

Carbon-Neutral Production of Methanol Via Direct Air Carbon Capture and Blue Hydrogen
(Technical Paper)

The Use of Direct Air Capture to Reduce Carbon Emissions for Process Plants
(STS Paper)

A Thesis Prospectus
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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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Prospectus

Introduction

Without a planet to live on, the technological advancements of the future will be pointless. It is absolutely necessary to address the global carbon emissions problem in order to ensure the longevity of future generations. In the last century, the concentration of CO₂ in the atmosphere has risen by 100 ppm, from 300 ppm to 400 ppm. This has directly led to average temperature increases across the globe (Ritchie & Roser, 2020). As the world began to industrialize, the reliance on carbon emitting fossil fuels quickly spiraled out of control without any concern for the consequences of these technological advancements.

In order to address the global emissions problem, new technologies and considerable amounts of research has already been done on carbon capture and sequestration (CCS). Currently, three main capture technologies exists: pre-combustion, post-combustion, and oxy-fuel carbon capture. Like the name implies, pre-combustion carbon capture involves removing the CO₂ in a fuel source prior to combustion. Similarly, post-combustion carbon capture involves removing the CO₂ from the exhaust gas that is produced from combustion. Oxy-fuel carbon capture involves combusting a fuel source in a nearly pure oxygen condition in order to make carbon capture easier following the combustion. While these technologies address further contributions to the global emissions problem, a solution to removing the excess CO₂ in the current atmosphere is needed. To address this issue, I will propose the design of a direct air capture (DAC) system that will capture CO₂ directly from the atmosphere and use it to produce methanol, an important product that is produced across the globe.

The effort to advance technology to reverse and heal the planet will not be enough to address the global emissions issue. Several economic, political, and societal factors heavily influence the slow transition away from fossil fuels and the slow adaptation of carbon-neutral

practices. Some of these factors include existing infrastructure, the market for fuel, as well as misconceptions about carbon capture in public media. In order to solve the issues of carbon emissions, these societal factors must simultaneously be examined with developments and advancements of CCS technology.

To address the global carbon emissions problem, I will use chemical process design and simulation to develop a DAC system that can reduce the concentration of CO₂ in our atmosphere while also producing a useful product at the same time. In addition to this design project, I will analyze Chevron's CCS project in Gorgon using Actor-Network Theory in order to understand what must be done to successfully integrate carbon capture in our society.

Technical Research Problem

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

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.

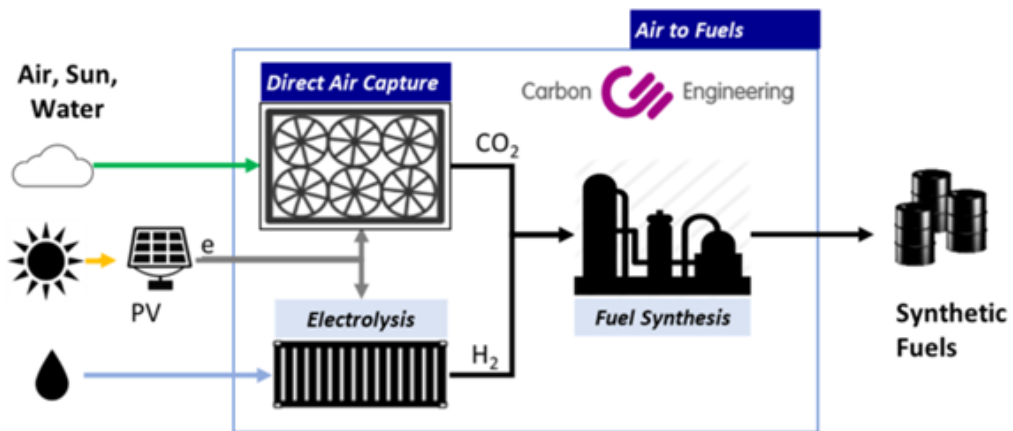


Figure 1. Overall Project Process

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.

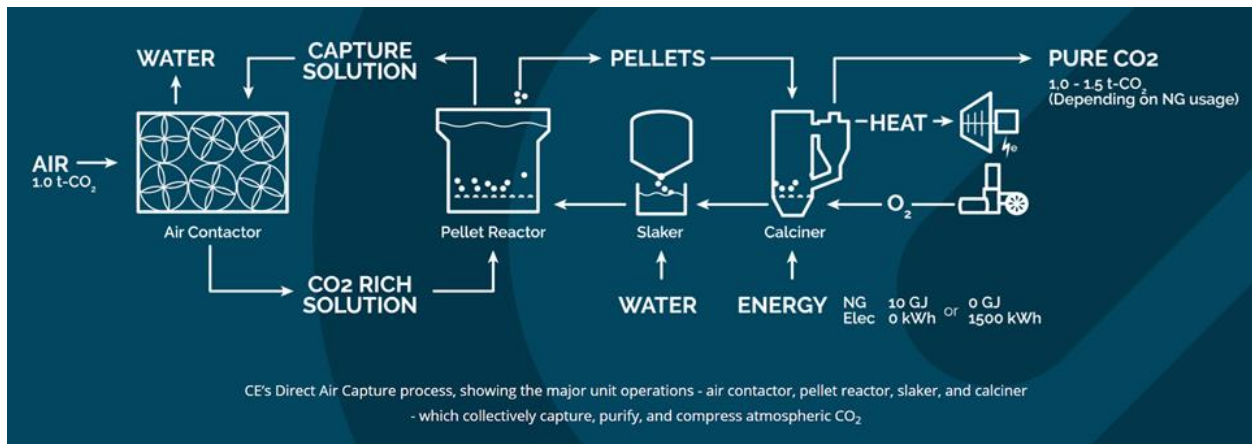
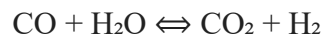


Figure 2. Process Flow Diagram for DAC

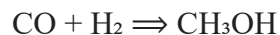
Thus far, only one company has implemented wide scale HT DAC (Fasihi, 2019), so there is opportunity for competitors to develop their own versions. This proposed project provides an avenue for improvement with the addition of downstream processing of CO₂. Therefore, providing a novel way to improve the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

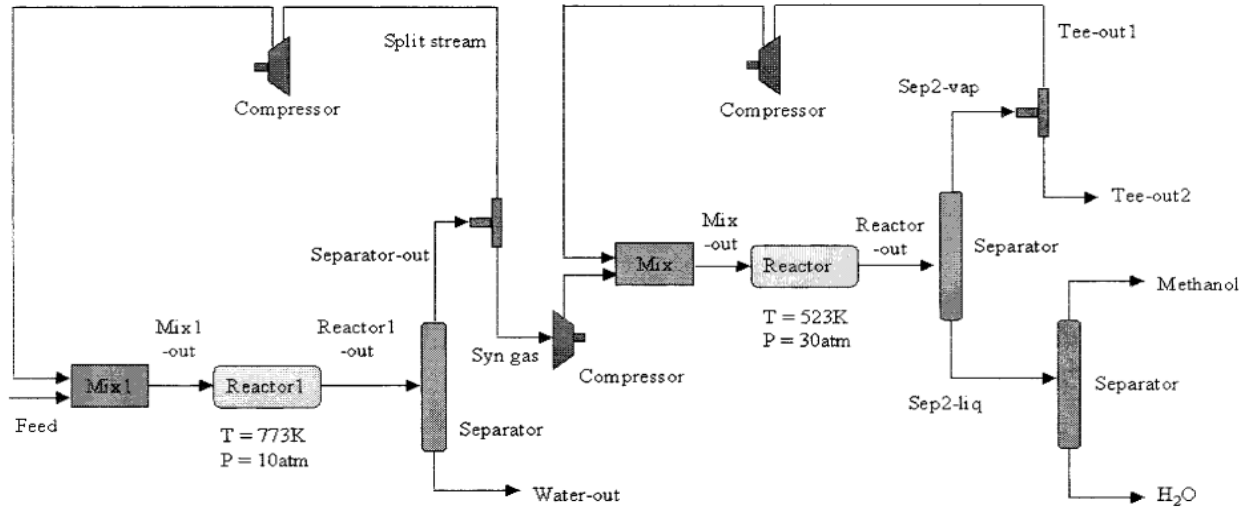


Figure 3. CAMERE Process Flow Diagram

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.

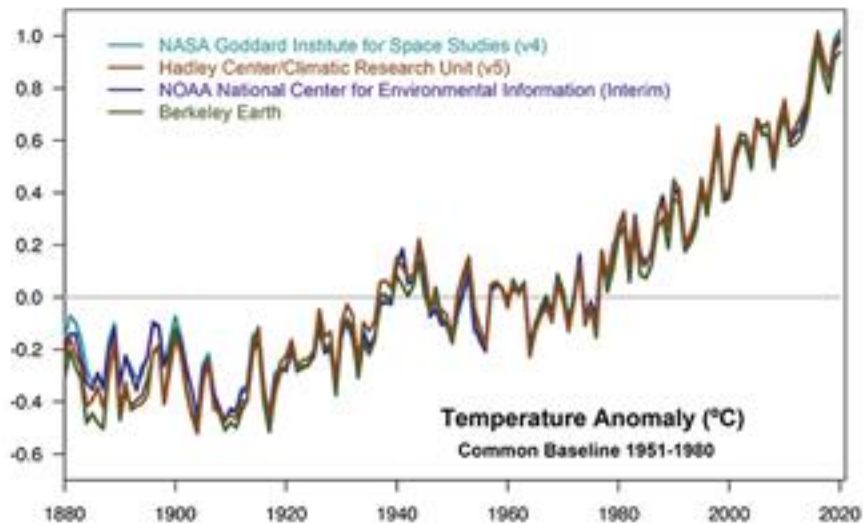


Figure 4. Global Temperature Trends Post-Industrialization

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 Research Problem

In 2009, Chevron Australia, in a joint venture with ExxonMobil and Shell, began construction on a natural gas plant on Barrow Island, off the coast of Australia. A radical part of

this project was the CO₂ capture system, the largest that was to be implemented in the world. The main plant is a liquified natural gas plant, with the CCS system injecting captured CO₂ back into a giant sandstone formation 2 km underneath the island. The project was originally estimated to cost 55 billion dollars, but Chevron increased the cost estimate by 15 billion after labor shortages, logistic challenges, and the strength of the Australian dollar in 2012. The CCS portion of the project was estimated to cost 2 billion dollars, and the Australian government invested 60 million into this project via the Low Emissions Technology Demonstrations Fund. The Australian Government also accepted liability for the CCS project in 2009.

The plant unfortunately did not meet the five-year emissions reduction target set as the plant began operation. There has been backlash because of this failure to reach the target from the Australian Government. The main issue and subsequent problems occurred in January of 2021, when a problem with the pressure management system led to sand clogging the injection system for the CO₂ to reach the sandstone formation beneath the island.

It is evident that multiple factors influenced the shut down of the plant and the subsequent backlash from the public. I argue that previous public opinion about CCS, the strength of the Australian dollar, and previous existing infrastructure all play a role in perpetuating and blowing the failure of the plant out of proportion. Using Actor-Network Theory, each network builder, both human and non-human, can be identified and characterized in order to paint a better picture of how this network was formed and ultimately failed. This will allow for future insight into how CCS technologies can be better implemented for success. In order to carry out this analysis, I will utilize news reports, press releases from Chevron, interviews, and public reports.

Conclusion

The end product of the technical problem will be the design of a large-scale DAC system that will produce methanol from the captured CO₂ via process design modeling and simulation. The STS research problem will analyze why the large-scale CCS project owned by Chevron on an island off the shore of western Australia was not able to meet the five-year target that was previously set as the plant began to run. Using Actor-Network Theory, the relevant human and non-human factors will be characterized to see how much they influenced the outcome of this case study. The combination of this technical report with the Chevron case study will give a practical solution to implementing CCS technologies in order to reverse our global emissions problem, while also addressing any societal, political, and economic factors that may hinder the achievement of practical solutions to greenhouse emissions.

Works Cited

- Ritchie, H., & Roser, M. (2020, May 11). CO₂ and greenhouse gas emissions. Our World in Data. Retrieved October 26, 2021, from <https://ourworldindata.org/co2-and-other-greenhouse-gas-emissions>.
- Broehm, Micah and Strefler, Jessica and Bauer, Nico. (September 25, 2015). Techno-Economic Review of Direct Air Capture Systems for Large Scale Mitigation of Atmospheric CO₂. Potsdam Institute for Climate Impact Research <http://dx.doi.org/10.2139/ssrn.2665702>
- Buis, A. (2020, October 12). *A degree of concern: Why global temperatures matter – climate change: Vital signs of the planet*. A Degree of Concern: Why Global Temperatures Matter. Retrieved October 17, 2021, from <https://climate.nasa.gov/news/2865/a-degree-of-concern-why-global-temperatures-matter/>.
- Cox, L. (2021, January 14). Western Australia LNG plant faces calls to shut down until faulty carbon capture system is fixed. The Guardian. Retrieved November 1, 2021, from <https://www.theguardian.com/environment/2021/jan/15/western-australia-lng-plant-faces-calls-to-shut-down-until-faulty-carbon-capture-system-is-fixed>.
- Department of Energy. (n.d.). Pre-combustion CO₂ Capture. National Energy Technology Laboratory. Retrieved November 1, 2021, from <https://netl.doe.gov/coal/carbon-capture/pre-combustion>.
- Fasihi, M., Efimova, O., & Breyer, C. (2019). Techno-economic assessment of CO₂ direct air capture plants. *Journal of Cleaner Production*, 224, 957–980. <https://doi.org/10.1016/j.jclepro.2019.03.086>
- Funk, C., & Hefferon, M. (2021, July 12). *U.S. public views on climate and Energy*. Pew Research Center Science & Society. Retrieved October 17, 2021, from <https://www.pewresearch.org/science/2019/11/25/u-s-public-views-on-climate-and-energy/>.
- Global Methanol Market Research Report (2021 to 2026) - by source, end-use industry, derivatives and region - researchandmarkets.com. Business Wire. (2021, September 1). Retrieved October 18, 2021, from <https://www.businesswire.com/news/home/20210901005564/en/Global-Methanol-Market-Research-Report-2021-to-2026---by-Source-End-use-Industry-Derivatives-and-Region--ResearchAndMarkets.com>.
- Gorgon CO₂ Injection Project. Chevron. (n.d.). Retrieved November 1, 2021, from <https://australia.chevron.com/-/media/australia/publications/documents/gorgon-co2-injection-project.pdf>.
- Gorgon Fact Sheet: Carbon Dioxide Capture and Storage Project. Carbon Capture and Sequestration Technologies @ MIT. (n.d.). Retrieved November 1, 2021, from <https://sequestration.mit.edu/tools/projects/gorgon.html>.

- Joo, O. S., Jung, K. D., Moon, I., Rozovskii, A. Y., Lin, G. I., Han, S. H., & Uhm, S. J. (1999). Carbon dioxide hydrogenation to form methanol via a reverse-water-gas- shift reaction (the CAMERE process). *Industrial and Engineering Chemistry Research*, 38(5), 1808-1812. <https://doi.org/10.1021/ie9806848>
- Keith, D. W., Holmes, G., Angelo, D. S., & Heidel, K. (2018). A Process for Capturing CO₂ from the Atmosphere. *Joule*, 2(8), 1573–1594 .<https://doi.org/10.1016/j.joule.2018.05.006>
- Oxy-combustion. netl.doe.gov. (n.d.). Retrieved November 1, 2021, from <https://netl.doe.gov/node/7477>.
- Yang, L., Pastor-Pérez, L., Villora-Pico, J. J., Gu, S., Sepúlveda-Escribano, A., & Reina, T. R. (2020, January 31). CO₂ valorisation via reverse water-gas shift reaction using promoted Fe/CEO₂-al₂o₃ catalysts: Showcasing the potential of advanced catalysts to explore new processes design. *Applied Catalysis A: General*. Retrieved October 18, 2021, from <https://www.sciencedirect.com/science/article/abs/pii/S0926860X20300351>.
- U.S. Energy Information Administration - EIA - independent statistics and analysis. Use of energy in industry - U.S. Energy Information Administration (EIA). (2021, August 2). Retrieved October 17, 2021, from <https://www.eia.gov/energyexplained/use-of-energy/industry.php>.