.

Young et al. [13] employed a different approach for estimating DAC costs that also incorporates the impact of how the DAC plant is powered, focusing on building bottom-up economic models of DAC plants powered by grid electricity, intermittent renewables, geothermal, nuclear, and other sources. The authors found that solid-sorbent DAC costs would fall between \$200-\$500/tCO_2 in a high uptake scenario by 2050. They also noted that pairing intermittent renewables with DAC would significantly increase the cost of CO_2 capture because it would require ramping the DAC plant based on the availability of power. Although using intermittent renewables would reduce DAC operational emissions, the high fixed costs and slow ramping rates of DAC make it ideal to run non-stop even considering the associated emissions of base load electricity. This underscores the need for technologies such as TES that provide DAC with the capability to utilize intermittent renewable resources without needing to disrupt operations.

Finally, there is significant work studying the cost evolution and potential applications for TES in different industries. Stack et al. [16] conducted an economic analysis of TES based on a firebrick storage medium and resistive wire heating system, finding a cost of \$10/kWh. Iyer et al.

[8] at RMI found that TES as constructed today likely costs in the range of $85/kWh to $210/kWh, having selected more conservative estimates for component costs beyond the storage medium such as transformers and blowers. They also found that IRA 45X storage incentives would help subsidize these costs to the extent of $45/kWh. Similarly, the PNNL Storage Grand Challenge report found that thermal energy storage would likely cost above $100/kWh storage until 2030. Ma et al. [18] explored the potential of using TES with solar power to provide industrial process heat with higher capacity factors. They identified potential suitable industrial applications such as bauxite calcination and industrial hot air supply. Finally, Sepulveda et al. [19] conducted a comprehensive study of the potential for long-duration energy storage technologies like TES to reduce electricity system costs and displace firm generation, finding that TES costs would need to fall below $1/kWh to have significant penetration on the grid. These findings demonstrate that TES has great potential for improving the utilization of renewables for medium to high-heat industrial processes as costs continue to come down. Though, these benefits will likely come at a cost to the plant operator.

Chapter 2

Methods

In our study, we needed to develop model that could simulate the plant level operational behavior of an optimal DAC and TES system and the larger, macroscopic interactions of this system with the rest of the electricity sector. Having a single model that could simulate both of these perspectives could reveal the larger impacts of different DAC configurations on plant level costs and electricity sector emissions. It could also reveal hidden relationships between how DAC deployment impacts the electricity market and costs of other clean energy technologies.

To accomplish this, we used the GenX model modified with custom modules for DAC and TES systems. We also created cost models for DAC and TES technologies to inform how plant level design and operations could be optimized. In the following section, we will provide an overview of the modeling techniques and the high-level design choices we used in setting up these DAC and TES electricity sector simulations. We will also detail our basic assumptions and sources used in developing our technology cost estimates.

Chapter 2.1 Electricity System Planning Model

GenX [20] is an open-source electricity sector optimization model developed by Princeton ZERO Lab and the MIT Energy Initiative. Given data on an electricity system such as available generators, basic transmission, and a set of decision variables for new build capacity, the GenX model will select the least cost electricity system solution that meets the defined engineering, policy, and market constraints using multi-integer linear programming techniques. To use this tool, we needed to design a simulation test bed incorporating where and how we wanted the DAC and TES modules to be built, which zones of the electricity sector we wanted to model, and what data we would use to represent the electricity market in this region.

2.1.1 Modifying GenX Capacity Expansion Model with DAC and TES

To incorporate DAC and TES into the larger GenX model, we built on previous work from Dr. Anriuddh Mohan to implement custom modules in the GenX codebase. This involved making several design decisions including how we would represent DAC and TES capacity sizing and operational costs, what decisions we wanted to implement as variables for the model to optimize, and how the DAC plant would fit within the larger electricity system optimization problem. Also, because captured carbon has little financial value, we had to set a fixed annual 1 $MtCO_2$ minimum capture constraint within our DAC system module to find the least cost system that could meet this carbon capture target. The specific design for these constraints is laid out in detail within the problem definition section. Our simulations model one year of operation in the Texas ERCOT grid system, providing the GenX model freedom to size the optimal capacity and hour-by-hour operational decisions for both DAC and TES systems, along with other technologies applicable to specific configurations that will be described later. For example, our model will be able to choose how far to charge or discharge the TES system at each hour of the year, minimizing the cost of heat to the DAC plant based on input electricity price data.

2.1.2 Modeling the ERCOT Power System

We chose to model our DAC scenarios within the Texas ERCOT grid system for three main reasons:

1. ERCOT is an isolated grid system independent of the rest of the US electric grid, so simulations on this grid provide more specific and pronounced insights into the impact of DAC on the electricity sector.
2. Texas has a high potential for DAC buildout given the large number of well-researched carbon sequestration sites in the state.
3. The ERCOT system has high percentage of renewable energy generation relative to the rest of the US, making it a good case study for demonstrating the potential increase emissions reductions when DAC can take advantage of clean electricity.

We split the ERCOT system into two zones representing East and West Texas. East Texas has a higher power demand with larger population centers such as Houston, Dallas, and Austin. West Texas has a smaller, rural population, but a significantly larger supply of intermittent renewable resources like solar and wind. Simplifying the ERCOT grid into this two-zone model made our simulations more tractable, while still maintaining underlying grid congestion between these two starkly different zones. We then added our DAC system into the West Texas zone based on early announcements for a DAC hub in the region [21] and the large number of potential carbon sequestration locations nearby.

2.1.3 Electricity Sector Data Aggregation

We used the PowerGenome tool [22], an open-source data aggregation package for electricity sector datasets, to generate data for a two-zone representation of the ERCOT grid system. PowerGenome draws from datasets available through the EIA, NREL, and EPA. It then organizes this data to provide transmission constraints, hourly load profiles, hourly generation profiles, cost estimates for standard, new-build generation units, and inputs for all existing generation units in the selected grid network region. This tool has been used in several previous projects within ZERO Lab in conjunction with GenX to provide accurate representations of various regions of the US electric grid.

2.2 Process Diagrams for DAC Case Study Configurations

There are four main configurations of DAC plant processes that we will model to understand the capabilities and value of thermal energy storage:

a. DAC with Heat Pump – the base case plant design representing a DAC system that draws power and heat directly from grid electricity using a large heat pump.
b. DAC with Thermal Energy Storage – the basic TES utilization scenario where all of the heating needs of the DAC plant are met by discharging the TES.
c. DAC with Thermal Energy Storage and a Heat Pump – a middle ground scenario where the plant has to optimize between the benefits of building TES and heat pump capacity.
d. DAC with Thermal Energy Storage and a Retrofitted Steam Turbine – an alternative approach where the DAC plant has a turbine collocated with the TES, allowing the plant to temporarily operate independent from the grid by drawing both heat and power from the combined TES + turbine system.

Together, these four configurations will provide a balanced understanding of the potential roles and impact that TES can serve within a DAC plant. Below, we'll provide a process flow diagram and relevant descriptions for the design choices in each DAC configuration.

A. DAC with Heat Pump

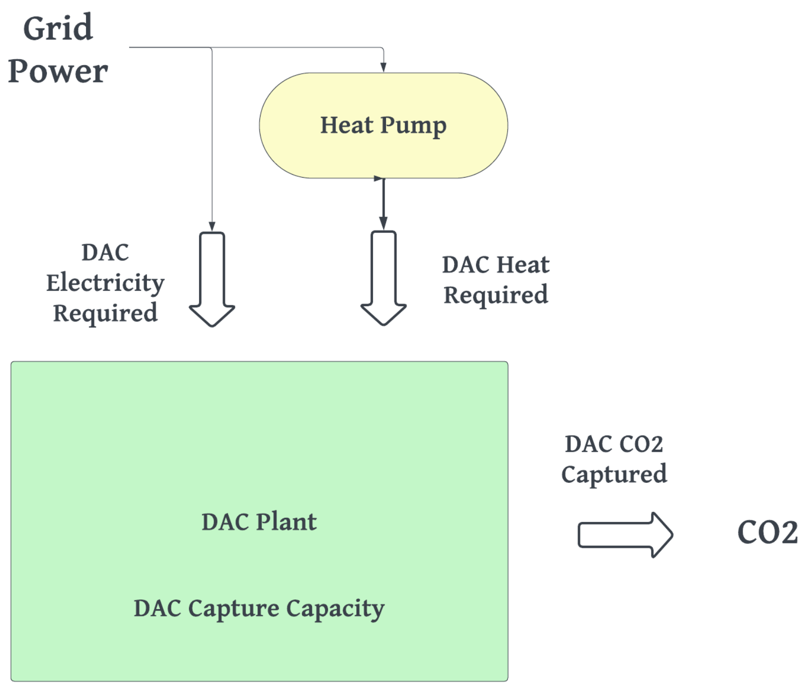


Figure 1 Process diagram of DAC with heat pump system

In this configuration, rather than relying on TES for heat, the DAC plant produces heat using a heat pump directly connected to the grid. We assume a heat pump with a COP of 2 and a cost of $500k/MW [23, 24]. In this scenario, the DAC plant will need to continuously pull electricity from the grid for both heating and power requirements. The only decision-making freedom the model has is whether or not to ramp down or shut off the DAC plant operations. This means that the DAC plant will have little protection against power price surges and no viable means of avoiding high carbon electricity beyond simply shutting down operations. This serves as a base case to compare with a DAC + TES system to measure the impact on operational costs and emissions.

B. DAC with Thermal Energy Storage

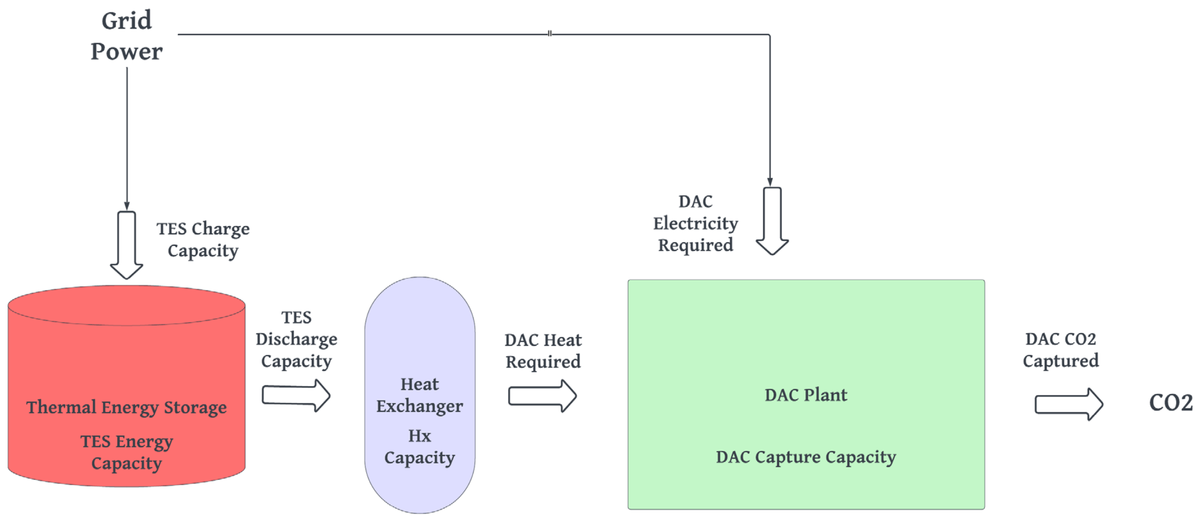


Figure 2 Process diagram of DAC with TES system

In this configuration, TES is collocated with a DAC plant to provide all its heating needs. The TES charges using power directly from the grid when prices are low, and it discharges heat to the DAC at a consistent rate, allowing the DAC to continue uninterrupted operations. Because periods of low-cost power often align with when renewables are most abundant, the TES charges using largely renewable power. This allows for the DAC plant to operate off low-cost, clean heat while continuing to operate steadily. Thus, the TES provides flexibility to the DAC in terms of when and how it will procure heat. The TES efficiency is 70% between the input grid power to the output heat [16]. Both the DAC and TES plant rely on the grid for their electricity needs such as powering blowers, auxiliary power systems, and controls. The cost of the TES are broken down in the following section on technology cost models.

C. DAC with Thermal Energy Storage and Heat Pump

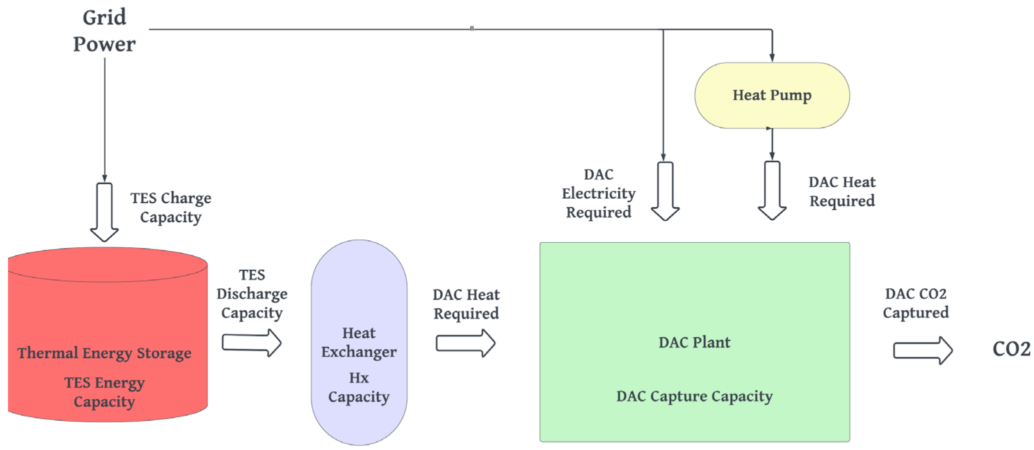


Figure 3 Process diagram of DAC with heat pump and TES system

To provide a middle ground between the previous configurations, we now consider a plant where the DAC has the option to draw heat either through the TES or the heat pump. At any point, the total heat discharged by the TES and produced by the heat pump need to equal the total heat requirements of the DAC. This design offers DAC the ability to build TES to use during periods of the day when power prices are high, while using the heat pump when power prices are low. By using both technologies, the plant has the potential to reduce how large of a TES system it needs to build out, while still having protection against high electricity prices and high carbon electricity. This combined TES + HP design has the potential to dramatically lower project costs while maintaining similar process emissions.

D. DAC with Thermal Energy Storage and Retrofitted Steam Turbine

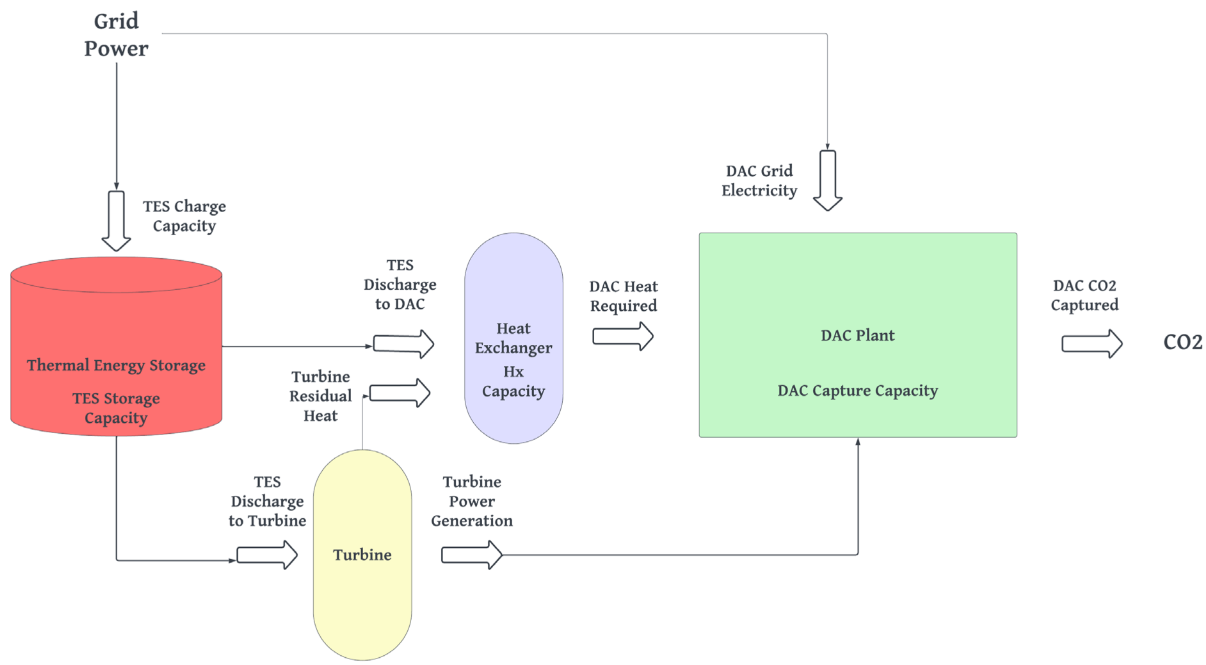


Figure 4 Process diagram of DAC with TES and turbine system

In this final configuration, the DAC plant has a TES that can now produce both heat and power by using a retrofitted steam turbine with a boiler connected to the TES. The steam turbine is sized to meet the full power needs of the DAC, allowing the DAC system to run completely independent of the grid during periods when power prices are high or when renewables aren't available. At each hour, some heat from the TES is directed to the boiler of the steam turbine to produce power for the DAC. The remaining heat discharged from the TES on a given hour is then sent directly to the DAC, bypassing the turbine. The residual heat from the turbine, along with heat directly discharged from the TES to the DAC, is then used to meet the total heating needs of the DAC operations at each time step. The DAC plant also has the option to supply power from the electric grid so that at any time step, it can optimize for the cheapest mix of power between the opportunity cost of discharging the TES and the electricity costs of drawing from the grid. Any excess power from the turbine not used by the DAC at each hour will be sent back into the grid network. Although this plant design is more expensive, it has the potential to make the greatest impact on reducing operational costs and process emissions because it is the least reliant on the electric grid at any given hour.

2.3 Component Modeling and Cost Analysis

In the following sections, we will discuss our cost models, assumptions, and reasoning for each of the components within our DAC configurations.

2.3.1 Direct Air Carbon Capture

The costs of DAC technology can be highly variable depending on the scale of the plant. We decided to model a solid sorbent DAC system because of its lower heat requirements (100°C), which lend themselves to more readily using thermal energy storage and heat pumps. We drew the following table of values for a 1MT DAC plant from the techno-economic analysis in Young et al [13]. These DAC model parameters are used across all the modeled plant configurations.

Table 1 DAC system requirements

Parameter	Unit	Value
Total Removals	$MtCO_2$/yr	1
Capital Costs per tCO2 (annualized)	$/year	800
Heat Requirement per tCO2	MMBTU/tCO2	9.8
Power Requirement per tCO2	MWh/tCO2	0.5
Maximum Capacity Factor	-	95%

2.3.2 Thermal Energy Storage

For a 1MT solid sorbent system DAC system as shown above, 85% of the hourly energy requirements are in the form of heat. TES systems can produce and store heat from grid electricity when power prices are cheap and renewable energy is abundant such as during mid-day. By introducing sufficient TES capacity, a collocated DAC plant can draw heat from the TES continuously, allowing it to continue operations uninterrupted while now using cleaner, lower-cost power. TES should thus be able to decrease the operational costs and the associated emissions of DAC processes and offer better system-wide utilization of low-cost, intermittent generation.

We modeled the TES system off of a silicon-carbide based thermal storage medium design as mentioned in Stack et al [16]. The TES charges by passing power from the grid through high resistance wires that convectively heat the thermal medium. It discharges heat in the form of steam using a heat exchanger. Our TES model has two design decision variables to size the TES: storage capacity ($/kWh) and charge capacity ($/kW), drawing on the same framework from Sepulveda et. al [19]. Major system component costs are grouped within these three decision variables as follows:

Table 2 TES component cost breakdown

Storage Capacity Components	Cost ($/kWh)	Charge Capacity Components	Cost ($/kW)
• Thermal Storage Medium • Insulation	10.3 0.4	• Resistance heater wire • Transformer • Grid connection	14 4 4.4

The individual cost estimations for each of these components are included within the Appendix. Additional component costs such as blowers, containment pipes, and valves are included within the balance of system costs represented as a set 50% adder to the previous equipment costs. EPC costs are then also included as 20% of the bare erect costs. Finally, we included a 90% contingency adder to form realistic estimations accounting for shipping costs, project delays, and other unexpected costs. These percentage adders are consistent with previous research on first of a kind project cost estimates in ZERO Lab and general guidelines for early-mover projects [25].

Table 3 TES system costs with adders

First of a Kind COST ESTIMATE	Cost Storage ($/kWh)	Cost Charge ($/kW)
Purchased Equipment Cost	11	22
including Bare Erect Cost adder (bare erect cost, includes balance of system costs)	16	34

including EPC adder (engineering, management, construction)	19	40
including contingency adder (unknown costs) at 90% of BEC	**34**	**71**

We use storage and charge capacity costs of \$34/kWh and \$71/kW respectively within our optimization models to optimize the size of our TES within the DAC plant. We conduct a sensitivity analysis on the impact of changing these cost estimations on our findings.

Assumptions:

- TES can size its storage capacity and max charge rates independently.
  - Reasoning: Storage capacity and max charging rates are determined by different system design decisions.
- Max discharge capacity costs can be included within the storage capacity costs.
  - Reasoning: The max discharge capacity is determined by the costs of a heat exchanger, which is largely based on the maximum heating needs of the DAC.
- The TES plant charging efficiency from electricity input to heat output is 70% [16].
  - Reasoning: The DAC plant charges by running current through high resistivity wires, which then heat up a thermal storage medium using convection. The thermal efficiency of this process in Stack et al. can vary between 70-90%.

2.3.3 Steam Turbine

By pairing the TES with a steam turbine, we can produce both heat and power for the DAC plant. This would not only provide more flexibility for the plant to meet its energy requirements, but also provide the DAC plant with more energy security, now able to operate independent of the grid system. We used ASPEN models developed by Dr. Hongxi Luo in ZERO Lab of several back-pressure steam turbines with different input water feed rates to find a trend in the efficiency and cost of these systems.

Using a regression over the costs of each simulated turbine, we found an average turbine cost of about \$600/kW. Other cases along with a breakdown of the ASPEN model are included in the Appendix.

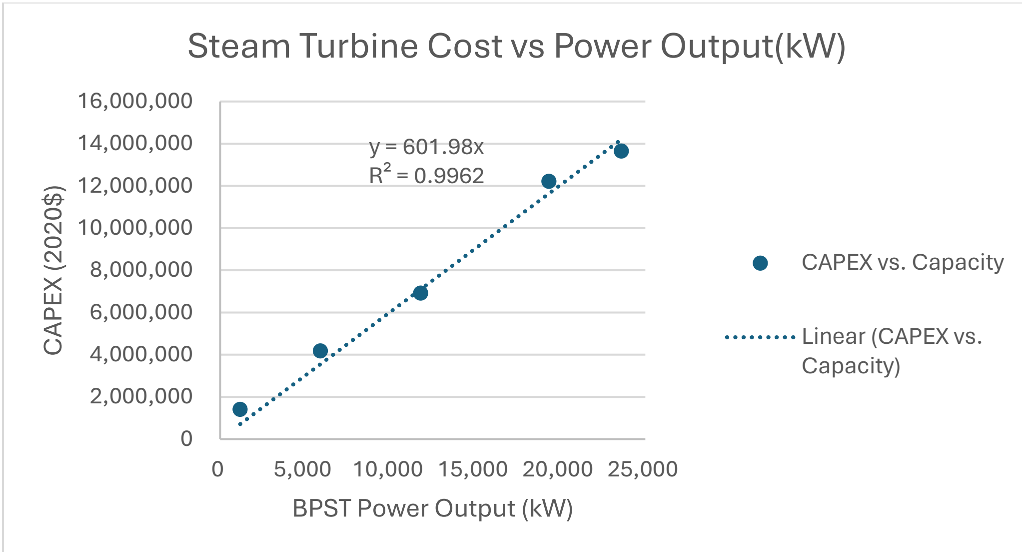


Figure 5 Regression over several steam turbine system costs results in an average turbine cost of about \$600/kW.

Using this metric, we could then size the turbine within GenX to identify the optimal size. After simulating different configurations of TES + turbine systems, we decided to fix the turbine power output capacity at 60MW such that it was capable of independently supplying the full power needs of the DAC without building excess turbine power capacity. This decision helped simplify our model and provided more clarity to our results.

2.3.4 Heat Pump

The heat pump modeled has a COP of 2 and a cost of \$500k/MW drawn from literature [23, 24]. The heat pump capacity and power consumption from the grid at each timestep is optimized by the GenX model to meet the required operation of the DAC plant in each system configuration.

2.4 Problem Formulation

Because GenX is a large multi-integer linear program (MILP), to incorporate our models, we needed to formulate each of these technologies into an optimization problem with decision variables and constraints. Below, we will provide a description and an accompanying mathematical problem formulation for the DAC and TES modules. We will then specify the relevant modifications for including a turbine collocated with the TES system. The code for these formulations is included in the Appendix.

2.4.1 Project Periods

When calculating costs for both the DAC and TES system, we annualize all project costs to determine DAC plant costs in a given year. We assume a project payback period of 15 years with a 4% interest rate, resulting in an annuity factor of 0.0899.

2.4.2 Direct Air Capture Formulation

The five decision variables that we optimize in the DAC module are the CO_2 removals at any hour (vCO2_DAC), the DAC system capacity (vCAP_DAC), the heat exchanger capacity (vHx_DAC), the heat pump capacity (vHP_DAC), and the power demand by the DAC to produce heat using the heat pump for each hour (vDAC_elec_heat). The main binding constraint of the DAC module is that the system needs to meet the annual CO_2 capture requirement of 1 $MtCO_2$. There is no incentive to capture CO_2 otherwise, so this constraint forces the DAC, TES, and other relevant technologies to be built to meet this requirement at the lowest possible cost.

DAC Variables:

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

$$vCAP\_DAC[y \ in \ Y] \ \geq \ 0$$

$$vCO2\_DAC[y \ in \ Y, t \ in \ T] \ \geq \ 0$$

$$vHx\_DAC[y \ in \ Y, t \ in \ T] \ \geq \ 0$$

$$vHP\_DAC[y \ in \ Y, t \ in \ T] \ \geq \ 0$$

$$vDAC\_elec\_heat[y \ in \ Y, t \ in \ T] \ \geq \ 0$$

DAC Constraints:

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

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

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

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

$$vDISCHARGE\_TES[y,t] + vDAC\_elec\_heat[y,t] * MMBTU\_per\_MW$$
$$= eDAC\_Heat\_Requirement[y,t]$$
$$vDAC\_elec\_heat[y,t] \leq vHP\_DAC[y], y \in Y, t \in T$$
$$eDAC\_Heat\_Requirement[y,t] \leq vHx\_DAC[y], y \in Y, t \in T$$
$$Total\_Power\_Balance += \sum_{y \in Y, t \in T} eDAC\_Power\_Requirement[y,t]$$
$$\text{Total\_Cost} += \sum_{y \in Y} \text{vCAP\_DAC[y]} * \text{Cost\_per\_ton\_CO2} + \text{v\_Hx\_DAC[y]} * \text{Cost\_per\_MMBTU}$$

2.4.3 Thermal Energy Storage Formulation

We modeled the TES unit like a battery as described in the technology section with a self-discharge capacity of 5% per day and an efficiency of 70%. To represent co-location with DAC, each TES unit is paired with a DAC plant by defining a DAC_ID index. The TES generates heat using grid power represented by vCHARGE_TES. It then stores this heat with the state of charge represented by vS_TES. Finally, it discharges this heat to the DAC plant given by vDISCHARGE_TES. The state of charge is maintained by updating vS_TES at every time step based on the net change in heat. The system is constrained by the amount of charging and storage capacity that is built, and the total system cost is calculated by the charge and storage capacity multiplied by their respective modeled costs.

TES Variables:

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

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

TES Constraints:

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

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

$$vCHARGE\_TES[y,t]\ \le vCAP\_CHARGE\_TES[y], y \in Y, t \in T$$

$$vDISCHARGE\_TES[y,t]\ \le vCAP\_DISCHARGE\_TES[y], y \in Y, t \in T$$

$$vS\_TES[y,t]\ \le\ vCAP\_ENERGY\_TES[y], y \in Y, t \in T$$

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

$$\mathrm{Total\_Cost} \mathrel{+}= \sum_{\mathrm{y}\ \in \mathrm{Y}} \mathrm{vCAP\_CHARGE\_TES[y]} * \mathrm{CHARGE\_CAP\_COST} + \mathrm{vCAP\_DISCHARGE\_TES[y]}\ *\ \mathrm{DISCHARGE\_CAP\_COST} + \mathrm{vCAP\_ENERGY\_TES[y]}\ *\ \mathrm{STORAGE\_CAP\_COST}$$

2.4.5 Modifications for Turbine

To modify this linear program to direct heat in the TES to a steam turbine, we needed to divide the vDISCHARGE_TES variable into two variables: vDISCHARGE_TES_Turbine and vDISCHARGE_TES_DAC. We then needed to constrain the amount of heat discharged to the turbine to not exceed the turbine's rated power capacity. Finally, we calculated the total heat supplied to the DAC, eDISCHARGE_TES, by summing the residual heat from the turbine with the heat directed to the DAC directly from the TES. We replaced all instances of vDISCHARGE_TES with eDISCHARGE_TES in the TES and DAC problem formulations.

Turbine Variables:

$$vDISCHARGE\_TES\_Turbine[y\ in\ Y, t\ in\ T]\ \geq\ 0$$

$$vDISCHARGE\_TES\_DAC[y\ in\ Y, t\ in\ T]\ \geq\ 0$$

Turbine Constraints:

$$vDISCHARGE\_TES\_Turbine[y,t] * power\_output\_ratio \leq Turbine\_Power\_Capacity[y], y \in Y, t \in T$$

$$eDISCHARGE\_TES[y,t] = vDISCHARGE\_TES\_DAC[y,t] + residual\_heat\_ratio * vDISCHARGE\_TES\_Turbine[y,t] y \in Y, t \in T$$

2.5 Differentiating Plant vs System Level Cost of Capture

In our simulations, we study two different perspectives for the cost of CO_2 capture: the plant level perspective and the system level perspective. The plant level cost of capture considers only the total cost required to capture 1MT of CO_2 without considering the emissions produced by the operation of the plant or the stress the plant's energy demand places on the electricity system. This perspective prioritizes the view of a private DAC operator focused on minimizing the cost of their plant's operations. The system level instead considers how the total, system-wide emissions changed after the addition of the DAC plant. The system perspective allows us to consider both the operational emissions and the wider, secondary impacts of implementing DAC technology on the electricity system.

To estimate the DAC plant's CO_2 removal cost, we totaled the annual fixed and operational costs of the plant and divided this by the 1MT annual capture target. To calculate the system's CO_2 removal cost, we had to first calculate the effective CO_2 removal of the DAC plant from the electricity system perspective. We defined the effective CO_2 removal of a DAC plant as the difference between the total system emissions in a system with the DAC plant versus without it. We could then calculate the system cost of CO_2 removal by dividing the total DAC system costs by the total effective CO_2 removed. The equations for calculating the plant level and system level costs are given below:

$$
\begin{aligned}
DAC\ Plant\ Costs \\
&= FixedCost_{DAC} + FixedCost_{TES} + FixedCost_{Turbine} \\
&+ \sum (electricity_{DAC} + electricity_{TES}) * cost_{electricity}
\end{aligned}
$$

$$
Cost\ of\ Capture_{Plant} = \frac{DAC\ Plant\ Costs}{1MtCO2}
$$

$$
Cost\ of\ Capture_{System} = \frac{DAC\ Plant\ Costs}{Effective\ CO2\ Removal}
$$

A script for this calculation is included in the Appendix.

Chapter 3

Results

We will break down the results of this research into four sections.

i) Operation of DAC Plant Configurations**:** demonstrates how TES impacts the flexibility of DAC systems using longitudinal data on simulated DAC operation with and without a collocated TES.

ii) Breakdown of DAC Plant Costs: compares how the cost of capture between our modeled plant configurations differ, breaking down the individual fixed and operating costs of each design.

iii) Analysis of System Emission Penalties: studies the relationship between the plant level cost of capture and the system-wide cost of emissions reduction for all four modeled DAC plant configurations.

iv) TES Cost Sensitivity Analysis: conducts a sensitivity analysis on how the cost of TES impacts the effective system-level emissions reduction of each DAC plant configuration and the plant level cost of capture of a DAC+TES system.

Together, these results will provide a comprehensive understanding of the potential benefits and tradeoffs of TES systems within DAC plants. This will ultimately help DAC developers weigh the tradeoffs between incorporating TES into their operations and help policy makers craft legislation that motivates the development of effective DAC systems.

3.1 Operation of DAC Plant Configurations

In these DAC plant simulations, we will show one week of longitudinal data for various plant level decisions. This will allow us to observe the relationships between TES and DAC operations and examine how plant level performance is impacted by the introduction of a TES system.

3.1.1 DAC + Heat Pump

We first simulated a DAC plant connected directly to the electric grid with a heat pump to serve as a base case.

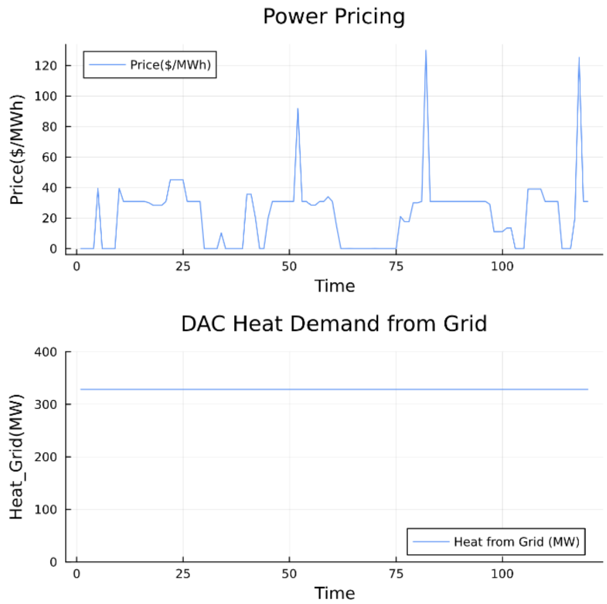


Figure 6 DAC plant has no flexibility to avoid high-cost electricity periods, increasing operational costs

The results illustrate how the DAC plant's inability to ramp quickly forces it to continue steady-state operations even during periods of high-cost power. Although it would be cheaper operationally for the DAC plant to shut down its operations during peaks in power, the opportunity cost relative to needing to build greater DAC capacity is too high. This finding strengthens the need for building some form of heat storage into the DAC plant to provide it more flexibility for when it draws electricity from the grid.

3.1.2 DAC with Thermal Energy Storage

Next, I added the TES module to the DAC plant simulation. This new plant design took much greater advantage of low-cost power by using the ramping capabilities of the TES unit.

Table 4 TES capacity in DAC + TES system

TES Energy Capacity (MWh)	TES Charge Capacity (MW)	TES Discharge Capacity (MW)
6145	1638	328

The optimal TES for each DAC plant was a 4-hour battery sized as shown above.

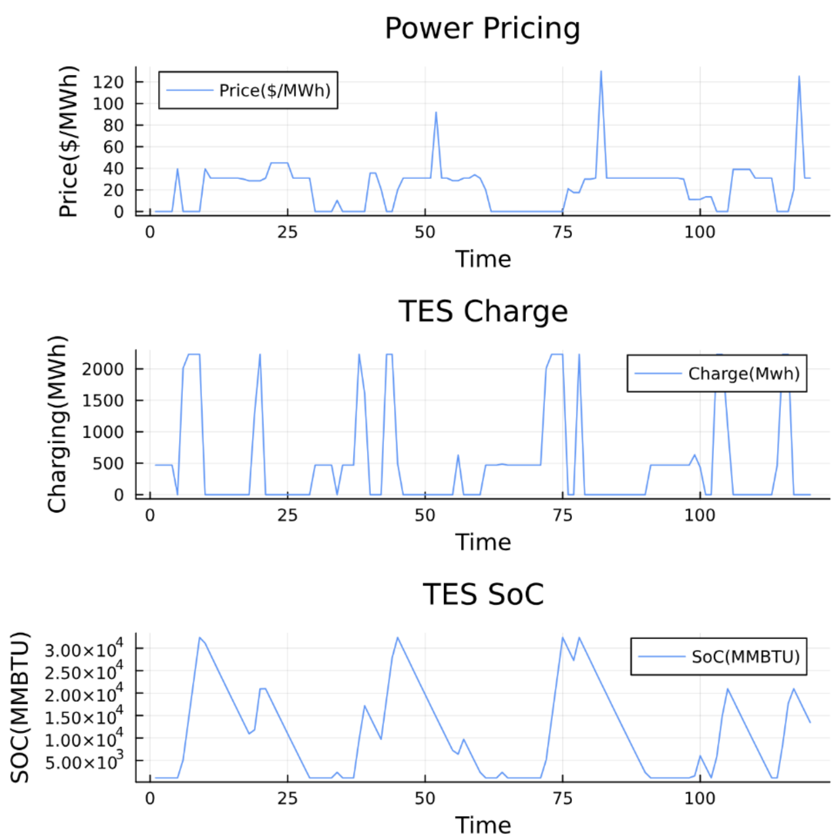


Figure 7 Operation of DAC plant with TES, charges during periods with low-cost power (Plots 1 and 2) and discharges gradually to the DAC (Plot 3).

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

3.1.3 DAC with TES and Heat Pump

Now, we can consider the plant design where the DAC unit can draw heat from both the TES and from the grid via a heat pump. This is an important addition because it's not always optimal to supply the full heating needs of the DAC plant from only the TES unit. Given that the heat pump has a higher efficiency than the TES, drawing power from the heat pump is preferred when electricity costs are low.

Table 5 TES capacity in DAC + TES + Heat Pump system

TES Energy Capacity (MWh)	TES Charge Capacity (MW)	TES Discharge Capacity (MW)
367	69	328

In the below results, we can see how the TES serves as a hedge against high power costs, only providing a small amount heat storage capacity to allow the DAC plant to avoid surges in power prices. We will see later in the results how this decision significantly impacts the operational emissions of the plant.

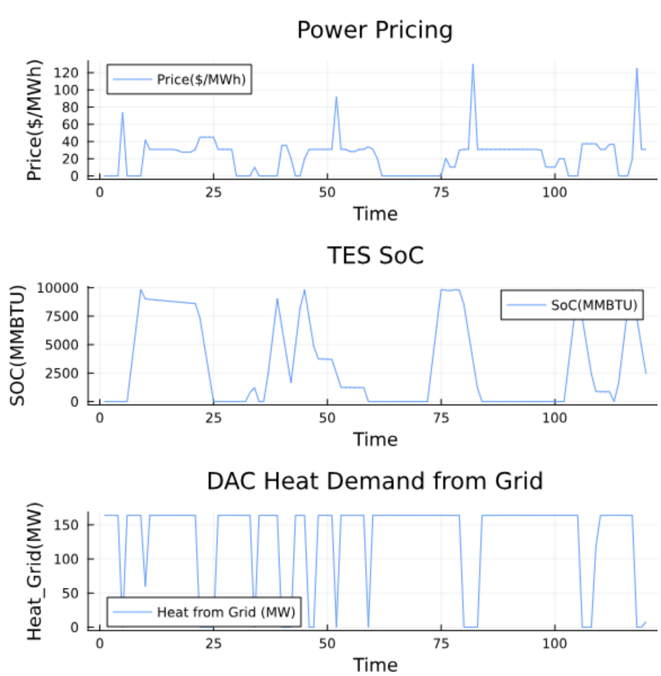


Figure 8 DAC plant operation with option to draw heat from both heat pump and TES unit.

3.2 Breakdown of DAC Plant Costs

The full cost of capture is the sum of the annualized fixed and operational costs divided by the annual CO_2 capture of the plant. Below, we break down the cost of capture for each respective plant configuration into its respective components.

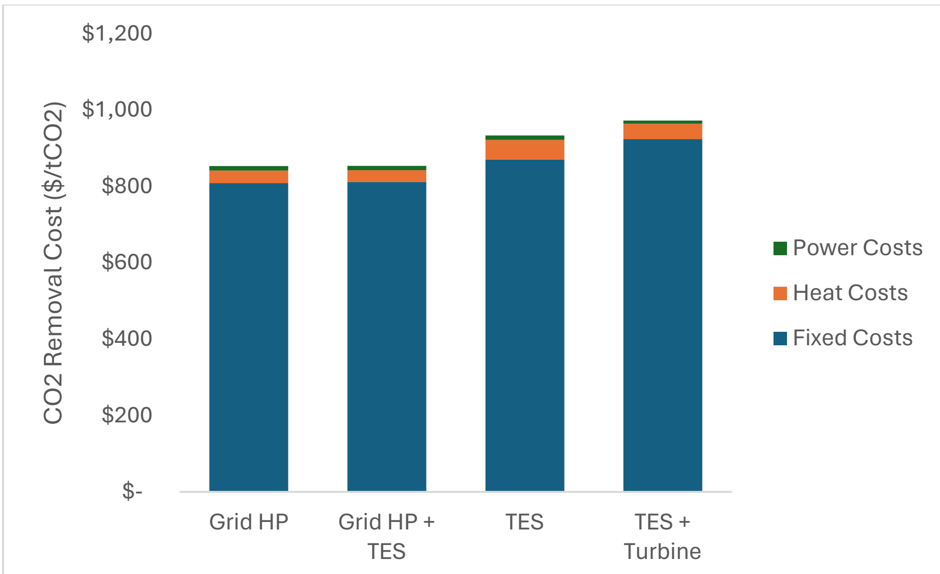


Figure 9 DAC fixed and operational costs. Axis below $500/t$CO_2$ are fixed costs

The fixed costs of the heat pump and heat pump + TES systems are significantly lower than the other two configurations because these plants avoided the high fixed costs of building the large TES. The TES and steam turbine increased the cost of capture by about $50/$CO_2$ each. Additionally, because the TES has a lower efficiency in generating heat than the heat pump, the cost of heat produced by the TES system is also more expensive. Although the addition of the turbine does slightly lower the power costs of the plant, this margin here is much smaller than the fixed costs of the turbine itself, resulting in the TES + Turbine system having the highest plant level cost of capture. From a private, plant perspective, TES and steam turbine technologies are significantly outcompeted by heat pumps for producing heat for DAC plants. Though, digging deeper into the operational emissions and system level effects of these different DAC systems, we start to see a much richer story.

3.3 Analysis of System Emissions Penalties

In this section, we'll explore the differences between the cost of capture for the private DAC plant versus cost of emission reductions for the grid system across all four DAC configurations. As described in the methodology, we define the effective system-wide emissions reduction as the reduction in total grid sector emissions after each DAC plant begins operations. The system-wide cost for emissions reductions is then calculated as the total plant costs for CO_2 removal divided by this effective emissions removal. Finally, we define the system penalty as the difference between the cost of CO_2 capture at the plant level versus the cost of CO_2 reduction at the system level. By analyzing how the overall system-wide emissions and the cost of capture changes between the operation of these different DAC plant configurations, we can get a better understanding of how effective each DAC plant is at actually reducing electricity sector emissions.

3.3.1 System Wide Emissions Impact

First, we'll examine the effective system emissions reduction of each DAC plant.

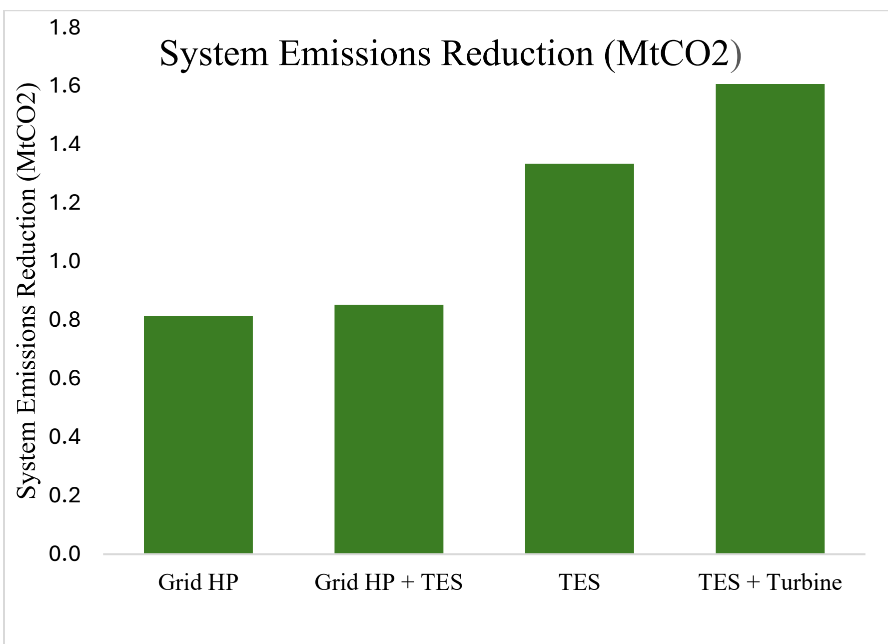


Figure 10 System-wide emissions reductions across all four DAC configurations.

The DAC plant configurations that rely most heavily on the heat pump for day-to-day operations have significantly lower total emissions reductions than the configurations that rely only on TES.

This difference is driven by when each respective plant draws power from the grid. Because heat pumps have no storage capacity, they are exposed to carbon-based electricity emissions that occur when renewables aren't available on the grid, so this leads to an increase in their operational emissions. On the other hand, TES systems charges during periods when intermittent renewables are most abundant at mid-day, so the systems that rely on TES heat have significantly less operational emissions. This difference translates directly into increasing the effective system-wide CO_2 removal of TES + DAC systems relative to TES + heat pump systems.

An interesting feature of this data is the ability for the TES-based DAC plants to drive emissions reductions in the system beyond the total CO_2 the DAC removed itself. Although the DAC plant only captured 1 $MtCO_2$, the system emissions lowered in the TES and TES + Turbine cases by between 1.3-1.6 $MtCO_2$. This occurs because the high demand for power by the TES during midday drives the development of more renewable resources to serve this power demand. By having more renewable resource in the energy mix, the system wide emissions are driven further down. These network effects between the DAC plant and the greater electricity system emphasizes the importance of considering system-wide market dynamics when modeling the role of DAC in our future grid.

3.3.2 Plant versus System-Wide Cost of Capture

Now, equipped with a better understanding of how our DAC configurations interact with the greater electricity system, we can compare how the cost of capture between each DAC configuration changes between the plant perspective and system perspective.

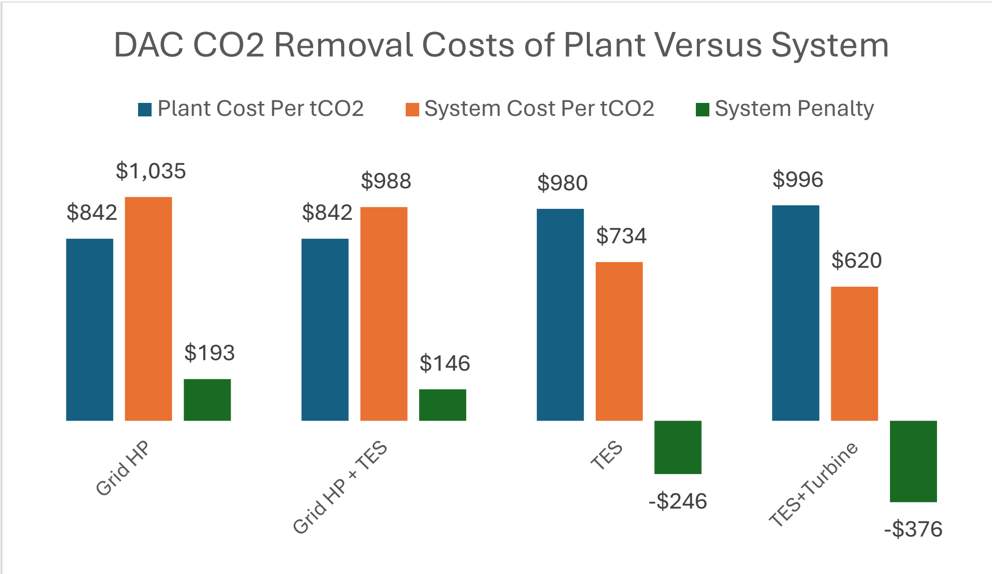


Figure 11 The cost per ton of CO_2 removal compared across four DAC plant configurations, demonstrating the gap between the cost of CO_2 removals from the plant vs electricity system perspective.

These four DAC plant implementations all remove 1MT of atmospheric CO_2 per year, resulting in their plant level costs being relatively similar. Though, because of the differences in their system level cost of emissions reduction, the system penalties between the configurations vary drastically. DAC plant configurations that rely on a heat pump have large system penalties because their emission reductions on the system level are significantly less than on the plant level. Meanwhile, DAC plants that utilize large TES units have negative system penalties, representing the bonus impact they have on reducing system emissions by creating demand for more intermittent. The TES + Turbine had the lowest system-wide cost of CO_2 reduction, driven by avoiding high-cost, carbon-based power sources for both the DAC heat and power needs. Though, this excess renewable generation should be considered within the context that the overall system-wide costs increased by $94M, not including the costs of the DAC and TES plants themselves. This represents the premium for the extra clean power generation buildout.

The significant differences between these system penalties demonstrates an important lesson: any load connected to the grid is capable of affecting the dynamics and future decisions of the larger system in significant ways. Studying these dynamics provides a more complete picture into the interactions between different technologies and the greater electricity market. For example, this system level analysis sheds light on the significant impact that TES can have on changing the way power demand from DAC affects the rest of the grid system. These effects will only be amplified as we increase the number of DAC plants. In future work, we will vary the annual removals from DAC, but in this paper, we only consider the 1MtCO2 requirement.

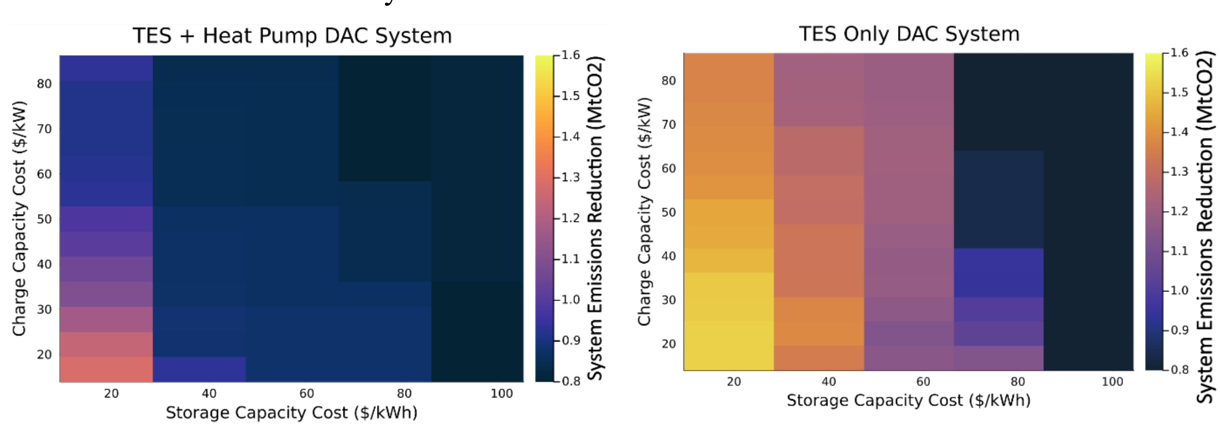
The vast deviation between how different DAC plants impact overall system emissions demonstrates a need for policies to incentivize the construction of DAC plants that maximize system-wide emissions reductions rather than just considering plant level reductions. This is challenging because calculating the impact of an individual DAC plant on overall energy system emissions is only possible in the context of a planning problem. But by using these modeling tools like in this study, we can identify effective configurations for DAC plants that create favorable system-level effects and create policies that incentivize the construction of such technology.

3.4 TES Cost Sensitivity Analysis

3.4.1 System Level Emissions Reduction

Previous research [16, 17] has shown large uncertainty in the future costs of TES storage. By understanding how DAC system emissions reductions are affected across different TES storage and charge capacity costs, we can see how our results may evolve over time and under different experience curves.

System Emissions Reduction in $MtCO_2$



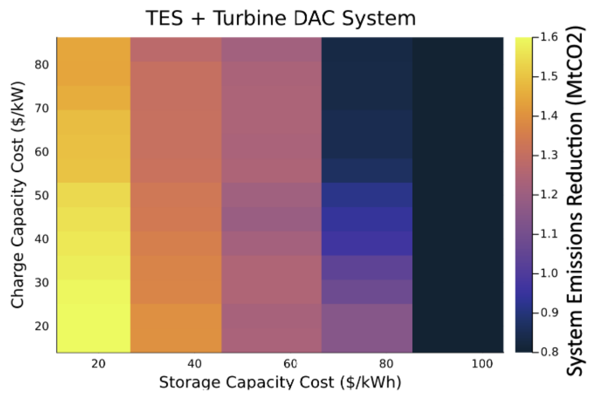


Figure 12 System-wide emissions reductions ($MtCO_2$) across TES cost uncertainty range

We ran simulations for each DAC configuration that uses TES across a range of storage and charge capacity costs to show how system-wide CO_2 reductions changed. From these heat maps, we can see that reductions in TES storage costs had a larger impact on driving system emissions reductions than changes in charge costs. This is because the DAC plant cannot take advantage of low charge capacity costs until it can build significant storage capacity. When the TES has a larger storage capacity at lower costs, it can store more clean electricity when available and send larger demand signals to the market to build extra renewable power. This drives an increase in emissions reductions. Without sufficiently low TES storage capacity costs, none of these effects would be possible. This is demonstrated by how past $100/kWh, regardless of the cost of charge capacity or the configuration of the DAC plant, TES offers no improvement in system emissions reductions over a heat pump system, which also reduces system emissions by 0.8 MtCO2.

Reductions in charge capacity costs do still play an important, secondary role in reducing system emissions when the cost of storage is low enough. This is most apparent in the TES + heat pump configuration. As the storage capacity costs decrease below $40/kWh, the DAC plant begins building greater TES storage and can begin taking advantage of improvements in charge capacity costs. As charge capacity costs decrease in these cases, we can observe significant increases in total emissions reductions, reflecting improvements in both DAC efficiency and an increase in clean energy generation. Though, this trend seems to be generally only true up to a four-hour duration battery.

3.4.2 Plant Level Cost of CO_2 Capture

Finally, we'll explore how changes in the costs of TES affect the private, plant level cost of capture in a TES only configuration.

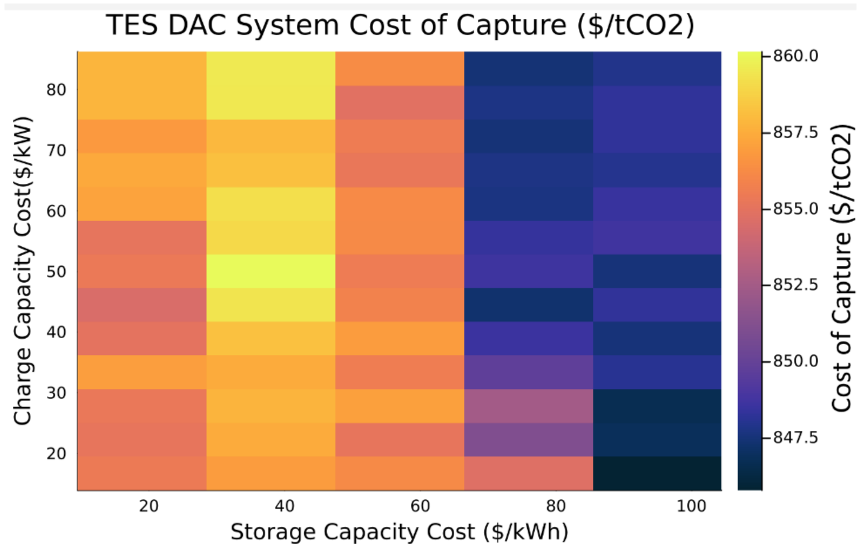


Figure 13 Large changes in TES costs only cause small variations to the overall plant cost of capture

Our heatmap results demonstrate how cost reductions in TES don't play a significant role in lowering the cost per ton of DAC CO_2 capture. Even between the lowest and highest cost TES scenarios, there is only about a \$15/tCO_2 difference in the cost of capture. This shows that despite the high, uncertain costs of TES today, future investments into TES within DAC plants won't offer significantly better returns even in the most extreme cost reduction scenarios. Thus, if a DAC operator intends to eventually incorporate TES into their plant, it makes sense to prioritize these investments sooner rather than later, while early-adopter benefits such as 45X tax credits are still available.

In summary, our results show that TES significantly increases the impact that DAC plants have on reducing system-wide emissions, nearly doubling the total emissions reduction when included with a turbine. But these benefits to the system come at a cost to the DAC plant, increasing the cost of capture by about \$50/tCO_2. Motivating DAC plants to modify their operations to benefit the larger electricity system will likely require changing how we incentivize the development of DAC technology. This leads into our discussion in the next section on DAC incentives structures.

Chapter 4

Discussion

4.1 Modeling Limitations

This study used a simplified model of the electricity system, only incorporating basic transmission and no distribution constraints between two zones of the ERCOT grid system. This was required to make our model tractable within a linear programming setting. With more transmission constraints, we would be able to model the relative impact of placing DAC plants at different nodes within the grid network, providing a deeper understanding of how the geographic placement and power requirements of the plant impact congestion on the larger electricity system. However, this level of granularity is not necessary for gaining insight into the higher-level implications of DAC development on multi-year planning timescales.

Additionally, this study assumed values for the current costs of DAC and TES capacity based on techno-economic analyses and component values available in literature. However, there is still a large amount of uncertainty in the cost of both technologies with the first large scale DAC systems still under development and TES only beginning to gain traction in industry. To develop a reasonable model, we selected conservative estimates for the cost of these technologies and incorporated cost multipliers to account for unexpected additionalities and project delays. We also conducted a sensitivity analysis for the TES cost estimates to gain a more thorough understanding of how our results would change under different pricing scenarios. As we continue to gain more certainty into the future costs and experience curves of these technologies, our models will gain more explanatory power.

The choice of modeling the DAC system within the ERCOT grid system also has inherent limitations. This system has an abundance of renewable power, clear divisions in regional land usage, and many available carbon sequestration sites. Many locations where DAC may be installed likely will not have as favorable conditions in at least one of these criteria. Regional differences will likely change how DAC and TES plants impact local grid systems compared with the observations in this study. Future research should expand modeling beyond the Texas ERCOT grid system to compare how other regions may be impacted by DAC development, providing greater insight into where geographically DAC could be a favorable technology.

Finally, there are limitations to using a model that simply optimizes for a minimal cost system. For instance, because there is no economic incentive in place within these models to prioritize the reduction of system-wide emission reductions beyond our 1 MtCO2 capture requirement, the model makes decisions that lead to higher emission output scenarios when they lead to lower systems costs. This was apparent in the TES + HP simulations where the DAC plant opted to use power from the grid for most of the year despite the higher operational emissions because it could avoid the cost of building greater TES capacity. It may be worthwhile in the future to modify our model to add a carbon incentive to see how the results change. There are also many factors beyond cost that are crucial to project development decisions such as a project risk, land use challenges, public perception, and political support. Although these considerations are more difficult to quantify than cost, they often play a critical role in determining a project's viability and likely impact the accuracy of our models.

4.2 DAC Incentives and Carbon Credits

As part of the Inflation Reduction Act, both DAC and TES technologies are subsidized through tax credits. The 45Q tax credit for DAC is available for projects that begin construction before 2033, and 45X Advanced Manufacturing tax credits for TES begin to phase down starting in 2029. These timelines demonstrate the US federal government's intention to drive rapid development of both DAC and TES technology in the coming years. Such development will be crucial to bringing down the costs of these respective technologies. Though, currently, there is little specificity as to how the operational emissions of DAC processes should be handled in terms of generating carbon credits or utilizing these tax credit incentives.

This modeling work has shown that DAC systems can vary greatly in their efficiency of reducing system emissions based on how they source heat and power. Although a broad tax credit structure is appropriate in the short term to drive development and innovation in the sector, it is critical to add nuance in the long term to incentivize the development of DAC plants that maximize system wide emission reductions.

In this direction, future incentives for DAC-based CO_2 removal should include bonus incentives based on how and where DAC plants are built. For example, larger tax credits should be given to DAC plants that take better advantage of renewable power by using TES or to plants that are built in locations that reduce strain on the electricity system.

In addition, carbon credit markets need to implement methods for incorporating the system-level impact of producing carbon credits. Our study has shown that the same gross CO_2 removal from two different plants can lead to vastly different emissions reductions on the system level. One approach to addressing this gap would be to rank the quality of a carbon credit based on the operational emissions and modeled system impact of the DAC plant from which it originated. Without such proactive policy measures, DAC could become a net-harm to achieving our decarbonization goals by allowing carbon removal credits to represent greater CO_2 removals than they've reduced in the energy system. Not only would this add noise to already complex decarbonization pathways, but it would also muddle decision making for hard-to-abate industries that are attempting to offset their emissions using these negative emissions services.

4.3 Future Work

There are many potential directions for further study of DAC and TES technology. One avenue of study would be to explore the impact of incorporating mandatory renewable procurement rules to investigate how the operation of these different DAC plant configurations changes when required to operate on renewable energy sources. For example, we could explore the impact of adding a renewable energy matching such that all power demand from DAC must come from newly built renewable generation. In these cases, TES would likely play a much larger role in lowering plant level operational costs by lowering the capacity of newly build renewable generation necessary to meet DAC energy requirements.

Another direction of research could examine the impact of adding larger and multiple DAC plants onto a given system to study how the impact of these plants changes as deployment scales. More specifically, a study could look into how a hub of DAC plants located in the same grid zone compares with DAC plants distributed across different grid zones in terms of system emissions reduction and costs. Such research would build deeper understanding of the synergies between closely located DAC plants and the strain that a DAC hub could place on the grid. This will be important to guiding decision-making towards current efforts for megaton scale DAC deployment.

Finally, our research could also lead into further study into the application of TES for other high-cost, inflexible industrial applications to find new opportunities where the technology can play a major role in creating cleaner and more reliable operations.

4.4 Final Thoughts and Conclusion

Both direct air carbon capture and thermal energy storage are technologies critical to the clean energy transition. The large energy requirements of DAC plants and the high costs of TES have resulted in skepticism towards both systems. By collocating TES within DAC plants, we've shown that we can significantly lower the operational emissions at the plant level, while boosting the emissions reduction impact of DAC on the electricity system. These findings demonstrate a powerful synergy between the two technologies that helps improve the economics and value proposition of each. Further research should be conducted to explore how these observations scale with larger and more numerous DAC plant deployments and different renewable energy procurement rules. By continuing to build a deep understanding of the relationships between these technologies and their potential role in our future energy system, we can work towards achieving decarbonization goals at the lowest cost and fastest pace, creating a clean, equitable energy future for all.

Appendix A

A1. Engineering Standards and Industrial Conventions

The independent project described in this thesis incorporated the following engineering and industrial standards:

- Programming Languages Used:
    - Julia JuMP Optimization Language
    - Python
    - Git
    - MATLAB
    - These languages were used for building optimization models, cleaning the resulting data, and creating visualizations
- International System of Units: Employed several SI units including GW, MMBTU, joule, and kilogram

Appendix B. Technology Cost Models

B.1 Thermal Energy Storage

Table 6 TES storage and charge capacity cost calculation

Minimum temperature (Celsius)[1]	500		Minimum output temperature into HX
Max temperature (Celsius)	1200		Maximum storage temp
Specifc Heat Capacity (kJ/kg K)	0.75		
Heat reqd (kWh)	10000		10 MWh system example
Heat reqd (kJ)	3600000 0		
Mass required (kg)	68571		
Volume required (m3) [70% volume fraction in container]	31		
Surface area (m2)	13.78		
Electrical power peak in (kW) [5 hour charge]	2000		
Peak heat out (kW) [20 hour discharge]	500		
Cost of SiC ($/ton)	1500		
High temperature insulation cost ($/m2)	300		
Electrical equipment charging cost ($/kW)	35		
Grid connection cost ($/kW)	11		
Transformer cost ($/kW)	10		
	$	**$/kWh**	**$/kW**
Thermal medium	102857	$ 10.29	
Insulation	4133	$ 0.41	

[1] Minimum temperature can be as low as 200 Celsius, which is within our uncertainty range.

Electrical equipment (transformer, substation, cabling)	112000		22
Total cost ($/kWh)	**218990**	**$10.70**	**22**

B.2 Steam Turbine

B.2.1 Turbine Process Flow Diagram

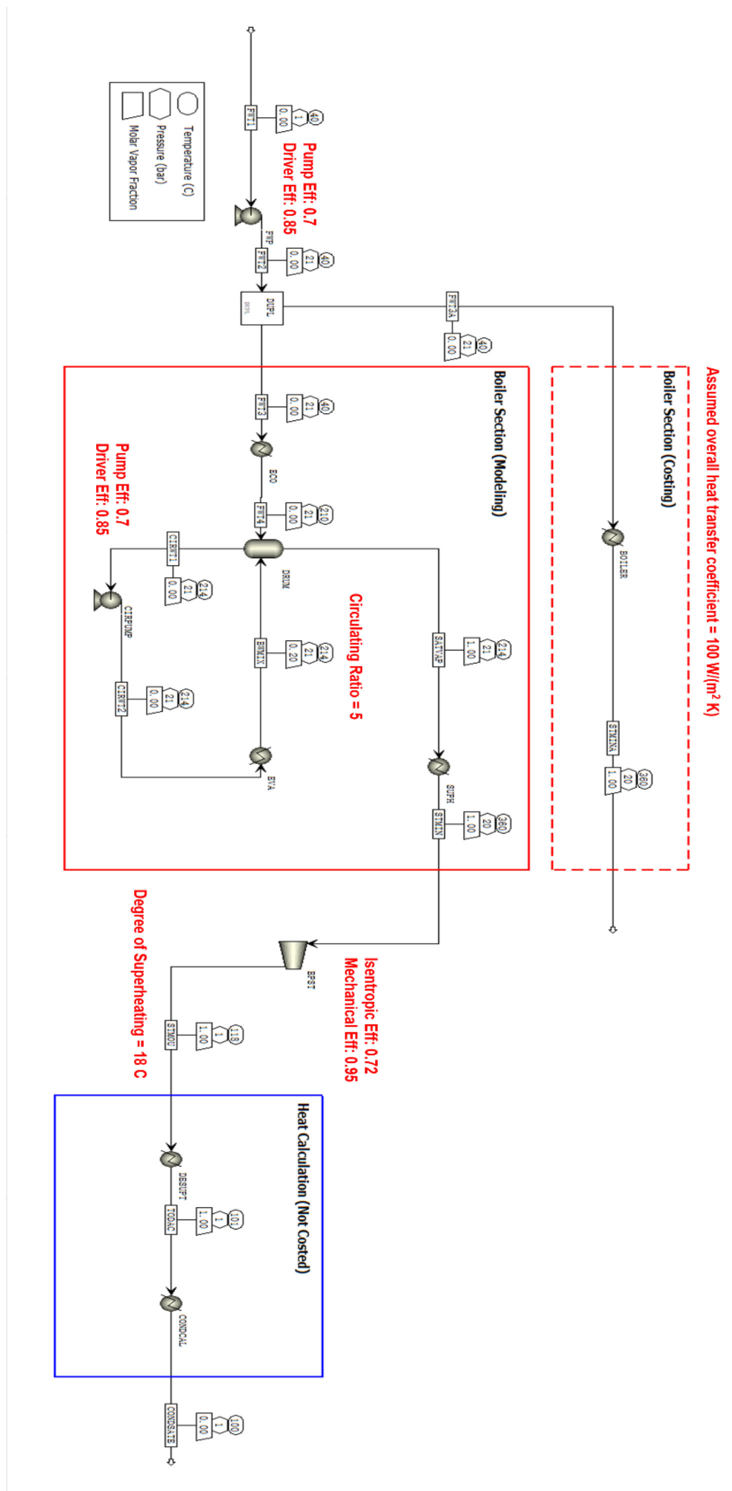


Figure 14 ASPEN model of steam turbine operation developed by Dr. Hongxi Luo

B.2.2 Additional Turbine Sizing Costs

Table 7 Turbine cost breakdown at water feed rate 165 tons/hour

Cost of Steam Turbine Components		
Name	Equipment Cost [USD]	Installed Cost [USD]
BPST	3,094,000	3,462,200
DRUM-flash vessel	242,500	542,300
FWP	58,600	129,300
BOILER	1,585,200	4,398,500
CIRPUMP	24,700	187,200
Total	5,005,000	8,719,500

Table 8 Turbine costs for different water feet rates

Case No.	Water Feed Rate (tonne/hr)	BPST Power Output (kW)	CAPEX (2020$)	Unit CAPEX ($/kW)
1	10	1,180	1,403,500	1,190
2	50	5,899	4,175,220	708
3	100	11,797	6,914,320	586
4	165	19,341	12,207,300	631
5	200	23,595	13,644,260	578

B.2.3 Additional Turbine System Performance

Table 9 Steam turbine performance characteristics

Steam Turbine Operational Performance (Water Feed Rate: 165 tons/hour)					
Process	Unit	Value	Process	Unit	Value
Total Boiler Duty	MMBtu/hr	468.06	Combined Efficiency	%	89.67
	MW	137.17	Captured CO_2 (Elec Cal)	tonne/hr	38.68
BPST Power Output	kW	19492.54	Captured CO_2 (Heat Cal)	tonne/hr	37.32
	MW	19.49	Difference	%	-3.66
Pump Electricity Input	kW	151.07			
	MW	0.15			

Net Output	kW	19341.46			
	MW	19.34			
Heat Available for DAC	GJ/hr	373.18			
	MW	103.66			

Appendix C: Code

All project code can be accessed on GitHub at https://github.com/vinaykonuru/GenX.

We used several scripts for setting up and automating simulations. Below is the list of custom modules and scripts we developed for this project:

- dac.jl – incorporates the decision variables and constraints of DAC into GenX
- dac_TES.jl – incorporates the decision variables and constraints of TES as well as additional constraints to collocate the TES with DAC
- long_operation.jl – plots the load demand and operational decisions of the TES and DAC over a one week period
- format_data.jl – calculates various plant level and system level metrics for the DAC and TES system across several case study simulations, such as total heat and power costs and system-wide emissions reductions, and compiles all of the data into a CSV
- analysis.jl – reads the compiled data from format_data.jl and develops heat maps used in sensitivity analysis

Appendix D: Guide to Building a DAC Unit

Over the past year, we've made progress on building a small-scale, pilot DAC unit to understand the fundamental bottlenecks and cost drivers of this technology and motivate more research towards optimizing its design. In this section, we will provide a summary of the work we've done thus far to serve as a guide for future students interested in continuing or extending the project.

D.1. System Modeling and Preliminary Design Choices

Developing a system design is an iterative process. Before beginning any calculations, we first needed to decide on a set of system requirements. We set out to build a DAC capable of capturing 0.5 kT of CO_2 per year. Based on our literature review, we decided on an adsorption-based process using Zeolite 13X impregnated with PEI as our sorbent based on the lower temperature requirements and cheaper costs of this design. After conversations with DAC startup OctaviaCarbon, we also decided on to build an axial fan-based system to drive air flow through our reactor.

This led to the following system requirements:

- Average capture cycle duration: 3 hours
- Minimum air flow rate: 250 CFM
- Minimum flow pressure: 0.04 psi

And the following design specifications:

- 14" diameter, 1" thick hollow aluminum reaction chamber
- 15" steel drum reaction vessel
- 6" diameter axial fan
- 10m Kanthal wire resistive heating coil
- 5kg of Zeolite 13x impregnated with PEI

D.1.1 Kozeny-Carman Equation Static Pressure Calculations

Many of the design specifications are based on tuning the static pressure requirement to push air through the packed sorbent bed. To calculate this pressure requirement, we used the Kozeny Carman Equation given below:

$$\frac{\Delta P}{L} = -\frac{180\mu}{\Phi^2 d^2}\frac{(1-\epsilon)^2}{\epsilon^3}\ \mu_s$$

To solve this calculation, we made the following assumptions about the sorbent:

- Zeolite 13X beads are uniformly 2mm in diameter
- Packing density of 0.7 in Zeolite 13x packed bed

Based on this equation, we developed a calculator that allowed us to identify different configurations of packed bed geometries with a low enough pressure drop to be met by available axial ducting fans.

D.1.2. CAD Design

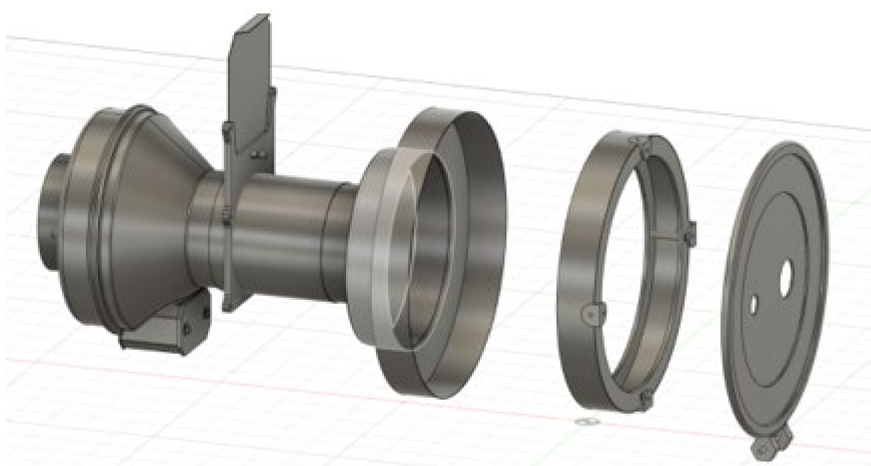


Figure 15 CAD Design of DAC System

Based on these preliminary design considerations, we implemented a CAD design of the DAC system. This helped greatly in sizing components to order from vendors and identifying challenges before purchasing parts. For example, identifying challenges in fitting the axial fan into the opening of our ducting system within the CAD design allowed us to get ahead of this problem in the construction stage by purchasing a duct diameter reducer.

D.2. Vendors

Sourcing and purchasing components can quickly become one of the most difficult parts of the build process. Oftentimes, vendors will have significantly different prices based on quantity, location, and available supply. This makes it important to compare several different vendors when sourcing parts.

D.2.1 Sourcing PEI

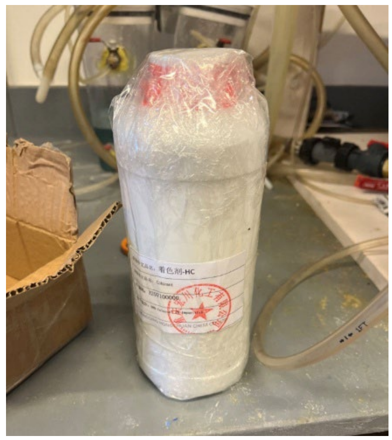


Figure 16 PEI from Shandong Zhishang Chemical Company on arrival in lab

PEI was the most challenging chemical to purchase because quoted prices varied significantly between vendors and across different branch structures. For our purposes, we needed to purchase about 2L of PEI. Lab-focused suppliers such as Sigma Aldrich tailored to smaller quantities of PEI, while bulk vendors often didn't list prices on their websites. After contacting and comparing the quotes of six different bulk vendors, we settled on purchasing from the Shandong Zhishang Chemical Company because they offered the most reliable service and the lowest costs. To verify we were receiving the correct product, we asked the supplier for the Certificate of Analysis (COA). Also, on arrival of the chemical, practicing standard lab safety protocol, we verified the listed properties.

D.2.2 McMaster Carr

Purchasing from McMaster Carr is a seamless and convenient process. We purchased components directly through the University's Prime Marketplace and had shipments arrive within two days. McMaster Carr also offers CAD components for nearly every part they offer, which leads to fewer surprises when translating from design into implementation. The biggest challenges with this vendor are that they have limited offerings and high prices. We found this McMaster Carr was best for smaller and more standardized components. We purchased our axial fan, steel drum, and many smaller bolts and fasteners from McMaster Carr, but left more customized ducting purchases to other vendors.

A.2.3 Ducting Vendors

Because we needed specific ducting sizes, we needed to source these components from a few different vendors. Ultimately, we sourced the majority of our duct work from FAMCO and Amazon. FAMCO components had the advantage of being sturdy and reliably fitting together. Amazon components were less reliable, but there was much greater selection available for finding more niche parts and getting replacements quickly.

D.2.4 Ethanol

We needed to purchase 10L of 70% ethanol for the wet impregnation procedure to synthesize our Zeolite-13x + PEI sorbent. After comparing five different vendors including Lab Alley and Sigma Aldrich, we settled on Government Scientific Source. They quoted about $17/liter plus chemical shipping costs. The shipments were quick, and the suppliers were responsive.

D.3. Sorbent Synthesis and Testing

Much of the available literature on sorbent impregnation procedures only synthesize between 1-5 grams of sorbent. We wanted to synthesize 200 grams per trial to achieve our 5kg target within 25 synthesis reactions. We tried several different impregnation procedures to find a reliable way of mixing larger quantities of Zeolites. Below, we’ve enumerated the procedure for synthesizing and testing the sorbent along with common pitfalls and challenges that we faced.

D.3.1 Sorbent Synthesis Procedure

This procedure draws from Karka et al. [26] with small modifications from our experiences to impregnate 200g of Zeolite 13x with a 40% loading ratio of PEI:

Figure 17 200 gram Zeolite sorbent synthesis trial after overnight impregnation

1. Measure out 200g of Zeolite-13X and place aside in a beaker.
2. Measure and pour 80mL of PEI into a separate beaker.
3. Measure 405mL of ethanol into a large flask and mix for 30 minutes with PEI or until fully dissolved.
4. Pour Zeolites and PEI + ethanol solution into a large beaker. Place a cap on the beaker to avoid ethanol evaporation and mix slowly with a stirring rod on a hot plate for 16 hours.
5. Remove Zeolites from the beaker. If the Zeolites are clumped together, soak them in a small portion of ethanol and mix until they separate.
6. Bake the Zeolites at 70 °C for 3-4 hours.
7. Remove the synthesized sorbent from the oven and it place in sealed jar,
8. Conduct breakthrough testing to measure adsorption capacity of the sorbent.

D.3.2 Sorbent Breakthrough Testing

To measure the adsorption capacity of the Zeolite sorbent, we followed breakthrough testing procedures provided by Micrometrics using the LI-COR CO2 Gas Analyzer [27]. Our procedure is given below:

Figure 18 Test bed for measuring CO2 adsorption capacity of sorbent sample (left) and CO2 desorption setup(right).

1. Record the mass of sorbent sample.
2. Place sorbent sample into sealed jar with holes in the lid for inflow and outflow tubes.
3. Add valves between the two tubes to allow airflow to bypass the sorbent jar when the valves are shut.
4. Connect inflow tube to humidity-controlled pump and outflow tube into the input of the CO2 gas analyzer.
5. Connect the gas analyzer to laptop and open the CO2 monitoring software.
6. Shut the inflow and outflow valves so airflow bypasses the sorbent, turn on the pump, and wait for the CO2 recordings on the laptop to stabilize. Record the ambient CO2 level in the lab.
7. Open the inflow and outflow valves so pumped air passes through the jar and over the sorbent. The CO2 levels recorded by the sensor should rapidly drop.
8. Begin recording data from the CO2 monitor, saving it to a CSV file.
9. End data recording when CO2 levels converge to ambient levels.
10. Using MATLAB, calculate the total adsorbed CO2 in the system by calculating the integral of the difference between recorded CO2 levels and ambient CO2 levels across all time steps. Convert this value into a mmol CO2/gram sorbent measurement and compare with expected data from literature.
11. Bake the sorbent sample for 3-4 hours at 100°C to regenerate and repeat testing procedure.

Our sorbent samples typically achieved between 0.15-0.2 mmol/gram sorbent across several trials.

D.3.3 Common Challenges + Pitfalls

- Ethanol evaporation: When leaving the sorbent soaking in the ethanol + PEI solution overnight, make sure to cover the beaker to avoid the ethanol from evaporating off before the PEI can penetrate the Zeolites

Figure 19 Example of overmixed sorbent sample, Zeolites were blended by stirring rod

- Mixture Rate: Avoid overmixing the sorbent solution with the stir bar to prevent breaking up the Zeolites. We want to spin the stir bar just fast enough to enable even impregnation
- Clean Up: PEI is a very sticky substance. Always wear gloves and make sure to wipe down the lab station and tools regularly to avoid sticky situations!

D.3. Construction

Translating our designs into construction proved to be an iterative process. We divided our construction by the four major subsystems of the DAC machine and built each separately. The four subsystems were the reaction chamber, the ducting, the heating system, and the desorption system.

D.3.1 Reaction Chamber

To build our reaction chamber, we had to cut the bottom out a steel drum using an angle grinder. We then drilled L-brackets into the steel drum to create a support for the internal packed bed. We constructed the packed bed chamber out of an aluminum sheet sourced from the Jadwin materials shop and fabricated in the machine shop.

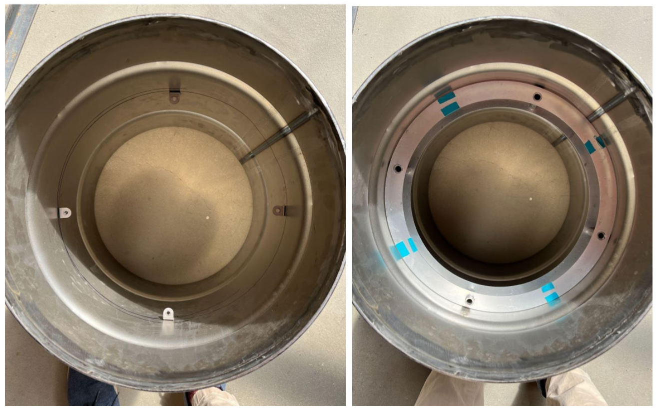


Figure 20 Steel drum with packed bed chamber sitting inside

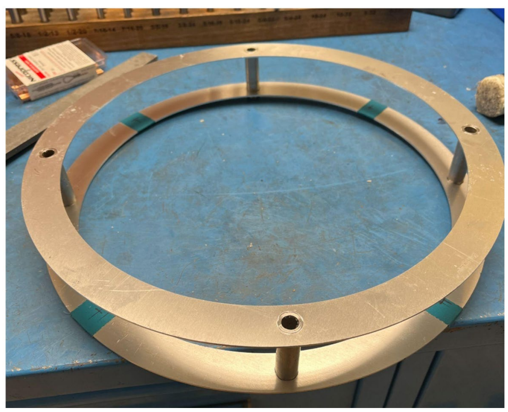


Figure 21 Packed bed without casing

D.3.2 Ducting

Figure 22 Flexible ducting connects the fan (far back) to the steel drum reaction chamber

The ducting work for the DAC involved sizing and fitting duct reducers to ensure that there was as little air flow leakage as possible between the fan and the reaction chamber. The ducting also has a blast gate damper to close off airflow to the reaction chamber when we need to regenerate the sorbent. We iterated on different designs for the ducting because of poor fits between the duct and the steel drum. One major improvement came from switching from hard-metal to flexible ducting, allowing us to more tightly secure the connection between our fan and blast gate damper. Though, there is still significant leakage between the reducer and the opening of the steel drum. There are no readily available reducers that will provide a better fit, so we plan to add padding around the reducer to reduce these flow losses.

D.3.3 Heating System

The heating system is an open problem for the DAC machine. The main design requirement is that we need a heating system capable of reaching an evenly distributed 100°C while still allowing air flow to pass through it. The original attempt at using a resistive heating system with Kanthal wire proved ineffective because we couldn't get the heat from the wire to dissipate through the body of sorbent in the packed bed. We also explored the possibility of using an induction heating system, placing copper tubes inside the packed bed and running current around it to create several sources of heat. Though, discussing with experts in induction heating, we found that the current requirements for this setup would be substantial, and even then, the heat would likely still not dissipate well. The third approach we are exploring now is to simply use an electric grill grate that we will conductively heat up using our resistive wires looped around its body. This will be allowing for the heat from the grill to evenly heat up the sorbent. The downside to this being that it will likely cause a significant increase in the static pressure of the system.

D.4 Future Work

Beyond the open problems with heating the sorbent and patching airflow leakage, future work for this project should focus on setting up a desorption system sized properly to the pressure requirements for the DAC. CO2 and temperature monitoring sensor circuits should also be built and placed inside the reaction chamber. Finally, the walls of the packed bed chamber should be refitted with a more cushioned material to allow for a tighter fit when placed inside the steel drum. Overall, this project has taught me about the engineering design process and given me a deeper appreciation for the unexpected challenges of building real systems. It has also given me more insight into where some of the open problems in direct-air capture technology lie such as the inherent tradeoff between solid and liquid sorbent systems, the problems of using resistive heating systems, and significant energy and air flow requirements for capturing CO_2 emissions. These lessons will help me as I continue to grow an engineer in the clean energy industry, motivating me to consider the deeper complexities of the systems that I interact with.

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