

**CARBON-NEUTRAL PRODUCTION OF METHANOL VIA DIRECT AIR CARBON  
CAPTURE AND GREEN HYDROGEN**

**ANALYSIS OF SOCIETAL IMPACTS ON CARBON CAPTURE TECHNOLOGY**

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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As the world searches for ways to mitigate the consequences of climate change, there has been an increasing effort to develop new technologies or methods to limit the amount of carbon emitted into the atmosphere. Since the Industrial Revolution, humankind has increased the ambient concentration of carbon dioxide by 48% which has led to a continuous increase in global temperatures due to the greenhouse gas effect (“The cause of climate change,” 2021).

Technologies such as carbon capture have been developed to combat the rise of carbon dioxide concentrations in the atmosphere. Carbon capture technologies have the potential to remove carbon dioxide emissions from either point sources such as smoke stacks from factories or from the ambient air through direct air capture (DAC). Additionally, new production methods have been researched to lower emissions while still generating products and profits. An example of this can be seen in the production of methanol, a highly efficient alternative fuel that offers lower emissions compared to conventional petroleum, but the production process emissions are large. The most common method for methanol production today involves the burning of syngas which can emit 0.9-1.0 metric tonnes of carbon dioxide per ton of methanol produced (“Methanol fuel in the environment,” n.d.). This has created both “operational inefficiencies” and environmental concerns as carbon is emitted into the environment, which represents both a loss of useful reagents for methanol production and an increase of emissions of a greenhouse gas (“Methanol fuel in the environment,” n.d.). This technical project seeks to solve both operational and environmental challenges by implementing a new process to produce carbon-neutral methanol fuel. This involves using carbon dioxide captured via DAC and procured green hydrogen to produce methanol. This technical project will focus primarily on the chemical processes to capture carbon dioxide from ambient air through DAC and the synthesis of methanol using the CAMERE process. While this technology and methodology are promising, there are many

barriers it faces including difficult economics, lack of public support, and political turmoil. In the current climate, this technology is highly dependent on government subsidies, so the implementation of this technology has been deeply politicized with many actors in play. With back-and-forth support of carbon capture, the development of the technology has been slowed over the recent years. Hence, the STS research focuses on the societal impacts on the development of carbon capture technology using Actor-Network Theory to determine the relevant actors and their motives. The topics of the technical project and STS research are tightly coupled and are directly related to each other.

### **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. Carbon-neutral implies that the equivalent amount of carbon dioxide emitted from burning methanol will be captured via DAC with no net emissions. An example of the process is shown in Figure 1.

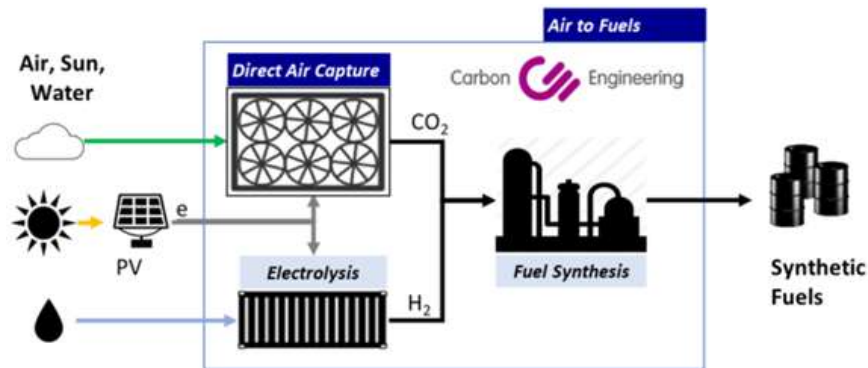


Figure 1. Overall process of the synthesis of methanol derived from green hydrogen and carbon captured directly from the air (“Air to fuels,” 2021).

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:

### DESIGN PROCESS #1- DIRECT AIR CAPTURE (DAC)

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

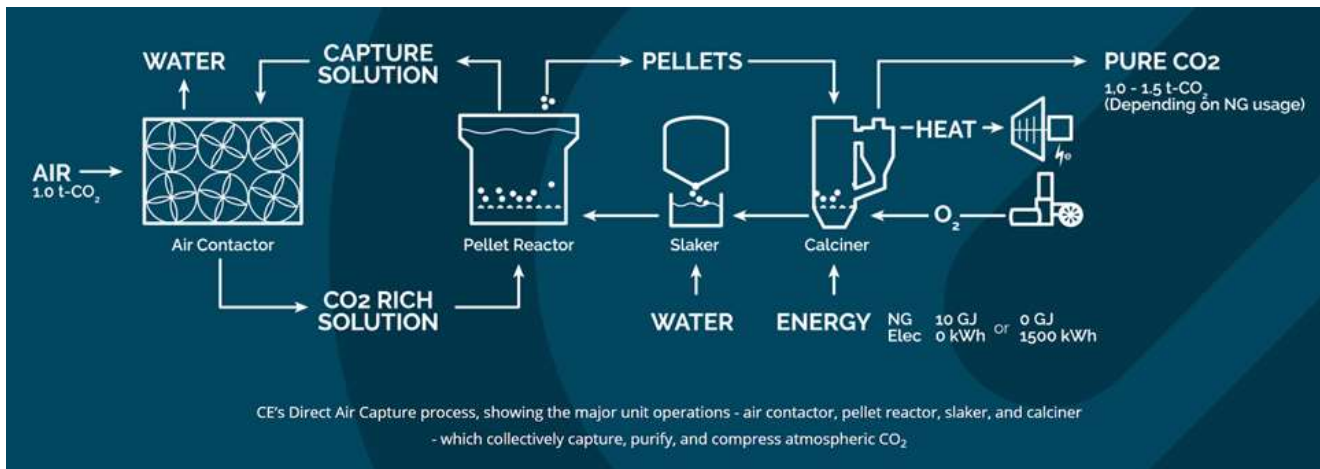


Figure 2. Process flow diagram for DAC to include the relevant unit operations which will separate carbon dioxide out from ambient air using sorbents and regenerative technology (Keith, 2018).

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.

Thus far, only one company has implemented wide scale HT DAC so there is opportunity for competitors to develop their own versions (Fasihi, 2019). This proposed project provides an avenue for improvement with the addition of downstream processing of carbon dioxide. Therefore, providing a novel way to improve the economics and utility of DAC as traditional DAC design either sequesters carbon in geological formations or is used in enhanced oil recovery.

## **DESIGN 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 carbon dioxide to carbon monoxide via the reverse water-gas shift reaction, the reaction is outlined below:

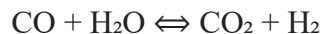


Figure 3. Water-shift reaction. Conversion of carbon dioxide and hydrogen to carbon monoxide and water (Brown, 2021).

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:

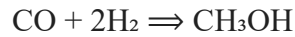


Figure 4. Hydrogenation of carbon monoxide. Method to produce methanol from carbon monoxide and green hydrogen (Brown, 2021).

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 (1999).

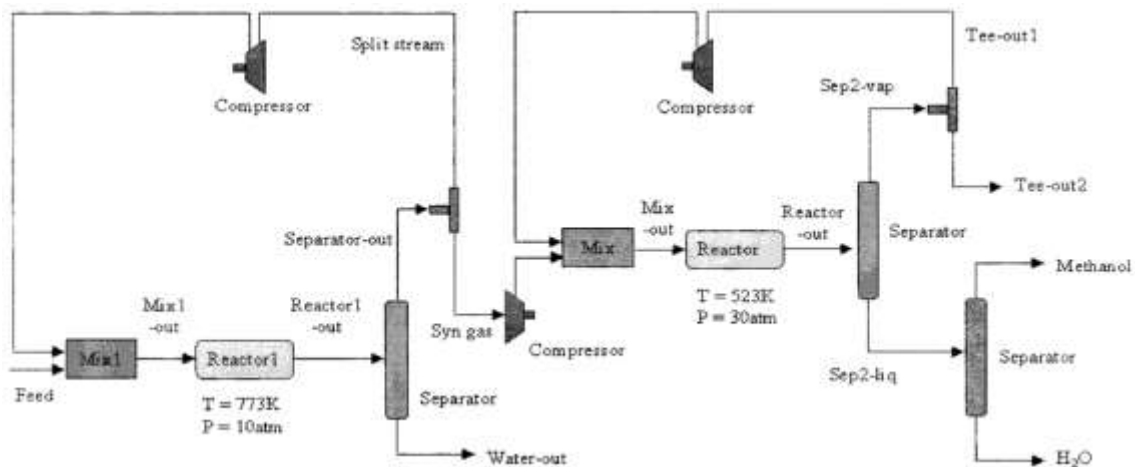


Figure 4. CAMERE process flow diagram which illustrates the unit operations necessary for this reaction. The end products will be methanol and water as shown above (Joo, 1999).

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. 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, Professor Eric Anderson, in the Chemical Engineering Department. The proposed DAC 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.

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.

### **WHY IS THE SKY NOT BLUE?**

With carbon emissions being so tightly coupled with modern development, there is a deep feeling of uncertainty on whether or not the world can reverse the devastating effects of climate change. Developing countries inherit the technology of the past because they are the most convenient, but also the most harmful. The responsibility falls onto developed countries which have the means to research and integrate new technologies to bring hope back to the climate change battle. When the world was halted in place due to the COVID-19 virus, the once heavily polluted skies of developing nations such as India and China impossibly became blue again. At this moment in history where the world was feeling a collective sense of despair, there was a glimpse of hope that redefined what could be possible.





Figure 5. New Delhi's India Gate in October 2019 (left) and April 2020 (right) illustrates the change in air quality in a matter of months due to the decrease in transportation emissions from COVID-19 shutdowns (Bourzac, 2020).

The importance of cleaning our skies cannot be understated, and new ways of thinking must be considered to solve this global problem. While abandoning modern transportation methods is an unlikely solution, the development of new technologies such as carbon capture could bring hope back to our skies.

## **USE OF ACTOR NETWORK THEORY TO UNDERSTAND PROGRESS**

With the immense potential carbon capture technology has, it still lacks the widespread implementation which begs the question: what has stopped its progress? To answer this, the framework of Actor Network Theory (ANT) will be used to understand the motivations and actions of relevant actors at play. Actor Network Theory was chosen for this analysis as it takes into account the relationships between power, politics, and space that human and non-human actors influence (Muller, 2015). Using ANT will provide a framework that aims to simplify the entangled relationships between different actors to uncover the reasons why carbon capture technology is not being utilized to reduce the effects of climate change, one of this generation's most pressing challenges. While critics claim that ANT provides an "endless chain of

associations without ever arriving at an explanation,” this theory will still be used as a stepping point to understand the most important actor-actor interactions (Muller, 2015).

The initial analysis using Actor Network Theory is rendered in Figure 6 below, with arrows representing relationships between human and non-human actors circled in red and blue, respectively.

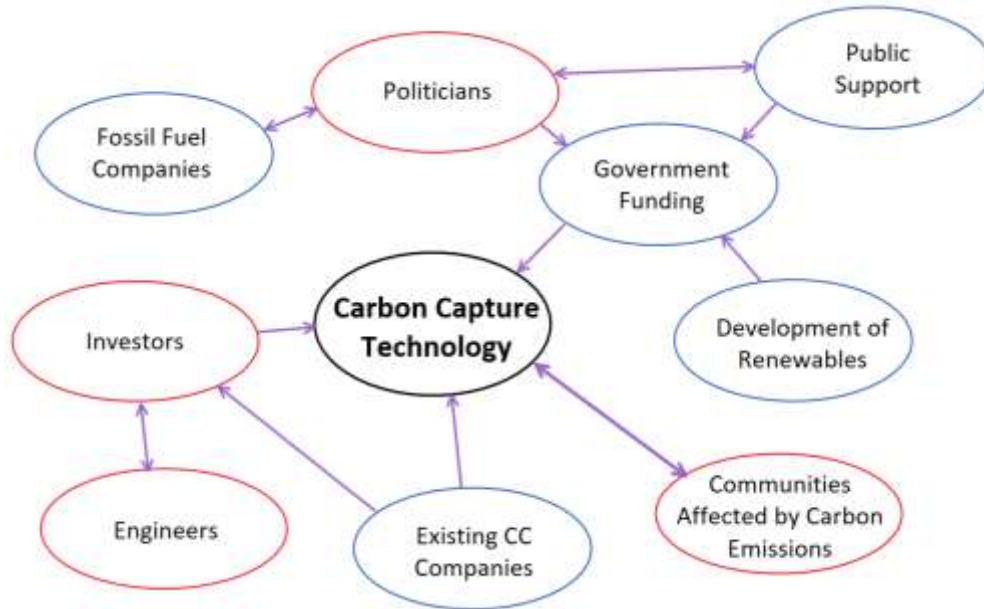


Figure 6. Actor Network Theory for carbon capture. Using Actor Network Theory to analyze actors, both human and non-human, influencing the development of carbon capture technology (Brown, 2021).

At the center of the analysis is carbon capture technology, and the main question to be answered is why the technology has not been widely implemented despite the maturity and research backing it. Through initial research, the largest barriers to development center around the allocation of funds and the impact of the technology on surrounding communities.

## ALLOCATION OF FUNDS

Despite the potential of the technology, carbon capture still requires government subsidies as the energy requirements and capital costs are relatively large at this stage of

development (National Academies of Sciences, E., & Medicine, 2019). With the introduction of government subsidies, politics and power become a central barrier for development. Government funding is influenced by politicians, who are driven from a number of actors, including donors to their constituents. For example, a state that has heavily invested in the fossil fuel industry to provide jobs for their residents may have conflicting interests and not support carbon capture projects. According to authors Friedman and Davenport, there is a long-held relationship between the Republican Party and the fossil fuel industry, on the account of the \$46 million donated to the GOP in the year 2020 alone (2021). Also, politicians are motivated by the needs of their constituents in the form of jobs. Senators like Rick Scott of Florida believe that mitigative technologies, such as carbon capture, are not worth the risk, if “you are killing the jobs.” (Friedman & Davenport, 2021). This sentiment runs deep within the GOP, and one of the focuses of this research is to understand these relationships between the fossil fuel industry, politicians, and their supporters. For those politicians who do support carbon capture technology, there is the issue of allocating resources to other projects as well. The development of other renewable technologies creates competition to secure funding. With this, carbon capture technology has been greatly politicized in that different parties wish to fund different applications of the technology. There is currently a debate on whether or not to support post-combustion carbon capture and storage technology. This essentially supports the fossil fuel industry by resupplying the oil reserves with captured carbon. While some view the technology as a responsible answer to the issue of current carbon emissions, others see it as a temporary fix that enables the fossil fuel industry to continue production and diverts the allocation of resources away from developing renewable energy sources (Nisbet, 2019).

## **DEVELOPMENT AND IMPACT ON SURROUNDING COMMUNITIES**

As aforementioned, the application of carbon capture technology can have very different effects, especially on the communities that surround the technology. There are many methods to carbon capture but storage for oil recovery and direct air capture illustrate the spectra of implications of carbon capture technology. On one end of the scale, carbon capture and storage for enhanced oil recovery essentially supplies reserves for future oil drilling. On the other hand, direct air capture could potentially create negative emissions and reduce the overall concentration of carbon dioxide in the atmosphere. As both are carbon capture technologies, they are inherently associated with each other despite the very different impacts of each application. In this research, the implications of carbon capture and sequestration will be analyzed as it is more widely implemented in industry today. Through understanding these effects, recommendations to reduce the effect on surrounding communities can be made for direct air capture as the technology becomes more developed in the future.

Across the country, there are environmental and social justice battles between industry giants and local communities occurring every day. This fight is evident in St. James Parish, a corridor located in southern Louisiana colloquially called Cancer Alley. With about 150 oil refineries, plastics plants, and chemical facilities along the Mississippi River, the residents of Cancer Alley suffer from higher rates of cancer and respiratory diseases than the national average ("Environmental racism...", 2021). Of the residents in the region, people from Black communities are disproportionately affected. According to the UN News, African American residents' risk of cancer is about 104 to 105 cases per million, but the risk is 60 to 75 cases per million in districts of predominantly white residents (2021). Cancer Alley has been deemed an environmental sacrifice zone which is an area where in and is usually inhabited by low-income

families and people of color (“Let’s talk about...”, 2021). This is illustrated in Figure X below, showing the sites of the industrial facilities surrounding the Mississippi River.

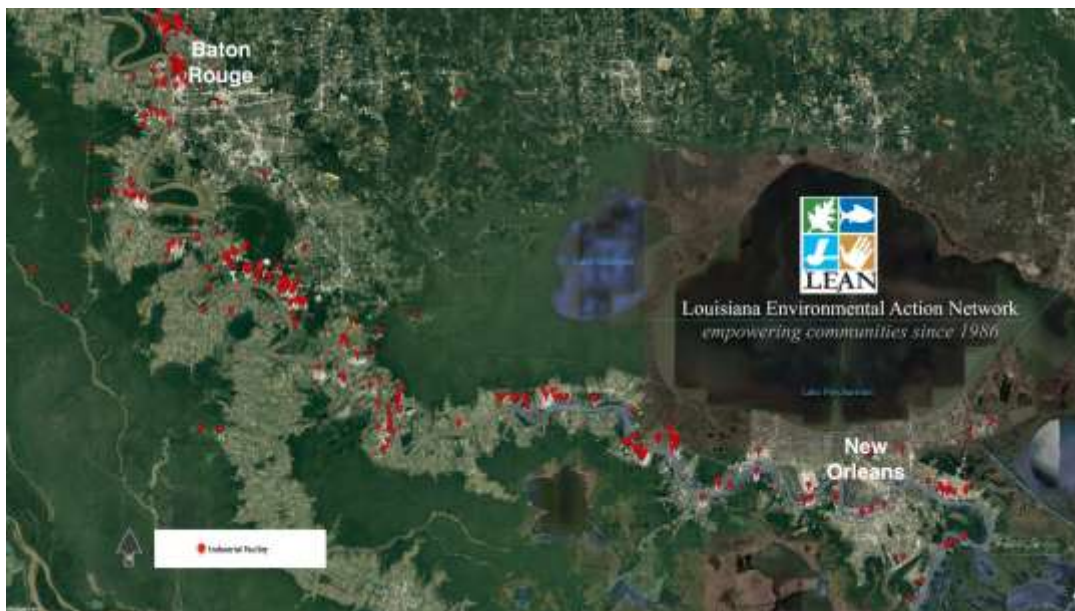


Figure 7. Illustration of the magnitude of polluting sources surrounding the Mississippi River in “Cancer Alley” with each red dot representing an industrial facility (Harris, 2020).

Carbon capture and sequestration has been utilized by the facilities in Louisiana with the support of state legislation which continues the reliance on fossil fuels in the region. With this, there has been push back from affected communities and environmental groups hoping to change the focus of legislation from supporting carbon capture to increasing public health measures. As a result of years of excessive pollution and governmental prioritization of industry, residents lack trust in their government and reject the development of the technology outright. This research aims to use Cancer Alley as a case study to understand how the motives and relationships between affected communities, industry, and the government impact the development of carbon capture technology as a whole.

Through the technical and STS research, this project aims to find a path forward for the development of carbon capture technology taking into account the viability of chemical

processes and its impact on society. While technologies like direct air capture are not used widespread, this research seeks to provide a technical proof of concept and an STS framework for future implementation.

## REFERENCES

- Air to fuels. (2021). *Carbon Engineering*. <https://carbonengineering.com/air-to-fuels/>
- Backstrand, K., Meadowcroft, J., & Oppenheimer, M. (2011). The politics and policy of carbon capture and storage: Framing an emergent technology. *Global Environmental Change*, 21(2), 275-281. <https://doi.org/10.1016/j.gloenvcha.2011.03.008>
- Bourzac, K. (2020, September 25). COVID-19 lockdowns had strange effects on air pollution across the globe. *Chemical & Engineering News*. 98(37). <https://cen.acs.org/environment/atmospheric-chemistry/COVID-19-lockdowns-had-strange-effects-on-air-pollution-across-the-globe/98/i37>
- Broehm, M., Strefler, J., & Bauer, N. (2015). Techno-economic review of direct air capture systems for large scale mitigation of atmospheric CO<sub>2</sub>. *Potsdam Institute for Climate Impact Research*. <https://dx.doi.org/10.2139/ssrn.2665702>
- Brown, R. (2021). *Hydrogenation of carbon monoxide*. [Figure 4]. *Prospectus*. (Unpublished undergraduate thesis). School of Engineering and Applied Science, University of Virginia. Charlottesville, VA.
- Brown, R. (2021). *Actor Network Theory for carbon capture*. [Figure 6]. *Prospectus*. (Unpublished undergraduate thesis). School of Engineering and Applied Science, University of Virginia. Charlottesville, VA.
- Brown, R. (2021). *Water-shift gas reaction*. [Figure 3]. *Prospectus*. (Unpublished undergraduate thesis). School of Engineering and Applied Science, University of Virginia. Charlottesville, VA.
- Buis, A. (2020, October 12). A degree of concern: Why global temperatures matter – climate change: Vital signs of the planet. *NASA Global Climate Change*. <https://climate.nasa.gov/news/2865/a-degree-of-concern-why-global-temperatures-matter/>.
- Environmental racism in Louisiana’s ‘Cancer Alley’, must end, says UN human rights experts. (2021, March 2). *UN News*. <https://news.un.org/en/story/2021/03/1086172>
- Fasihi, M., Efimova, O., & Breyer, C. (2019). Techno-economic assessment of CO<sub>2</sub> direct air capture plants. *Journal of Cleaner Production*, 224, 957–980. <https://doi.org/10.1016/j.jclepro.2019.03.086>
- Friedman, L., & Davenport, C. (2021, August 13). Amid extreme weather, a shift among Republicans on climate change. *The New York Times*. <https://nyti.ms/3m7Ew5I>

- Funk, C., & Hefferon, M. (2021, July 12). U.S. public views on climate and Energy. *Pew Research Center Science & Society*. <https://www.pewresearch.org/science/2019/11/25/u-s-public-views-on-climate-and-energy/>.
- Hanschke, H. (2021, February 8). How Elon Musk will award \$100 million in carbon capture contest. *NBC News*. <https://www.nbcnews.com/science/environment/how-elon-musk-will-award-100-million-carbon-capture-contest-n1257084>
- Harris, J. (2020, November 4). Letter to the editor: ‘Cancer Alley’ story is inaccurate, made up. *Daily Advertiser*. <https://www.theadvertiser.com/story/opinion/2020/11/04/letter-editor-cancer-alley-story-inaccurate-made-up/6160882002/>
- 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>
- Let’s talk about sacrifice zones. (2021, May 13). *The Climate Reality Project*. <https://www.climateRealityproject.org/blog/lets-talk-about-sacrifice-zones>
- L’Orange Seigo, S., Dohle, S., & Siegrist, M. (2013). Public perception of carbon capture and storage (CCS): A review. *Renewable and Sustainable Energy Reviews*. 38, 848-863. <https://doi.org/10.1016/j.rser.2014.07.017>
- Keith, D. W., Holmes, G., Angelo, D. S., & Heidel, K. (2018). A process for capturing CO<sub>2</sub> from the atmosphere. *Joule*, 2(8), 1573–1594. <https://doi.org/10.1016/j.joule.2018.05.006>
- Methanol fuel in the environment. (n.d.). *Methanol Fuels*. <https://methanolfuels.org/about-methanol/environment/>
- Muller, M. (2015, January 28). Assemblages and actor-networks: Rethinking socio-material power, politics, and space. *Geography Compass*, 9(11), 27-41. <https://doi.org/10.1111/gec3.12192>
- NASA, NOAA analyses reveal 2019 second warmest year on record. (2020, January 15). *NASA Global Climate Change*. <https://climate.nasa.gov/news/2945/nasa-noaa-analyses-reveal-2019-second-warmest-year-on-record/>
- National Academies of Sciences, E., & Medicine. (2019). *Negative Emissions Technologies and Reliable Sequestration: A Research Agenda*. Washington, DC: The National Academies Press. <https://doi.org/10.17226/25259>.
- Nisbet, M. C. (2019). The carbon removal debate: Asking critical questions about climate change futures. Institute for Carbon Removal Law and Policy. <https://www.american.edu/sis/centers/carbon-removal/upload/carbon-removal-debate.pdf>



The causes of climate change. (2021, August 30). *NASA Global Climate Change*.  
<https://climate.nasa.gov/causes/>

Tremel, A., Wasserschied, P., Baldauf, M., Hammer, T. (2015). Techno-economic analysis for the synthesis of liquid and gaseous fuels based on hydrogen production via electrolysis. *International Journal of Hydrogen Energy*. 40(35),  
<https://doi.org/10.1016/j.ijhydene.2015.01.097>

Use of energy explained. (2021, August 2). *U.S. Energy Information Administration (EIA)*.  
<https://www.eia.gov/energyexplained/use-of-energy/industry.php>.

Yang, L., Pastor-Pérez, L., Villora-Pico, J. J., Gu, S., Sepúlveda-Escribano, A., & Reina, T. R. (2020, January 31). CO<sub>2</sub> valorisation via reverse water-gas shift reaction using promoted Fe/CEO<sub>2</sub>-al<sub>2</sub>o<sub>3</sub> catalysts: Showcasing the potential of advanced catalysts to explore new processes design. *Applied Catalysis A: General*. 593(5). 117441.  
<https://doi.org/10.1016/j.apcata.2020.117442>