Optimization of the Carbon-Neutral Production of Methanol Via Direct Air Carbon Capture

Analysis of Occidental Petroleum's Proposed Direct Air Carbon Capture Project

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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

Global carbon emissions are rising rapidly, risking catastrophic changes to the environment including food shortages and losses of biodiversity. Hundreds of gigatons are still to be produced from existing fossil fuel infrastructure. Almost every model used by the Intergovernmental Panel on Climate Change (IPCC) describing a safe climate trajectory involves not only reducing carbon emissions but necessitates "negative emissions," or burying captured CO₂ (*Pulling CO₂ Out of the Air and Using It Could Be a Trillion-Dollar Business*, 2019). A 2017 paper in Nature Climate Change estimates that even if optimistic emission reductions are successful, 120-160 gigatons will still need to be sequestered before 2050 to stay below the 2°C increase in global average temperature limit set by the Paris Climate Agreement (Mac Dowell et al., 2017).

Carbon capture utilization and sequestration (CCUS) technologies are a "readily deployable technology solution" to reach the goals set by the Paris Climate Agreement. CCS strategies suggest geological sequestration where CO₂ is injected deep underground. Although drawbacks of CCUS include large capital investments and energy costs, utilization of the CO₂ in manufacturing can help create markets and lower financial barriers for companies to adopt carbon capture (Mac Dowell et al., 2017). To address the economic drawbacks of carbon capture technologies, I will propose the optimization of a relatively new method called direct air carbon capture and the subsequent synthesis of methanol to lower production costs and minimize emissions.

Although carbon capture technology may be necessary to help our climate, there are hidden environmental risks to consider. Government subsidies for CCUS allow polluting fossil fuel plants to continue operations and prolong the shift to renewable energy. Risks associated with geo-sequestration include surface gas leaks, acidification of groundwater, and geological instability (Hardisty, 2011). Enhanced oil recovery (EOR) is the most common use of CO₂, enabling increased oil production and emissions (Geraci, 2017). Occidental Petroleum's proposed direct air carbon capture project is one sociotechnical case where EOR will be subsidized on a large scale by government funding. It is important to understand these factors to make informed decisions about future carbon capture policies and implementation.

Technical, economic, and environmental factors will all need to be considered simultaneously to successfully implement CCUS. Using chemical process modeling and

simulation, I will address this issue by optimizing a direct air carbon capture plant and the subsequent production of methanol designed to produce 0.98 Mt of CO₂ per year that will examine the economic feasibility of this technology. Furthermore, I will apply actor-network theory to analyze the human and non-human actors in the argument surrounding Occidental Petroleum's proposed direct air carbon capture project.

Technical Project Proposal

The average temperature on Earth has risen 0.08° Celsius per decade since 1880, but this rate has more than doubled since 1981, rising 0.18° C per decade in recent years. The effects of global warming are driving regional and seasonal temperature extremes. These extremes have played a role in melting glaciers, intensifying hurricanes, extreme heat waves, and drastically altering the habitats that many life forms depend on for survival (Lindsey et al., 2022). Following the Industrial Revolution, carbon dioxide (CO₂) emissions from man-made sources have been increasing. Now, 87 percent of all anthropogenic carbon dioxide emissions come from burning fossil fuels (*Main sources of carbon dioxide emissions*, 2017). Greenhouse gases, such as carbon dioxide, are the leading cause of climate change, and while diverging from fossil fuels towards renewable energy is the ultimate goal, carbon capture technologies represent an important tool in emission reduction.

Direct air capture (DAC) is a new type of technology that serves to decrease ambient carbon dioxide concentrations as opposed to traditional carbon capture technologies which target point source emissions. In this project, a direct air carbon capture system and methanol production plant are designed based on "Carbon-Neutral Production of Methanol Via Direct Air Carbon Capture," a technical report submitted in 2022 by Brown, Huynh, Lee, Park, and Smith. DAC is achieved by the chemical reaction cycles shown below, while methanol production is achieved by catalytic hydrogenation of CO and H₂ syngas produced from reverse water-gas shift reactions.

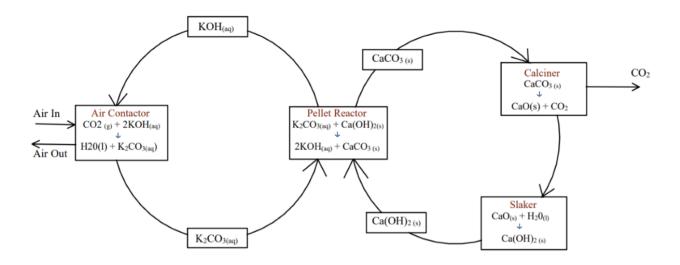


Figure 1. Process chemistry and thermodynamics for Carbon Engineering's aqueous direct air capture system (Keith et al., 2018).

This project is still of interest for several reasons. First, the methanol market is expected to grow from \$36,803 million in 2022 to \$54.630 million in 2030 (*Methanol Market Report*, 2022). Second, most DAC systems are in early stage or experimental in nature, thus the government provides a \$180 tax credit (Q45) for each ton of CO₂ captured directly from air (Cooper et al., 2022). These two factors combined creates a strong economic driving force for reconsidering this project. Moreover, some parts of the process were blackboxed and not optimized; the true potential of DAC methanol production could not be comprehensively evaluated under such conditions.

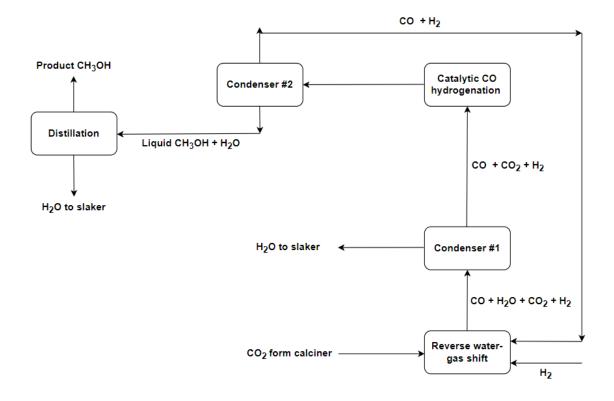
Our group aims to complete one of the blackboxed designs, the power island, and optimize the methanol production process. The power island consists of a natural gas turbine and a heat recovery steam generator (HRSG), according to Carbon Engineering's plant report. Heat recovery systems are designed to create additional steam to contribute to the turbine. To ensure no additional CO₂ is emitted from the turbine, all combusted fuel from the turbine will be sent to the CO₂ absorbers, which are also blackboxed in the 2022 design report. All amounts of fuel and products of the turbine process will be evaluated and electricity supplied to the turbine will be calculated and costed, as well. The steam resulting from the generator is combined with steam from the slaker unit, passed through the superheater to extract heat from the calciner off-gases, and then used to drive a steam turbine that generates the remainder of the power required for the plant. As done in Carbon Engineering's Aspen simulation, we will also reduce the complexity by

using independent steam cycles for the gas turbine and the slaker/superheater (Keith et al., 2018). Material and energy balances for this process will be found and cost evaluated in this report.

The previous design had a water knockout system for the CO₂ product stream out of the calciner and precedes the methanol synthesis process. However, this system is costly in terms of both capital and utilities. The excess water comes from the combustion of natural gas in the calciner. To address this issue, the calciner will be redesigned as a heat exchanger-reactor, in which combustion takes place at the outer shell of the calciner, providing heat for the reaction at the inner shell. Water from the distillation bottom and condenser #1 will be recycled back to the slaker to increase Ca(OH)₂ production. New material and energy balances and economic analysis will be derived based on the improved model.

Similar to the 2022 design report, the scale up of this project will be designed with a capacity to produce 0.98 Mt of CO₂ per year based off of an internal pilot plant designed by Carbon Engineering with a capacity of approximately one tonne of CO₂ per year. The goal of the methanol synthesis is to yield 412 million kilograms of methanol per year at a production schedule of 6000 hours per year.

This project will be done as part of a two-semester team project fulfilling the requirements of CHE4474 Process Synthesis, Modeling, and Control. Modeling of process flow diagrams will be performed using ASPEN software. Two members of the team will likely focus on the power island and two members will focus on the methanol synthesis process. However, in order to create a seamless design and report, all team members will aid in work for the process as a whole and likely will shift focus as the semester progresses to work more on areas which require more complex modeling and design effort.



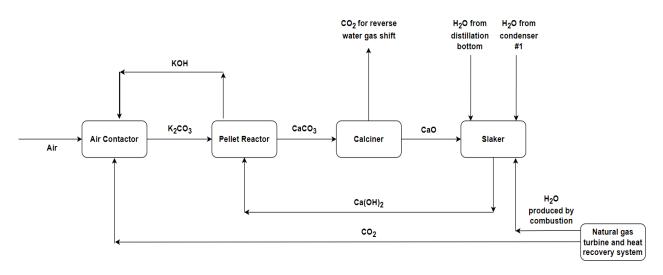


Figure 2. Overview of carbon capture and methanol synthesis system based on Carbon Engineering's design. The methanol synthesis block is redesigned without the water knockout system.

STS Project Proposal

Occidental Petroleum seeks to build a series of massive industrial projects in Texas and up to 70 direct air capture plants globally by 2035. To further offset capital investment cost, Occidental plans to use the captured CO₂ in enhanced oil recovery (EOR) to extract oil from its depleted reservoirs located near a planned carbon capture plant site (Valle, 2022). Currently, EOR is the largest industrial use of captured CO₂, whereby pressurized fluids are injected into existing reservoirs to bond with the oil and improve the flow to the surface. EOR can reverse the decline of mature oil fields and recover up to 60% of the oil in a reservoir while sequestering 90 – 95% of the injected CO₂ in the ground (*Could Squeezing More Oil Out of the Ground Help Fight Climate Change*?, 2019). An estimated 60% of total U.S. crude oil production is attributed to EOR, making it the most common oil recovery practice in the United States (Geraci, 2017).

While Occidental's carbon capture proposal and EOR operation has been mostly celebrated as a success for reducing fossil fuel-related emissions, this view fails to consider the lack of public attention regarding EOR, the dangers to groundwater which will disproportionately affect people of color and environmental justice communities, the lack of oversight and regulation, and the long-term effects on CO₂ emissions. These considerations highlight the importance of the role played by the government, environmentalists, and fossil fuel lobbyists in developing new carbon capture and EOR operations. In 2018, environmentalist actors wrote a letter titled "Congress Must Stop Subsidizing Enhanced Oil Recovery," signed by over 30 environmental, health, and social justice organizations targeting the Section 45Q Tax Credit which subsidizes EOR, pointing to concerns over "water protection, insufficient climate protections, and a lack of financial accountability for companies claiming the credit" (Redman, 2018). Although the U.S. Environmental Protection Agency regulates EOR, "regulations of EOR activities are outdated and do not effectively safeguard groundwater." Underfunded state regulatory programs and scarce media attention on EOR have resulted in little review of its regulations since the 1980s (Geraci, 2017). If governmental policies and new technologies continue to serve only wealthy petrochemical company profits and short-term benefits, the consequences on the climate will be catastrophic.

I argue that the motives of fossil fuel companies, exploitable legislative policies, lack of regulatory oversight and public awareness surrounding the dangers of EOR are what led to the general support for Occidental's carbon capture proposal. Actor-Network theory considers both

human and non-human elements equally as actors within a network, arguing that the concern is mapping the way in which actors define and distribute roles and how association between actors determines the power of the network. A network builder (often, engineers) assemble a network to accomplish a goal or solve a problem (Cressman, 2009). I will apply the concept of Actor-Network theory to argue how human and non-human actors play a role in the public opinion and future development of Occidental's carbon capture and EOR plans. For this analysis, I will utilize evidence from the letter, "Congress Must Stop Subsidizing Enhanced Oil Recovery," the 45Q tax credit, a dynamic life cycle assessment of CO₂-EOR (Núñez-López, 2019), and the report of groups affected by related water scarcity and groundwater threats.

Conclusion

The technical project discussed in this paper will deliver a full design of the carbon-neutral production of methanol via direct air carbon capture capable of yielding 412 million kilograms of methanol per year with detailed modeling and simulation work to support this goal. The STS research paper will aim to determine why there is a controversy surrounding the Permian's largest operator of CO₂-EOR requesting billions of dollars of public funding for their proposed carbon capture development project. This will be accomplished by applying Actor-Network theory to characterize how relevant human and non-human actors influence the development of CCUS plants. The combined results of this research will address the issue of developing carbon capture technology from a sociotechnical lens, emphasizing the vital considerations for the long-term sustainability of carbon capture and proposing a plant design for carbon-neutral utilization of direct air capture CO₂.

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