TRAPS: Tunable Rapid-Uptake AminoPolymer Aerogel Sorbent for Direct Air Capture of CO_2

primary project goal

The Palo Alto Research Center Inc. (PARC), in collaboration with Lawrence Livermore National Laboratory (LLNL), is developing a novel solid sorbent for direct air capture (DAC) of carbon dioxide (CO_2). The innovative sorbent, Tunable Rapid-uptake AminoPolymer Aerogel Sorbent (TRAPS) builds on PARC's proprietary polymer aerogel synthesis platform, which will be adapted to produce a polyamine aerogel with a combination of high CO_2 capacity, rapid uptake kinetics, resistance to degradation, and low cost. During the project, PARC is developing the novel TRAPS sorbent and LLNL is testing the performance of the sorbent under DAC-relevant conditions in a lab-scale fixed-bed reactor. TRAPS will yield substantial improvements to process cost, energy consumption, and sorbent lifetime, drastically improving the economic viability of DAC.

technical goals

- PARC will develop a synthesis process to produce polyamine aerogels achieving, at 400 parts per million (ppm) CO_2 in air, high equilibrium CO_2 capacity, rapid uptake rate, and oxidative stability greater than benchmark silica-supported poly(ethylenimine) (PEI).
- PARC will produce sorbent at scales required for fixed-bed performance evaluation and characterize its physical properties to inform the future design of a DAC contactor.
- LLNL will demonstrate the performance of the sorbent under DAC-relevant conditions (400 ppm CO_2) in a lab-scale fixed-bed reactor.
- LLNL will develop a high-level model to assess the performance and cost of a notional DAC process incorporating the sorbent.
- Develop a techno-economic assessment (TEA) to compare against commercial technologies.

technical content

PARC's development of TRAPS solid sorbent for DAC technology will deliver simultaneous advances in all areas identified by the National Academy of Sciences (NAS), with the potential to achieve a disruptive process cost below $100/tonne CO_2, using estimates from the NAS report. The aerogel structure (Figure 1) that results from PARC's proprietary polymerization process provides numerous benefits to the TRAPS sorbent for DAC applications, including:

1. High equilibrium-loading of CO_2 4 mmol/g due to minimization of inert content in the aerogel.
2. High uptake rate (45-minute full cycle) achieved by controlling aerogel structure through synthesis. High specific surface area combined with high amine incorporation provides a large number of accessible surface sites for sorption. Porosity in the mesopore size regime enables efficient gas transport.

program area:
Carbon Dioxide Removal

ending scale:
Laboratory Scale

application:
Direct Air Capture

key technology:
Sorbents

project focus:
Polyamine Aerogel Sorbent for DAC

participant:
Palo Alto Research Center Inc.

project number:
FE0031951

predecessor projects:
N/A

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N/A

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percent complete:
55%

3. Improvement in oxidative stability over conventional ceramic-supported PEI sorbents is expected due to the covalent integration of amines and control of chemical environment.
4. Low sorbent cost due to use of commodity precursors and scalable processes. In the NAS study, the sorbent budget, $50/kg, is higher than the expected cost of the sorbent. The expected long-term cost of TRAPS is in line with cost models that use a carbon price of $100/tonne CO_2.
5. Low minimum sensible heat load due to low content of inert materials.
6. System-integration benefits—the sorbent will be compatible with a variety of schemes for heat integration and regeneration.

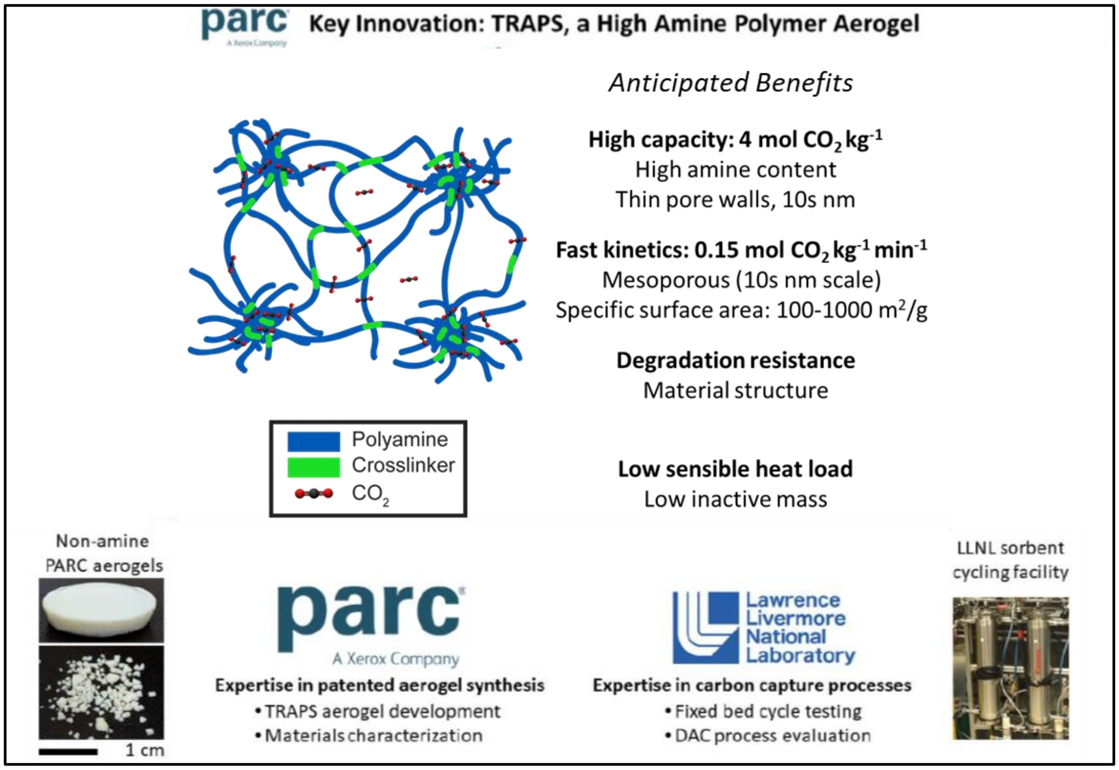

Figure 1. TRAPS concept overview.

Sorbents for DAC are deployed in a variety of contactor designs. PARC's polymerization process has been used to produce aerogels in a variety of form factors ranging from 25–100 µm particles to 0.3 x 10 x 10 cm^3 monoliths. TRAPS could be produced as binder-free pellets, fluidizable particles, or cast onto macroporous substrates. Due to the intrinsic toughness of polymers, TRAPS particles are advantaged in crush- and attrition-resistance over brittle ceramic sorbents.

TABLE 1: DAC SORBENT PROCESS PARAMETERS

Sorbent	Units	Current R&D Value	Target R&D Value
True Density @ STP	kg/m^3	—	1000
Bulk Density	kg/m^3	—	450
Average Particle Diameter	mm	—	Controllable
Particle Void Fraction	m^3/m^3	—	0.3
Packing Density	m^2/m^3	—	0.24 x 10^9
Solid Heat Capacity @ STP	kJ/kg-K	—	1.2
Crush Strength	kg_f	—	2
Attrition Index	-	—	0.4
Thermal Conductivity	W/(m-K)	—	0.14
Manufacturing Cost for Sorbent	$/kg	—	—

Adsorption			
Pressure	bar	—	.0004 CO_2
Temperature	°C	—	25
Equilibrium Loading	g mol CO_2/kg	—	4
Heat of Adsorption	kJ/mol CO_2	—	90-45
CO_2 Adsorption Kinetics	gmol/time	—	0.15 mmolCO_2/g/min
Desorption			
Pressure	bar	—	0.5
Temperature	°C	—	110
Equilibrium CO_2 Loading	g mol CO_2/kg	—	0.4 (remaining)
Heat of Desorption	kJ/mol CO_2	—	90-50
CO_2 Desorption Kinetics	gmol/time	—	0.3 mmolCO_2/g/min

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:

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

technology advantages

- Enable cost less than $100/tonne CO_2, leveraging unique pore characteristics to improve lifetime capture capacity of sorbent.
- Significantly lower energy consumption due to reduced sensible heat load.

- Enable cycle life greater than 10,000 by tuning the chemical environment around amine sites in the aerogel.
- High equilibrium loading is achieved by minimizing inert material in the aerogel.
- High uptake rate 45-minute full cycle is achieved by controlling aerogel structure through synthesis.
- Improvement in oxidative stability over conventional ceramic-supported PEI sorbents.
- Low sorbent cost is enabled by using a demonstrated, scalable polymerization process; high-volume, low-cost precursors; and rapid ambient drying of the aerogel.

R&D challenges

- Adapting synthesis to incorporate amine.
- Maximizing amine content without sacrificing pore structure.
- Achieving long cycle life is a challenge for solid sorbents, in general.

status

PARC prepared amine sorbents using the TRAPS aerogel process and explored two classes of post-processing conditions within each downselected post-process condition to maximize amine content and surface area. Physical properties of the sorbents were studied, including preliminary multi-cycle sorbent stability using thermogravimetric analysis. The initial materials exhibit CO_2 uptake at low CO_2 partial pressures. PARC manufactured sorbent material at the ~5-g-scale for packed-bed testing at LLNL; the porosity was robust for pelletization and handling. PARC is currently investigating the impact of surface area on CO_2 adsorption/desorption and understanding the quantitative correlation between process conditions and amine content.

available reports/technical papers/presentations

Mahati Chintapalli, "TRAPS: Tunable Rapid Uptake AminoPolymer Aerogel Sorbent for Direct Air Capture of CO_2" Direct Air Capture kickoff meeting presentation, Pittsburgh, PA, February 2021. *http://www.netl.doe.gov/projects/plp-download.aspx?id=11045&filename=TRAPS%3a+Tunable+Rapid+Uptake+AminoPolymer+Aerogel+Sorbent+for+Direct+Air+Capture+of+CO2.pdf*.

Mahati Chintapalli, "TRAPS: Tunable Rapid Uptake AminoPolymer Aerogel Sorbent for Direct Air Capture of CO_2" Project kickoff meeting presentation, Pittsburgh, PA, April 2021. *http://www.netl.doe.gov/projects/plp-download.aspx?id=11043&filename=Tunable+Rapid+Uptake+Amino+Polymer+Aerogel+Sorbent+for+Direct+Air+Capture+of+CO2.pdf*.

Mahati Chintapalli, "TRAPS: Tunable Rapid Uptake AminoPolymer Aerogel Sorbent for Direct Air Capture of CO_2" PARC, A Xerox Company, 2021 NETL Carbon Management Research Project Review Meeting, Pittsburgh, PA, August 2021. *https://netl.doe.gov/sites/default/files/netl-file/21CMOG_CDRR_Chintapalli.pdf*