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

DE-FE0031951

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PARC, a Xerox Company

U.S. Department of Energy

National Energy Technology Laboratory
Carbon Management Project Review Meeting
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Project Overview

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

Mahati Chintapalli
Jonathan Bachman
Gabriel Iftime
Norine Chang
Youkabed Ostadhossein

parc
A Xerox Company

Materials Development
Materials Downselection

Lawrence Livermore National Laboratory

Nathan Ellebracht
Elwin Hunter Sellars
Melinda Jue
Wenqin Li
Simon Pang

Fixed bed testing
Process model

- 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

Technology Background

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

PARC aerogels:

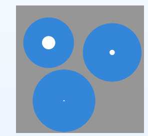
- Moderate porosity
- Ambient dried/scalable
- High surface area
- Thin pore walls
- Tunable chemistry
- Variety of formfactors

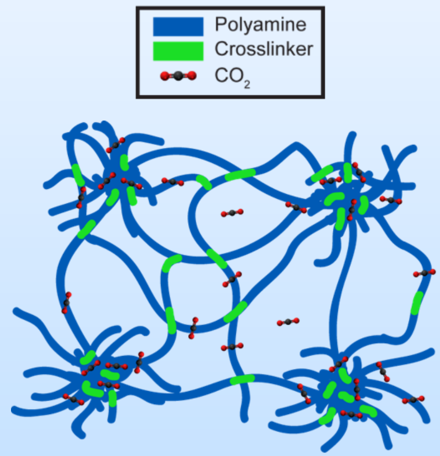
Non-sorbent aerogels

Develop Sorbent

Key Innovation: Polyamine aerogel

Bottom-up porosity, vs. pore-functionalized sorbents





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:

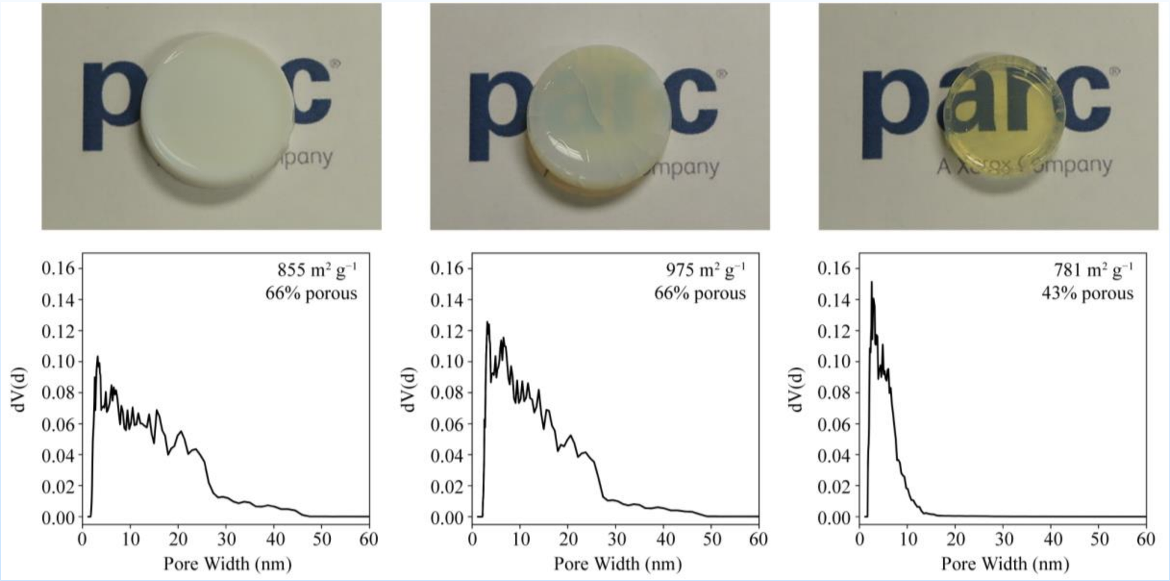
- Adapting synthesis to incorporate amine
- Maximizing amine content without sacrificing pore structure
- Achieving long cycle life is a challenge for solid sorbents, in general

Technology Background: Polymer aerogel platform

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: presentation of functional groups (CO_2 capacity)
- Porosity:
  - gas transport (CO_2 cycle rate, lifetime)
  - thermal transport (heat capacity/thermal conductivity)

Project Scope

Envisioned operation:

Adsorption at ambient conditions

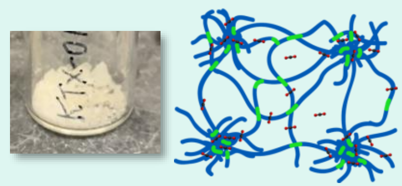
Desorption at < 110 °C (conditions to be explored)

Prior work:

High surface area polymer aerogels in other materials

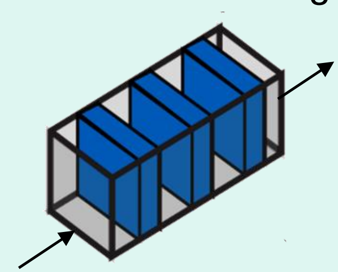
This project

Develop a high capacity CO_2 sorbent and demonstrate performance



Future development

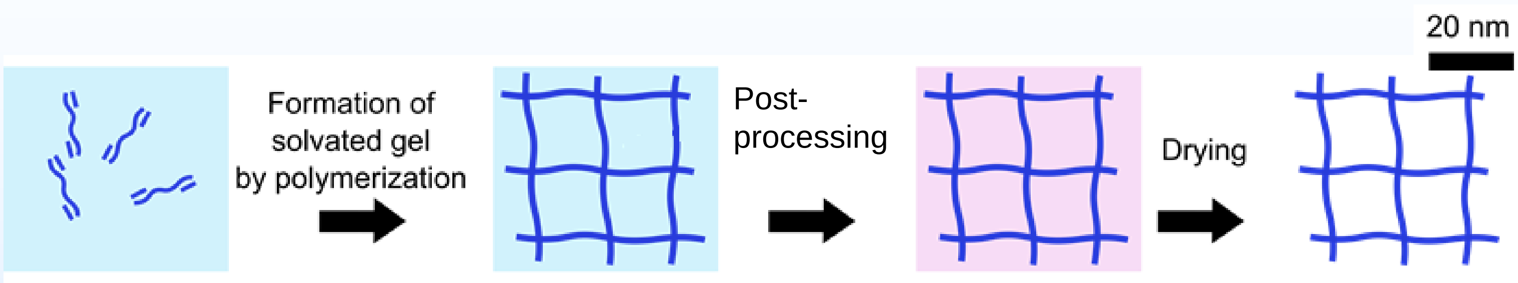
Sorbent integrated into a contactor design



- 1 Budget Period, 2/16/2021 to 3/31/2023 (with no cost extension)
- Key milestone: 4 mmol/g capacity, 0.015 mmol/g/min rate, cycle life better than PEI/SBA-15
- Qualitative objectives:
  - Make sorbent combining MOF-like performance and polymer-like manufacturability
  - Mature the technology to the point where a contactor can be designed

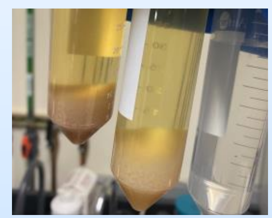
Sorbent production process

Monomer(s)
+ solvent
+ cross-linkers
+ additives



Cast, as-polymerized monoliths

Crushed solvated gels



Post-processed, dried powder

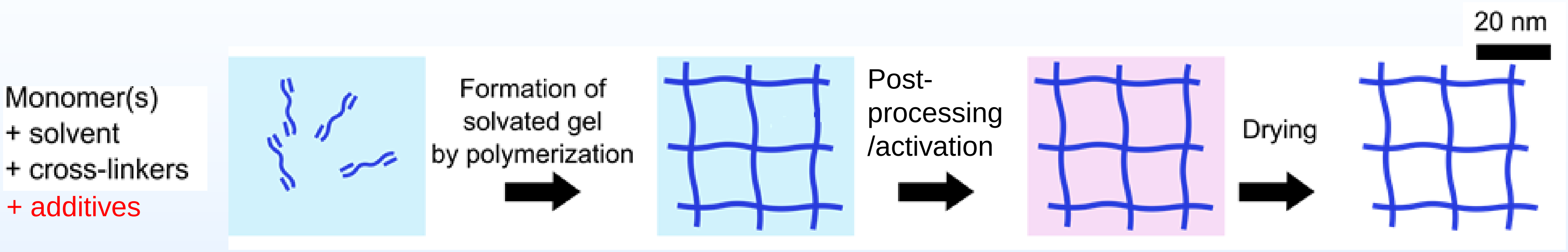
Options for structured sorbent production (future work)

Cast, as monolith → **Post-process** → **Use as directly as structured sorbent**

Cast, as monolith → **Crush to powder** → **Post-process** → **Wash coat onto structure**

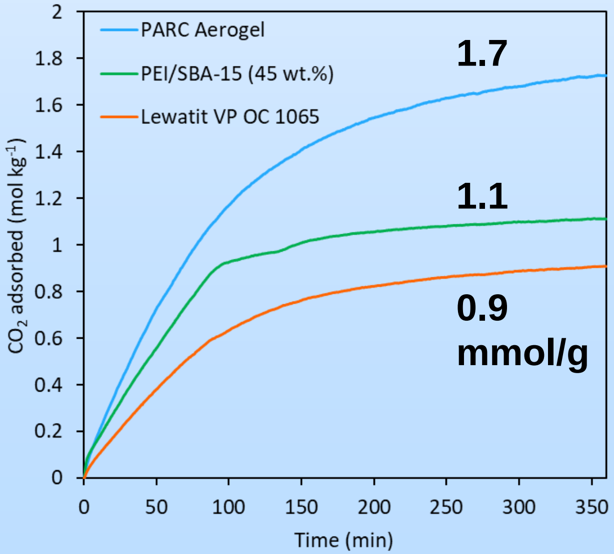
- For lab scale experiments, we crush and use as a powder for expediency
- Direct structuring is interesting for durability, performance, and reduction of parasitic heat loads

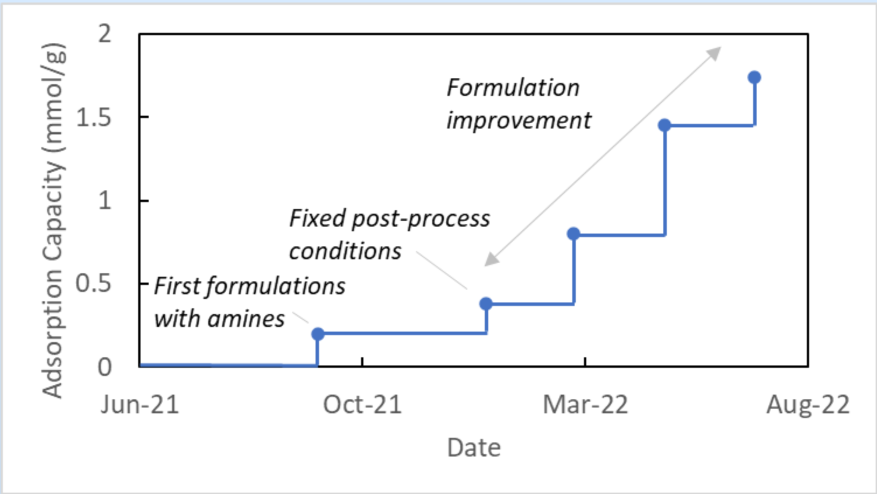
Achieved higher capacity than benchmark sorbents via formulation



- Established a fixed procedure for post-processing/activation
- Explored numerous variations in polymerization formulation and processing
- Initial characterization focus: Adsorption capacity at ~400 ppm, by TGA

Adsorption in 410 ppm CO_2 in N_2 @ 25°C

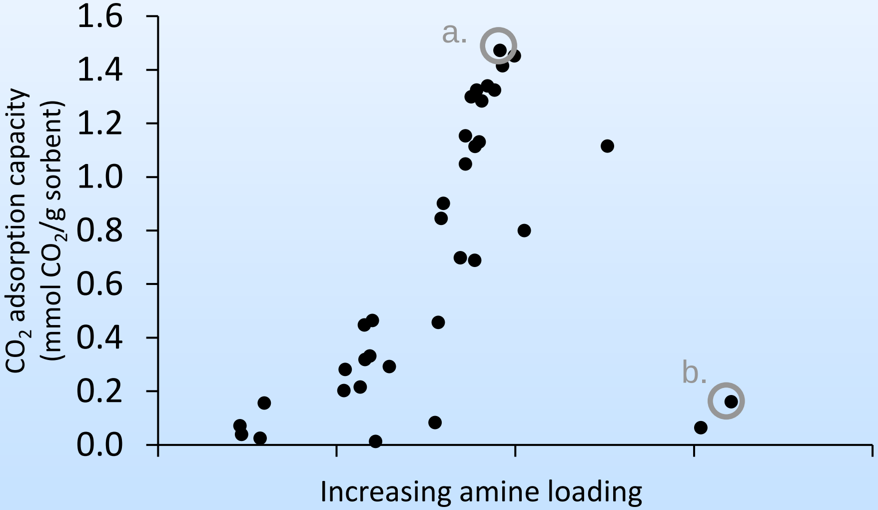




Amine loading drives capacity improvement

- Improvement to properties could be driven by several factors:
  - Total amine loading
  - Amine utilization: pore structure changing accessibility, or other mechanisms

Adsorption capacity vs. amine loading across formulations



- Pore characteristics vary unpredictably across range
- Equilibrium adsorption is driven by amine loading
- Too much amine leads to pore collapse and loss of capacity

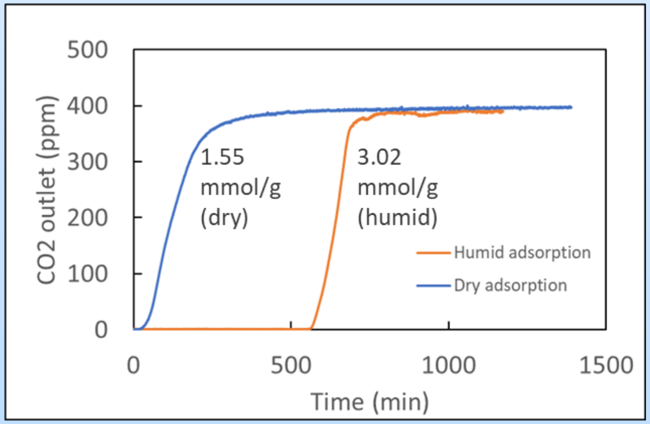
- Next steps:
  - Does cycle rate correlate to pore structure?
  - Get better resolution around the turn-off point

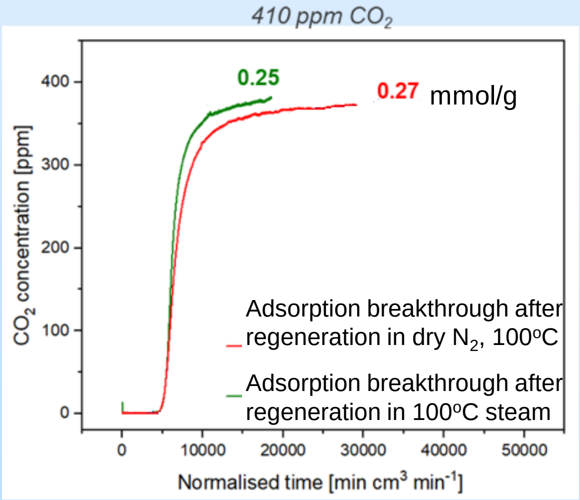
	Samples like a.	Samples like b.
Porosity %	20 - 50	Non-porous
Pore size (nm)	~1 nm – 1 micron	N/A
Specific surface area	50 - 500	N/A

High capacities achieved under humid adsorption

- Fixed bed testing experiments performed by LLNL
  - Adsorption under dry and humid conditions
  - Desorption under N_2, humidity, or steam
- ~2x adsorption enhancement under humid conditions, consistent with bicarbonate forma
  - Consistent with bicarbonate adsorption mechanism (1:1 CO_2 to amine)
- Initial exposure to steam regeneration shows retention of adsorption capacity
- Best sample in humid adsorption: **3.6 mmol/g** at 410 ppm CO_2 & 25 °C

Breakthrough curves in
dry and humid adsorption conditions

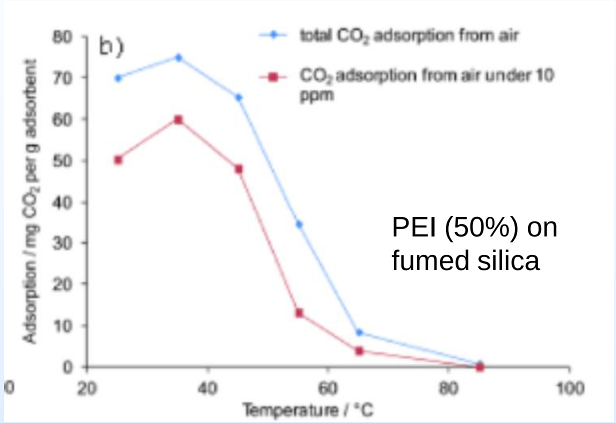




*older generation sample with lower capacity

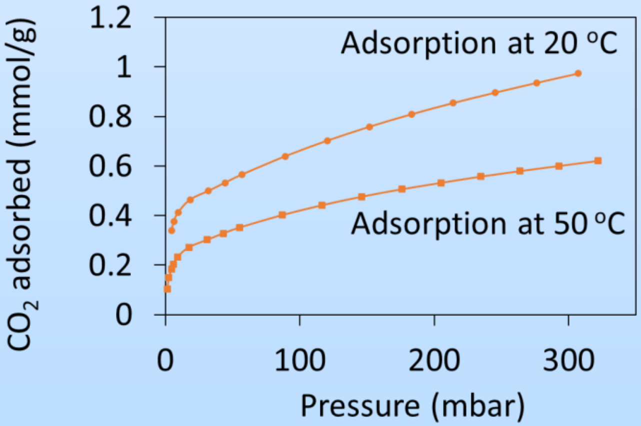
Adsorption decreases with temperature due to porous structure

- Some supported amine sorbents requite thermal activation to maximize adsorption capacity
  →kinetic barrier to gas interaction
- Our sorbent shows monotonic decrease in adsorption with temperature
  →Porous structure makes amines accessible
- Elevated temperature is not needed to maximize adsorption in air:
  beneficial for reducing oxidation



ChemSusChem 2014, 7, 1386−1397

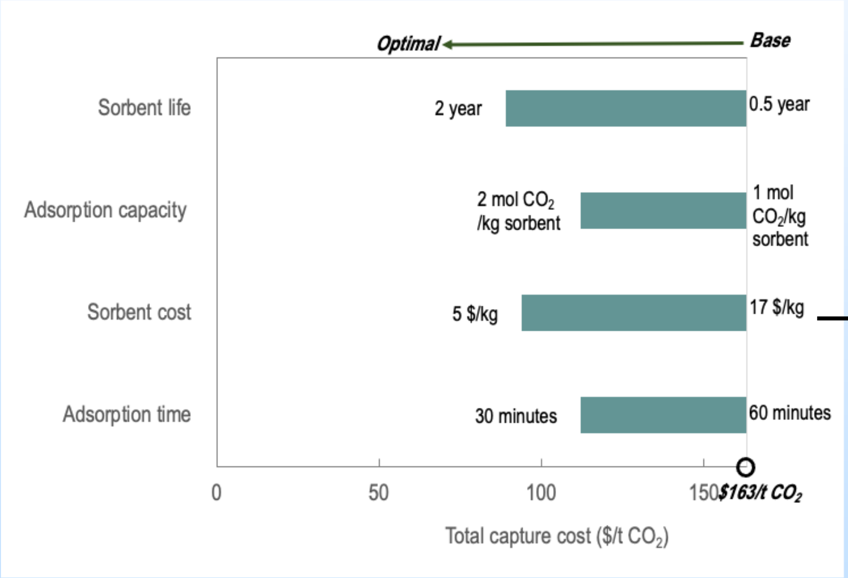
Adsorption isotherms at different temperatures for PARC sorbent



Pathway to $\$100/tCO_2$

High level process model by LLNL shows current cost to capture of ~$160/t-$CO_2$

- Current sorbent outperforms baseline capacity
- Further validation underway for sorbent **cost at scale**, **lifetime**, and **cycle rate**



- Current sorbent production estimate: $25/kg
- Materials dominate—50% of cost
- Scaled process conditions under validation

- Sorbent accounts for 60% of cost
- Energy accounts for 30% of cost
- Pumps, fans, etc: 10% of cost

Environ Sci Technol 2020; 54: 7542–7551.

Technology next steps: Characterization & Contactors

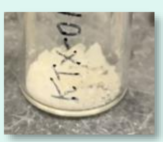
This project next steps

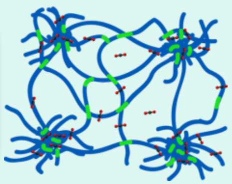
*Cycle rate

*Working capacity

*Lifetime

*Optimized process conditions



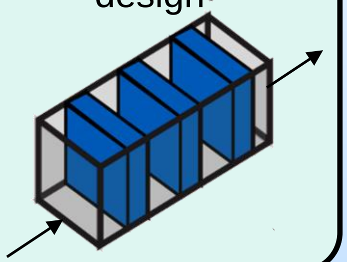


Point-source capture offshoot
EERE-AMO:
DE-EE0009420

Moisture-swing offshoot
ARPA-E:
DE-AR0003300

Future development

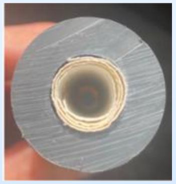
Sorbent integrated into a contactor design



1. Production of structured, scaled-up sorbents
   - Coat powders onto supports, or…
   - Cast resin into support: send us supports!
   - Scale-up + refine production cost model

Crushed to powder

vs.



Cast onto support (flexible membrane)

2. Integration and testing of low pressure drop contactor designs
   - Seeking next phase DOE or commercial funding

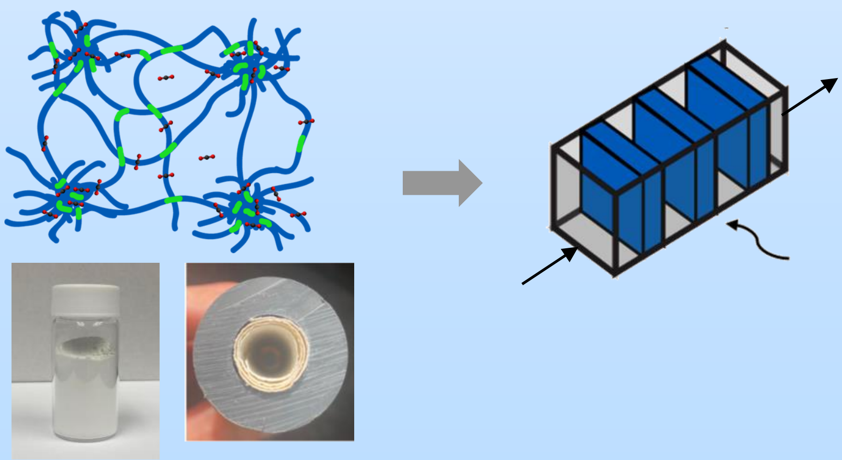
3. Exploration of tech-to-market pathways
   - Materials licensing vs. module development
   - Licensing / Joint venture / Spin-out

Conclusions

- Produced all-polymer porous material with equilibrium capacity 3.6 mmol/g under humid adsorption conditions
- Sorbent has potential to be compatible with steam-regeneration

- Characterization of process-dependent properties under-way:
  - Cycle time
  - Working capacity
  - Lifetime

- Seeking funding to raise TRL from lab scale material to bench-scale structured contactor
- Seeking partnerships to enable commercialization



Acknowledgements

- **FECM**: DE-FE0031951, Andy O'Palko, Nicole Shamitko-Klingensmith, Naomi O'Neil
- **PARC**: Jon Bachman, Gabriel Iftime, Norine Chang, Youkabed Ostadhossein
- **LLNL**: Nathan Ellebracht, Simon Pang, Elwin Hunter Sellars, Melinda Jue, Wenqin Lu

Appendix

Organization Chart

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 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 Dr. Simon Pang
6: Conceptual DAC process design		Dr. Wenqin Li

Gantt Chart – Tasks Led by PARC

PARC

Revision 06/06/2022

	Q1	Q2	Q3	Q4	Q5	Q6	Q7	End
Due date in SOPO	(8/30/2021)	########	2/28/2022	5/31/2022	8/31/2022	########	2/28/2022	3/31/2023
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		✓M						
2.2 - Aerogel formulation with high amine content				✓M				
Task 3.0: Lab Scale Aerogel Characterization								
3.1 - Develop and validate test procedures								
3.2 - Detailed sub-gram scale testing				✓M	M†			
Task 4.0: Aerogel Scale-up and Physical Charac								
4.1 - Scale-up formulations			✓M					
4.2 - Measure sorbent physical properties						**M†**		

Gantt Chart – Tasks Led by LLNL

LLNL

Revision 06/06/2022

	Q1	Q2	Q3	Q4	Q5	Q6	Q7	End
Due date in SOPO	(8/30/2021)	########	2/28/2022	5/31/2022	8/31/2022	########	2/28/2022	3/31/2023
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†**

Technology Background (2-3 Slides)

Use the guidance from this slide for individual technology development efforts.

a. Describe how the technology is envisioned to work in operation, including a simple schematic labeled with preferred operating conditions (e.g., pressures and temperatures), and any other requirements
b. Describe fundamental science driving technology (chemistry, thermodynamics, etc.)
c. Discuss technology development efforts prior to current project (e.g., previous lab and/or bench-scale testing)
d. List and briefly describe the technical and/or economic advantages of your technology.
e. List and briefly describe the technical and economic challenges of your technology.

Technology Background (2-3 Slides)

Use the guidance from this slide for field related sites and pilot projects.

- Technology /Site Selection
- For capture and conversion projects, describe fundamental science behind the technology selected (chemistry, thermodynamics, etc.)
- For storage projects, describe the rational or approach to site selection – just the major factors that controlled the decisions.
- For capture/conversion/use projects, discuss technology development efforts prior to current project (e.g., previous demonstration/scale)
- For storage projects, briefly outline the site characterization efforts
- List and briefly describe the technical and/or economic advantages of your technology or site.

Technical Approach/Project Scope (1-2 Slides)

a. Experimental design or project steps and work plan
b. Project schedule – just provide key milestones; do not include a detailed Gantt chart
c. Project success criteria
d. Project risks and mitigation strategies