Energy-Efficient Direct Air Capture System for High-Purity CO_2 Separation

primary project goal

The University of Cincinnati (UC) is developing a revolutionary carbon dioxide (CO_2) capture system optimized for direct air capture (DAC). The technology utilizes an adsorption-regeneration cycle with a proprietary aminopolymer-silica hybrid adsorbent. UC is being assisted by BASF Catalysts and Daeyoung C&E in developing the sorbent-washcoated monolith structure and Trimeric for the economic analysis.

technical goals

- Perform a computational fluid dynamics (CFD) analysis to model fluid mechanics and adsorption kinetics to establish baseline adsorbent geometry.
- Manufacture sorbent in-house. Establish long-term lab-scale performance criteria.
- Manufacture sorbent-washcoated monolith structure.
- Design, construct, and test air contactor structure.
- Design, construct, and test full DAC system.
- Evaluate performance of adsorbent-washcoated monolith in air contactor/DAC system.
- Perform a techno-economic analysis (TEA) and life cycle analysis (LCA) and construct a state-point data table for the whole system.

technical content

UC is developing a new adsorbent material with a proprietary hybrid blend of aminopolymer and silica with a washcoated monolith structure. The new adsorbent is slated to be used in a DAC system that constructed in partnership with BASF Catalysts and Daeyoung C&E. Trimeric is assisting in carrying out a full-scale TEA and LCA for the complete DAC system. The scope of work for this project consists of the determination of CO_2 adsorption kinetics (via process modeling through a CFD study); sorbent manufacturing; development of the sorbent-washcoated monolith structure; the design, fabrication, and operation of a passive air contactor; performance evaluations; and TEAs and LCAs. The DAC system design makes use of a novel air contactor system that is slated to maximize CO_2 throughput with minimal external energy requirements (less than 80 kJ/mol CO_2 for desorption). The sorbent is being designed to be resistant to both oxidative and thermal degradation with cost-effective scalability. The air contactor is being designed for high air throughput with minimum pressure drop. The process parameters of the complete DAC sorbent system are shown in Table 1, while a schematic of the air contactor system is shown in Figure 1.

program area:
Carbon Dioxide Removal

ending scale:
Bench Scale

application:
Direct Air Capture

key technology:
Sorbents

project focus:
Sorbent-Washcoated Monolith in Air Contactor System

participant:
University of Cincinnati

project number:
FE0032128

predecessor projects:
N/A

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partners:
BASF Catalysts LLC; Daeyoung C&E Co.; Trimeric

start date:
10.01.2021

percent complete:
20%

TABLE 1: DAC SORBENT PROCESS PARAMETERS

Sorbent	Units	Current R&D Value	Target R&D Value
True Density @ STP	kg/m^3	2,050	2,050
Bulk Density	kg/m^3	810	810
Average Particle Diameter	mm	0.05	0.02-0.05
Particle Void Fraction	m^3/m^3	0.3	0.3-0.4
Packing Density	m^2/m^3	470,000	TBD
Solid Heat Capacity @ STP	kJ/kg-K	1.30	1.30
Crush Strength	kg_f	Not applicable	TBD
Attrition Index	-	~7-10	~7-10
Thermal Conductivity	W/(m-K)	Not available	TBD
Manufacturing Cost for Sorbent	$/kg	4-8	4-8
Adsorption			
Pressure	bar	1.013	1.013
Temperature	°C	0-40	0-40
Equilibrium Loading	g mol CO_2/kg	1.8-2	1.8-2
Heat of Adsorption	kJ/mol CO_2	66	66
CO_2 Adsorption Kinetics	gmol/(kg sorbent×min)	~0.05-0.08	~0.05-0.08
Desorption			
Pressure	bar	0.3-1	0.3-1
Temperature	°C	70-100	70-100
Equilibrium CO_2 Loading	g mol CO_2/kg	~0.1	~0.1
Heat of Desorption	kJ/mol CO_2	~120	~120
CO_2 Desorption Kinetics	gmol/(kg sorbent×min)	~0.4-0.6	~0.4-0.6
Proposed Module Design		*(for equipment developers)*	
Flow Arrangement/Operation	—	Flow though monolith in air contactor, adsorption-desorption cycles	
Flue Gas Flowrate	kg/hr	~4-16	
Space Velocity	hr^{-1}	5,000-20,000	
Volumetric Productivity	$gmol_{CO2}/(hr \times V(L)_{absorber\ bed})$	~2	
CO_2 Recovery, Purity, and Pressure	% / % / bar	>90% >95%	1.0325
Adsorber Pressure Drop	bar	0.002	
Degradation	% capacity fade/cycle	0.005	
Estimated Adsorber/Stripper Cost of Manufacturing and Installation	$\frac{\$}{kg/hr}$	Not available	

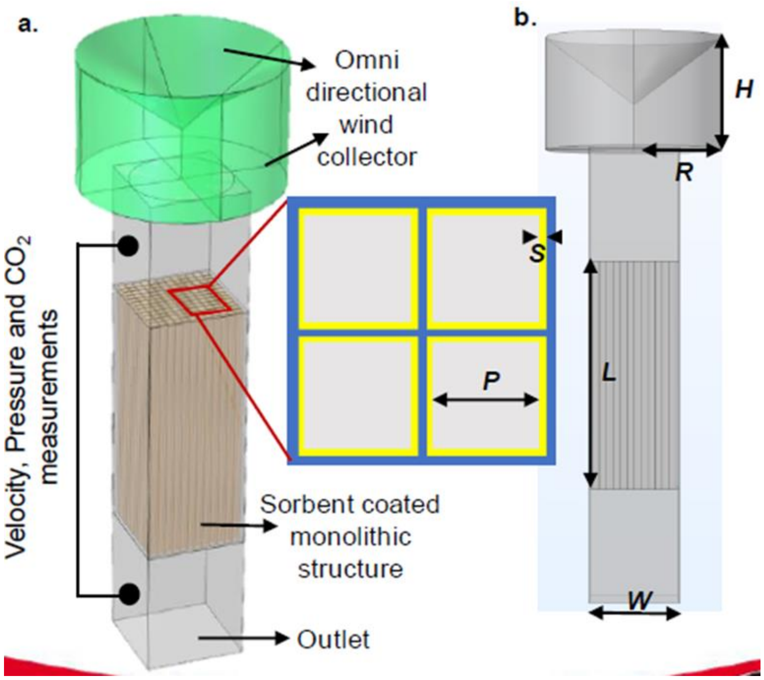

Figure 1: Passive air contactor (a) isometric view and (b) side view.

One of the core strengths of the new adsorbent mixture is the resistance to oxidative and thermal degradation. Figure 2 highlights the performance of the proposed sorbent compared to that of a conventional one of similar chemical makeup. The modified aminopolymer/silica blend suffers significantly less weight loss over time and is able to maintain high performance for more than 30 times longer than the conventional sorbent blend.

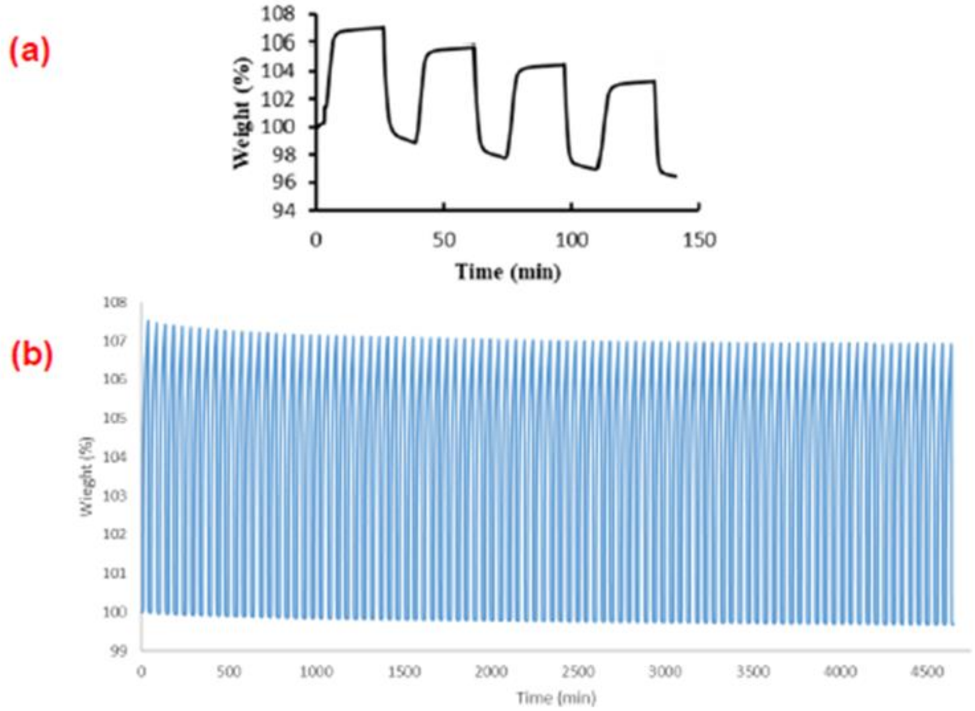

Figure 2: Degradation performance (@ 25°C, 400 ppm CO_2 in dry air) of (a) conventional aminopolymer/silica and (b) modified aminopolymer/silica.

A TEA is being performed as a part of this study. Predicted and target economics results are shown in Table 2.

TABLE 2: DIRECT AIR CAPTURE ECONOMICS

Economic Values	Units	Current R&D Value	Target R&D Value
Cost of Carbon Captured	\$/tonne CO_2	150	100
Cost of Carbon Avoided	\$/tonne CO_2	n/a	n/a
Capital Expenditures	\$/tonne CO_2	n/a	n/a
Operating Expenditures	\$/tonne CO_2	n/a	n/a

Definitions:

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

Cost of Carbon Avoided – Projected cost of capture per mass of CO_2 avoided under expected operating conditions.

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.

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.

Feed Gas Assumptions –

Pressure	Temperature	Composition						
		vol%					ppmv	
		CO_2	H_2O	N_2	O_2	Ar	SO_x	NO_x
14.7 psia	50-105 °F	0.04	variable	78.09	20.95	0.93	trace	trace

Other Parameter Descriptions:

Chemical/Physical Sorbent Mechanism – Chemical adsorption by complex formation.

Sorbent Contaminant Resistance – Selectivity toward CO_2 over H_2O and resistance to O_2.

Sorbent Attrition and Thermal/Hydrothermal Stability – Sorbent attrition is dependent on sorbent coating onto monolith and the monoliths are being prepared using the proprietary formulations of BASF and Daeyoung C&E. Thermal stability is warranted by controlling temperature and pressure conditions for desorption.

Flue Gas Pretreatment Requirements – N/A.

Sorbent Make-Up Requirements – Sorbent make-up rate is determined from long-term cyclic evaluations of the sorbent.

Waste Streams Generated – Waste gases (mostly water).

technology advantages

- Lower degradation rate: longer lifespan.
- Low required desorption energy input (<80 kJ/mol).
- Air contactor requires no external energy input.
- High CO_2 purity (>95%).
- High CO_2 adsorption selectivity.
- Low air-side pressure drop.

R&D challenges

- Development of the sorbent-washcoated monolith structure.
- Establishing the CO_2 adsorption kinetics.

status

The project has begun. A CFD analysis for the air contactor design is underway and lab-scale evaluation of the CO_2 sorbent is progressing.

available reports/technical papers/presentations

Lee, J., 2022, "Energy-Efficient Direct Air Capture System for High-Purity CO_2 Separation." Project Kickoff Meeting. DOE/NETL. Pittsburgh, PA. March 7. *https://netl.doe.gov/projects/plp-download.aspx?id=12948&filename=Energy-Efficient+Direct+Air+Capture+System+for+High+Purity+CO2+Separation.pdf*.