# TRAPS: Tunable Rapid-uptake AminoPolymer Aerogel Sorbent for direct air capture of $CO_2$

DE-FE0031951


Mahati Chintapalli

PARC, a Xerox Company



U.S. Department of Energy

National Energy Technology Laboratory

Carbon Management and Natural Gas & Oil Research Project Review Meeting

Virtual Meetings August 2 through August 31, 2021

# Project Overview

– Funding: $0.8M DOE & $0.2M Cost Share
– Period of performance: 18 months (Feb 2021 – Aug 2022)
– Team:

parc
A Xerox Company

Lawrence Livermore National Laboratory

– Objectives:
  - Synthesize sorbent with high equilibrium capacity (4 mmol/g), rapid uptake rate (0.15 mmol $g^{-1}$ $min^{-1}$), and long oxidative stability
  - Characterize sorbent in a fixed bed reactor at >25 g scale
  - Model performance and cost of a DAC process with the sorbent

# Team and Facilities

## PARC Team





Dr. Jonathan Bachman
Dr. Mahati Chintapalli (PI)
Dr. Gabriel Iftime
Dr. Stephen Meckler
Kay Xia

## Livermore Team



Dr. Nathan Ellebracht (Team Lead)
Dr. Wenqin Li
Dr. Simon Pang

Preliminary characterization @ PARC

Pore characteristics

Sorption


Fixed bed characterization @ LLNL

Gemini: custom fixed bed sorbent testing instrument

# Technology Background

Temperature swing sorbent based on PARC's porous polymer synthesis platform

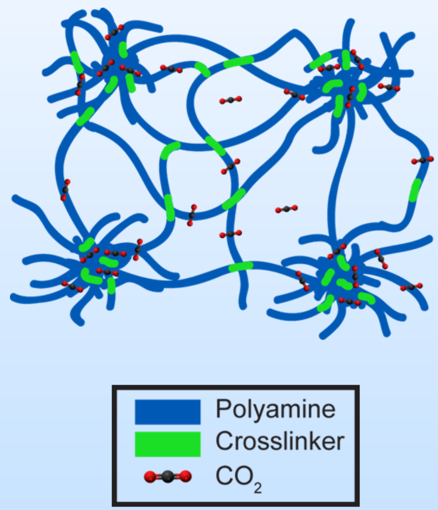
**PARC aerogels:**

- Moderate porosity
- Ambient dried/scalable
- High surface area
- Thin pore walls
- Tunable chemistry
- Variety of formfactors

Develop Sorbent

**Non-sorbent aerogels**


**Key Innovation: Polyamine aerogel**




*Anticipated Benefits*

**High capacity: 4 mol $CO_2$ kg$^{-1}$**
High amine content
Thin pore walls, 10s nm

**Fast kinetics: 0.15 mol $CO_2$ kg$^{-1}$ min$^{-1}$**
Mesoporous (10s nm scale)
Specific surface area: 100-1000 $m^2/g$

**Degradation resistance**
Material structure

**Low sensible heat load**
Low inactive mass

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

# Technology Background

**Envisioned operation:**

Adsorption at ambient conditions

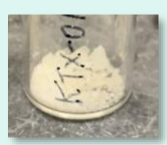
Desorption at < 110 $^{o}C$ (conditions to be explored)

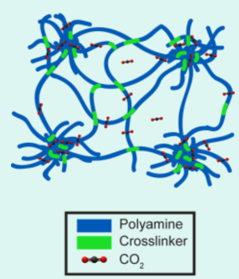
**Prior work**:

High surface area polymer aerogels in other materials


**This project**

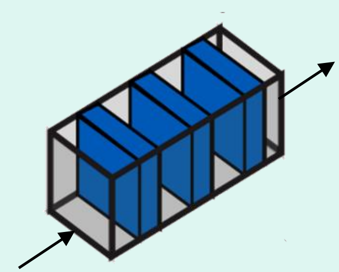
Develop a high capacity $CO_2$ sorbent and demonstrate performance






**Future development**

Sorbent integrated into a contactor design



# Technical Approach/Project Scope

PARC led

**Aerogel formulation development**

Maximize incorporation of amine monomer

**Lab scale characterization**

Show feasibility of meeting target properties

**Scale-up and physical properties**

(1) Produce sorbent for fixed bed testing
(2) Measure attrition/crush strength

LLNL led

**Fixed bed sorbent testing**

Demonstrate Target properties

**Conceptual process design**

Develop projections of cost and energy efficiency

Success Criteria:

- Measure sorbent and physical properties in State Point Table
- Achieve $CO_2$ adsorption up to 4 mmol/g at 0.15 mmol/g/min and desorption down to 0.4 mmol/g at 0.3 mmol/g/min, at 400 ppm in air
- Conceptual process design and cost and performance projections to enable next stage development: integrated prototype and field testing

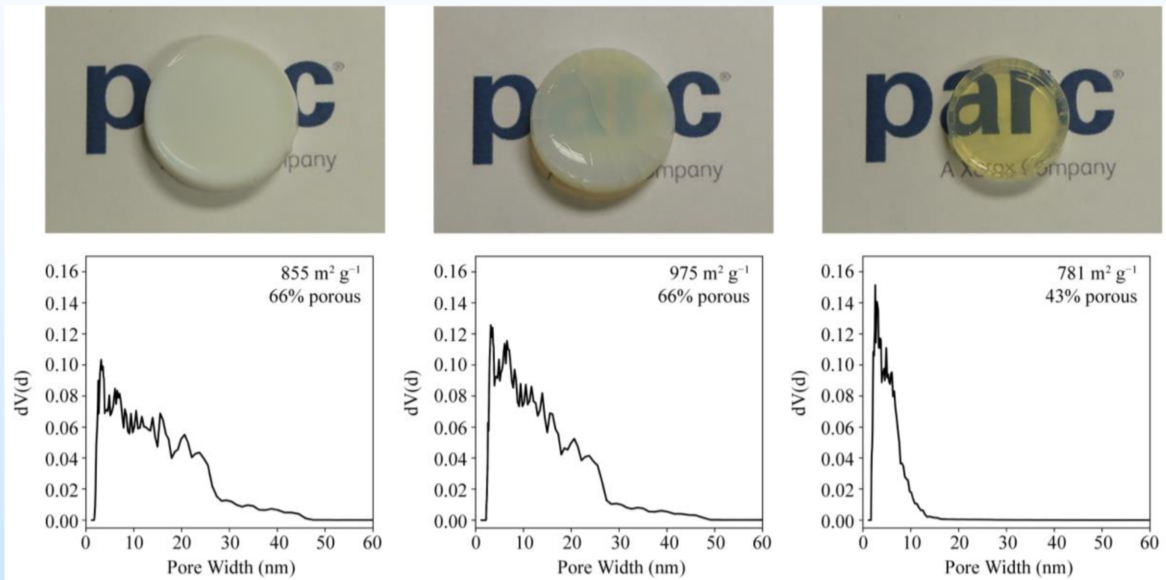
# Current Status

## Technology status prior to project

Conventional method

PARC synthesis method

Non-sorbent, ambient-dried materials

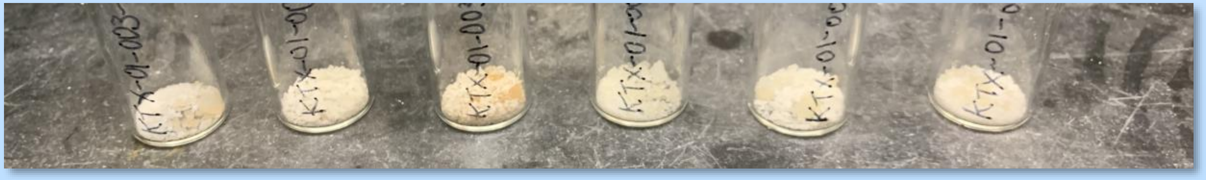



- Pore size and porosity control through proprietary synthesis conditions
- Surface area: surface functionalization, $CO_2$ uptake
- Porosity: heat capacity and thermal conductivity, durability

# Polymer aerogel synthesis adapted to incorporate amine


New to this project: adapted solvent exchange (“post-processing”)

- Project Challenge 1 addressed
- Explored two classes of post-processing and conditions within each
- Down-selected post-process conditions to maximize amine content and surface area
- Gen 1 process conditions fixed to enable exploration of formulation space → Challenge 2



# Testing capabilities established

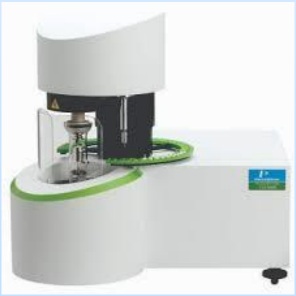
- Physical characterization: $N_2$ adsorption, elemental analysis, FTIR
- Adsorption isotherms: $CO_2$ adsorption isotherms
  - Capability established at PARC
  - Next steps: extend to lower pressure measurements
- Preliminary cycling: TGA in dry and 30% RH
  - Installation of automatic cycling planned for Aug
- Fixed bed breakthrough testing (LLNL)
  - First materials sent

**Preliminary characterization @ PARC**

Pore characteristics
Isotherms

+

Sorption



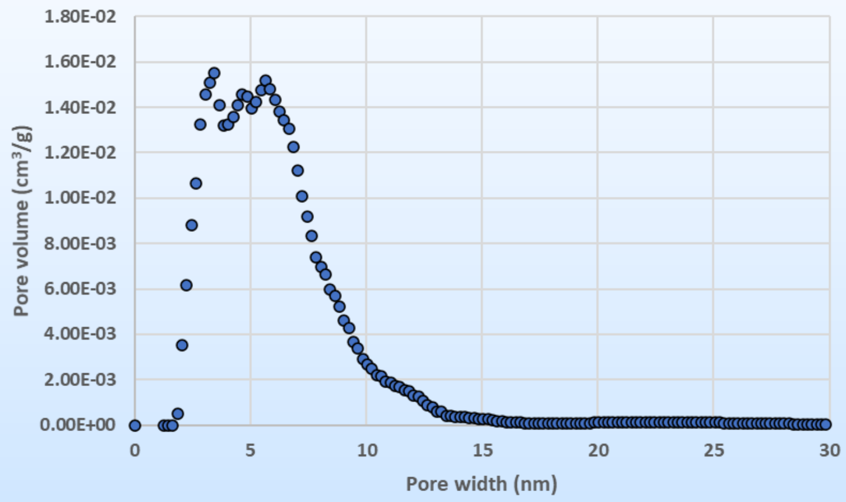
**Fixed bed characterization @ LLNL**


Gemini: custom fixed bed sorbent testing instrument

# Produced amine-containing materials with high surface area

| Gel composition | Process Conditions | Surface area (m²/g) |
|---|---|---|
| No amine | None/NA | 964 |
| Low amine | none | 470 |
| | Process 2.0 | 275 |
| | Process 1.0 | 346 |
| Baseline amine | none | 199 |
| | Process 2.0 | 24 |
| | Process 1.0 | 123 |
| | Process 2.1 | **522** |

Baseline amine formulation, Process 2.1, pore size distribution

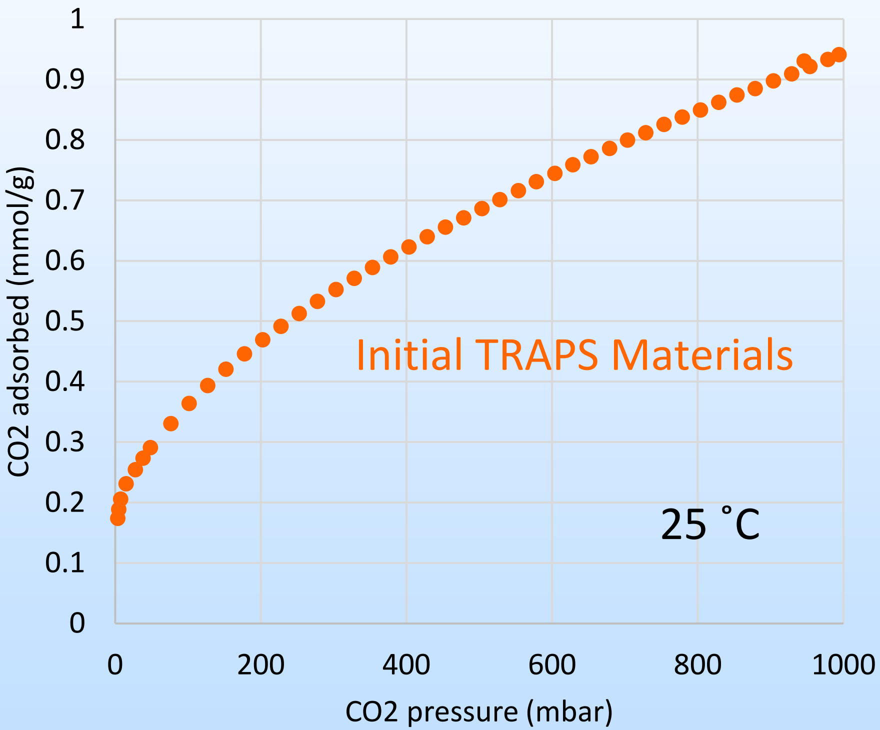



- Process 2.0 yields lower specific surface area than Process 1.0
- The lower surface area is reversible via Process 2.1
- Process 2.1 leads to highest amine content and most promising pore structure
- **Surface area of 522 m²/g** is significantly higher than typical ceramic-supported sorbents

**Investigations in progress:**

- Impact of surface area on $CO_2$ adsorption/desorption
- Quantitative correlation between process conditions and amine content

# Initial sorption experiment shows $CO_2$ uptake




- Initial, unoptimized material shows $CO_2$ uptake

**Next steps**

- Improve uptake with formulation and process conditions
- Explore sorption at different temperatures
- Upgrade instrument to study low pressure regime

# Synthesized material for breakthrough testing

- Materials exchanged with LLNL for benchmarking and breakthrough testing in a fixed bed column
- Produced material at ~5 g scale for breakthrough testing
- Porosity is robust to pelletization and handling

Un-pelletized Pelletized

| Sample | BET surface area ($m^2/g$) |
|---|---|
| Un-pelletized | 250 |
| Pelletized | 230 |

# Plans for future development

This project: TRL 2 → TRL 3

Primary focus: validating materials performance (capacity, kinetics, longevity)

**Today**:

High specific surface area amine-containing materials generated

**End of Project:**

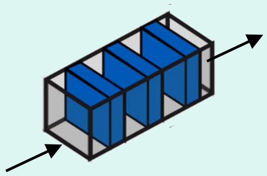
Concept validation & data to inform integrated prototype design

**Next Steps:**

Integrated prototype, field testing, pilot testing

**Future development**

Sorbent integrated into a contactor design

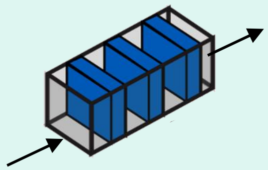


- Contactor designs
- Integration with energy sources
- Integration with downstream processes
    - Utilization
    - Compression/sequestration

# Opportunities for Collaboration

**Future development**

Sorbent integrated into a contactor design



- Contactor designs
- Integration with energy sources
- Integration with downstream processes
  - Utilization
  - Compression/sequestration

Partnerships for further technology development:

- Detailed design of integrated DAC system
- Passive or low pressure drop systems
- Field and pilot unit construction and testing
- Technology commercialization

Collaboration with PARC/Xerox: engage@parc.com

- Multidisciplinary research: materials, hardware systems, software
- Cleantech strategic business unit for technology commercialization

# Summary Slide

**Achievements in first quarter:**

- Adapted synthesis process to incorporate materials with amine
- Downselected post-process conditions
- Initial materials exhibited $CO_2$ uptake at low pressures
- Materials with specific surface area >500 $m^2/g$ were obtained

**Next steps:**

- Characterization of $CO_2$ adsorption/desorption performance:
  - Lab scale
  - Fixed bed testing
- Shift focus to Formulation Challenges 2 and 3:
  - Maximizing amine content and pore structure
  - Formulation for cycle life/degradation resistance

# Appendix

# Organization Chart

parc
A Xerox Company

**Dr. Mahati Chintapalli** *PI*

parc
A Xerox Company

**Dr. Stephen Meckler**
*Technical lead*

**Dr. Jonathan Bachman**
*Materials characterization Lead*

**Kay Xia**
*Material synthesis intern*

**Dr. Gabriel Iftime**
*Synthesis advisor*

Lawrence Livermore National Laboratory

**Dr. Nathan Ellebracht**
*LLNL Lead*
*Process design*

**Dr. Wenqin Li**
*Process design lead*
*Cost assessment*

**Dr. Simon Pang**
*Materials assessment*
*Process design*

| Task | Key Personnel | |
|---|---|---|
| | parc A Xerox Company | Lawrence Livermore National Laboratory |
| 1: Project management | Dr. Mahati Chintapalli | Dr. Nathan Ellebracht |
| 2: Develop aerogel formulations | Dr. Stephen Meckler<br>Kay Xia | |
| 3: Lab scale aerogel characterization | Dr. Jonathan Bahcman | |
| 4: Aerogel scale-up & Physical characterization | Dr. Stephen Meckler | |
| 5: Fixed bed sorbent testing | | Dr. Nathan Ellebracht<br>Dr. Simon Pang |
| 6: Conceptual DAC process design | | Dr. Wenqin Li |

# Gantt Chart – Tasks Led by PARC

**Task 1.0: Project Management and Planning**

1.1 - Project Management Plan

1.2 - Technology Maturation Plan

1.3 – Quarterly update reports

**Task 2.0: Develop Aerogel Formulations**

2.1 - Develop baseline aerogel formulation

2.2 - Aerogel formulation with high amine content

**Task 3.0: Lab Scale Aerogel Characterization**

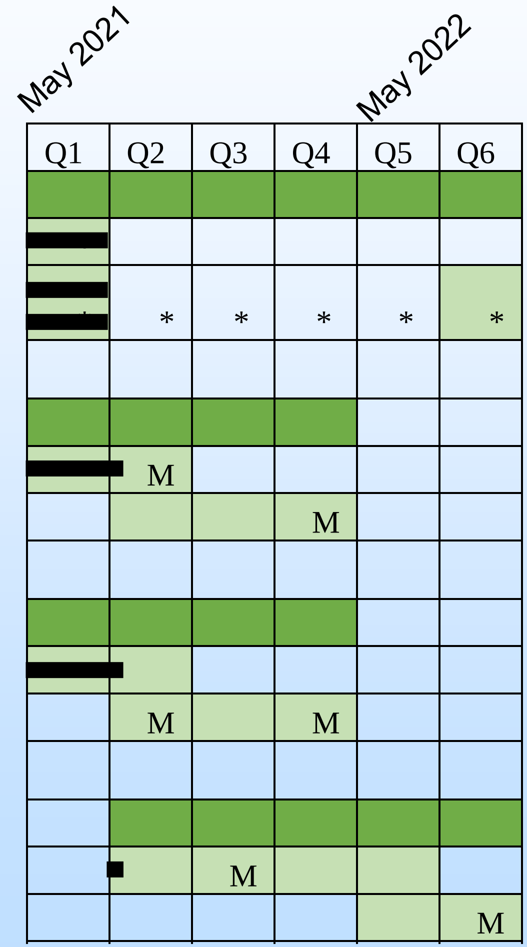
3.1 - Develop and validate test procedures

3.2 - Detailed sub-gram scale testing

**Task 4.0: Aerogel Scale-up and Physical Characterization**

4.1 - Scale-up formulations

4.2 - Measure sorbent physical properties



# Gantt Chart – Tasks Led by LLNL

May 2021 | May 2022

| | Q1 | Q2 | Q3 | Q4 | Q5 | Q6 |
|---|---|---|---|---|---|---|
| | | | | | | |
| **Task 5.0: Fixed Bed Sorbent Testing** | | | | | | |
| 5.1 - Fixed bed testing of sorbents | | | | M | M | |
| 5.2 - Optimization of fixed bed process conditions | | | | | | M |
| | | | | | | |
| **Task 6.0: Conceptual DAC process design** | | | | | | |
| 6.1 - Develop and analyze high level process flow | | | M | | | |
| 6.2 - Develop a cost projection | | | | M | | M |