Dual Function Materials for Direct Air Capture of CO$_2$

primary project goal

Susteon Inc. is teaming with Columbia University, Applied Catalysts, and Kiewit Engineering to advance the development of a "reactive" direct air capture (DAC) process that is capable of capturing and converting carbon dioxide (CO$_2$) from air into valuable products. The reactive DAC process involves selective chemisorption of CO$_2$, followed by sorbent regeneration through reversible desorption or, optionally, catalytic conversion of adsorbed CO$_2$ into methane (CH$_4$; also referred to as renewable natural gas [RNG]), using waste or renewable hydrogen (H$_2$).

In Phase I of this Small Business Innovation Research (SBIR) project, the research team optimized existing dual-function materials (DFMs), originally developed for treating flue gas from large point sources, for application in removing CO$_2$ from air. The DFM exhibited a high CO$_2$ adsorption capacity and capture kinetics in ambient air. The technical and economic feasibility of the "reactive" capture DAC process was demonstrated successfully in Phase I.

Phase II is focused on further optimizing the DFMs and process cycle; developing a high-fidelity bench-scale (1 kg/day) prototype unit to perform parametric and long-term testing; optimizing DFM on the selected support structure to achieve maximum CO$_2$ adsorption capacity, low pressure drop, and conversion into methane; developing a process model to accurately represent the process; and performing and refining the techno-economic assessment (TEA) obtained in Phase I to evaluate the commercial potential of the process.

technical goals

- Develop optimum DFM washcoat formulation on commercial monolith support through lab- and bench-scale testing.
- Develop an efficient method of heating the DFM layer on the monolith using Joule heating.
- Develop a commercial manufacturing process for DFM structures by working with a commercial catalyst manufacturer.
- Design and build a bench-scale unit capable of 1.0 kg/day of CO$_2$ capture.
- Conduct parametric testing in the bench-scale unit to determine optimum DAC-DFM process conditions for CO$_2$ adsorption, RNG production, and optimum process cycle design.
- Conduct long-term testing to establish DFM aging and performance degradation.
- Refine and validate the current process model using bench-scale data to develop a high-level process design for a pilot-scale (50 kg CO$_2$/day) system scale-up and testing in the next phase.
- Perform a TEA and LCA.

technical content

DAC of CO$_2$ is a promising technology that can potentially contribute to mitigation of CO$_2$ emissions at scale. DAC technology can be also used to provide sustainable CO$_2$ as feedstock for CO$_2$ conversion technologies to produce

program area:
Carbon Dioxide Removal

ending scale:
Bench Scale

application:
Direct Air Capture

key technology:
Sorbents

project focus:
Dual Function Materials for Capture and Conversion of CO$_2$ into Methane

participant:
Susteon Inc.

project number:
SC0020795

predecessor projects:
N/A

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partners:
Columbia University; Kiewit Engineering Group Inc.

start date:
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percent complete:
47%

synthetic fuels, chemicals, and construction materials. In this project, Susteon is advancing the development of a "reactive" DAC system that is capable of capturing, as well converting, CO_2 from air into valuable products.

In Phase I of this project, Susteon successfully demonstrated this process-intensified reactive DAC process using DFMs for capture of CO_2 from air and its subsequent conversion into CH_4 using renewable/waste hydrogen for regeneration. The DFM porous solid material, consisting of a novel combination of an adsorbent and a catalyst, has shown high CO_2 capacity under DAC conditions, and even greater capacity in the presence of atmospheric moisture, in laboratory experiments. Regeneration can be achieved using mild temperatures (200–300°C), minimizing the temperature difference between chemisorption and sorbent regeneration and mitigating the need for heating and cooling of the reactor beds, which are typically needed in most adsorption-based processes. The "green" CH_4 formed in this process can be sold as RNG, which qualifies for various carbon credits and incentives, similar to biogas, landfill gas, etc. This reactive DAC process is designed to intensify both the capture and utilization of atmospheric CO_2, creating a platform technology for production of a variety of green hydrocarbon products from air (i.e., CH_4, methanol, dimethyl ether, olefins, diesel, aviation fuel, etc.). As shown in Figure 1, air is fed into an adsorption reactor containing DFM, which rapidly captures CO_2 from ambient air. Once the bed is saturated with CO_2, it is heated to about 170°C and regenerated with an H_2-containing gas stream to directly react CO_2 to produce CH_4 using the Sabatier reaction ($CO_2 + 4H_2 = CH_4 + 2H_2O$). This project is aimed at demonstrating the production of RNG at a cost comparable or better than the current RNG prices in California with low-carbon fuel standards (~$15/MM British thermal units [Btu]), creating a business opportunity for further development and deployment of this DAC technology.
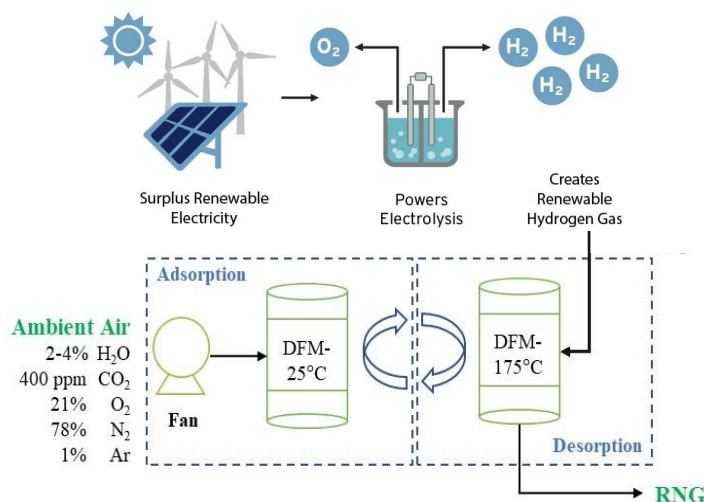

Figure 1: Block flow diagram for the overall DAC-DFM process using renewable H_2.

In Phase I, working with research institute partner Columbia University, Susteon identified, synthesized, and tested a ruthenium (Ru)-promoted sodium oxide dispersed on alumina as the DFM for this process. DFM optimization in Phase I led to identification of 0.25% Ru + 10% Na_2O supported on a high-surface area Al_2O_3 DFM, which exhibited a high CO_2 adsorption capacity and capture kinetics in ambient air. The extent of CO_2 capture (% removal of 400 parts per million [ppm] CO_2 in air) was significantly higher in the presence of atmospheric moisture (relative humidity in air), unlike physical sorbents like zeolites, aluminas, metal organic frameworks (MOFs), and even amine-based CO_2 capture sorbents. This DFM also showed a very fast mass transfer rate during adsorption and desorption/methanation without any noticeable aging/degradation. The preliminary TEA of the DFM-based DAC system (Figure 2) with 1 tonne CO_2/day basis indicated a combined power and heat requirement of 2,300 kWh/tonne CO_2, which involves (a) CO_2 capture under ambient conditions without needing to heat or pressurize air followed by (b) heating the DFM for initiating methanation to 120–200°C. The methanation reaction being significantly exothermic (-164 kJ/mol) creates opportunities to utilize and integrate this heat to further lower the overall energy need. The DFM material is used on a structured support (e.g., cordierite monoliths used in automobile catalytic converters) to minimize pressure drop.
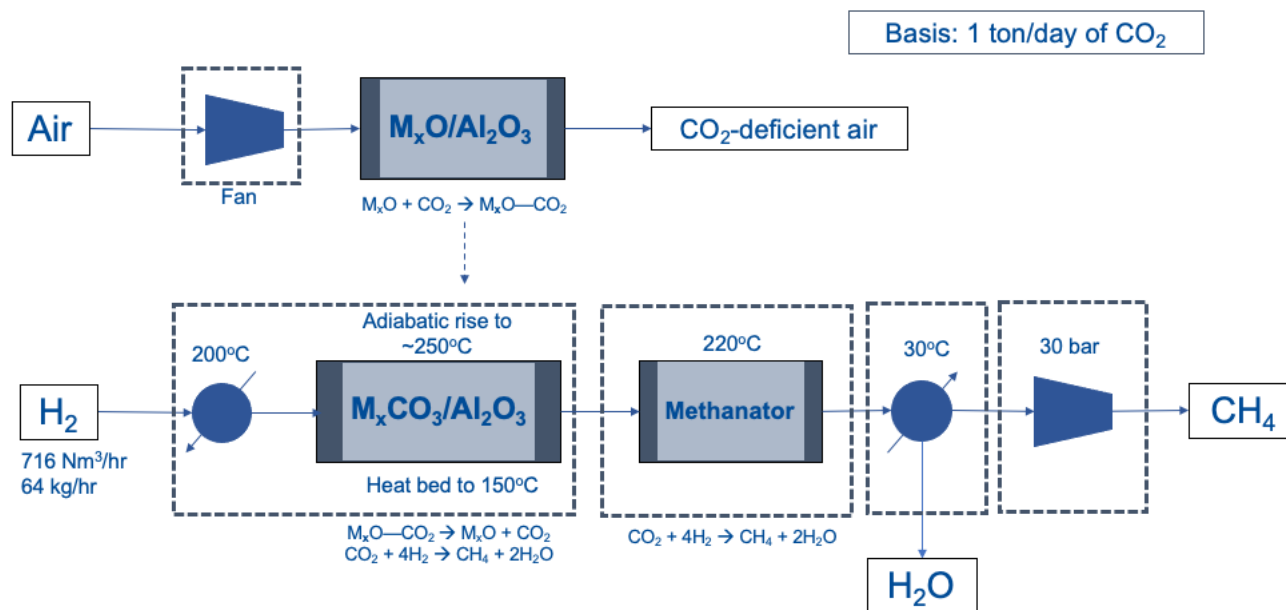
Figure 2: DAC-DFM with CO_2 capture at ambient conditions (25°C).

The Phase II project is aimed at further optimizing the DFMs and process cycle and building a high-fidelity bench-scale prototype unit to demonstrate this process and obtain engineering data needed for a pilot system design in a follow-on phase. DFM optimization focuses on the formulation and dispersion of DFM on the commercially available structured supports to achieve maximum DFM stability, CO_2 adsorption capacity, and rapid kinetics of CO_2 adsorption and methanation reactions. This work involves further reducing the Ru loading to lower overall cost of CO_2 capture. A novel Joule heating method is being integrated in the structured support to selectively heat the DFM layer between adsorption and regeneration steps. Bench-scale testing is being conducted to determine DFM process conditions that yield the fastest CO_2 adsorption rate, highest CO_2 capacity, maximum CH_4 production, and lowest-energy consumption for reactive DAC. The process model is validated using lab- and bench-scale data and employed to develop a high-level process design for a 50-kg/day engineering-scale reactive DAC system, as well as techno-economic analysis (TEA) and life cycle analysis (LCA) studies on a commercial-scale system. Lab- and bench-scale test results are used to further refine the process model developed in Phase II.

Definitions:

STP – Standard Temperature and Pressure (15°C, 1 atm).

Sorbent – Adsorbate-free (i.e., CO_2-free) and dry material as used in adsorption/desorption cycle.

Manufacturing Cost for Sorbent – "Current" is market price of material, if applicable; "Target" is estimated manufacturing cost for new materials, or the estimated cost of bulk manufacturing for existing materials.

Adsorption – The conditions of interest for adsorption are those that prevail at maximum sorbent loading. Measured data are preferable to estimated data.

Desorption – The conditions of interest for desorption are those that prevail at minimum sorbent loading. Operating pressure and temperature for the desorber/stripper are process-dependent. Measured data are preferable to estimated data.

Pressure – The pressure of CO_2 in equilibrium with the sorbent. If the vapor phase is pure CO_2, this is the total pressure; if it is a mixture of gases, this is the partial pressure of CO_2.

Packing Density – Ratio of the active sorbent area to the bulk sorbent volume.

Loading – The basis for CO_2 loadings is mass of dry, adsorbate-free sorbent.

Kinetics – A characterization of the CO_2 adsorption/desorption trend with respect to time, as complete in the range of time as possible.

Flow Arrangement/Operation – Gas-solid module designs include fixed, fluidized, and moving bed, which result in either *continuous*, *cyclic*, or *semi-regenerative* operation.

Estimated Cost – Basis is kg/hr of CO_2 in CO_2-rich product gas; assuming targets are met.

Atmospheric Air Feed-Gas Assumptions – Update values below to describe the air feed-gas pressure, temperature, and composition entering the capture system:

Pressure	Composition						
14.7 psia	vol%					ppmv	
	CO₂	**H₂O**	**N₂**	**O₂**	**Ar**	**SOₓ**	**NOₓ**
	0.04	variable	78.09	20.95	0.93	trace	trace

Chemical/Physical Sorbent Mechanism – Both chemisorption and physisorption occur during the adsorption step.

Sorbent Contaminant Resistance – To be determined.

Sorbent Attrition and Thermal/Hydrothermal Stability – To be determined.

Flue Gas Pretreatment Requirements – N/A.

Sorbent Make-Up Requirements – To be determined.

Waste Streams Generated – N/A.

Process Design Concept – See Figure 1 for block flow diagram and Figure 2 for more detailed DAC-DFM reaction scheme.

Proposed Module Design – To be determined.

TABLE 2: DIRECT AIR CAPTURE ECONOMICS

Economic Values	Units	Current R&D Value	Target R&D Value
Cost of Carbon Captured	$/tonne CO_2	312	205
Produced RNG	tonne/day	18.2	32.4
Net Cost of Carbon Captured[i]	$/tonne CO_2	197	0
Capital Expenditures	$/tonne CO_2	187	86.1
Operating Expenditures	$/tonne CO_2	125	115

[i]Projected cost of capture less revenue from RNG sales based on the current RNG price of $15/MMBtu (including carbon credits), and a renewable hydrogen price of $2/MMBtu.

Definitions:

Cost of Carbon Captured – Projected cost of capture per mass of CO_2 captured under expected operating conditions.

Net Cost of Carbon Captured – Projected cost of capture less revenue from RNG sales per mass of CO_2

Capital Expenditures – Projected capital expenditures in dollars per tonne of CO_2 captured.

Operating Expenditures – Projected operating expenditures in dollars per tonne of CO_2 captured.

Calculations Basis – The economic values in Table 2 result from a process model on a 100 tonne/day captured CO_2 basis. The model developed in Aspen Plus was used to generate process material and energy balances, equipment sizing, and costs with the following assumptions:

- 25°C ambient temperature.
- 101.325 kPa ambient pressure.
- 60% relative humidity air.
- 1 kPa pressure drop in shell and tube heat exchangers.
- Compressor/blower specification: Polytropic with 70% efficiency and 90% drive motor efficiency.
- 10°C approach to cooling water on aftercooler heat exchanger.

- RGibbs reactor model for all reactions, including adsorption, desorption, and methanation.

Scale of Validation of Technology Used in TEA – The DAC economic values in Table 2 result from analysis of fundamental lab-scale data gathered at Technology Readiness Level (TRL) 3, implying a significant level of uncertainty in the process design and cost for a commercial system. This analysis is undertaken in the early stages of the technology development cycle to establish the feasibility of this novel technology with respect to technical soundness, operational flexibility, and economic viability.

Qualifying Information or Assumptions – Initial preliminary TEA results are based on the current RNG price of $15/MMBtu (including carbon credits), and hydrogen price of $2/MMBtu.

technology advantages

- Provides a saleable product from CO_2 with a strong market demand; for this project, it is RNG, which is in heavy demand to meet the low-carbon standards for CH_4 and power.
- Eliminates the need for CO_2 disposition infrastructure; compression, pipelines, storage sites, and long-term monitoring as CO_2 is directly converted into a saleable product, which can be distributed in existing natural gas infrastructure.
- Provides a platform for delivering renewable methane (RNG) from atmospheric CO_2 (Power-to-Gas) for downstream utilization to produce "green" hydrocarbons like methanol, Fischer-Tropsch fuels, olefins, etc. This could be accomplished by incorporating appropriate catalysts during the regeneration.
- Provides a market mechanism by utilizing current subsidies/incentives for low/negative carbon products (so called "Green Premiums") for offsetting the cost of DAC by revenue generated by selling the products manufactured from CO_2.

R&D challenges

- Designing an efficient process cycle for adsorption, heating, desorption, methanation, and cooling to maximize capital productivity and minimize the overall capital expenses (CAPEX) and operating expenses (OPEX) for the technology.

status

Susteon is currently working on a process model to predict key performance parameters involved in their DAC process, such as overall capture efficiency, energy consumption, CH_4 yield, and DFM degradation rates. Additionally, the bench-scale test system design, equipment sizing, and procurement are also currently being completed.

available reports/technical papers/presentations

Raghubir Gupta, "Dual Function Materials for Direct Air Capture of CO_2," Phase II Project kickoff meeting presentation, Pittsburgh, PA, September 2021. *https://www.netl.doe.gov/projects/plp-download.aspx?id=12122&filename=Dual+Function+Materials+for+Direct+Air+Capture+of+CO2.pdf*.