MIL-101(Cr)-Amine Sorbents Evaluation Under Realistic Direct Air Capture Conditions

Project Number (See Federal Project Manager for help)

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National Energy Technology Laboratory

Direct Air Capture Kickoff Meeting

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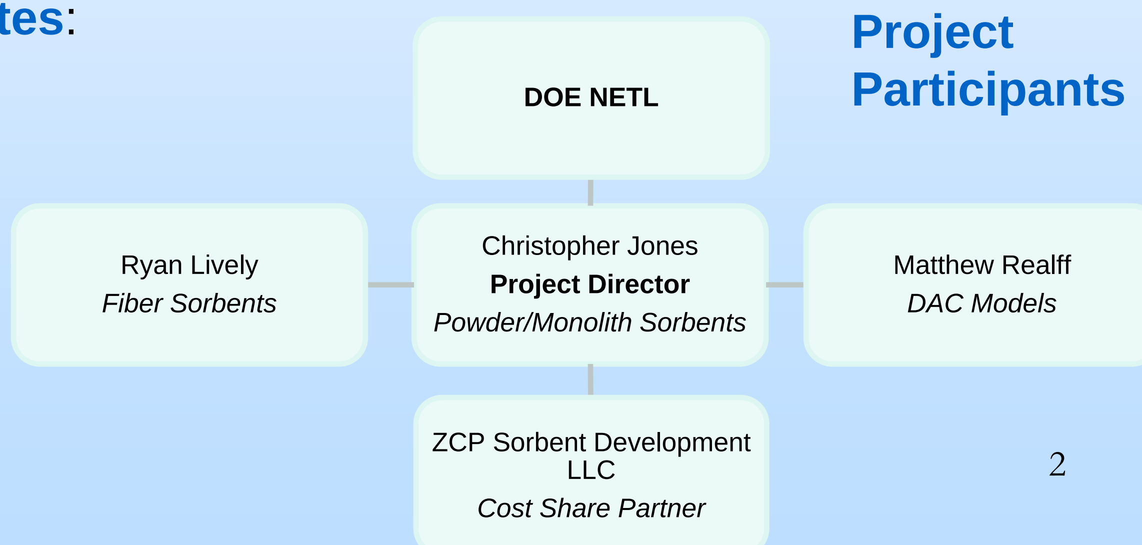
Program Overview

Funding	FY 2020		FY 2021		FY 2022		Total	
	DOE Funds	Cost Share	DOE Funds	Cost Share	DOE Funds	Cost Share	DOE Funds	Cost Share
Applicant			$548,435		$206,731		$755,166	
Sub-recipient A, if proposed				$138,000		$53,482		$191,482
Total ($)			$548,435	$138,000	$206,731	$53,482	$755,166	$191,482
Total Cost Share %			20.10%		20.55%		20.23%	

Overall Project Performance Dates:
10/01/20-3/31/22

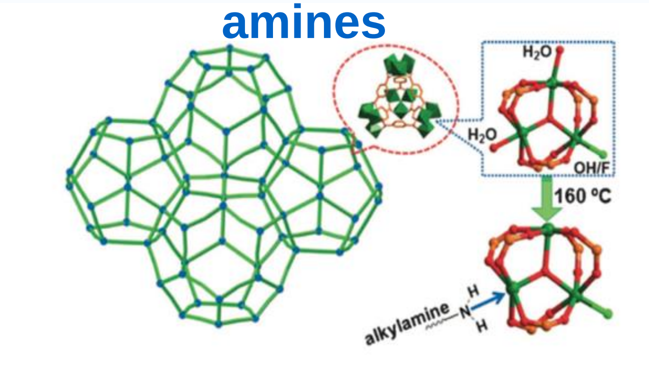
Overall Project Objective:
- assess the performance of a small family of MIL-101(Cr)-amine hybrid sorbents for CO_2 capture at sub-ambient conditions

Project Participants



Technology Background

MIL-101(Cr) loaded with amines



Literature data recorded at ambient conditions

Equilibrium Loading	gmol CO_2/kg	2.8 (TREN-MIL-101(Cr)) 1.35 (PEI-MIL-101(Cr)) (measured at 25 °C)
Heat Adsorption	kJ/gmol CO_2	70 (measured)
CO_2 Adsorption kinetics	gmol/time	1.68 x 10^{-5} mol/g/min (initial adsorption rate, measured at 25 °C)

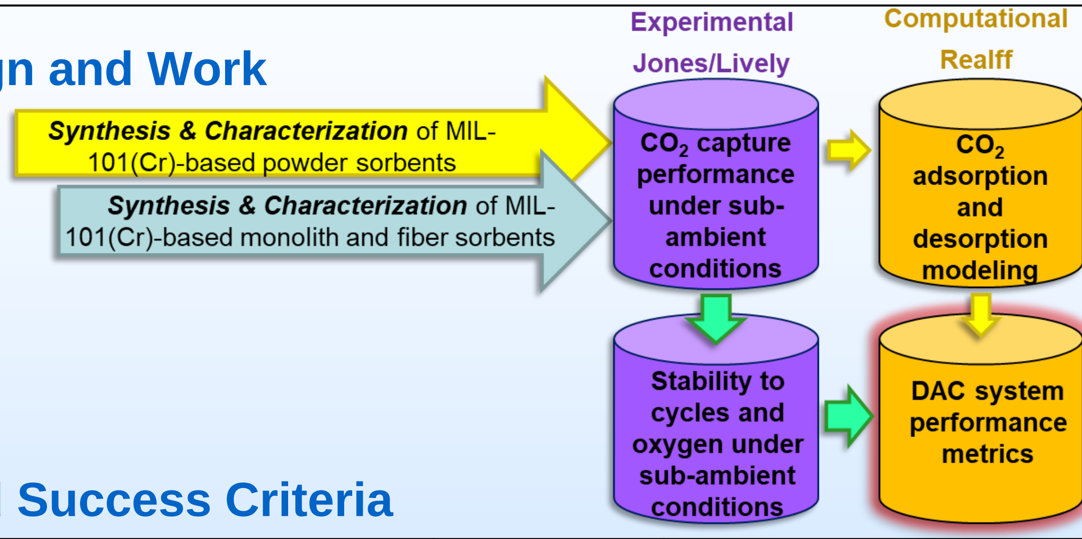
Proposed Technological Approach:

Advantages	Challenges
• High BET surface area • Tunable pore characteristics • High pore volume • High density of open metal sites • Stable over a wide range of conditions • High efficiency at CO_2 concentration of 400 ppm • Greatly benefited from functionalization with amines	Polymeric amines become rigid at sub-ambient temperatures, leading to high diffusional resistances and slow kinetics

Hu, Y.; Verdegaal, W. M.; Yu, S. H.; Jiang, H. L., Alkylamine-Tethered Stable Metal–Organic Framework for CO_2 Capture from Flue Gas. ChemSusChem **2014**, 7 (3), 734-737.

Technical Approach/Project Scope

Experimental Design and Work Plan



Key Milestones and Success Criteria

Task/ Subtask	Milestone Title & Description	Planned Completion Date	Success Criteria
3.2/4.2	Development of MIL-101(Cr)-based fibers and monolith sorbents. MIL-101(Cr) sorbent macrostructures, with at least two different compositions, successfully fabricated and structurally characterized.	Month 9	Successful synthesis of MIL-101(Cr)-amine fiber and monolith sorbents.
5/8	Evaluation of performance and stability of powder MIL-101(Cr)-based sorbents at sub-ambient conditions. CO_2 capacities will be measured for at least three sorbent powder types. Cyclic stability and rate of oxidative degradation will be measured for at least 1 sorbent at 3 different conditions.	Month 18	1-2 MIL-101(Cr)-based powder sorbents identified as promising sorbents at sub-ambient conditions: good compromise between CO_2 capacity, kinetics and stability (towards multiple cycles and oxygen).
9	Translation of most promising powder MIL-101(Cr)-based sorbents to fiber and monolith forms. Developed macrostructures should have CO_2 capacity of at least 75% of the powder sorbent capacity.	Month 18	Performance of fiber or monolith is at least 75% of the powder performance.
10	Employ models of adsorption and desorption behavior to estimate DAC system performance metrics; report swing capacity and energy consumption per ton CO_2.	Month 18	Adsorption and desorption models represent experimental data and estimated DAC system metrics allow assessment of suitability for next stage of process development.

Team and Facilities

Georgia Tech Team

Christopher Jones

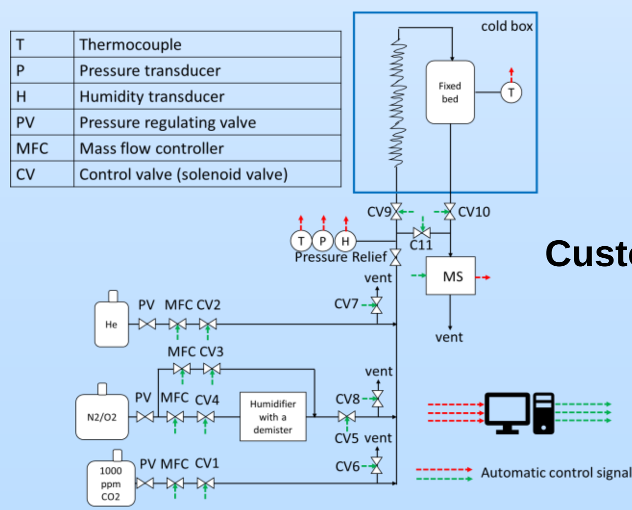
Ryan Lively

Matthew Realff

Georgia Tech Sub-ambient Laboratory

Volumetric system

Thermogravimetric system



Custom-built fixed bed

Progress and Current Status of Project

Brief Description of the Equipment Used/Built in the Project

Equipment	Experimental conditions	Information acquired
Thermogravimetric system	-20 – 25 °C, dry gas feed	CO_2 equilibrium adsorption and desorption capacities and kinetic profiles
Volumetric system	-20 – 25 °C, dry gas feed	CO_2 adsorption isotherms
Fixed bed	-20 – 25 °C, humid gas feed with RH between 0 to 80%	Breakthrough capacity, adsorption and desorption kinetic profiles

Significant Accomplishments/Performance Achieved to Date

- Setting up the sub-ambient laboratory
- Increased CO_2 uptake in presence of amines – results consistent with literature
- Greater CO_2 uptake in presence of a smaller amine (TEPA) as compared to PEI at sub-ambient conditions
- First step towards sorbent optimization based on DAC location: low-molecular weight sorbents maybe more effective at sub-ambient temperatures

Material	CO_2 uptake at 400 ppm CO_2 and -20 C (mmol/g)	CO_2 uptake at 400 ppm CO_2 and 20 C (mmol/g)
MIL-101(Cr)	0.002	<0.001
50% TEPA-MIL-101(Cr)	0.38	1.37

Opportunities for Collaboration

Synergistic effects of collaboration:

- CO_2 utilization technologies can provide more incentives for CO_2 capture
- Better sorbent and contactor design could result from collaborating with teams with similar research goals

Areas of complementary work that others may contribute to this technology:

- Develop more economical ways to synthesize MIL-101(Cr) and sorbent amines at larger scales
- Geological and geographical studies of potential locations for deployment to lower the cost and reduce uncertainties of the installation of plants
- Improve the efficiency and economy of CO_2 utilization or geological sequestration
- LCA analysis could help better understand the global impacts of this technology