TRAPS: Tunable Rapid-uptake AminoPolymer Aerogel Sorbent for direct air capture of CO$_2$
DE-FE0031951

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PARC, a Xerox Company

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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](parc.png) ![Lawrence Livermore National Laboratory](LLNL.png)

- 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

Non-sorbent aerogels

Key Innovation: Polyamine aerogel

Anticipated Benefits
- High capacity: 4 mol CO$_2$ kg$^{-1}$
- Fast kinetics: 0.15 mol CO$_2$ kg$^{-1}$ min$^{-1}$
- Degradation resistance
- Low sensible heat load
- High amine content
- Thin pore walls, 10s nm
- Mesoporous (10s nm scale)
- Specific surface area: 100-1000 m$^2$/g
- 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 °C (conditions to be explored)

Prior work:
High surface area polymer aerogels in other materials

This project
Develop a high capacity CO₂ 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

- Pore size and porosity control through proprietary synthesis conditions
- Surface area: surface functionalization, CO$_2$ uptake
- Porosity: heat capacity and thermal conductivity, durability

Non-sorbent, ambient-dried materials
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\textsubscript{2} adsorption, elemental analysis, FTIR
- Adsorption isotherms: CO\textsubscript{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

- 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 CO₂ adsorption/desorption
- Quantitative correlation between process conditions and amine content
Initial sorption experiment shows CO$_2$ uptake

Initial TRAPS Materials

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

<table>
<thead>
<tr>
<th>Sample</th>
<th>BET surface area (m²/g)</th>
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</thead>
<tbody>
<tr>
<td>Un-pelletized</td>
<td>250</td>
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<tr>
<td>Pelletized</td>
<td>230</td>
</tr>
</tbody>
</table>
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

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
Achievements in first quarter:
• Adapted synthesis process to incorporate materials with amine
• Downselected post-process conditions
• Initial materials exhibited CO₂ uptake at low pressures
• Materials with specific surface area >500 m²/g were obtained

Next steps:
• Characterization of CO₂ 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
Organization Chart

Key Personnel

Dr. Mahati Chintapalli  PI

Dr. Stephen Meckler  Technical lead

Dr. Jonathan Bachman  Materials characterization Lead

Kay Xia  Material synthesis intern

Dr. Gabriel Iftime  Synthesis advisor

Dr. Nathan Ellebracht  LLNL Lead  Process design

Dr. Wenqin Li  Process design lead  Cost assessment

Task

1: Project management  Dr. Mahati Chintapalli  Dr. Nathan Ellebracht

2: Develop aerogel formulations  Dr. Stephen Meckler  Kay Xia

3: Lab scale aerogel characterization  Dr. Jonathan Bachman

4: Aerogel scale-up & Physical characterization  Dr. Stephen Meckler

5: Fixed bed sorbent testing  Dr. Nathan Ellebracht  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

<table>
<thead>
<tr>
<th>Task 5.0: Fixed Bed Sorbent Testing</th>
<th>Q1</th>
<th>Q2</th>
<th>Q3</th>
<th>Q4</th>
<th>Q5</th>
<th>Q6</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1 - Fixed bed testing of sorbents</td>
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<tr>
<td>5.2 - Optimization of fixed bed process conditions</td>
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<table>
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<tr>
<th>Task 6.0: Conceptual DAC process design</th>
<th>Q1</th>
<th>Q2</th>
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<td>6.2 - Develop a cost projection</td>
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