AIR2CO2: Advanced Integrated Reticular Sorbent-Coated System to Capture CO_2 from the Atmosphere

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U.S. Department of Energy

National Energy Technology Laboratory

Carbon Management and Natural Gas & Oil Research Project Review Meeting

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Program Overview

$1 MM program (20% cost share)

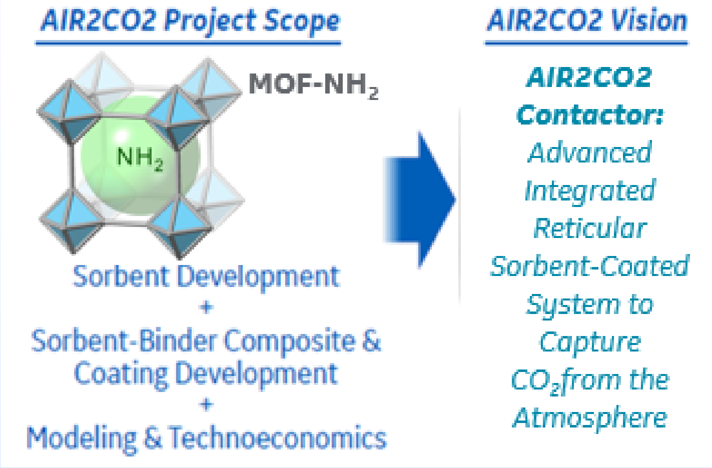
15-month program: 10/1/2020 to 12/31/2021

Project Participants:

- GE Research
- University of California, Berkeley

Overall Project Objectives:

Demonstrate AIR2CO2 material system that integrates pioneering metal-organic framework (MOF) sorbents and sorbent-binder composite coatings to capture and release atmospheric CO_2.



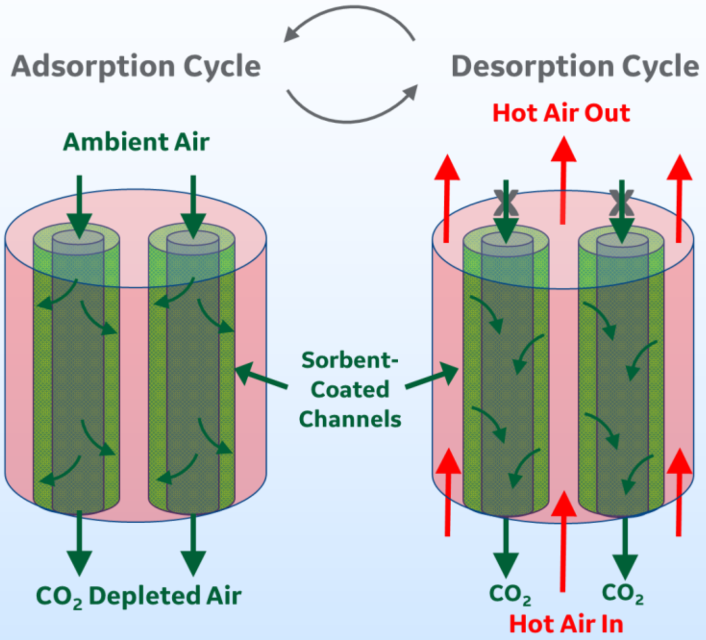
GE Research

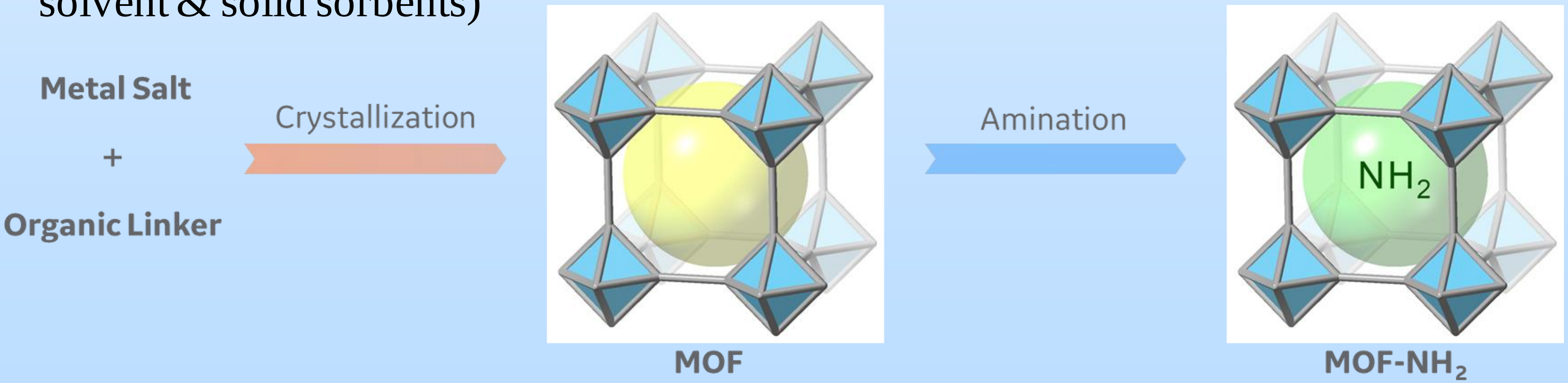
Berkeley
UNIVERSITY OF CALIFORNIA

Technology Background

Two contactors operate in alternating adsorption and desorption modes to continuously remove CO_2 from air. Technical/economic advantages include:

- high amine loading of MOFs (3.3 gmol/kg)
- high thermal stability inherent to MOFs
- MOFs can be designed to exhibit high hydrolytic stability
- High CO_2 capacity, fast sorption kinetics, and novel contactor designs would reduce energy requirements by 60-70% vs state of the art DAC systems (liquid solvent & solid sorbents)





Technical Approach/Project Scope

Experimental design and work plan

Develop a sorbent-binder formulation that provides an adherent, thermally-stable coating to efficiently capture CO_2 from a simulated air stream under DAC relevant conditions.

Project schedule

- Manufacture 1 kg of benchmark sorbent
- Build AIR2CO2 lab-scale test apparatus
- Develop sorbent-binder composite coating; target CO_2 capacity = 3.2 mol/kg MOF
- Develop system and techno-economic models
- Integrate next generation sorbent-binder composite coating into contactor structure

Project success criteria

Demonstrate DAC performance with improved adsorption equilibrium loading, lower heat of desorption, and rapid sorption kinetics to enable a scalable, compact AIR2CO2 contactor design that reduces equipment size and pressure drop, and results in 60-70% lower energy requirements than current state-of-the-art solutions.

Project Risks & Mitigation Strategy

Perceived Risk	Mitigation/Response Strategy
Technical/Scope Risks:	
Insufficient sorbent capacity, slow CO_2 capture/release kinetics & thermal/hydrolytic instability	Tailor chemical architectures and synthetic approaches across MOF material class to maximize amine functional group density, minimize heat of desorption, and strengthen chemical stability.
Sorbent integration process and materials incompatibility result in rapid system degradation	Iterate on binder/slurry coating formulations and additive printing processes to improve structure, adhesion, coating thickness, and thermal transfer
Suboptimal AIR2CO2 contactor form and function results in large pressure drops	Leverage GE Additive expertise and explore DMLM & Binder Jet 3D designs to balance surface area, wall thicknesses & hydraulic diameters
Management, Planning, and Oversight Risks:	
Ineffective selection of sorbent materials, contactor designs & coating processes	Leverage Six Sigma statistical tools and detailed success criteria to downselect and advance technologies
EH&S Risks:	
Potential for sorbent decomposition results in downstream extractables/contaminants	Sorbent cycle life and CO_2 release effluent will be characterized, and possible by-products of side reactions analyzed
Potential for chemical hygiene, high temperature, or mechanical hazard near misses or incidents	GE and UCB will employ rigorous institutional standards & processes; leverage EHS personnel to ensure safety and compliance
External Factor Risks:	
COVID-19 pandemic hinders partnering & supply chain	Leverage virtual communication tools to facilitate technical sharing; proactively work with vendors and sourcing to ensure timely delivery

Progress and Current Status of Project

Test Equipment:

AIR2CO2 lab-scale test apparatus designed and assembled at GE Research for evaluation of MOF-binder composite formulations under DAC relevant conditions.

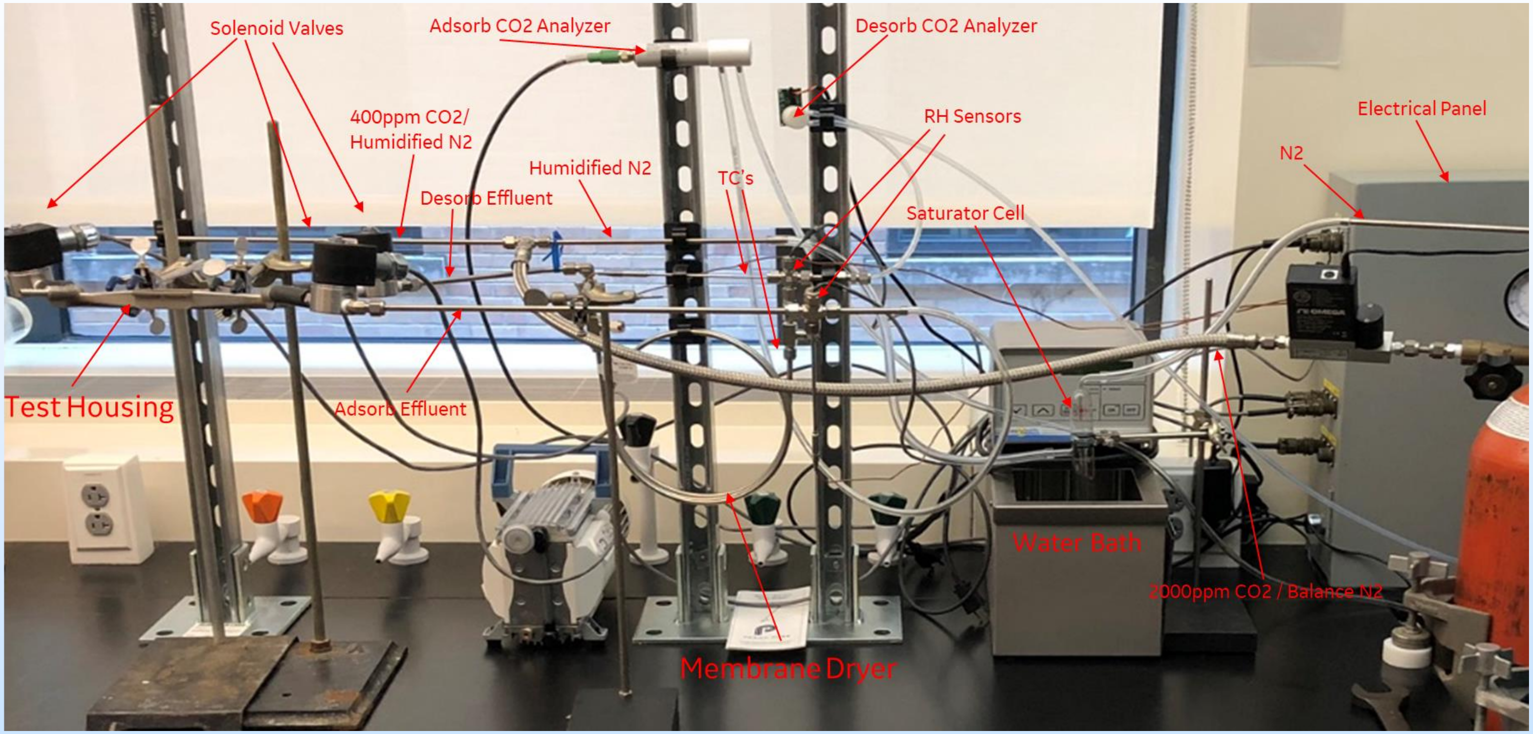
Significant accomplishments:

- ✓ 1 kg benchmark MOF successfully scaled
- ❑ Next generation, high-capacity sorbent under development
- ✓ AIR2CO2 lab-scale test apparatus commissioned
- ✓ Coating formulation developed which demonstrates 80% of native sorbent sorption performance and excellent adhesion to substrate.

Performance achieved so far:

Leading MOF-binder composite formulations exhibit only a ~20% decrease in sorption capacity versus the powdered sorbent. This is consistent with projected performance of the envisioned AIR2CO2 contactor relative to the powdered MOF as outlined in the state point data table.

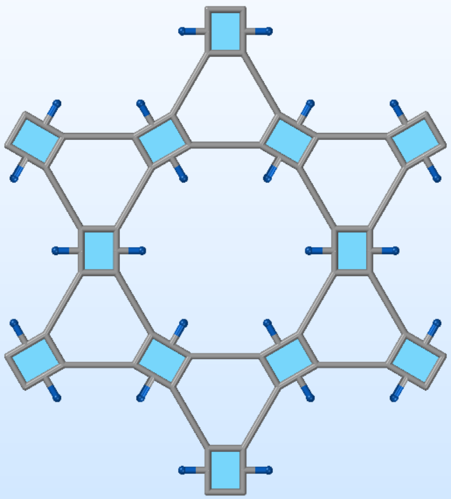
AIR2CO2 Test Apparatus



- Up to 100 sccm 400 ppm CO_2 in N_2 gas flow rate; $T_{ads} = 20°C$; $T_{des} = 120°C$
- Up to 80% RH achievable
- Sorption chamber holds up to 4 MOF-binder composite coated coupons for CO_2 capture performance testing
- Flanges being designed to house 3D components described below for evaluation.

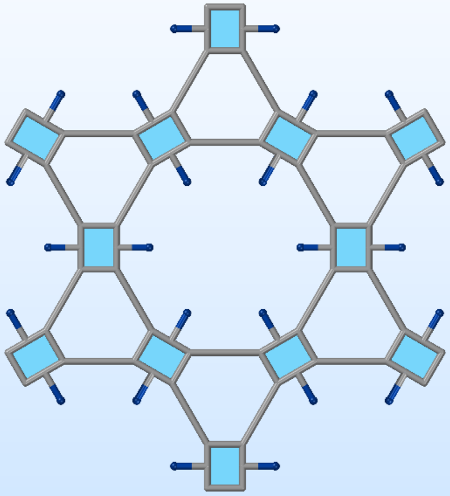
Sorbent Progress

Benchmark Sorbent **Next-Generation Sorbents**



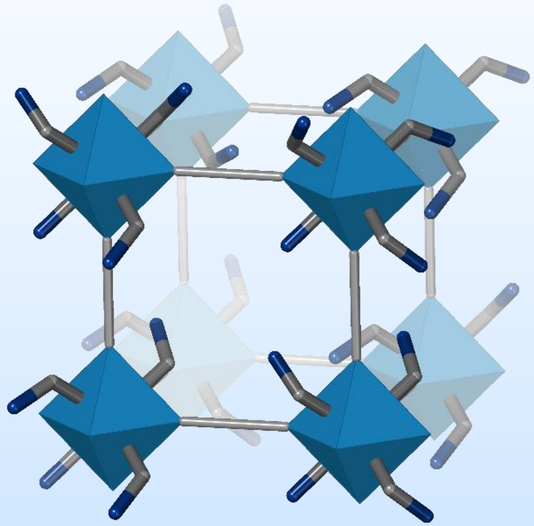
MOF-NH_2-A

- Developed in 2019
- 1 kg fabricated for benchmarking composite and device performance



MOF-NH_2-B

- Synthetic variation from MOF-NH_2-A ensuring ability to scale up
- Increased DAC capacity several fold

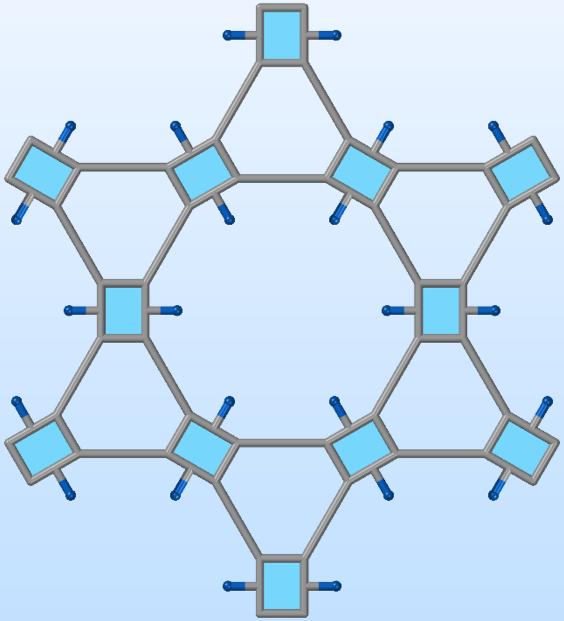


MOF-NH_2-N

- Redesigned with increased chemical stability while using the same chemisorption mechanism
- Optimization in progress

Sorbent Progress

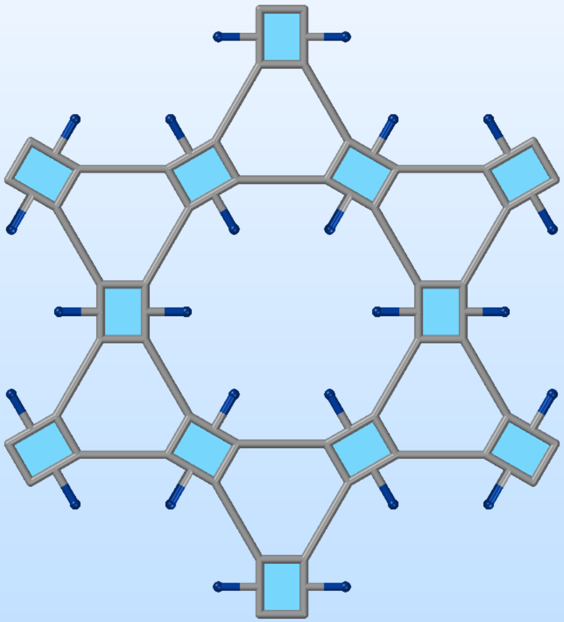
Benchmark Sorbent: MOF-NH_2-A



- Kilogram-scale synthesis finished during Q4 2020 with optimized preparation procedure and full analyses. Total delivery of MOF: 1193 g
  - Average yield: 63 ± 6%
- Amine loading: 3.4 ± 0.6 gmol/kg
- BET surface area: 1464 ± 78 m^2/g
- DAC Capacity at 25 °C
  - Dry CO_2: 0.04 gmol/kg
  - Humid CO_2:
    - 0.14 gmol/kg (RH 10%, binary sorption)
    - 0.24 gmol/kg (RH 20%, breakthrough)
    - Capacity increases with RH, in agreement with composite results
- Mechanism: carbamate-bicarbonate formation

Sorbent Progress

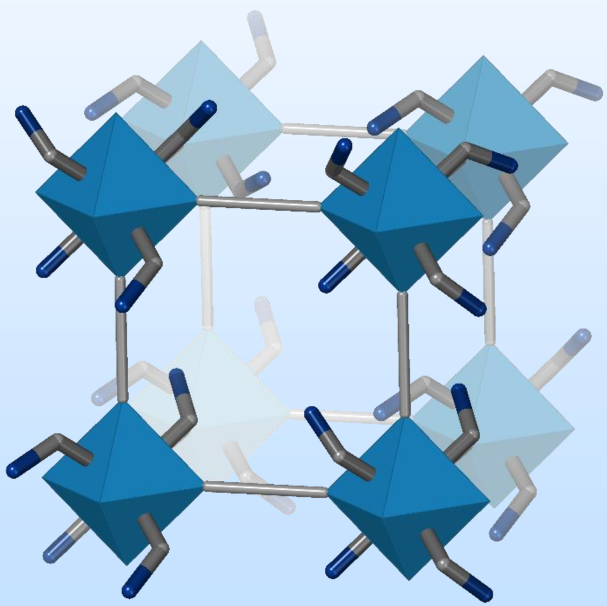
Next-Generation Sorbent Candidate: MOF-NH_2-B



- 17 synthetic variations based on MOF-NH_2-A introducing:
  - Amines with different pK_a (pK_b) to tune affinity to dilute CO_2 in air
  - Other functional groups to tune:
    - Chemical stability
    - Water uptake and sorption chemistry
  - Multivariate systems
- Variation with highest DAC capacity at 25 °C:
  - Dry CO_2: 0.27 gmol/kg (3.3 gmol/kg amine)
    - 6.8-fold increase compared to benchmark MOF-NH_2-A
  - Humid CO_2:
    - Testing in progress

Sorbent Progress

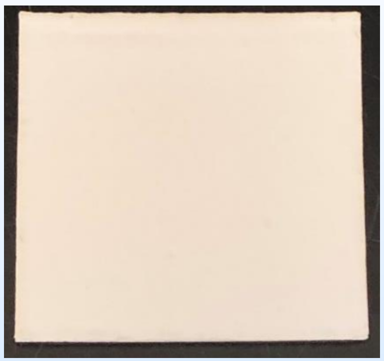
Next-Generation Sorbent Candidate: MOF-NH_2-N



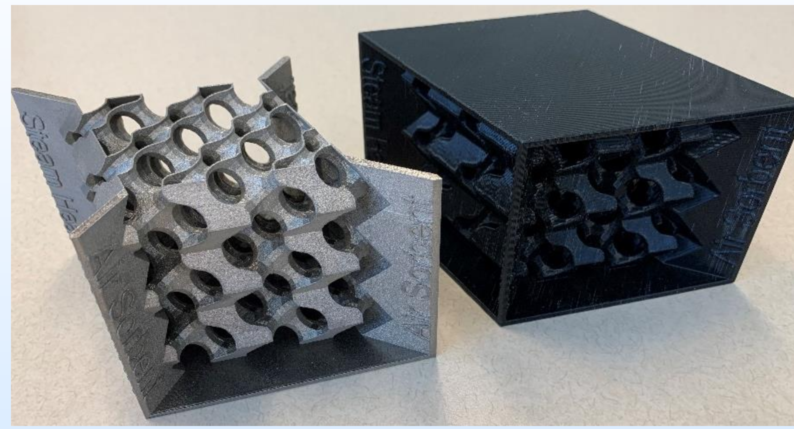
- Redesigned covalent amine-functionalized MOF chemisorbent for DAC
  - Permanently porous MOF framework, chemical stability up to pH > 14
    - Compared to benchmark sorbent: pH ≤ 10
    - Synthesis simplified and time shortened
  - Covalent functionalization of alkylamines on SBUs
    - Target amine loading: 5–6 gmol/kg
    - Amine reactivity much higher than benchmark
    - Increased capacity key to achieving target CO_2 capacity.
  - Currently finalizing synthesis and characterization

(MOF-NH_2-A)-Binder Composite Development & Coating

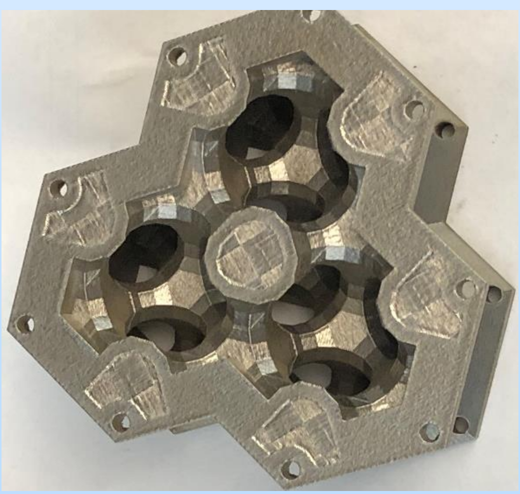
2” x 2” MOF-binder composite coated coupon

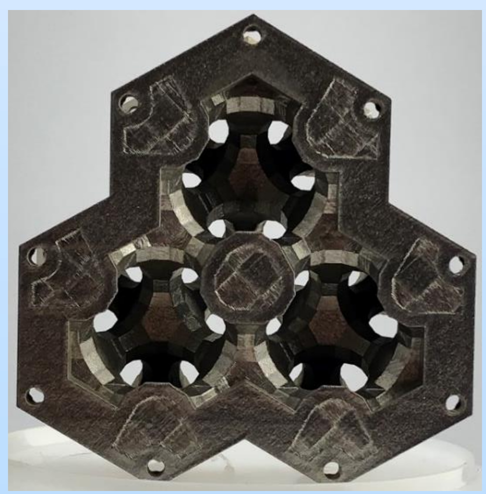


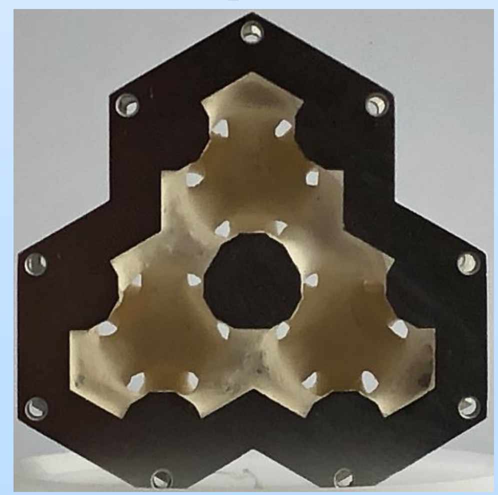
Inconel & ABS contactor prototypes



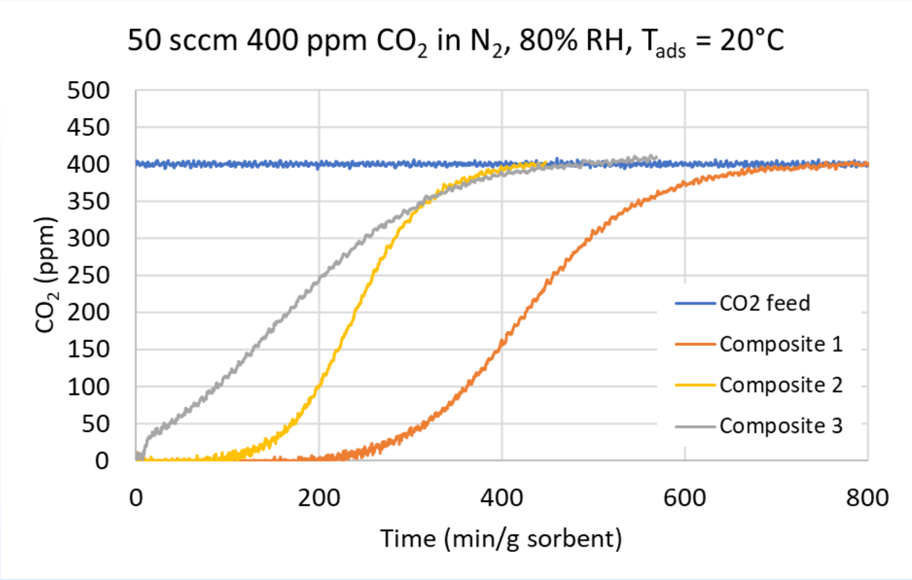
As made and MOF-binder composite-coated 3D contactor components.

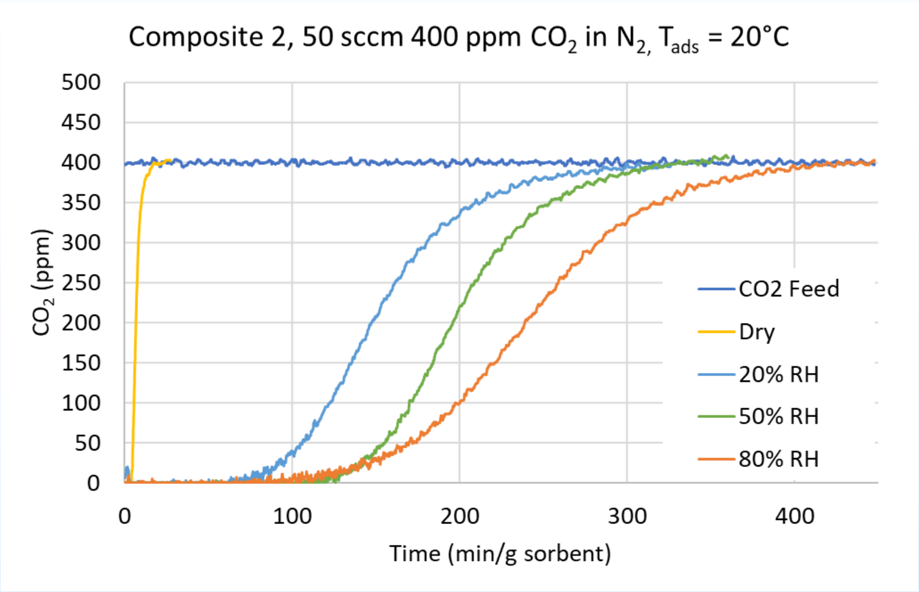






DAC Performance Evaluation





Various MOF-binder composite formulations tested for adhesion and CO_2 capture performance under DAC conditions (T_{ads} = 20°C, 20-80% RH, 400 ppm CO_2 in N_2, 20-100 sccm total gas flow rate, T_{des} = 120°C + vacuum).

MOF-binder composite coating maintains adhesion to substrate and exhibits 80% of the CO_2 capture capacity of the native MOF powder as initially proposed.

Composite 1 exhibits 0.38 mol CO_2/kg MOF-NH_2-A capacity at 80% RH

Opportunities for Collaboration

Synergistic effects of collaboration:

Integration of other high-capacity sorbents into novel contactor geometries would provide multiple pathways to advance the technology.

Potential areas for collaboration:

Sorbent manufacturing and scale-up

Multi-component sorption measurements and modeling

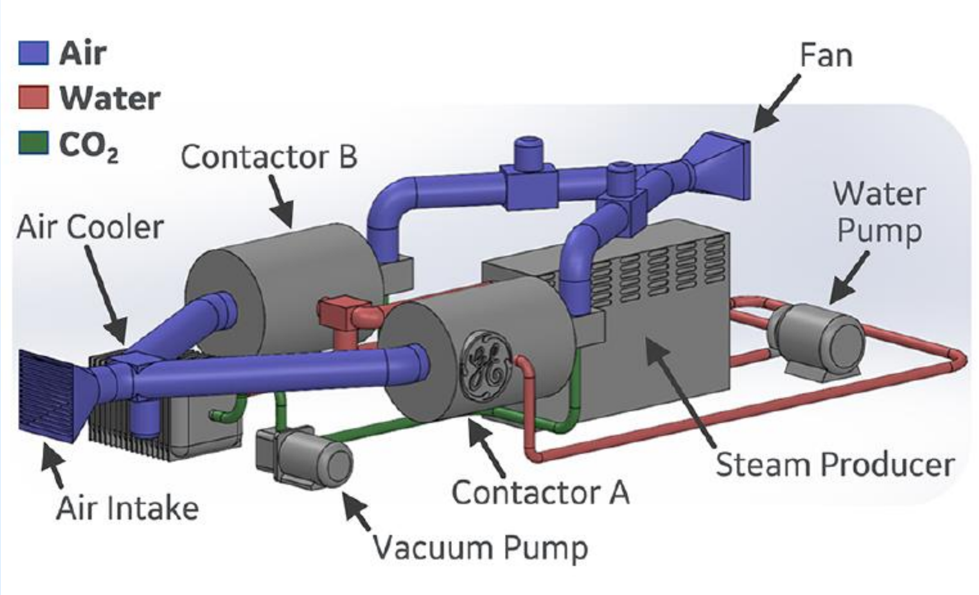
Artificial intelligence-guided molecular screening

Systems design and integration

End-user applications, including CO_2 sequestration and utilization (fertilization, food & beverage, sustainable aviation fuels)

Plans for future testing/development/ commercialization

a. AIR2CO2 Q4/5: Evaluation of new MOF-binder composite coatings, cyclability, thermal stability
b. Post-AIR2CO2: Bench-scale testing of coated, additively printed parts; techno-economics; 1 kg CO_2/day demo
c. Scale-up potential: Demonstration scale with full size additive contactor.



Summary Slide

Key findings:

- CO_2 capacity of MOF-binder composite increases with increasing humidity of the feed gas over a range of 20-80% RH.
- A pressure drop of <50 Pa across the AIR2CO2 contactor geometry is achievable based on coated, additively-printed designs.

Lessons learned:

- MOF water uptake has significant contribution to desorption energy

Future plans:

- Bench-scale testing of coated, additively-printed parts
- Techno-economic analysis of alternating adsorption-desorption bench-scale system

MOF-binder composite coatings achieve 80% of native sorbent performance and have been demonstrated on additively-printed components.

Appendix

– These slides will not be discussed during the presentation but are mandatory.

Team and Facilities

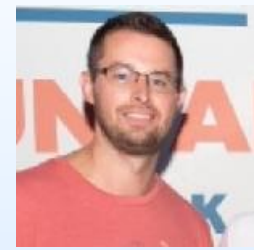
GE Research – contactor design & fabrication, coating development, coating performance testing, system modelling

Dr. David Moore
PI

Dr. Vitali Lissianski

Dr. Mark Doherty

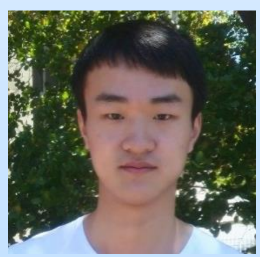
Mr. Dan Erno



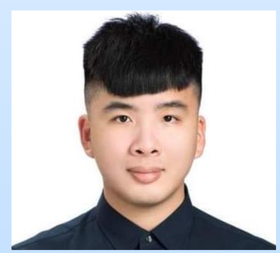
Mr. Mark Buckley

UC Berkeley – sorbent development & characterization, powder performance testing

Prof. Omar Yaghi
Co-PI



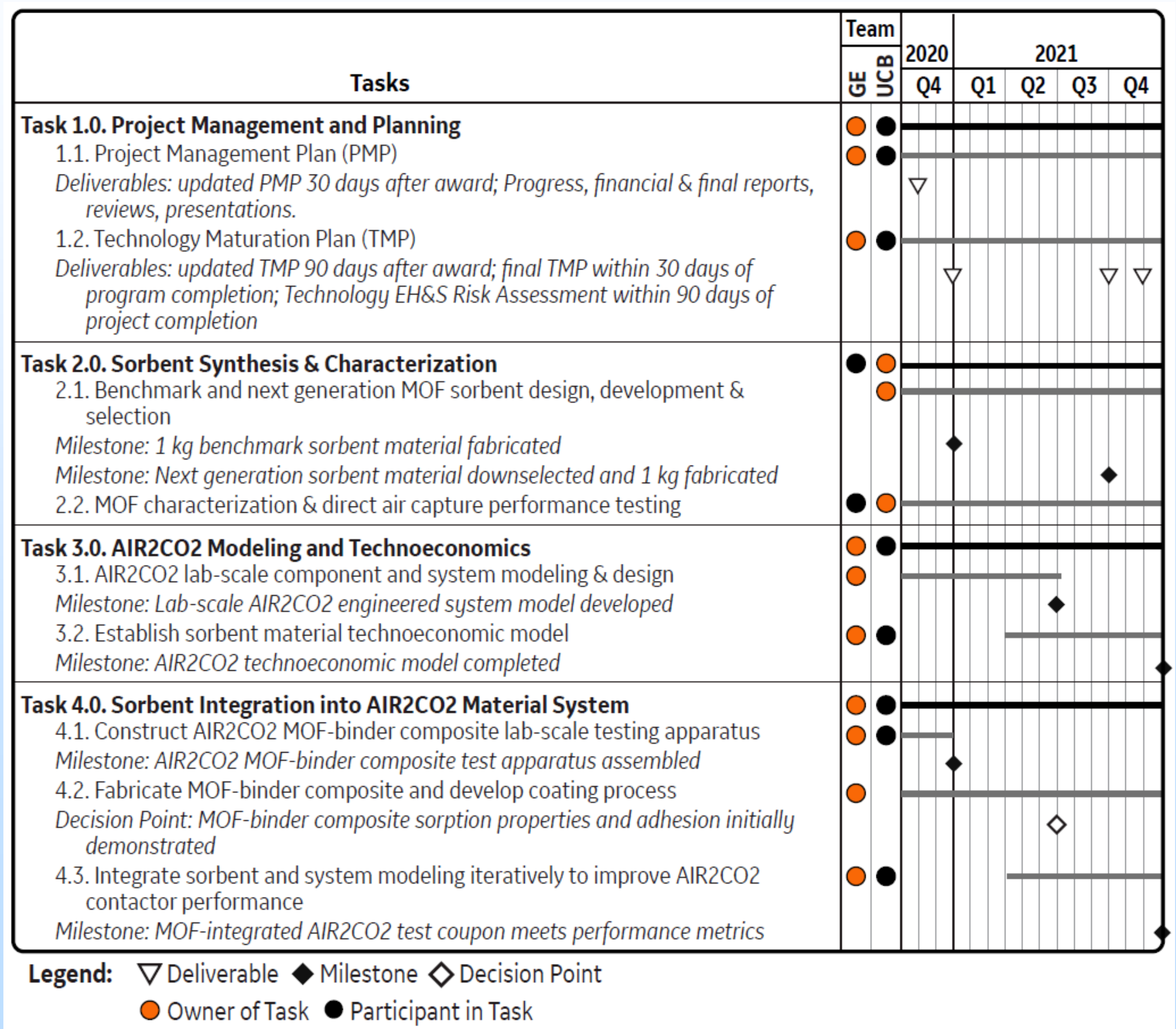
Mr. Hao Lyu



Mr. Oscar Chen

Dr. Ayan Zhumekenov

Gantt Chart


Tasks
Team
GE
UCB
2020
2021
Q4
Q1
Q2
Q3
Q4
Task 1.0. Project Management and Planning
1.1. Project Management Plan (PMP)
Deliverables: updated PMP 30 days after award; Progress, financial & final reports, reviews, presentations.
1.2. Technology Maturation Plan (TMP)
Deliverables: updated TMP 90 days after award; final TMP within 30 days of program completion; Technology EH&S Risk Assessment within 90 days of project completion
Task 2.0. Sorbent Synthesis & Characterization
2.1. Benchmark and next generation MOF sorbent design, development & selection
Milestone: 1 kg benchmark sorbent material fabricated
Milestone: Next generation sorbent material downselected and 1 kg fabricated
2.2. MOF characterization & direct air capture performance testing
Task 3.0. AIR2CO2 Modeling and Technoeconomics
3.1. AIR2CO2 lab-scale component and system modeling & design
Milestone: Lab-scale AIR2CO2 engineered system model developed
3.2. Establish sorbent material technoeconomic model
Milestone: AIR2CO2 technoeconomic model completed
Task 4.0. Sorbent Integration into AIR2CO2 Material System
4.1. Construct AIR2CO2 MOF-binder composite lab-scale testing apparatus
Milestone: AIR2CO2 MOF-binder composite test apparatus assembled
4.2. Fabricate MOF-binder composite and develop coating process
Decision Point: MOF-binder composite sorption properties and adhesion initially demonstrated
4.3. Integrate sorbent and system modeling iteratively to improve AIR2CO2 contactor performance
Milestone: MOF-integrated AIR2CO2 test coupon meets performance metrics
Legend:
Deliverable
Milestone
Decision Point
Owner of Task
Participant in Task