

Carbon-Neutral Production of Methanol via Direct Air Carbon Capture and Green Hydrogen

Direct Air Capture and the Proponents and Resisters of Technology

A Thesis Prospectus
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By

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On my honor as a University student, I have neither given nor received unauthorized aid on this assignment as defined by the Honor Guidelines for Thesis-Related Assignments.

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Introduction

The objective of this project is to design a chemical synthesis process to produce methanol in a carbon-neutral fashion. With global warming being a growing concern on Earth over the last few decades, it is important for humanity to find ways to reduce its carbon footprint and emission of greenhouse gases. Every year the temperature of the Earth rises due to the increase in greenhouse gases in the atmosphere, one of the biggest influences being the burning of methanol which releases copious amounts of CO₂. So, what if we could create a process to consume the exact amount of carbon that is put into the atmosphere? This project will allow methanol to become a more sustainable fuel by no longer increasing the amount of carbon in the atmosphere when burned. The process will utilize various unit operations that begin with a direct air capture (DAC) technology and renewable energy sources and will finish with a reverse water shift gas reaction and hydrogenation of methanol. The completed technical portion of this paper will cover the process more thoroughly, along with unit operation modeling, equipment design, process and control diagrams, an economic analysis, and safety, social, and environmental concerns. The STS research portion of this paper seeks to evaluate the integration of this new DAC technology into the already existing industries and markets. With this technology potentially providing a sustainable method to produce a commonly used fuel, it is important to know how this technology will be perceived across all parts of society. This paper will utilize the framework of Sustainable Transitions, as defined by Hess (2013) to understand the various aspects of policy making and market shifts by international regimes to see their impacts on the development of DAC technology.

Technical Topic

The purpose of this project is to design a carbon-neutral methanol synthesis process that incorporates the utilization of renewable hydrogen and carbon capture technology. An example outline of the process is shown in Figure 1.

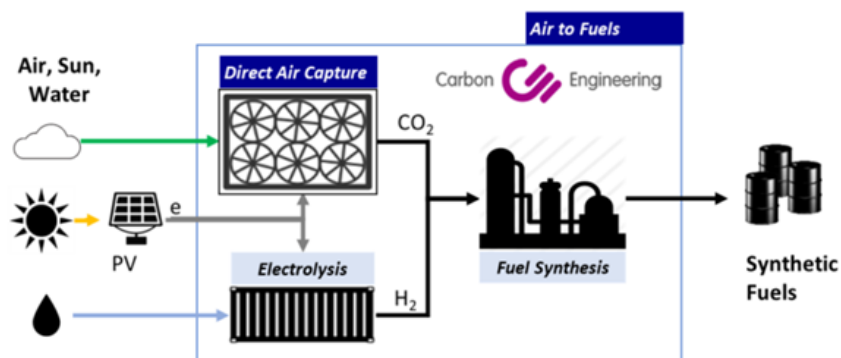


Figure 1. Overall Project Process

Hydrogen will be acquired through a third-party source, which produces its hydrogen via large-scale electrolysis supported by renewably generated electricity. Carbon dioxide will be obtained through a direct air capture system, which will be designed in this project. Next, methanol synthesis will take place with the combination of a reverse water gas shift reaction, RWGS, and the hydrogenation of carbon monoxide. The RWGS reaction will convert carbon dioxide into carbon monoxide, and carbon monoxide will be hydrogenated to form methanol as a final product. Both of these processes will be described in greater detail below:

Designed Process #1 - Direct Air Carbon Capture (DAC)

The first technology that will be designed in this project is a direct air carbon capture system (DAC), which will produce pure CO₂ from ambient air. The DAC system features an air contacting system which will introduce air to a liquid alkaline solution, capturing the CO₂. Then, a pellet reactor will be used to initiate the separation of CO₂ from the absorbent species. Lastly, a calciner will produce a pure stream of carbon dioxide gas, and a slacker will be used to regenerate the absorbing species upstream, see Figure 2 (Keith, 2018).

There are two choices for DAC technology: high-temperature aqueous solutions (HT DAC) and low-temperature solid sorbent (LT DAC) systems, where the HT DAC system is cited to be the most robust and developed of the two (Broehm, 2015). HT DAC improves upon LT DAC as the capacity is higher and it is a continuous process (Keith, 2018). Therefore, HT DAC will be used in this design process.

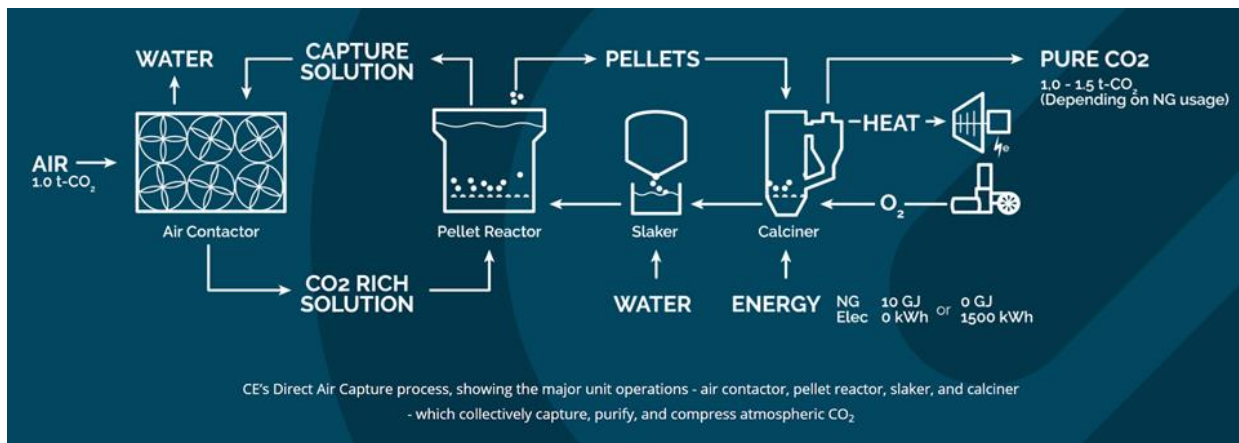


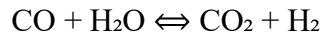
Figure 2. Process Flow Diagram for DAC

Thus far, only one company has implemented wide scale HT DAC (Fasihi, 2019), so there is opportunity for competitors to develop their own versions. This proposed project provides an avenue for improvement with the addition of downstream processing of CO₂. Therefore, providing a novel way to improve the economics and utility of DAC as traditional

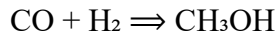
DAC design usually sequesters carbon in geological formations, or the carbon is used in enhanced oil recovery.

Process #2: Methanol Synthesis

The second step in our design process will be a methanol synthesis, which will occur via two chemical reactions. The sequence of these reactions can be referred to as the CAMERE Process. The first step is to convert the CO₂ to CO via the reverse water-gas shift reaction, the reaction is outlined below:



In order to get the desired reverse reaction, catalysts are needed (Yang, et al. 2020). The hydrogenation of the carbon monoxide is the next step to form the desired product, methanol. The hydrogenation reaction occurs as follows:



This reaction also requires a catalyst, which is used to drive the reaction to produce the desired product. As both reactions involve a selective choice of catalysts that is essential for product formation, respective catalysts used will be one of our critical design choices. Design of the unit operations as well as the scale of the process will determine what catalysts are used. The figure below displays an example methanol synthesis process flow diagram from a study performed by Joo et al., 1999.

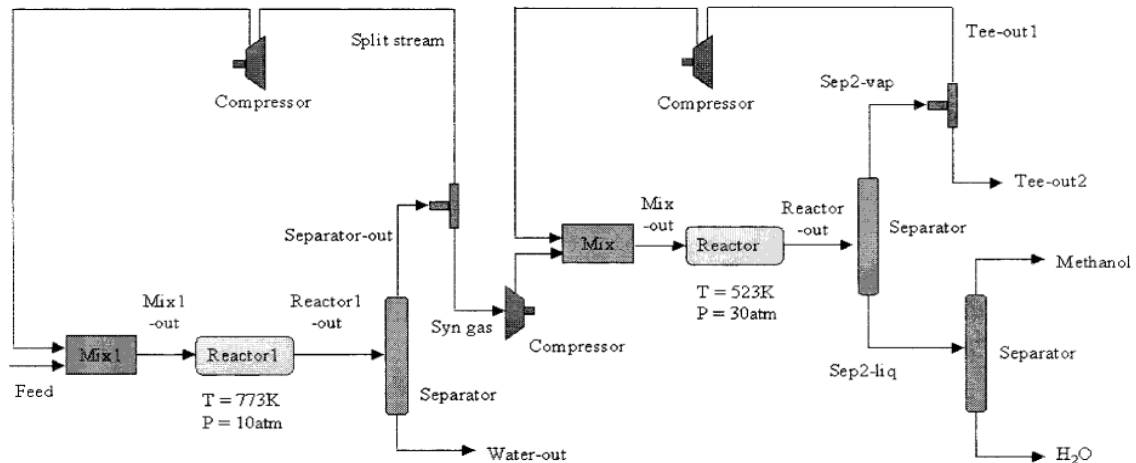


Figure 3. CAMERE Process Flow Diagram

This study was performed to minimize operation costs but can serve as a basis for this section of the project. The CAMERE process utilizes two reactors, one for the RWGS reaction

and one for hydrogenation of carbon monoxide, and various separators through the process to produce methanol.

Currently, the world's energy supply and chemical processes are heavily reliant on fossil fuels (U.S. EIA, 2021). Although efficient and energy dense, these fuels are unsustainable, and catalyze global climate change due to associated emissions of greenhouse gases, relevant trends can be seen in figure 4.

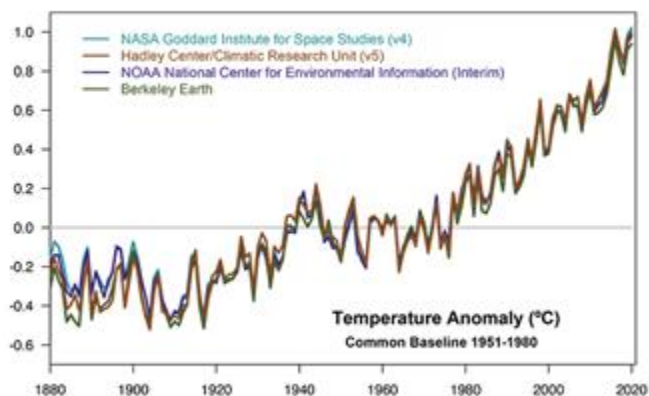


Figure 4. Global Temperature Trends Post-Industrialization

A significant issue with the reduction of greenhouse gas emissions is the transition to more sustainable fuels as large transportation infrastructure requires a high-level of energy density that cannot be achieved by alternatives. In addition, many chemicals used in manufacturing are produced from sources that use fossil fuels. So, novel methods of production of fuels and chemicals are needed as energy production costs increase and the depletion of current fossil fuel sources continues. With continued shifts in public opinion on climate change, there is a hopeful outlook that investment in sustainable energy and chemical production methods is economically feasible (Funk, 2021).

Moreover, based on recent research, the methanol market is expected to have a compound annual growth rate of 3.55% through 2026, worth 41.54 billion USD (Global, 2021). To this end, this project aims to design a sustainable methanol production process to be later used as a carbon-neutral, energy-dense fuel, or supplement chemical manufacturing supply chains. Simultaneously, this project functions to further work within direct air capture and alternative fuel production processes, both of which are relatively novel fields in the energy sector.

The outlined capstone project will be completed over a course of two semesters as part of CHE 4474/4476 curriculum under technical advisor, Eric Anderson. The proposed process will

be based upon research from a carbon capture company called Carbon Engineering which is derived from in-house experimental data, pilot plant data, commercial vendor information, and commonly-known thermodynamic information. The process will be subsequently modeled using a simulation software package, Aspen, with specified operating conditions. To begin modeling the methanol synthesis, publicly available experimental data is available that optimizes for different qualities such as maximizing product quantity and purity levels. We can reference literature to see what other studies have defined as optimal to serve as a starting point for our research.

The work will be divided into the group by the following subtopics: direct air capture, methanol synthesis, and byproduct formation. The main deliverables in the Fall of 2021 will include a prospectus, pitch, and design basis memorandum. In the Spring of 2022, progress report presentations and a final written report will be due. Within these deliverables, the process will have a well-defined heat and material balance analysis, process flow and control diagrams, equipment design, process economics, and analysis of safety, social, and environmental concerns. Using a Gantt chart to track progress, the team will meet weekly to discuss achievements and setbacks faced during the week and goals for future meetings.

STS Topic

Direct air capture technology is currently a very novel idea that is still in its infant stages. With any new technology that has the potential to make significant impacts on the world, it is important to research factors that have been slowing down or accelerating this transition to the new technology. As defined by Hess (2013) there are three crucial mechanisms of mobilization that contribute to Sustainability Transitions (ST): incumbent regime mobilization, grassroots mobilizations, and countervailing industry mobilization. Hess (2013) defines each of these groups as those who resist policies that threaten their short-term profitability, social movement organizations that form support for ST policies, and industrial powers that can provide financial support and resources to grassroots groups, respectfully. This paper will use those three mechanisms to guide the research on how this technology has already developed in various nations, particularly in North America, and predictions of where it can go in the future.

As of 2019, there exists only 11 DAC plants in the world, one of which is in the United States in Alabama (Larsen, Herndon, Grant, & Marsters, 2019). Aside from being a method to produce and sell CO₂, it could be said that the primary goal of DAC is to combat climate change. In December of 2015, the Paris Agreement was signed by 196 parties across the globe with the long-term goal of limiting the temperature increase of the planet. The parties all agree to assist each other financially as well as share technologies to accelerate development of DAC (*The Paris Agreement*). One of these larger nations involved is the US. Larsen, Herndon, Grant, & Marsters (2019) in their report cite the US as being a major actor for several reasons: the US has the potential to position itself as the leader in this new sector and help disperse the technology around the globe, over four billion dollars a year of federal funding is spent on technology

research, and the US has one of the largest economies with the ability to implement policy that will influence the global markets. The authors list a few key actions the US would need to take for DAC technology to get the jump start that it needs: enact and fund a comprehensive research, development, and demonstration program for DAC, pursue federal procurement, overcome non-cost barriers (i.e., storage), and lower the cost of investment to finance DAC plants and establish infrastructure.

It would be easy to believe that one of the biggest competitors for DAC could be the fracking industry, especially if the DAC technology seeks to produce oil and gas, but recent events show that this may not be the case. Canada's largest oil sands companies have formed an alliance to work to what they call the "Oil Sands Pathways to Net Zero initiative." These companies make up 90% of Canada's oil sands production. They will be working with Canada's federal government and the Alberta government to achieve Canada's climate goals. While the exact goals and methods of the alliance are unclear, it is noted that the 'vision is anchored by a major Carbon Capture, Utilization and Storage truckline.' The CO₂ captured in this process has the potential to further enhance the current oil recovery applications, thus it becomes beneficial for large fracking companies to invest in this type of technology to advance their own processes (Post, 2021).

Fracking also currently faces other hurdles. Globally, there are temporary prohibitions on fracking in a few nations such as France, Germany, and Ireland. While nations like the UK, Spain, and China have established timetables to phase out fossil fuel use (Newell & Simms, 2020). Over time as these nations begin to phase out fossil fuels and influence other nations to do so as well, this will open up room to integrate DAC technology and development.

While the proponents of DAC are strong, there are also significant regimes that will act as barriers against DAC's development. Brudinis, Krevor, Dowell, Brandon, & Hawkes (2018) address a few of these groups. Production costs and storage were some of the few issues listed, particularly storage in nations such as China, Japan, and South Korea. They also mention supply chain and building rate; even if supply was steady and the equipment was readily available, skilled labor to perform the necessary duties is hard to come by. While there are policies that do exist to promote DAC in nations like Australia and Canada, there exists concerns about the clarity and direction of the policies from major oil and gas companies. These large companies, like BP, fear "uncertainty about investment disparities" and the impacts of these policies on their business. The last actor that these authors talk about is the general public. The public shows to have an understanding that climate change exists, but not a clear understanding of how to combat it and which methods work the best. The general public lacks the knowledge of where the risks truly lie, and it is due to the lack of adequate communication between the experts designing the technology and the public. This leads to misplaced public concern of public investments. They believe that the investments going toward DAC research reduced the budget for renewable alternatives that do not reduce emissions as effectively.

There are other groups that are against this type of technology. They make claims that there are more cost-effective ways to curtail emissions, future carbon-removing systems will be more effective, and this technology allows for an ‘easy out for big polluters’ (*The Direct-Air Capture Debate*, 2021). These ideas can be contributed to ‘greenwashing,’ or the newly coined ‘carbon washing.’ Fairs (2021) makes claims that companies tend to take advantage of ‘vague and meaningless terminology.’ Companies like to use terms such as carbon-negative, without truly understanding the meaning. This leads to false claims that are made by companies where their products are not actually carbon-negative and not even carbon-neutral. Although this is supportive of the goals of reducing the effects of greenhouse gases, it can have the reverse affects. Allowing large ‘polluting enterprises’ to appear climate friendly, despite the nature of their processes and the harm it creates.

Next Steps

As this paper is developed through both the fall and spring semester with a technical team; my priority in the technical portion is to research the methanol synthesis process. The technical portion of this paper will continue to be researched and improved upon through the academic year. By the end of the fall semester, a few things will be determined. The desired product purities and quantities should be determined alongside the acquisition methods of necessary raw materials and equipment primarily based on economic viability. These decisions will also be guided by the scale of the project. In the spring semester, the technical portion of this paper will be significantly more thorough and defined. Selection of the plant site will be talked about, operating conditions will be simulated to determine the optimums for the desired product purity, and a final economic analysis report will be made to prove the value of the design. The STS portion of this paper has the potential to be developed indefinitely with the numerous regimes and policies that can play significant roles in the development of this technology. Moving forward it can be beneficial to research individuals that can have significant impacts, either as large donors or leading researchers. Looking further into hurdles that fracking faces as well as more grassroot type organizations that are supporting this technology.

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