Economically Viable Carbon Capture for Electro-Decarbonization of the US Economy

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Motivation. Intergovernmental Panel on Climate Change (IPCC) reports heavily rely on carbon capture, utilization, and storage (CCUS) in all models and scenarios assessing policies toward net-zero emissions by 2050 to limit warming to 1.5º [1]. While carbon capture through geologic sequestration is ready; economic, technological, and institutional factors impede large-scale deployment of CCUS in the electricity system [2] and the rest of the economy. Market mechanisms like a price on carbon are required to incentivize the adoption of capture. Moreover, meeting the IPCC target of net zero emissions by 2050 implies curtailing emissions in sectors where decarbonization is slow. Industrial commodities and chemicals like iron, steel, and cement account for over 15% of global emissions [3]. However economic viability [4] impedes large-scale CCUS deployment. CCUS is urgently needed as a stopgap on existing fossil fire infrastructure with decades of lifespan remaining [2]. **We develop a mathematical framework that evaluates economic viability of large-scale deployment of capture methods across sectors under possible policy scenarios, distinguishing between capturing carbon at the source and Direct Air Capture (DAC).** This model will initially focus on the energy and chemical sectors but is generalizable to emissions-intensive sectors like transportation and heating. We will also investigate the interplay in choosing between capturing carbon at the source and DAC. Figure 1 describes the methods and contributions of this project.

CCUS can enable economic viability of decarbonization strategies across sectors spanning the entire economy, and particularly in the chemicals sector. The carbon intensity of the electrical grid is less than that of fossil fire processes like steam cracking [5]. Steam cracking is breaking down large hydrocarbons like ethane into smaller hydrocarbons like ethylene using steam from fossil fire powered furnaces. Energy policy in the near future aims to decrease the carbon intensity of the electrical grid by increasing penetration of renewable energy sources [6]. NYU is leading the Decarbonizing Chemical Manufacturing Using Sustainable Electrification (DC-MUSE) initiative. DC-MUSE aims to electrify chemical manufacturing at scale [6]. Thirty percent of US industrial CO_2 emissions comes from the chemical industry, and 93% of the chemical processes use fossil fuel heat [6]. To better understand the variety of chemical and industrial processes that exist for each industrial product, we will leverage our ongoing collaboration with the Modestino group at NYU Chemical Engineering. DC-MUSE represents both an electrical and chemical engineering challenge as chemical production requires robust reliability of electrical energy and improvements in energy storage. Renewables present an additional challenge due to their intermittence [6]. Electrified production becomes economically attractive when a carbon price is implemented. Incorporating a carbon price, capture at the source, and DAC in our framework will demonstrate the viability of electrifying processes. Modeling CCUS across the economy will inform investment priorities in DC-MUSE.

Vision. This project will develop an optimization-based framework to explore what technological, economic, and regulatory conditions can accelerate large-scale deployment of CCUS technologies.

First, we develop an economy-wide framework which incorporates availability of DAC and capture at the source. Our preliminary work focuses on fuel-fired power plants and the chemical manufacturing sector; we envision generalizing our work to energy-intensive industries and major

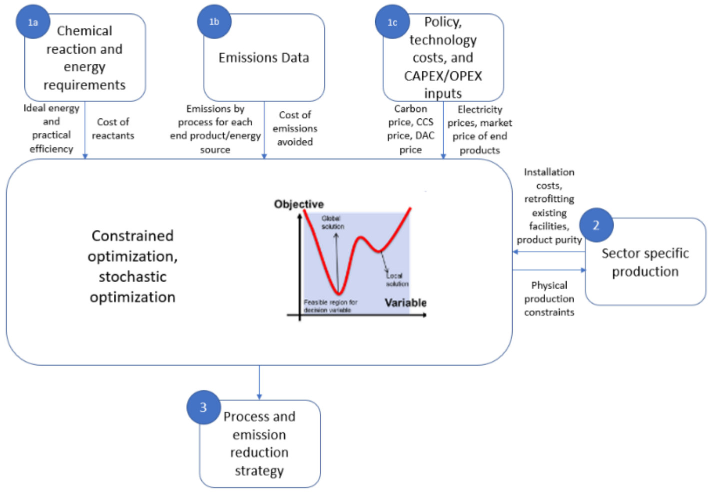

Figure 1 In steps 1a-c, we collect chemical process engineering data, emissions data by process and industry, and cost inputs of detailing technology, policy, and manufacturing. In step 2, we input data of all considered decarbonization investments alongside traditional fossil fire technology across processes and industries along with their associated production constraints. Using optimization, in step 3 our framework will output an emission allocation strategy distributed across capture at source, DAC, and paying a carbon price. Our model will also select a process out of all candidate inputs in step 2 for each industry and commodity.

emitters, including, for example, the agriculture sector. For each process, we have an emissions function relating production output with carbon emissions produced. The framework depends on emitters accounting for the emissions they produce using a combination of DAC, capture at the source, or paying a carbon price.

Second, we will investigate the interplay between the level of carbon prices and penetration of CCUS technologies. We will investigate how changes in the price of DAC affect model recommendations. We will use stochastic and robust optimization to investigate the effect of CCUS price and carbon price uncertainty on capture investment planning and strategy.

Model results will inform preferences between capture at the source and DAC under different scenarios. Results will inform viability of removing carbon on location with infrastructure maintained by the emitter versus at a location away from the source where no installations are necessary. DAC is currently more expensive but is also more convenient for the emitter. We investigate what sets of assumptions lead the model to favor DAC over capture at the source and vice versa.

Research Questions. In this project, we ask:

1. In which industries and in which specific processes is the implementation of capture at the source and/or DAC most economically viable at scale? How does policy (carbon price) and technology price affect the sensitivity of the model?
2. In the chemical industry, is electrified production currently viable at scale compared to conventional fossil fire sources like steam cracking? If electrified production is not currently viable, under what model parameters does electrified production become viable? For each desired end product, which electrified process is most cost effective at scale?

3. What technological gaps stand in the way of deployment at scale. What should be the investment priorities for emitters to accelerate adoption of CCUS?

Approach. We will develop an optimization model to capture the interplay of CCUS and carbon emitters across industries and processes [Figure 1]. Carbon emissions arise from the production process of each emitter. We will represent emitters as profit maximizers, each with their own technological constraints pertaining to their industry. For example, chemicals manufacturing is distinct from power generation, and thus carbon emissions arise at different points in their respective supply-chains. We will express profits as the difference between revenues, cost of production, and cost of emissions.

Step 1. Evaluate static viability of CCUS: We begin by considering each emitter (for example Natural Gas Combined Cycle (NGCC)) individually in an analysis with real-time electricity price data. We have defined linear emissions functions for all emitters we are currently evaluating. The fossil fire emitters currently in our model are NGCC, Pulverized Coal (PC), and Integrated Gasification Combined Cycle (IGCC). They can all implement capture at source [7] or rely on DAC. We calculate profit by subtracting the cost of power from revenue at each timestep.

The chemical we have already begun modeling is ethylene. We calculate gross margin (GM) in chemicals manufacturing by subtracting cost of reactants and cost of energy from revenue at each timestep. Subtracting cost of reactants can potentially increase gross margin when the chemical reaction produces end products alongside the desired chemical that can be sold for more than the cost of input reactants. For both industries, we can subtract the cost of carbon, DAC, or capture at the source depending on policy chosen to get profit or GM respectively. The electrification of chemical production reduces the emissions emitters must account for compared to fossil fire processes like steam cracking. It is complementary to the goals of CCUS.

For each emitter, we calculate the reduced profit using each of capture at the source, DAC, and carbon price at each timestep, on average, and the standard deviation. We perform a sensitivity analysis on the cost of DAC, capture at source, and carbon price under various realistic scenarios. We collect average cost and standard deviation under each scenario for each emitter.

Step 2. Dynamic optimization: Extending the model in step 1, we combine the variable elements of our static model into a dynamic optimization model. Our model accommodates potential non-linear emissions functions if increased complexity becomes necessary. Emitters must account for the entirety of their emissions with a combination of paying a carbon price, implementing capture at the source, or paying for DAC.

Capture at the source may not be applicable for all industries, for example, in the future we may seek to model livestock as an agricultural process. For capture at the source, emitters pay a lump sum to retrofit an existing facility which is priced out in the model as an annuity payment. We incorporate the knowledge that older plants are generally more costly to retrofit for capture at the source using an exponential function with plant age as the independent variable and cost to retrofit as the dependent variable. We also assume there is a maximum percentage of total carbon emitted that producers can recover using capture at the source (with the chemical constraint that 100%

purity can never be reached). Like capture at the source, chemical electrification requires an initial infrastructure investment by the producer that can be priced out as an annuity.

The model will produce an optimal strategy to split emissions between capture at source, DAC, and carbon price. If we are evaluating a chemical that can be produced using several different processes, the model will select the most economical process.

Step 3. Sensitivity Analysis on Carbon Price, Price of DAC, and Price of Capture at Source: Using the model from step 2, we will use stochastic optimization to evaluate how robust model outputs are to variations in input parameters. We will assess the economic viability of capture at source and DAC under different carbon price schemes. We will assess the relationship between paying for DAC and investing in capture at source across industries and emitters at different price thresholds. In this step we aim to understand the interplay between different CCUS alternatives across sectors and under different conditions.

Case Study and Data. Our preliminary optimization model is being coded in Julia with an objective function and constraints representing satisfying demand; physical production constraints (for example ramp-up and ramp-down constraints); accounting for all emissions using a combination of paying the carbon price, capture at source, and DAC; emissions functions relating end product production and CO_2 production; and cost of emissions for all processes. The decision variables are the ratios of paying the carbon price, capture at source, and DAC for each process in each industry as well as power output/final product output from each process in each industry. For example, if we have four different processes that produce ethylene and we need to satisfy a total demand for ethylene, the decision variable is the ethylene output from each of the four methods. It is expected to be cost-prohibitive for a producer to use more than one method as each requires initial sunk costs. We expect the model to satisfy product demand by selecting a single process.

After we develop our step 1 analysis and step 2 model, we will assume all processes source energy at cost from the electrical grid. Our model will use years of real-time and day-ahead LMP data down to 5 minute intervals from independent system operators (ISOs) across the country including NYISO (New York), MISO (Midwest), CAISO (California), ERCOT (Texas), and PJM (Eastern seaboard). We will investigate in which areas of the United States are DAC and/or capture at the source likely to be the most viable. We will also seek to establish any seasonality trends or time period trends (for example if DAC and/or capture at the source is more likely to be viable in the winter or in the evenings respectively).

We will source linear emission function data from IPCC reports [7]. We will source capture at source and DAC cost data in US$/t$CO_2$avoided from IPCC reports and research papers [7]. DAC cost data specifically will come from a paper by Carbon Engineering detailing an operational pilot plant running at 200 US$/t$CO_2$ that is not currently selling to businesses or the general public [8]. We will run scenarios with decreased costs of capture at source and DAC representing technological advancements and evaluate model results.

For chemicals manufacturing which is highly seasonal, we will use weekly commodity spot price time series data from WRDS. For each chemical product, the reactions we intend to evaluate will be chosen by literature review and with collaboration from subject matter experts in the Modestino group. Every chemical reaction has an ideal energy requirement and a variable process efficiency representing the ratio between the physical minimum energy required for a chemical reaction and the current minimum energy possible with existing technology for a chemical reaction. Efficiency is a unitless measure between 0 and 1. We will use the ideal energy requirement and the efficiency to calculate the cost of electricity for a given chemical reaction.

An existing data challenge is finding time series data for carbon intensity across different electrical grids. We are currently using government data with time invariant average carbon intensity in each state. We are seeking data that is more granular in both time and location.

Educational and Workforce Training Opportunities. The results of this project will aid the design of a section on CCUS technologies under the PI's yearly undergraduate energy course taught by Professor Dvorkin in NYU Tandon School of Engineering. Moreover, the project will provide the opportunity for graduate and undergraduate students across disciplines to conduct research on CCUS technologies and public policies. The opportunity will be available to students across disciplines through the semester-long Capstone program of the NYU Center for Urban Science and Progress (CUSP). Students from the NYU Electrical and Computer Engineering department will benefit from semester-long senior-design projects. Finally, the project will provide funding for graduate research assistants under the NYU Graduate Student Employment and Training (GSET) Program. Past projects include the design and implementation of a photovoltaic-powered aquaponic farm (nominated for the NYU-wide entrepreneurship competition); the design of a programmable inverter for scheduling loads based on time-of-use tariffs; and a demonstration of turning carbon into vodka using an award-winning technology from Air Co [9].

Research findings will provide material for the following outreach initiatives. The PI and his group will participate in NYU's Applied Research Innovations in Science and Engineering (ARISE) program for female students hosted by NYU's Center for K-12 STEM Education that runs for six weeks every summer. As part of this program, the PI currently advises two female high-school students (both work on graph theory methods for peer-to-peer transactions). The PI will also maintain his participation in NYU's #SUMMEROFSTEM program (general STEM overview program) for K-12 students.

Team. The project will be led by Alice Nuz with support from Dr Charalampos Avraam, and will be supervised by Prof. Yury Dvorkin at NYU. Alice Nuz is a PhD student in Electrical and Computer Engineering at NYU working on DC-MUSE and decarbonization using CCUS. Prior to beginning her PhD, she worked as a data scientist at BMO Capital Markets. Dr. Charalampos Avraam is a Smart Cities Postdoctoral Associate at the Center for Urban Science + Progress (CUSP) of NYU supervied by Prof. Yury Dvorkin, focusing on the economic, technological, and societal implications of disruptions in energy, food, and water infrastructures. Prof. Yury Dvorkin is an Assistant Professor and Goddard Junior Faculty Fellow in the Department of Electrical and Computer Engineering at NYU Tandon School of Engineering with an affiliated appointment at NYU's Center for Urban Science and Progress.

Conflicts of interest. The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this proposal.

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