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

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U.S. Department of Energy

National Energy Technology Laboratory

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Project Overview

- Funding
  - DOE Funds: $755,166 (79.73%)
  - Cost share (ZCP Sorbent Development, LLC): $191,482 (20.23%)
- Funding Period: 10/01/2020-03/31/2022
- Project Participants:
  - Georgia Institute of Technology
  - ZCP Sorbent Development, LLC

	FY 2021		FY 2022		Total	
	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%	

Project Overview

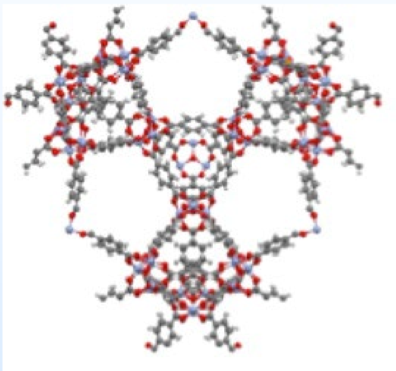
- Overall Project Objectives

  - Explore DAC performance of amine functionalized MIL-101(Cr) MOFs and build models of their adsorption behavior over a wide range of temperatures (-20 ^{o}C to 25 ^{o}C) and relative humidities (0% to 100%).

  - Develop and test the sub-ambient DAC materials in the forms of composite polymer/MOF fibers and on the surface of monoliths. (advance from TRL 2 to TRL 3)

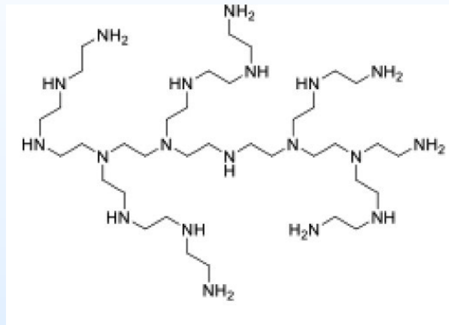
Technology Background

PEI impregnated MIL-101(Cr) MOFs for ambient DAC (Darunte et al., 2016) 25 °C



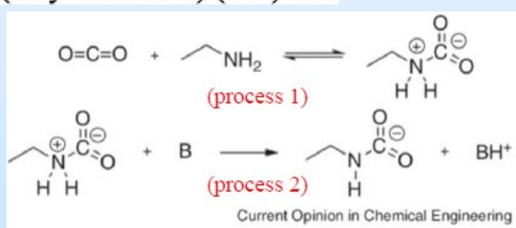
MIL-101(Cr)

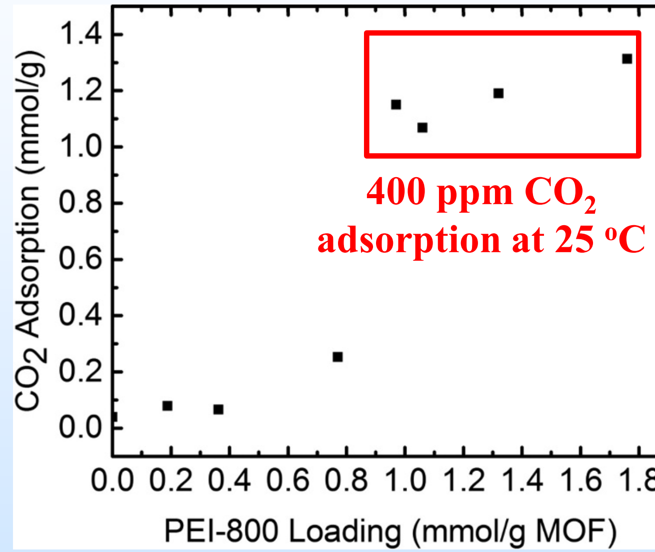
+



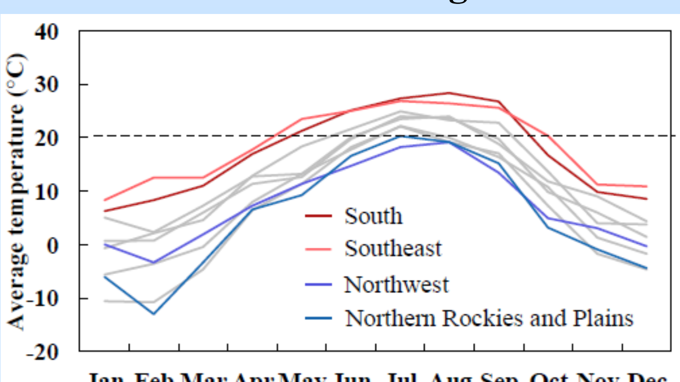
Poly (ethylene imine) (PEI)-800

DAC at 25 ^oC





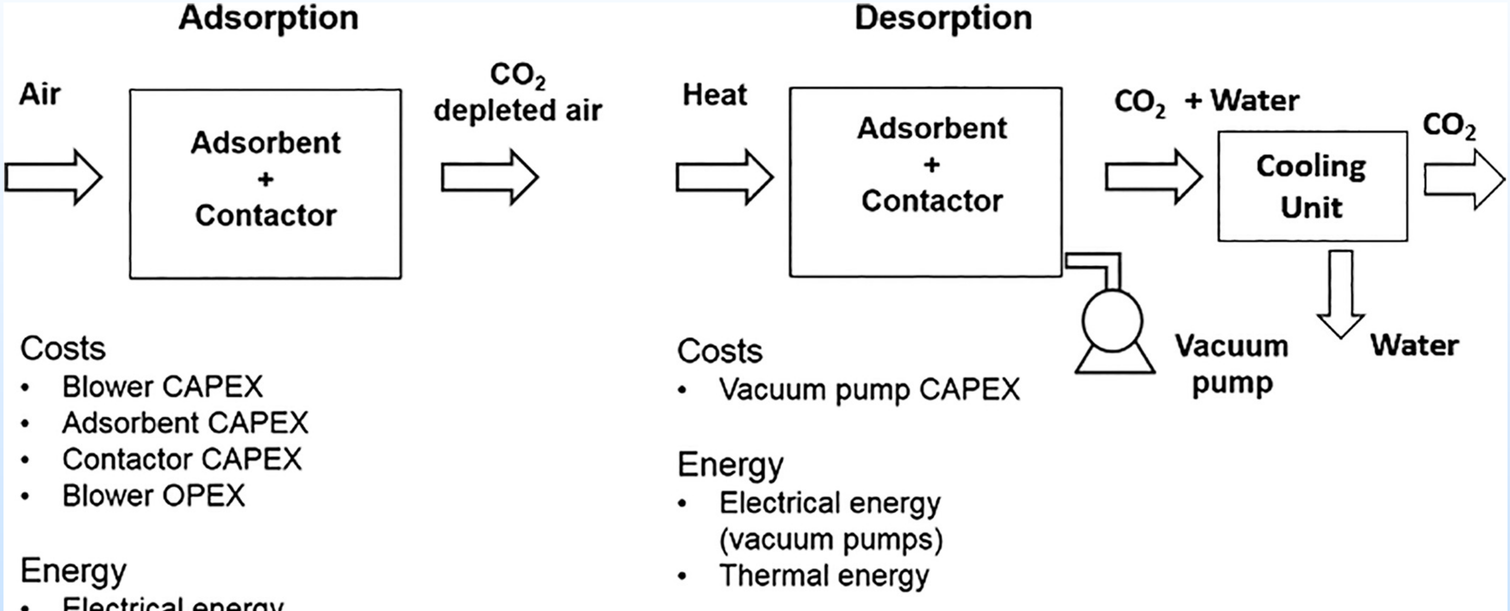
Average monthly temperatures for US Climate regions



Aim to investigate the CO_2 adsorption capabilities of MIL-101(Cr)-amine sorbents over wide range of adsorption temperature (-20 to 25 ^oC) and RH (0 to ~100%) conditions.

Technology Background

Sub-ambient DAC cycles with small T swing (e.g. -20 ^oC to 25 ^oC)



Sinha et al. *AIChE J.* **2019**, 65, e16607

- T/VSA using solid sorbents in a structured contactor (fibers or monoliths)
- Heat delivery mode TBD

Innovation: design of sorbents/processes for operation in practical, temperate outdoor adsorption temperature range of -20 to 25 °C, in all humidities.

Technology Background

Sub-ambient DAC cycles with small T swing (-20 ^{o}C to 25 ^{o}C; ΔT ~ 45 ^{o}C)

Today's state-of-the-art:

- 99% of all published DAC studies conducted at T $\geq$ 25 °C
- >50% of all published DAC studies conducted in absence of humidity
- Warm DAC gives improved kinetics, but requires handling of large water sorption loads

Proposed Innovation:

- Practical, outdoor DAC requires operation at cooler/colder temperatures & in all humidities
- Cool/cold operation may allow for more physisorption as well as less water sorption due to lower humidity; both offer potential for lower desorption energies

Project Schedule (Key Milestones)

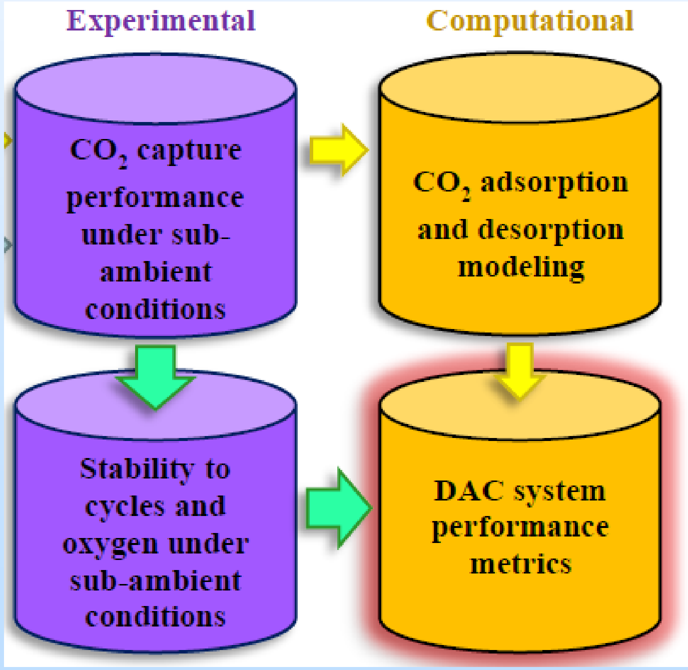
Task/ Subtask	Milestone Title & Description	Planned Completion Date
1	Project Management Plan	Month 1
3.2/4.2	Development of MIL-101(Cr)-based fibers and monolith sorbents. MIL-101(Cr) sorbent macrostructures, with at least two different compositions, successfully fabricated and structurally characterized.	Month 9 ↓ **Month 13 (extended)**
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
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
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

Experimental Design & Work Plan

Characterization of MIL-101(Cr) powder, monolith, and fiber sorbents

Equipment for lab-scale experiments	Expected experimental conditions	Information acquired
Thermo-gravimetric System (TGA)	-20 to 25 ^oC, dry gas feed	CO_2 equilibrium adsorption and desorption capacities, adsorption and desorption kinetic profiles
Volumetric System (SAP)	-20 to 25 ^oC, dry gas feed	CO_2 adsorption isotherms
Fixed bed breakthrough System + MS and IR detectors	-20 to 25 ^oC, humid gas feeds with relative humidity between 0 and ~80%	Breakthrough & equilibrium capacities, adsorption and desorption kinetic profiles

Integration of lab-scale sub-ambient CO_2 adsorption testing with analytical computational studies



Project Success Criteria

Milestone	Decision Point	Date	Success Criteria
2	Development of MIL101(Cr)-based fibers and monolith sorbents. MIL-101(Cr) sorbent macrostructures, with at least two different compositions, successfully fabricated and structurally characterized.	Month 9 ↓ **Month 13 (extended)**	Successful synthesis of MIL-101(Cr)-amine fiber and monolith sorbents.
3	Evaluation of performance and stability of powder MIL-101(Cr)-based sorbents at sub-ambient 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).
4	Translation of best performing powder MIL-101(Cr)-amine sorbents to fiber and monolith forms.	Month 18	Performance of fiber or monolith is at least 75% of the powder performance.
5	Employing models of adsorption and desorption behavior to estimate DAC system performance metrics.	Month 18	**Adsorption and desorption models** represent experimental data and estimated DAC system metrics allow **assessment of suitability for next stage of process development**.

Project Risks & Mitigation Strategies

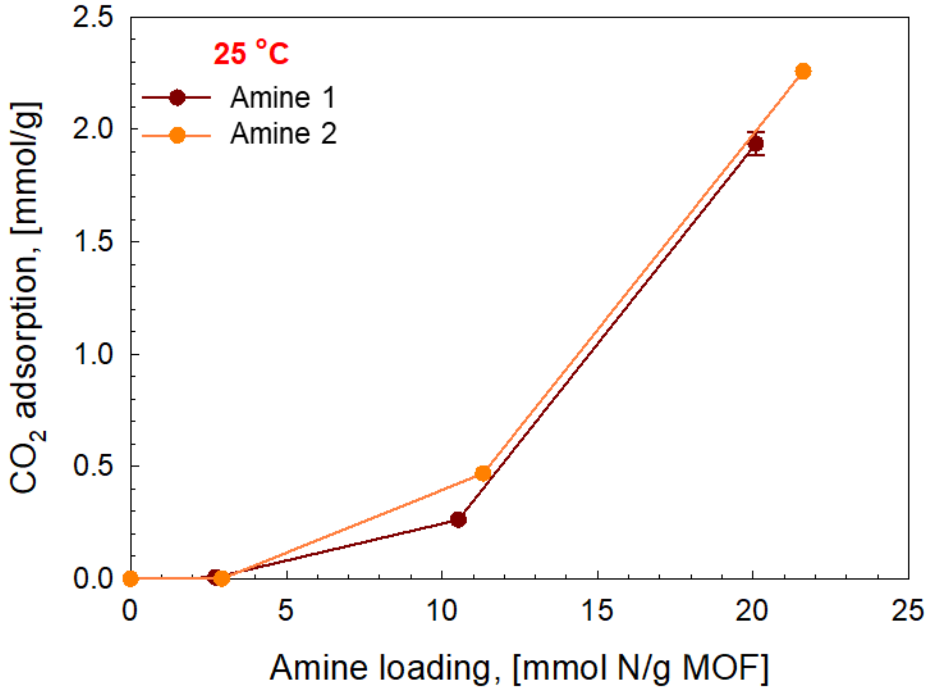
Perceive Risk	Risk Rating			Mitigation/Response Strategy
	Probability	Impact	Overall	
	(Low, Med, High)			
Financial Risks:				
Existing equipment failure, replacement funds not in budget	Low	Med	Low	Many experiments will be carried out on existing equipment that is regularly maintained and failure is unlikely.
Cost/Schedule Risks:				
Delayed hiring of personnel	Med	High	Med	PIs will seek applications for project before notification of award. PIs will seek applicants already at Georgia Tech. (Delays due to slow worker approval)
Delayed delivery of new equipment	Med	High	Med	If new equipment is delayed, existing equipment will be retrofitted with chillers to begin work on the project and limit delays. (Delays due to slow equipment delivery)

Perceive Risk	Risk Rating			Mitigation/Response Strategy
	Probability	Impact	Overall	
	(Low, Med, High)			
Technical/Scope Risks:				
Unable to grow MIL-101(Cr) on monolith materials	Low	Med	Low	Previous literature indicates MIL-101(Cr) can be grown on alumina; work can continue if no other monolith materials enable MIL-101(Cr) growth. Extrusion and 3D printing of MIL- 101(Cr) monoliths is also feasible.
Amine-MIL-101(Cr) sorbents not stable at low T	Med	Med	Med	Additional amines can be investigated. Previous work has found PEI-MIL-101(Cr) to be stable for adsorption at room temperature and work could continue with PEI.
Management, Planning, and Oversight Risks:				
Team collaboration and communication is poor	Low	Med	Low	Jones, Lively, and Realff work together in the same building at Georgia Tech and have successfully worked together before.
ES&H Risks:				
Accident associated with experimental testing	Low	High	Low	Laboratory designed for adsorption experiments. Gas cylinder management is already in place. Liquid nitrogen is already used and all experimentalists receive proper training.

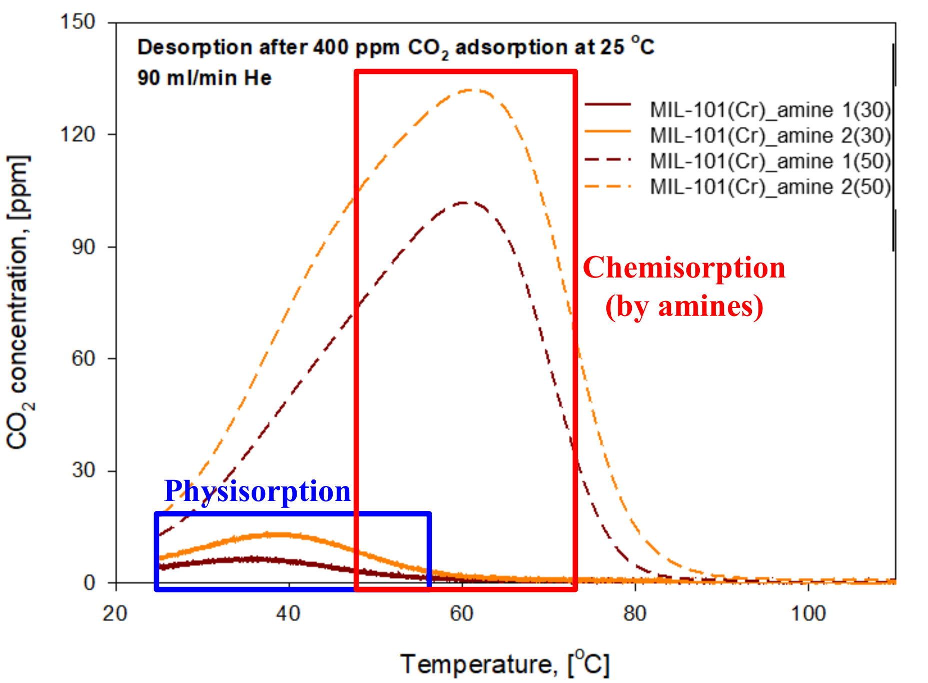
Development of MIL-101(Cr) Powders Sorbents and Baseline Testing

Amine impregnated MIL-101(Cr) (400 ppm CO_2 capture at 25 °C)

By SAP



CO_2-Temperature Programmed Desorption

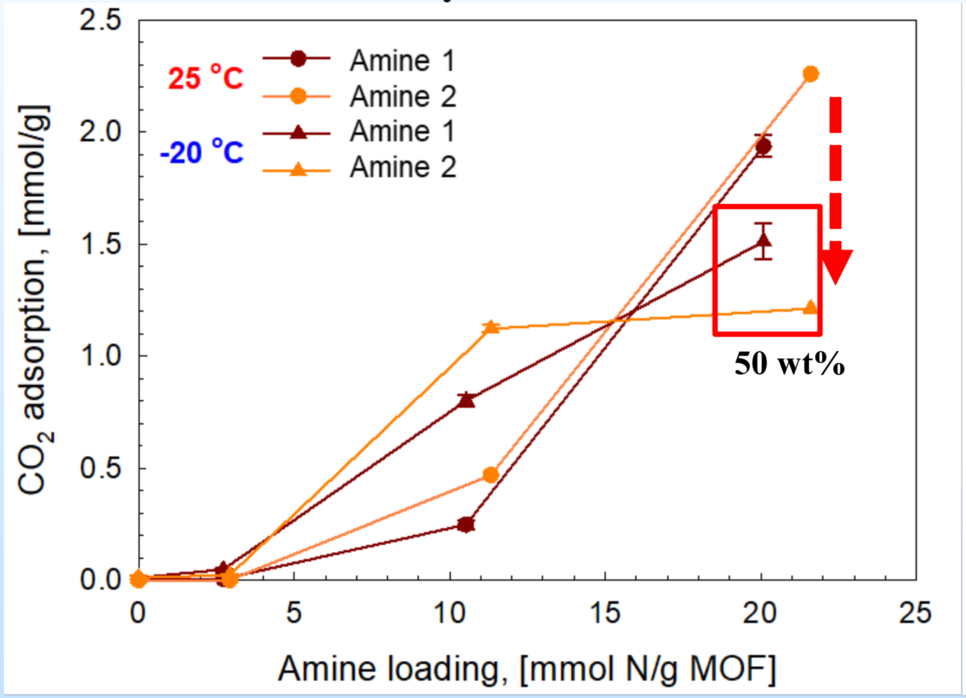


30 wt% loading: physisorption dominant
50 wt% loading: chemisorption dominant

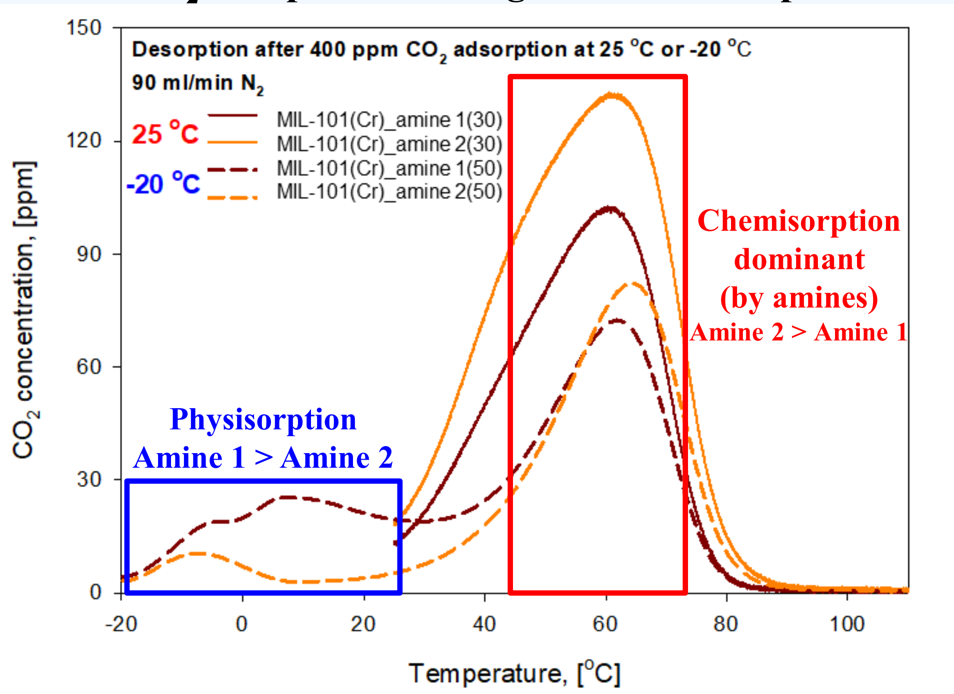
Development of <u>Powder</u> MIL-101(Cr) Sorbents at <u>Sub-ambient Conditions</u>

Amine impregnated MIL-101(Cr) (400 ppm CO_2 capture at -20 °C)

By SAP



CO_2-Temperature Programmed Desorption



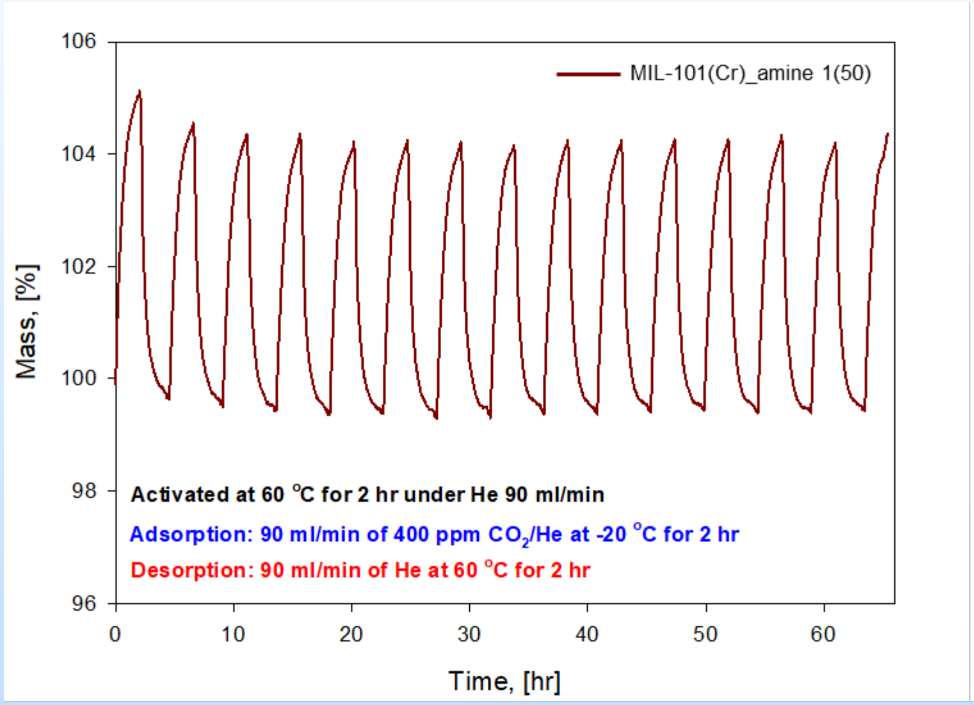
Reduced CO_2 adsorption: Reduced amine mobility at -20 °C (chemisorption dominant)
Amine 1 > Amine 2: "Frozen" Amine 1 has more free volume to physically capture CO_2 than Amine 2 due to structural differences

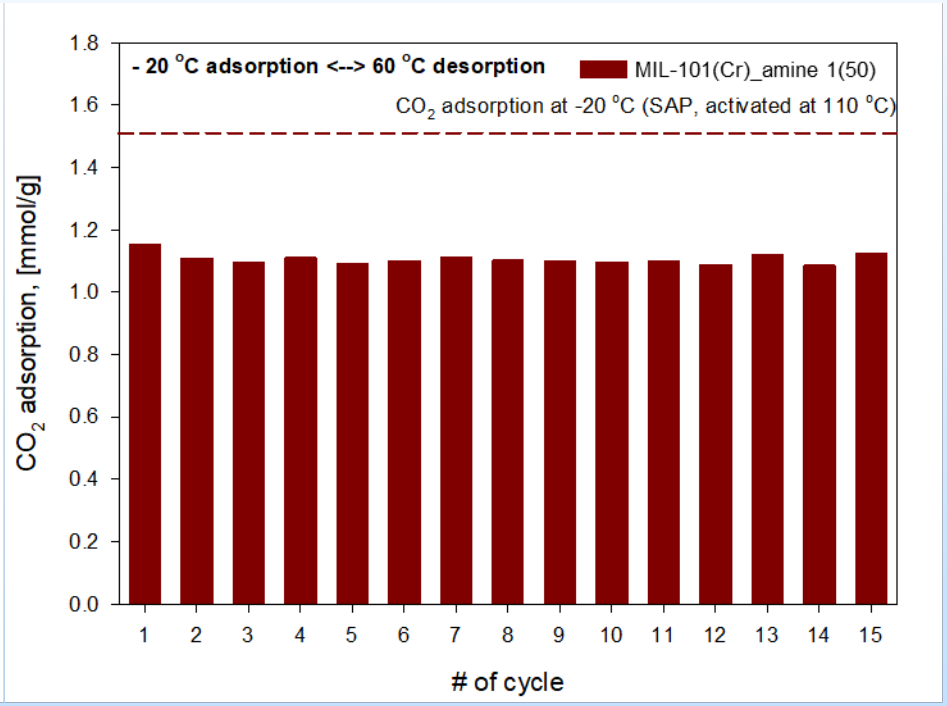
Due to higher physisorption, Amine 1 shows better adsorption capacity and is easier to regenerate

Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

Cyclic test (400 ppm CO_2 capture at -20 °C (2 h), desorption at 60 °C (2 h))

50 wt% Amine 1 impregnated MIL-101(Cr) powders



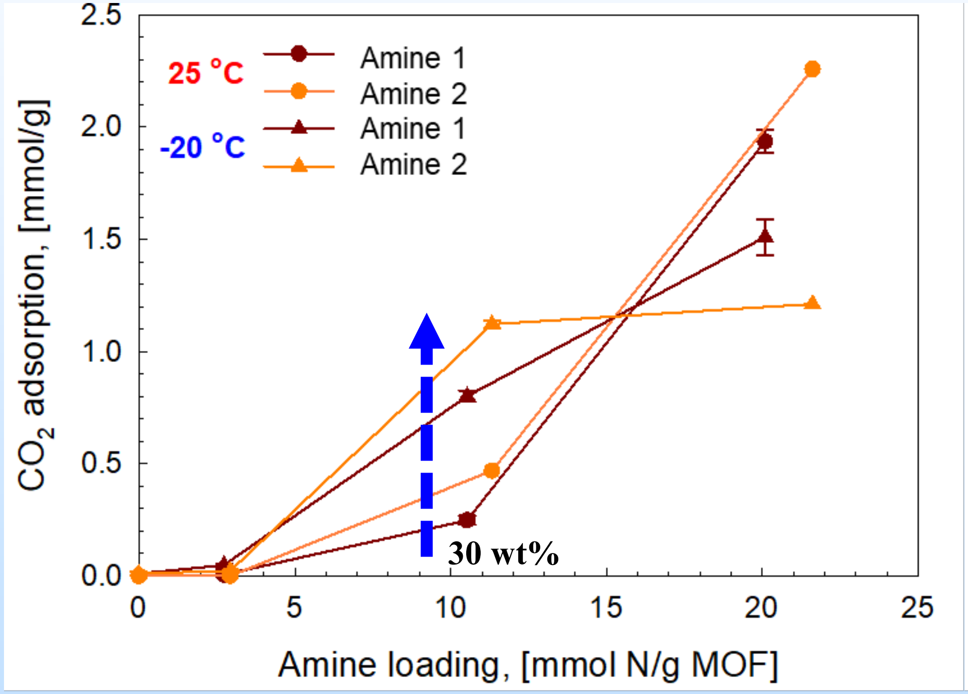


60 °C is sufficient to regenerate MIL-101(Cr)_amine 1(50)

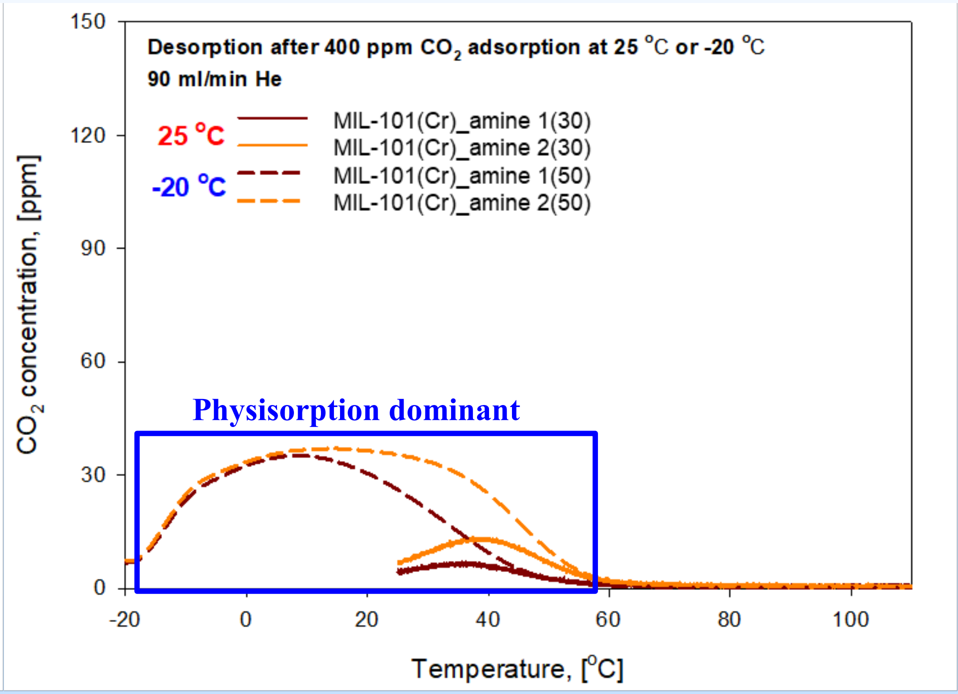
Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

Amine impregnated MIL-101(Cr) (400 ppm CO_2 capture at -20 °C)

By SAP



CO_2-Temperature Programmed Desorption

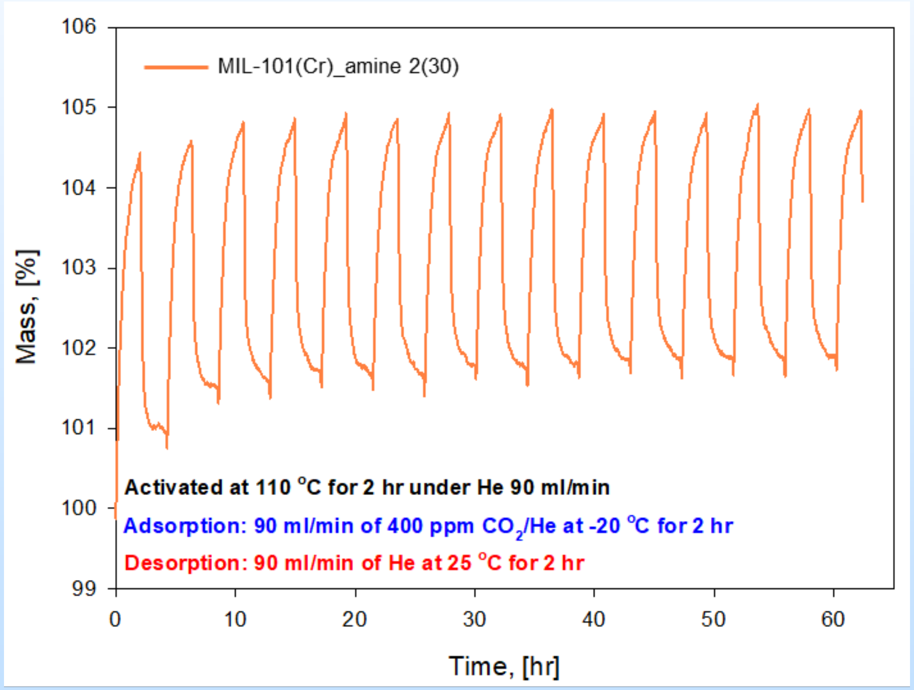


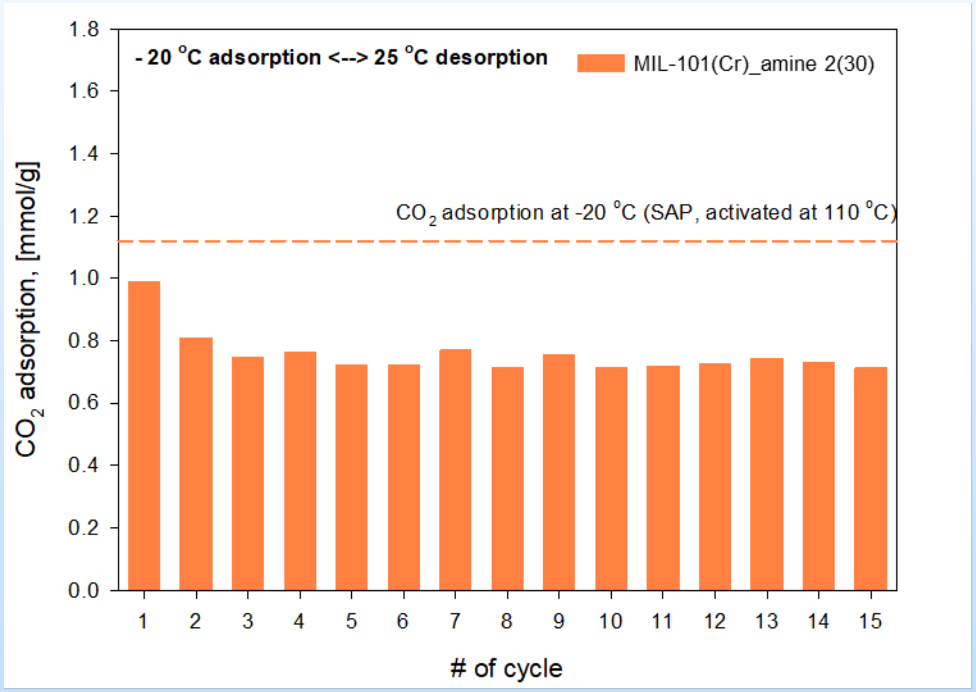
MIL-101(Cr)_amine 2(30) may be a preferred sorbent for sub-ambient DAC due to *promising adsorption capacity* and *low regeneration temperature* (physisorption dominant)

Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

Cyclic test (400 ppm CO_2 capture at -20 °C (2 h), desorption at 25 °C (2 h))

30 wt% Amine 2 impregnated MIL-101(Cr) powders





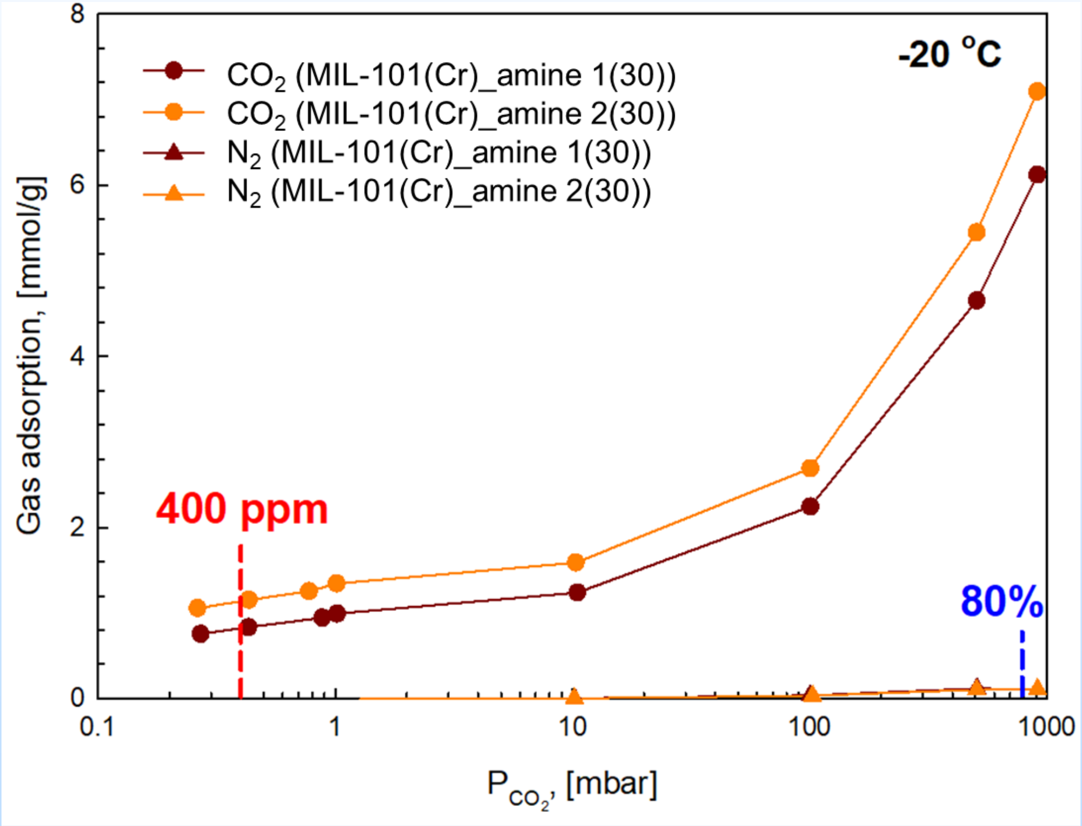
25 °C is sufficient to regenerate MIL-101(Cr)_amine 2(30) = ΔT of 45 °C

Small temperature swing

Still seek small capacity improvements

Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

Single gas (CO_2 and N_2) adsorption isotherm of 30 wt% amine impregnated MIL-101(Cr) at -20 ^oC



Selectivity:

10 – 14
(mol/kg CO_2 / mol/kg N_2)

20,000 – 30,000
(mol/kg CO_2 * x_{N2} / mol/kg N_2 * x_{CO2})

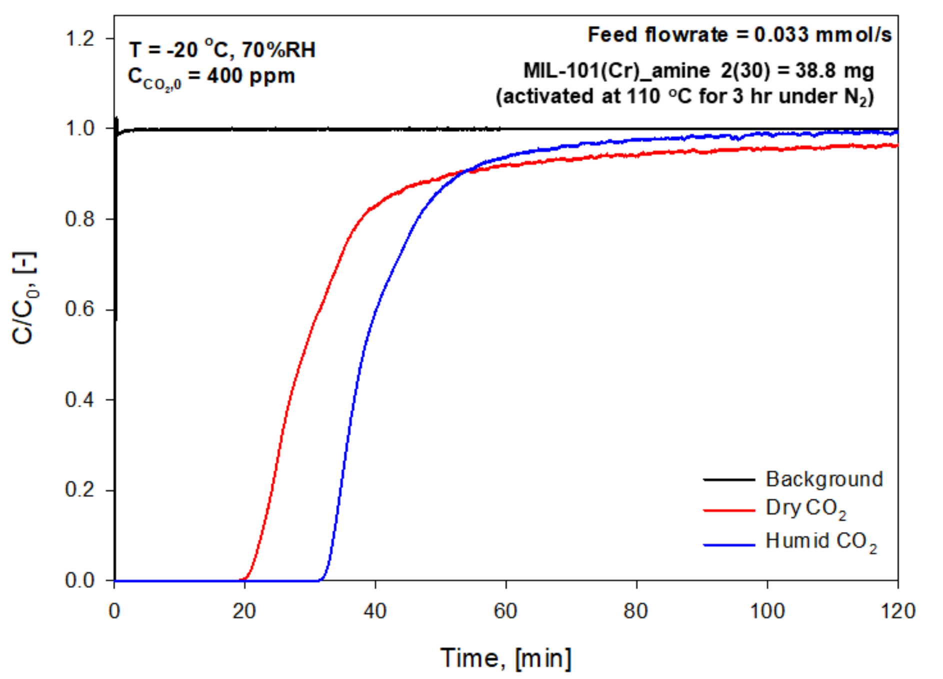
Selective 400 ppm CO_2 capture over 80% N_2 at -20 ^oC

Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

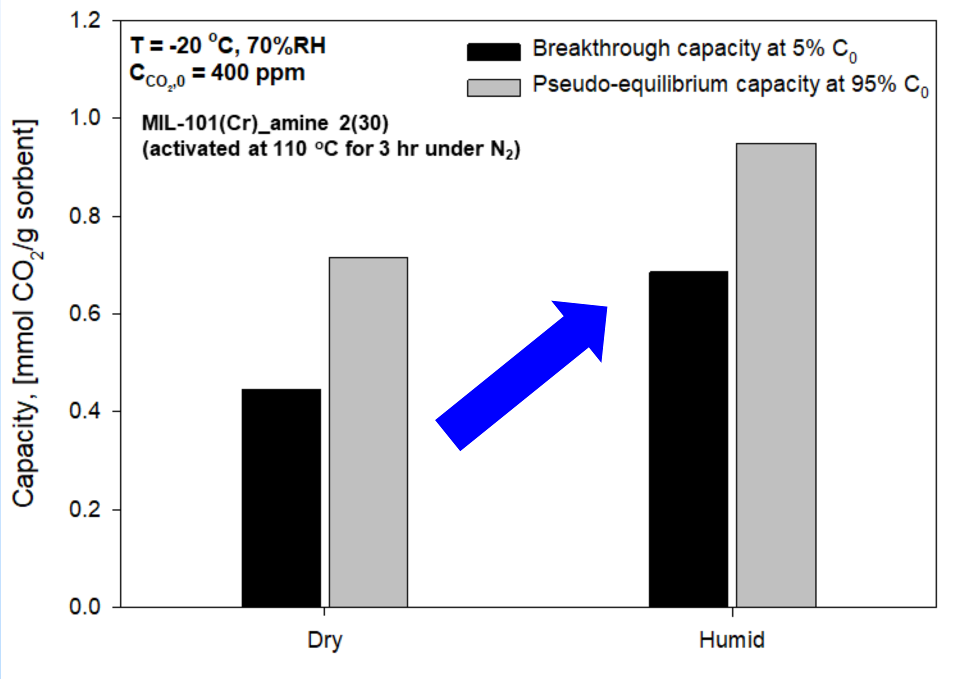
Sub-ambient DAC fixed bed test (dry and 70%RH at -20 ^oC)

MIL-101(Cr)_amine 2(30)

CO_2 breakthrough curve



CO_2 capture capacity



Moisture has positive effect on capacity of sub-ambient DAC with MIL-101(Cr)_amine 2(30)

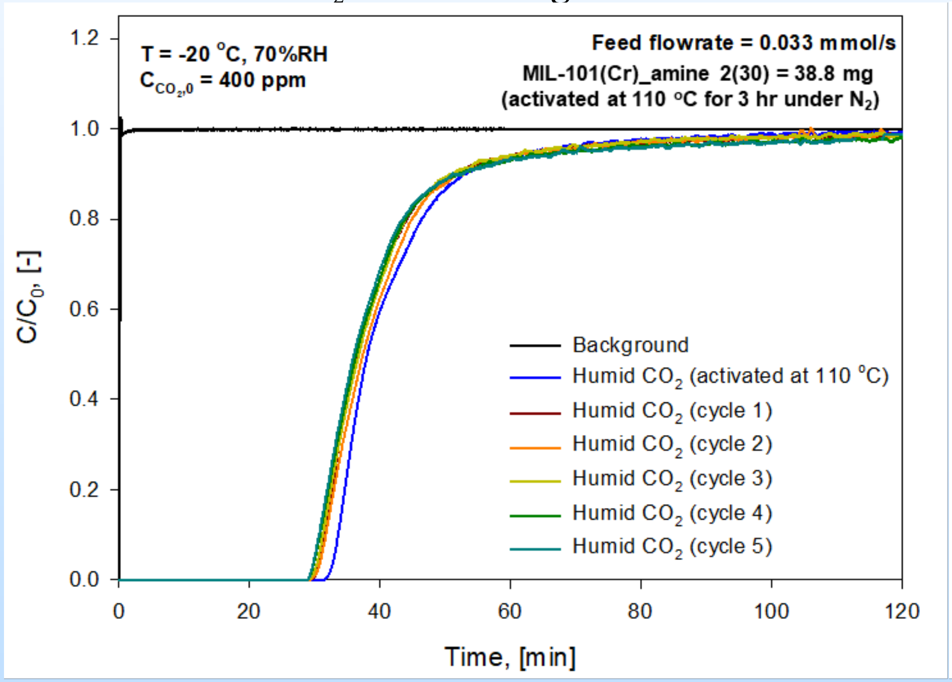
Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

Cyclic fixed-bed tests under humid conditions (70% RH at -20 °C)

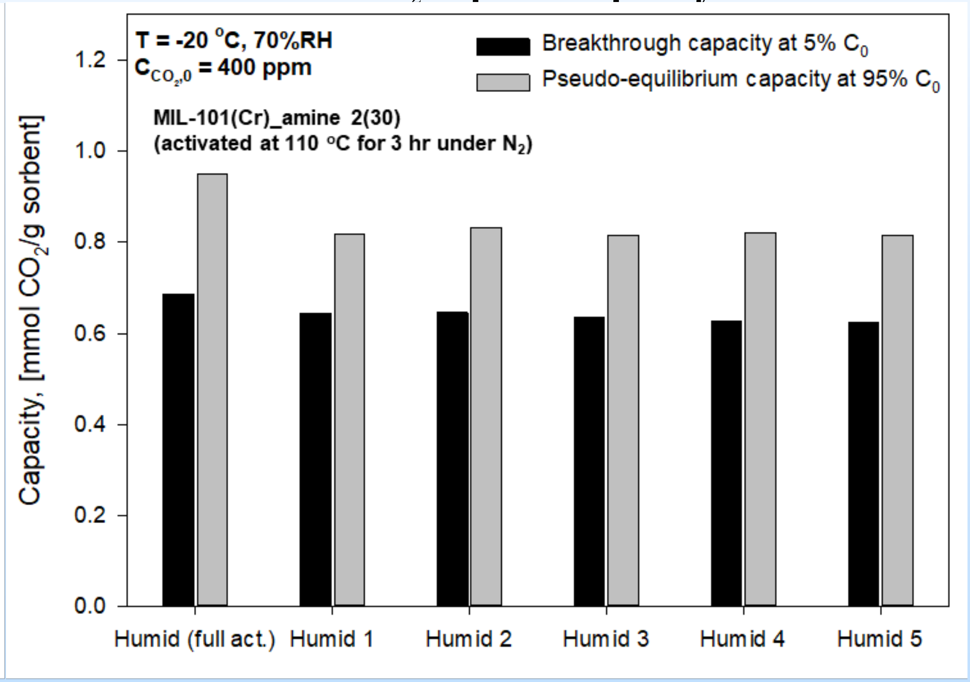
400 ppm CO_2 adsorption at -20 °C (2 h), desorption at 25 °C (2 h)

MIL-101(Cr)_amine 2(30)

CO_2 breakthrough curve



CO_2 capture capacity

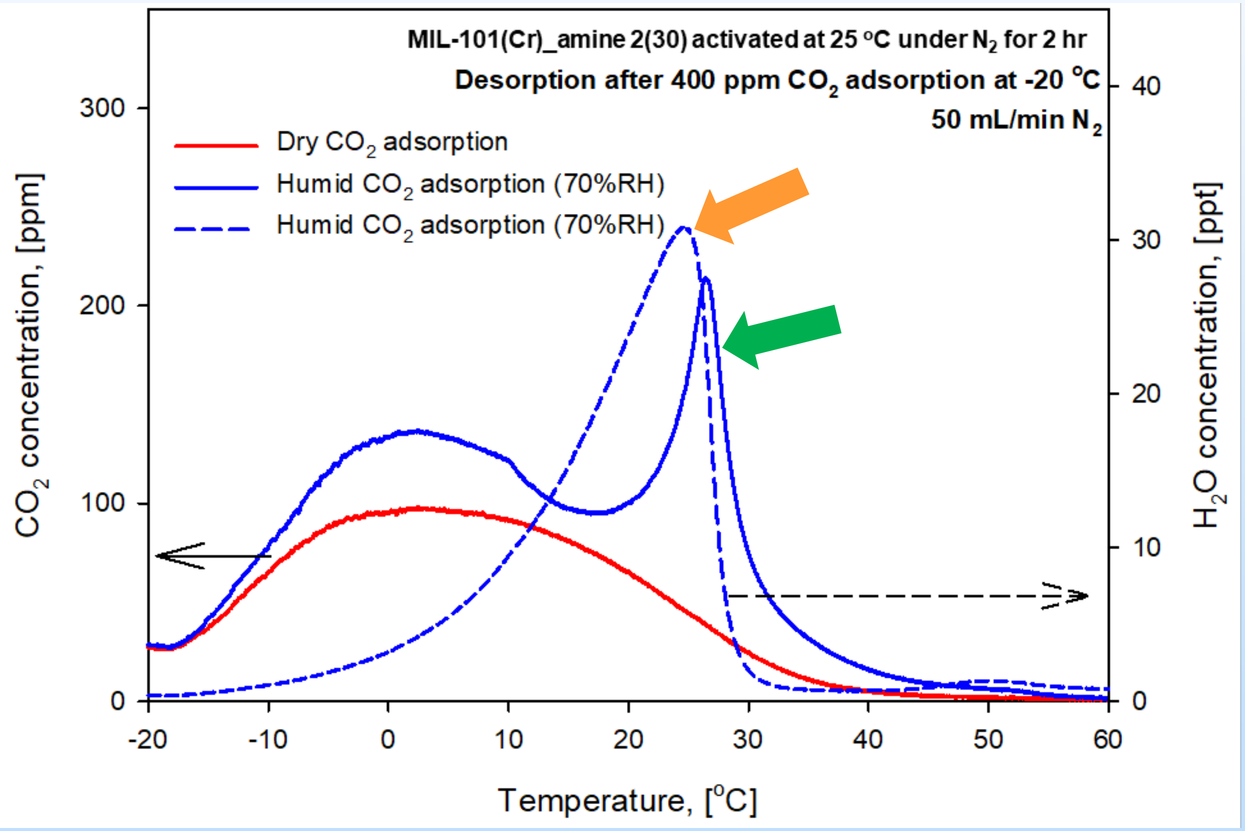


30 wt% Amine 2 impregnated MIL-101(Cr) powders (physisorption dominant) can be effectively regenerated at 25 °C even under humid conditions.

Development of Powder MIL-101(Cr) Sorbents at Sub-ambient Conditions

CO_2/H_2O-TPD experiments (adsorption dry and humid at -20 °C)

MIL-101(Cr)_Amine 2(30)



Enhanced CO_2 adsorption under humid conditions mostly attributed to new peak from 20 °C and 35 °C

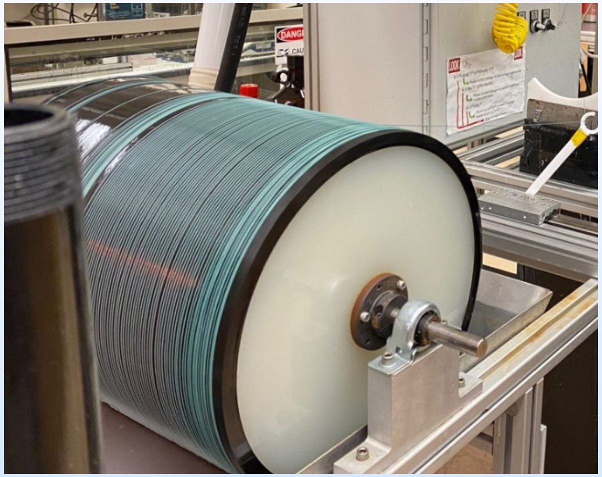
New CO_2 peak starts to appear after significant water desorption.

Thus, desorbed CO_2 may be related to HCO_3^- formation?

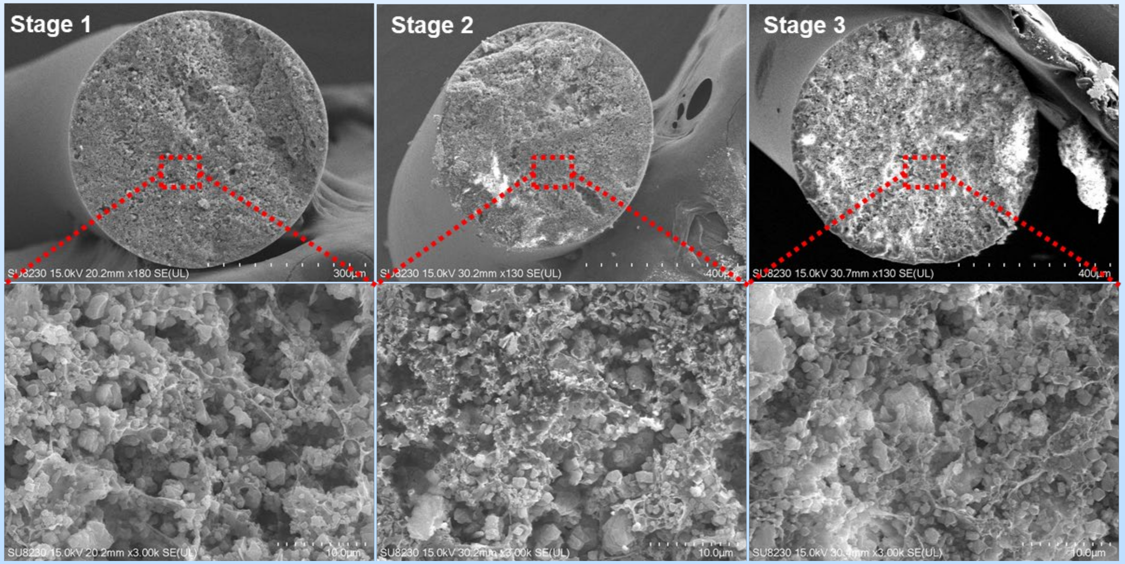
In situ IR may be deployed to probe this hypothesis.

Development of Preliminary Testing of MIL-101(Cr)-amine <u>Fiber</u> Sorbents

MIL-101(Cr)/CA fiber spinning

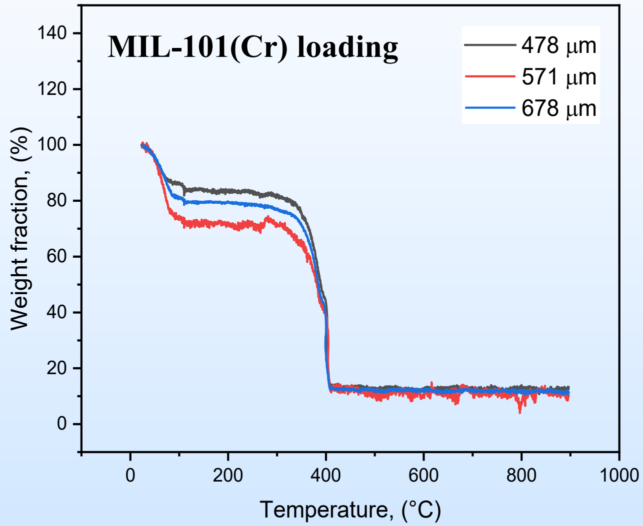


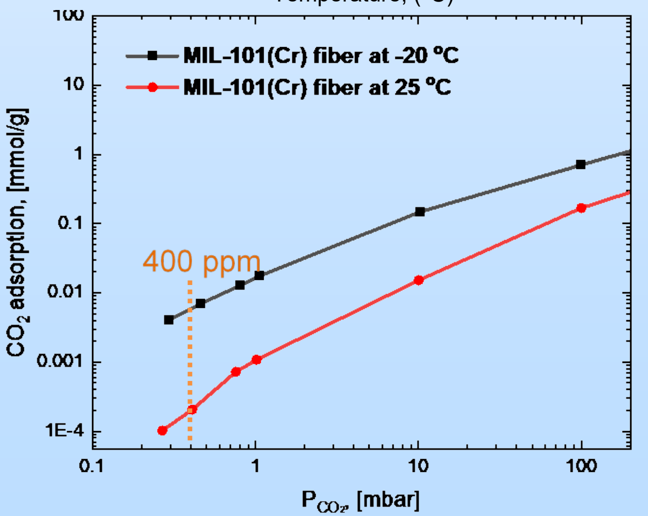
Stages	Flow rate, [mL/hr]	Take-up rate, [m/min]	Air gap, [cm]	Diameter, [μm]
1	**150**	10	5	**480**
2	**200**	10	5	**571**
3	**250**	10	5	**678**



Development of Preliminary Testing of MIL-101(Cr)-amine Fiber Sorbents

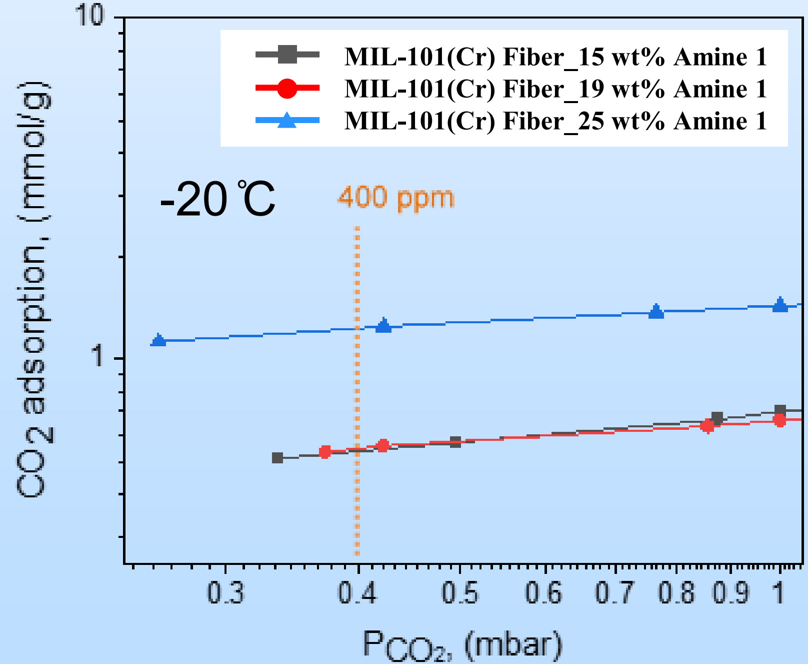
MIL-101(Cr)/CA fibers





Amine 1 impregnated MIL-101(Cr)/CA fibers

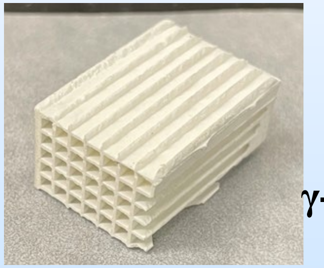
Weight percent of Amine 1 in MeOH solution, (wt%)	Amine 1 loading by EA, (wt%)	CO_2 adsorption, (mmol/g fiber)
5	**15**	0.53
10	**19**	0.54
20	**25**	1.23



Development of Preliminary Testing of MIL-101(Cr)-amine <u>Monolith</u> Sorbents

Synthesis of MIL-101(Cr) on monolith (Ramos-Fernandez et al., 2011)

5.1937 g



γ-alumina coating

Immersed in 33 wt% γ-alumina and 67 wt% water
Calcination at 550 ^{o}C for 3 h

5.9503 g

Seeding

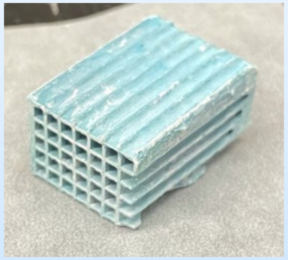
Immersed in 1 wt% MIL-101(Cr) EtOH for 1 h
Solvent was removed in oven (75 ^{o}C for 1 h)

5.9958 g

8 h at 220 ^{o}C

1.2 g $Cr(NO_3)_3 9H_2O$
0.5 g $C_6H_4(CO_2H)_2$
in 15 mL H_2O

6.0114 g

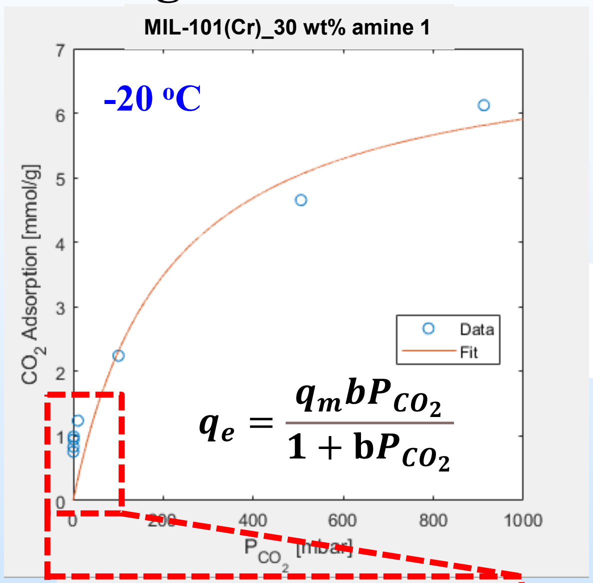


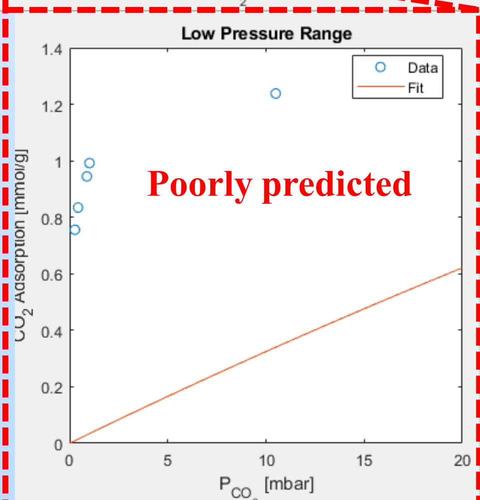
Will be analyzed by TGA to determine MIL-101(Cr) loading
Precursor solution will be altered to enhance MIL-101(Cr) loading

Enrique V. Ramos-Fernandez, Mariana Garcia-Domingos, Jana Juan-Alca˜niz, Jorge Gascon, Freek Kapteijn. "MOFs meet monoliths: Hierarchical structuring metal organic framework catalysts." *Applied Catalysis A: General* 391(2011) 261-267.

CO_2 Adsorption Isotherm Modeling of MIL-101(Cr)-amine <u>Powder</u> Sorbents

Langmuir Isotherm

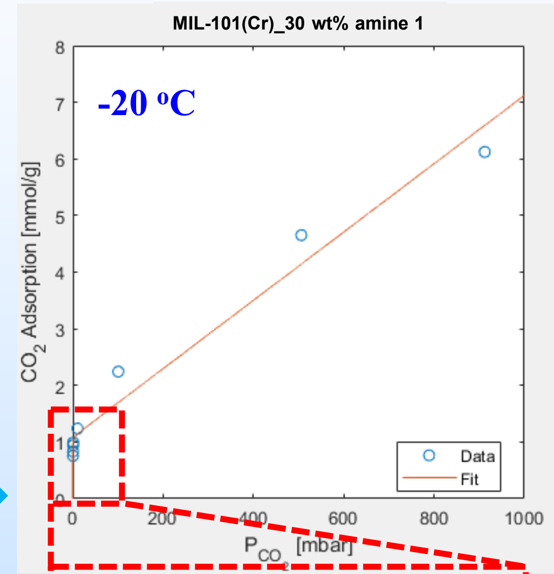


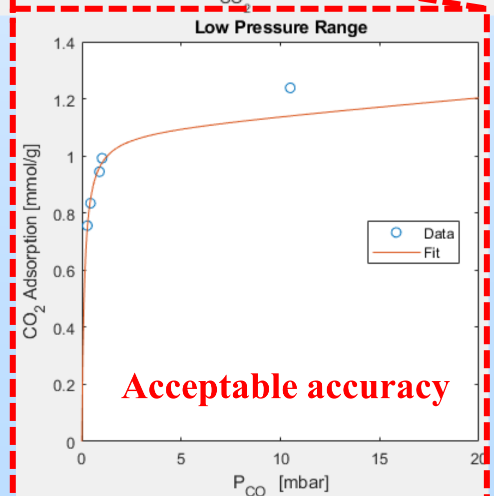


$$q_{eq} = \frac{q_m b P_{CO_2}}{1 + b P_{CO_2}} + c P_{CO_2}$$

Weighted Langmuir with Linear Term

Modified Langmuir Isotherm





Plans for future testing/development/ commercialization

Tasks for future scale-up & testing:

a. This project

   -- assess preferred mode of incorporation into structured contactors (fiber vs. monolith)

   -- complete & use process model to assess preferred operational conditions

b. After this project

   -- assess preferred modes of desorption (T, V, heating modes, etc.)

   -- use technoeconomic model to find cost minima

Plans for future testing/development/ commercialization

Tasks for future scale-up & testing:

c. Scale-up potential

-- sorbent components all commercially available at small scale; assess & develop supply chains for sorbent at larger scales

-- build and test automated low temperature DAC rig

Summary Slide

MIL-101(Cr) powder sorbents

a. Amine impregnated MIL-101(Cr) powders showed promising CO_2 uptake even at -20 ^oC due to enhanced physisorption at cold temperatures.

b. MIL-101(Cr)_amine 2(30) is a preferred sorbent for sub-ambient DAC due to promising adsorption capacity (1.1 mmol/g at -20 ^oC) and low regeneration temperature, 25 ^oC (physisorption dominant).

c. Sub-ambient DAC capacity of MIL-101(Cr)_amine 2(30) was enhanced under humid conditions and stable working capacities (0.82 mmol/g) were obtained over 5 small humid temperature swing cycles (-20 ^oC ↔ 25 ^oC) showing promising stability to humidity.

d. The effects of moisture may be further investigated with in situ cryogenic IR.

MIL-101(Cr) based fiber sorbents

a. Large-scale MIL-101(Cr)/CA (cellulose acetate) fiber was spun and subsequentially infused with Amine 2.

b. 25 wt% Amine 1 infused MIL-101(Cr)/CA fiber sorbents showed promising 400 ppm CO_2 uptake (1.2 mmol/g) at -20 ^oC.

c. The amine loading will be further increased to maximize the CO_2 uptakes.

MIL-101(Cr) based monolith sorbents

a. MIL-101(Cr) was successfully grown on the surface of the cordierite monolith support.

b. The MIL-101(Cr) loading on the monolith will be thermogravimetrically quantified and the synthesis process will be optimized to further increase MIL-101(Cr) loading on the monolith.

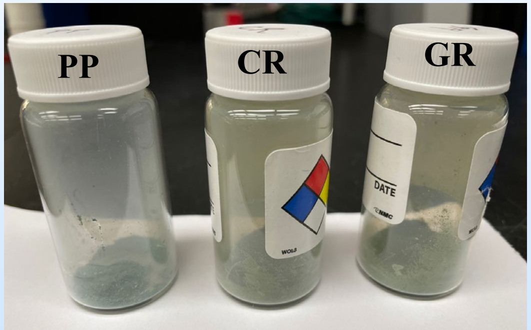
CO_2 adsorption isotherm modeling

a. Since the Langmuir isotherm model was not able to capture the CO_2 adsorption behavior over the whole Pco_2 range, a weighted Langmuir with linear term model was chosen for the thermodynamic modeling, showing acceptable accuracy.

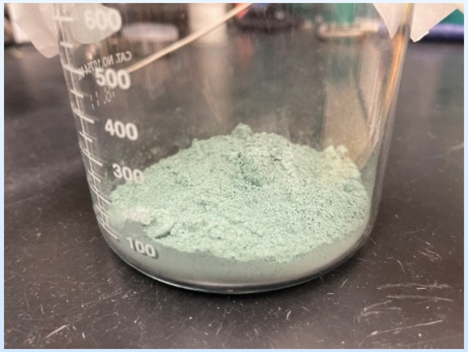
Appendix

Synthesis of MIL-101(Cr) (small and large batch)

Small batch (0.6 g)



Large batch (10 g)



	Material	Surface Area (m^2/g)
Small batch (0.6 g)	MIL-101(Cr)_PP*	3650
	MIL-101(Cr)_CR	3557
	MIL-101(Cr)_GR	3271
Large batch (10 g)	MIL-101(Cr)_MS	2350
Literature [1]		3340

*PP, CR, GR, and MS are the initials of researchers

Small batches MIL-101(Cr) reproduced results from literature*.

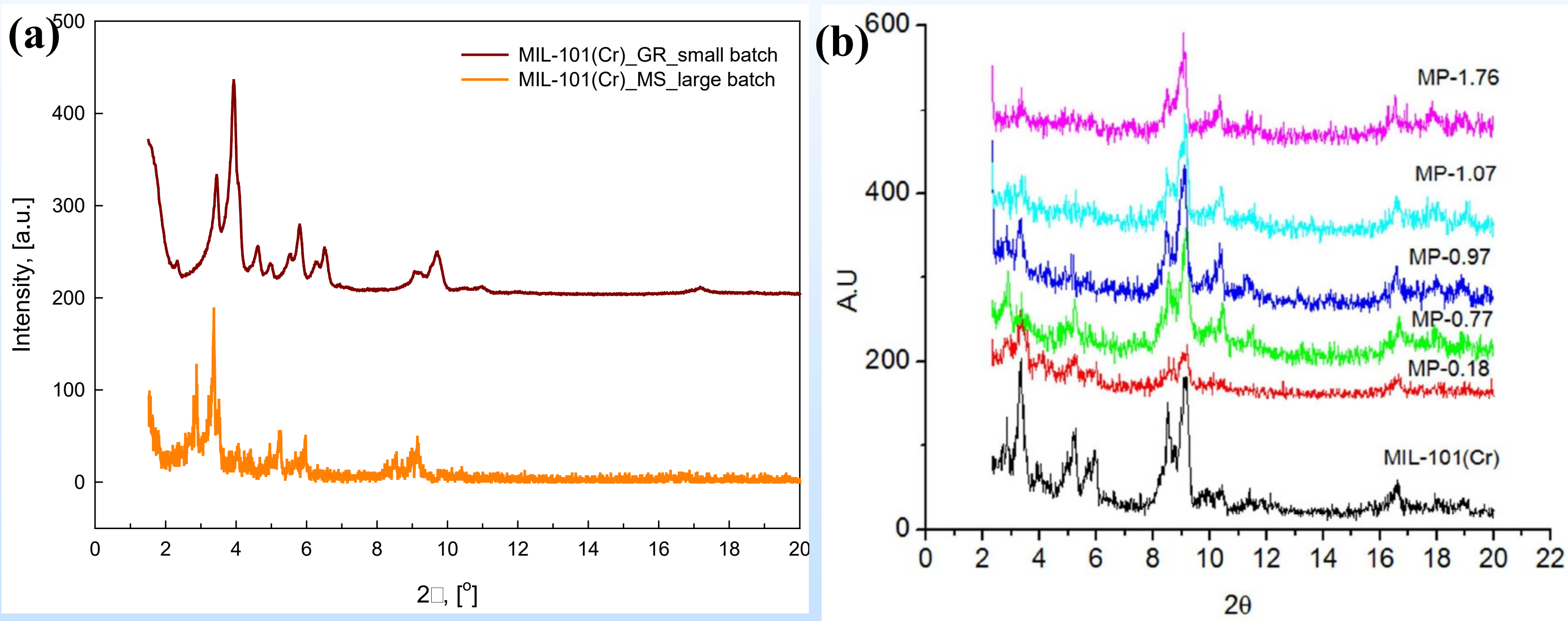
Scaling up of MOFs synthesis somewhat reduced the BET surface area.

*** Darunte, Lalit A., Aloysius D. Oetomo, Krista S. Walton, David S. Sholl, and Christopher W. Jones. "Direct air capture of CO_2 using amine functionalized MIL-101 (Cr)." *ACS Sustainable Chemistry & Engineering* 4, no. 10 (2016): 5761-5768.**

Appendix

Characterization of MIL-101(Cr) (XRD)

Darunte et al., 2016



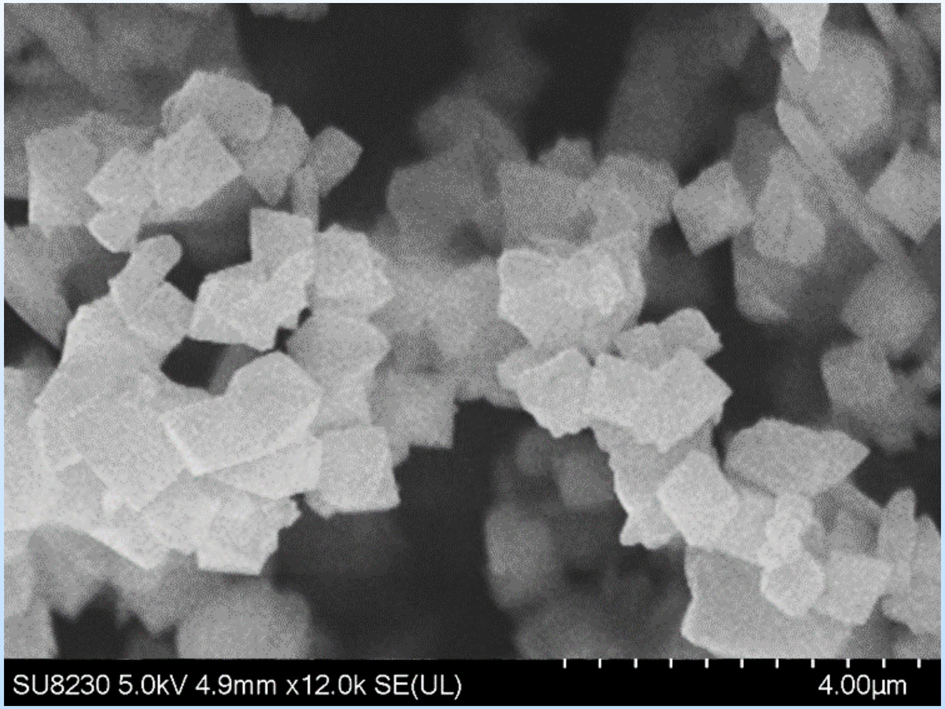
Synthesized MIL-101(Cr) with high crystallinity

* **Darunte, Lalit A., Aloysius D. Oetomo, Krista S. Walton, David S. Sholl, and Christopher W. Jones. "Direct air capture of CO_2 using amine functionalized MIL-101 (Cr)."** ***ACS Sustainable Chemistry & Engineering*** **4, no. 10 (2016): 5761-5768.**

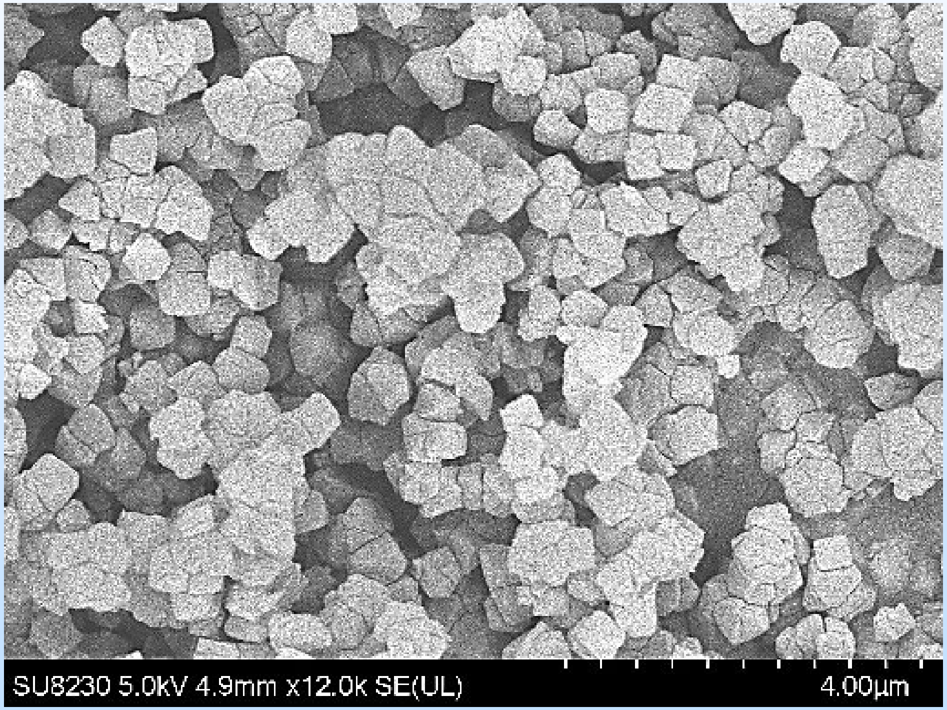
Appendix

Characterization of MIL-101(Cr) (SEM)

Large batch

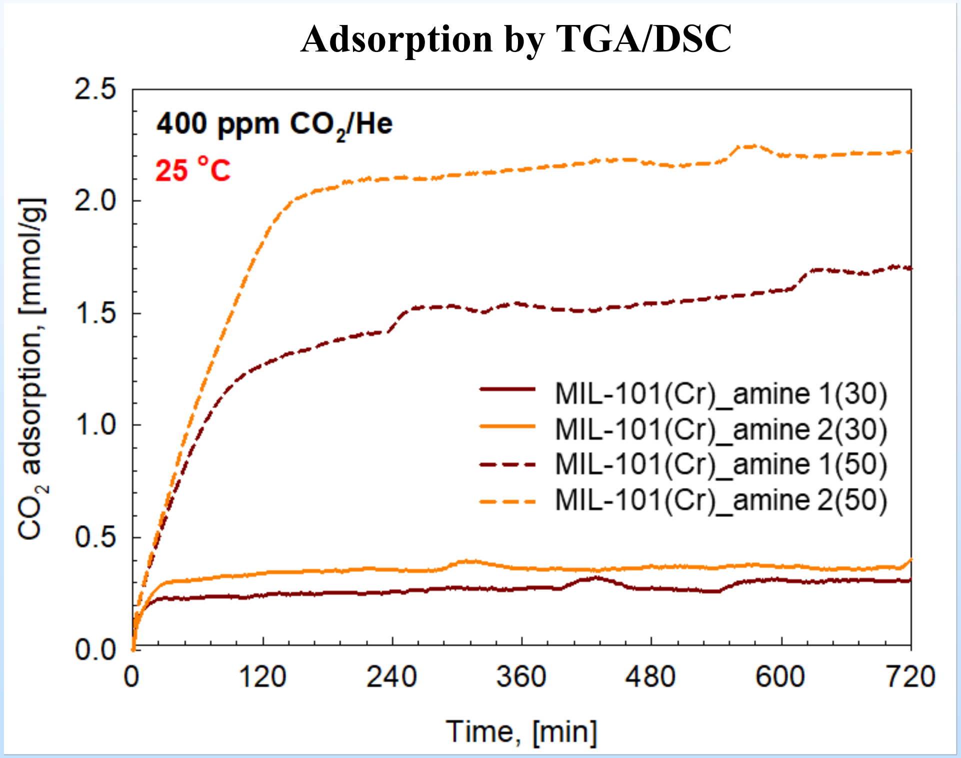


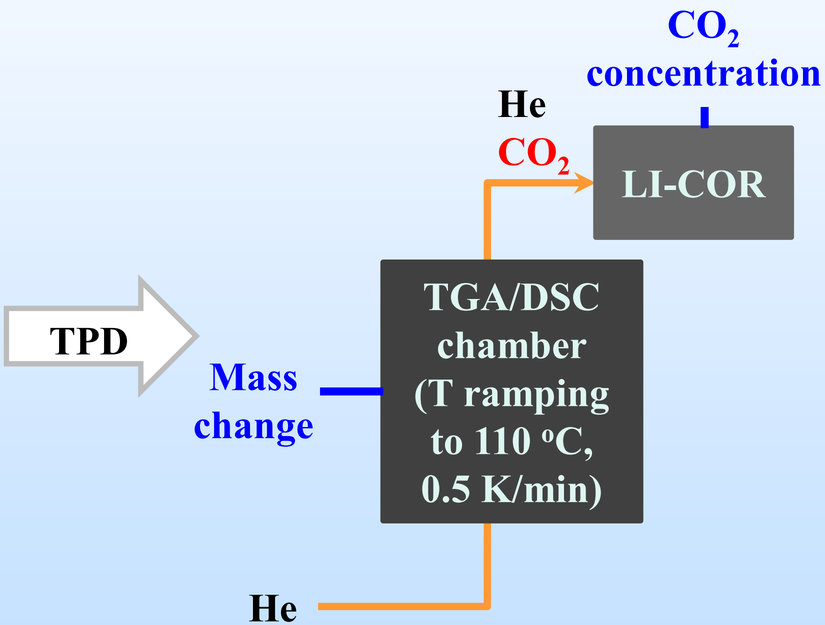
Small batch



Appendix

Temperature Programmed Desorption (TPD) of amine impregnated MIL-101(Cr)





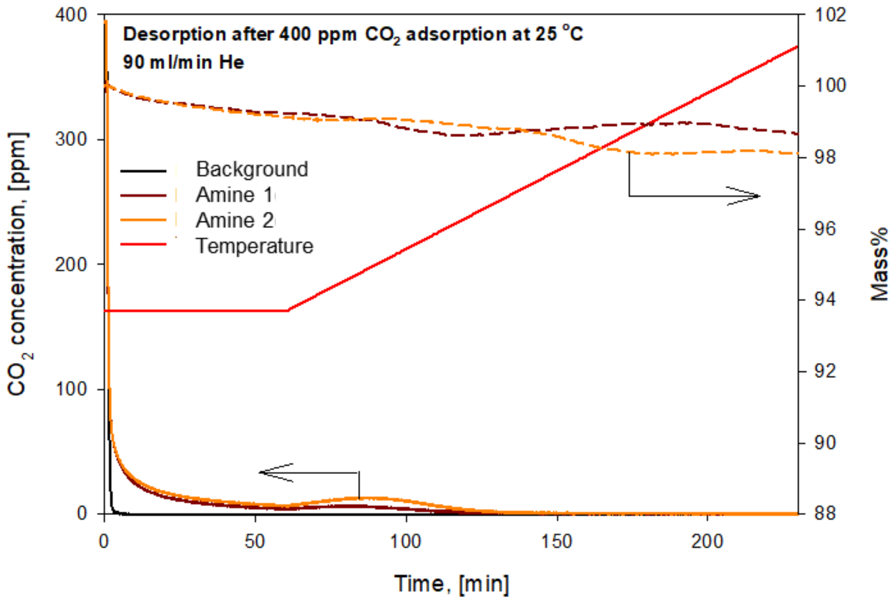
Study the interaction of CO_2 with amine impregnated MIL-101(Cr)

Appendix

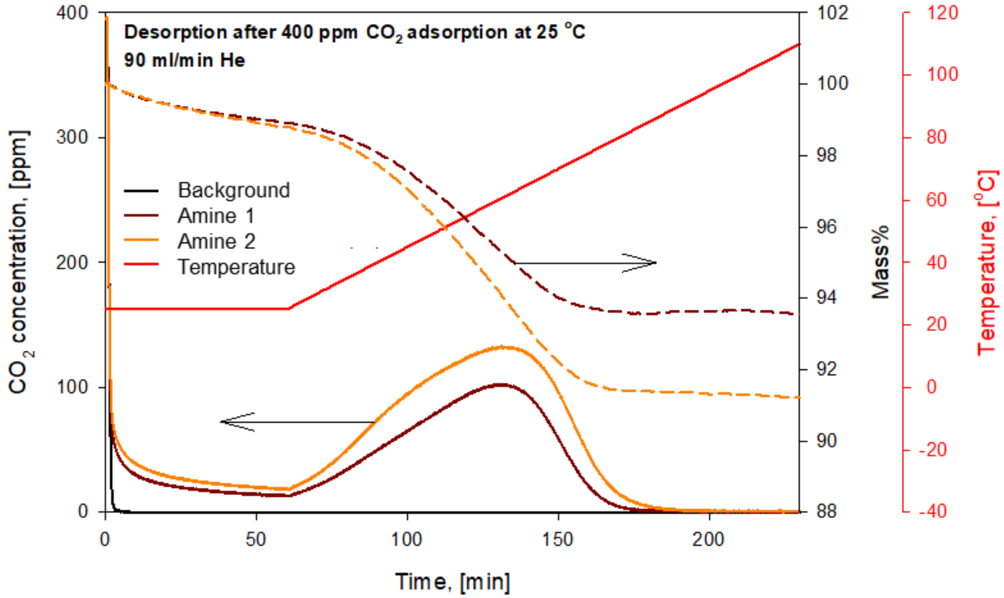
Temperature Programmed Desorption (TPD) of amine impregnated MIL-101(Cr)

Desorption after 400 ppm CO_2 adsorption at 25 °C

30 wt% loading



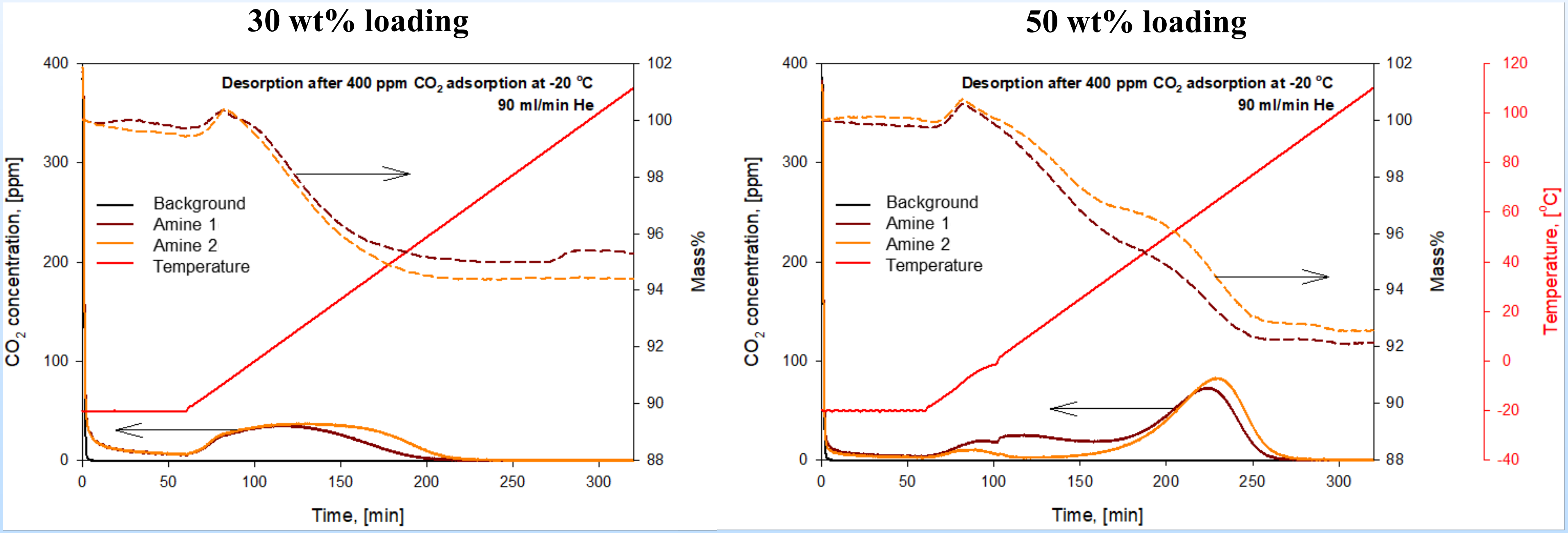
50 wt% loading



Appendix

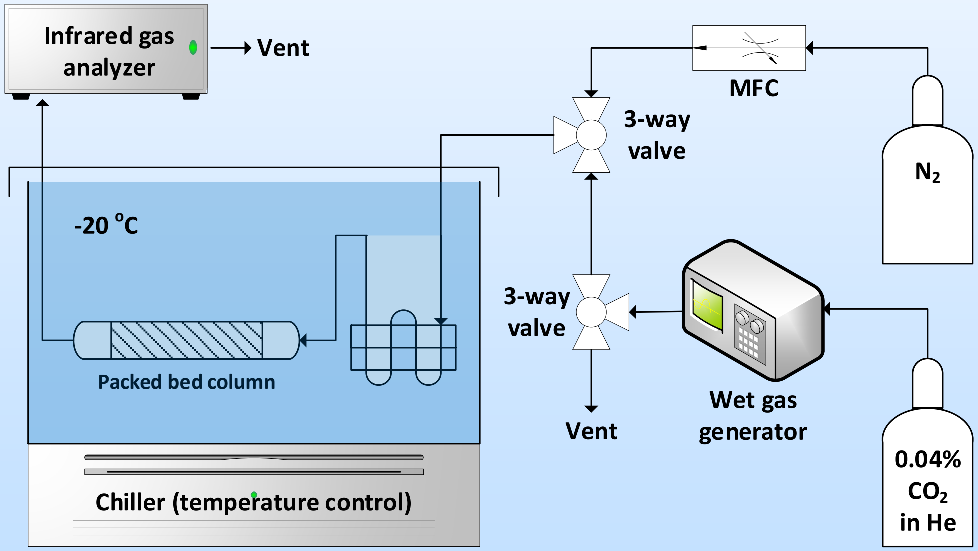
Temperature Programmed Desorption (TPD) of amine impregnated MIL-101(Cr)

Desorption after 400 ppm CO_2 adsorption at -20 °C



Appendix

Sub-ambient DAC Fixed Bed Experiments (MIL-101(Cr)_amine 2(30) powders)



Dry

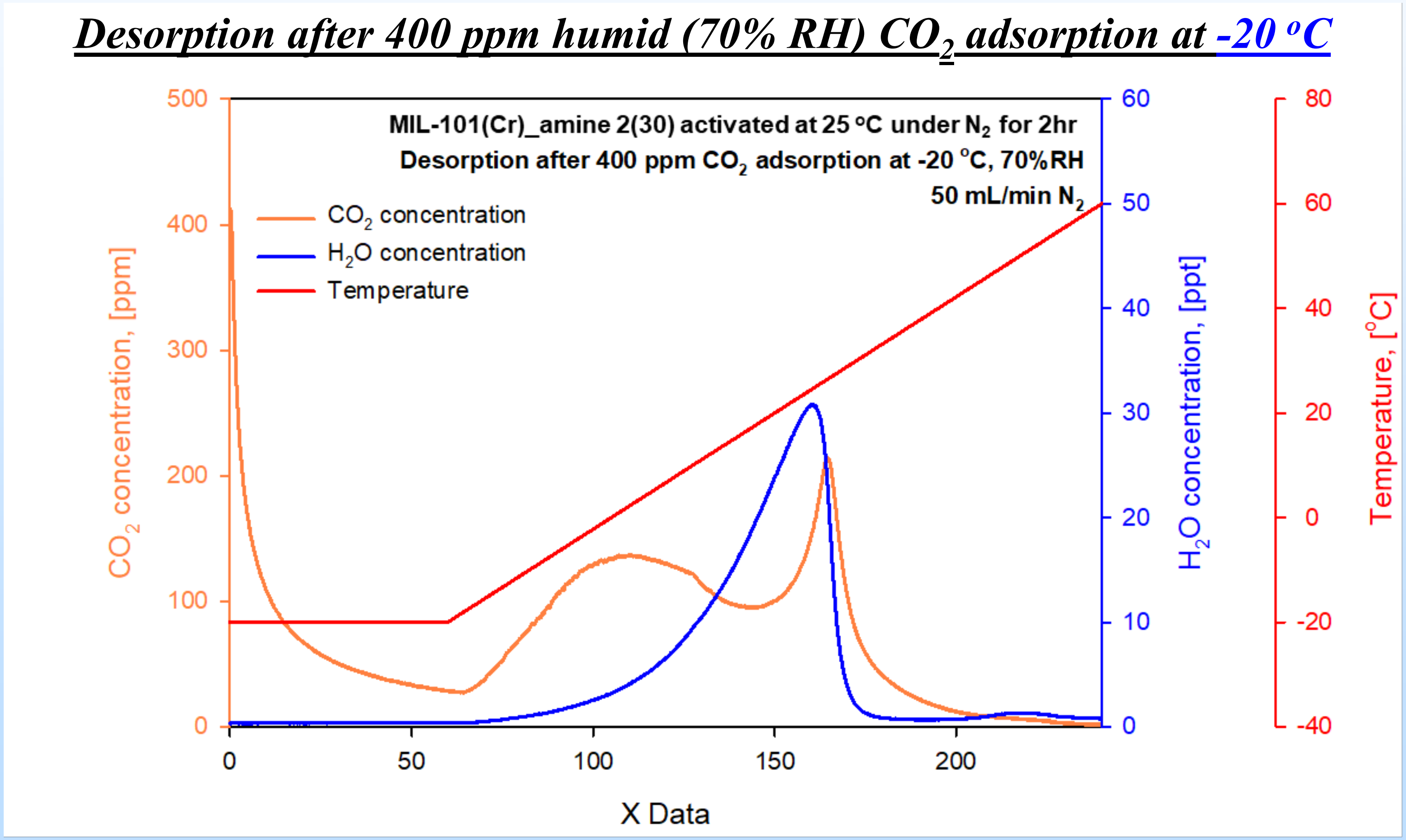
1. Activation (110 °C with N_2 for 3 hr)
2. Adsorption of dry 400 ppm CO_2/He at -20 °C

Humid

1. Activation (110 °C with N_2 for 3 hr)
2. Pre-humidification (wet N_2, 70%RH) at -20 °C
3. Adsorption of humid (70%RH) 400 ppm CO_2/He at -20 °C

Appendix

CO_2/H_2O-TPD of 30 wt% amine 2 impregnated MIL-101(Cr) (Fixed bed experiment)



Appendix

Direct Langmuir model fitting results

$$q_e = \frac{q_m b P_{CO_2}}{1 + bP_{CO_2}}$$

T (°C)	Fiber	Langmuir Fit			Note
		q_m	b	R^2	
25	MIL-101(Cr)	8.8971	2.79E-04	0.9999	
	MIL-101(Cr)_50 wt% amine 1	2.6399	6.95E+00	0.9246	
	MIL-101(Cr)_30 wt% amine 1	3.0281	8.35E-03	0.9017	
	MIL-101(Cr)_10 wt% amine 1	5.1196	5.39E-04	0.9990	
	MIL-101(Cr)_50 wt% amine 2	3.3967	4.53E+00	0.7530	
	MIL-101(Cr)_30 wt% amine 2	2.9704	1.77E-02	0.7849	
	MIL-101(Cr)_10 wt% amine 2	6.5815	3.36E-04	0.9998	
-20	MIL-101(Cr)	13.1907	7.34E-04	0.9996	
	MIL-101(Cr)_50 wt% amine 1	1.8174	1.17E+01	1	Overfit
	MIL-101(Cr)_30 wt% amine 1	7.1520	4.76E-03	0.8618	
	MIL-101(Cr)_10 wt% amine 1	11.2552	8.36E-04	0.9980	
	MIL-101(Cr)_50 wt% amine 2	1.3545	5.04E+00	1	Overfit
	MIL-101(Cr)_30 wt% amine 2	8.0579	5.45E-03	0.8037	
	MIL-101(Cr)_10 wt% amine 2	13.3880	7.58E-04	0.9992	

Appendix

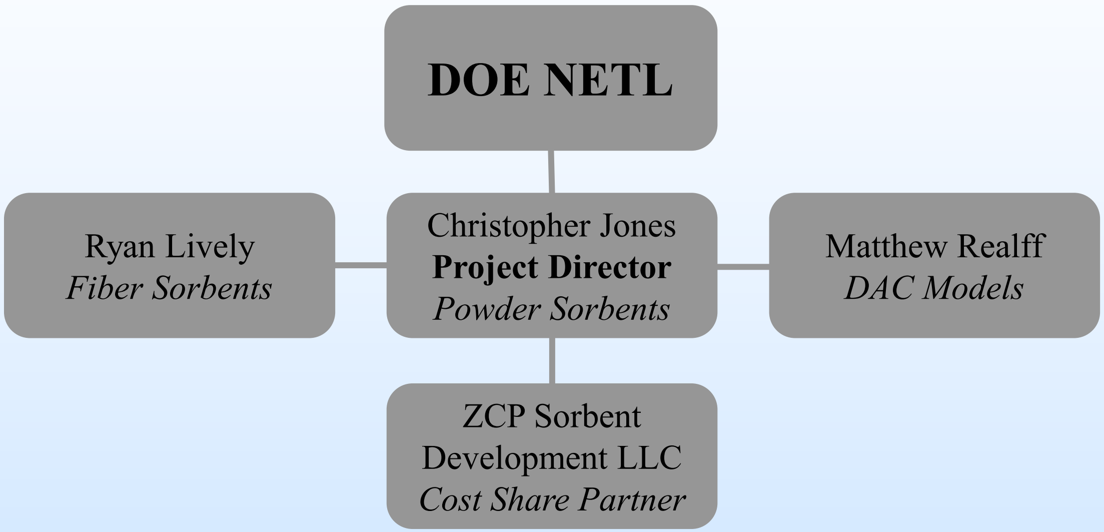
Weighted Langmuir with linear model fitting results

(Weight = 10^4 for the First 4 Data Points and Weight = 10^2 for the Fifth Data Point)

T (°C)	Fiber	Weighted Langmuir Plus Linear Term Fit				Note
		q_m	b	c	R^2	
25	MIL-101(Cr)	3.4556	4.94E-04	8.038E-04	0.9999	
	MIL-101(Cr)_50 wt% amine 1	2.3592	1.17E+01	3.535E-02	0.9974	
	MIL-101(Cr)_30 wt% amine 1	0.5813	2.04E+00	2.852E-03	0.9564	
	MIL-101(Cr)_10 wt% amine 1	0.0536	3.09E-01	1.856E-03	0.9955	
	MIL-101(Cr)_50 wt% amine 2	2.8165	1.02E+01	1.391E-03	0.9685	
	MIL-101(Cr)_30 wt% amine 2	0.8227	3.28E+00	2.867E-03	0.9579	
	MIL-101(Cr)_10 wt% amine 2	0.1396	1.55E-02	1.569E-03	0.9995	
-20	MIL-101(Cr)	3.4048	2.38E-03	3.267E-03	0.9999	
	MIL-101(Cr)_50 wt% amine 1	498.60	1.49E-01	-6.632E+01	1	Overfit
	MIL-101(Cr)_30 wt% amine 1	1.0894	7.98E+00	6.033E-03	0.9730	
	MIL-101(Cr)_10 wt% amine 1	0.1257	1.58E+00	5.512E-03	0.9886	
	MIL-101(Cr)_50 wt% amine 2	380.45	1.16E-01	-3.999E+01	1	Overfit
	MIL-101(Cr)_30 wt% amine 2	1.4423	9.80E+00	6.779E-03	0.9745	
	MIL-101(Cr)_10 wt% amine 2	0.1143	6.49E-01	6.195E-03	0.9896	

$$q_{eq} = \frac{q_m b P_{CO_2}}{1 + b P_{CO_2}} + c P_{CO_2}$$

Organization Chart



- School of Chemical & Biomolecular Engineering, Georgia Institute of Technology
  - **Primary PI, Christopher Jones**: project director and communicate with DOE, developing MOFs powder sorbents and supporting MOFs on monolithic contactors for DAC
  - **Co-PI, Ryan Lively**: designing and fabricating MOFs bearing fiber sorbents for DAC, process development
  - **Co-PI, Matthew Realff**: DAC modeling and techno-economic/life cycle analysis
- ZCP Sorbent Development, LLC
  - Provide cost share by directly funding personnel in the project

Gantt Chart

Task	Team Member	Task Description	M	Year 1 Q1	Year 1 Q2	Year 1 Q3	Year 1 Q4	Year 2 Q1	Year 2 Q2	Task Start Date	Task End Date
1	**CWJ**	**Project Management, Planning and Reporting**	M1								
2	**CWJ**	**Development of MIL-101(Cr) powder sorbents**									
2.1		Synthesis of sorbent powder samples								10/01/20	02/28/21
2.2		Baseline testing of powder sorbents								11/01/20	02/28/21
3	**RPL**	**Development and preliminary testing of MIL-101(Cr)-amine fiber sorbents**									
3.1		Preparation of MIL-101(Cr) fibers								10/01/20	02/28/21
3.2		Preparation and characterization of amine loaded MIL-101(Cr) fibers	M2							02/01/21	06/30/21
3.3		Preliminary testing of CO_2 adsorption performance over MIL-101(Cr)-based fiber sorbents								06/01/21	11/30/21
4	**CWJ RPL**	**Development and preliminary testing of MIL-101(Cr)-amine monolith sorbents**									
4.1		Synthesis of MIL-101(Cr) on monolith supports								10/01/20	04/31/21
4.2		Preparation and characterization of amine loaded MIL-101(Cr) monoliths	M2							02/01/21	06/30/21
4.3		Preliminary testing of CO_2 adsorption performance over MIL-101(Cr)-amine monolith sorbents								06/01/21	11/30/21
5	**CWJ**	**Development of powder MIL-101(Cr)-based sorbents at sub ambient conditions**									
5.1		CO_2 adsorption testing of powder MIL-101(Cr)-based sorbent at sub-ambient conditions								12/01/20	10/31/21
5.2		Stability of powder MIL-101(Cr)-based sorbents to humidity	M3							03/01/21	11/30/21

M indicates milestone.

- Work in progress; - To be completed (original schedule); - To be completed (extended schedule)

Gantt Chart

Task	Team Member	Task Description	M	Year 1 Q1	Year 1 Q2	Year 1 Q3	Year 1 Q4	Year 2 Q1	Year 2 Q2	Task Start Date	Task End Date
6	CWJ RPL	**Development of MIL-101(Cr)-amine monolith sorbent via 3D printing**									
6.1		Development of 3D printing procedure for MIL-101(Cr) monoliths								10/01/20	05/30/21
6.2		Testing of CO_2 adsorption performance for 3D printed MIL-101(Cr)-amine monolith sorbents								05/01/21	12/31/22
6.3		Investigation of effect of monolith properties on CO_2 adsorption performance								09/01/21	03/31/22
7	MJR	**Build models of the adsorption and desorption behavior of MIL-101(Cr)-amine materials**									
7.1		Model equilibrium adsorption behavior								02/01/21	10/31/21
7.2		Model kinetics of adsorption behavior								02/01/21	10/31/21
7.3		Model equilibrium desorption behavior								02/01/21	10/31/21
7.4		Model kinetics of desorption behavior								02/01/21	10/31/21
8	CWJ	**Measuring stability of MIL-101(Cr)-based sorbent powders at sub-ambient conditions**									
8.1		Stability of amine-MIL-101(Cr) sorbents to cyclic operation at sub ambient conditions								10/01/21	03/31/22
8.2		Stability of amine-MIL-101(Cr) sorbents to oxygen	M3							10/01/21	03/31/22
9	CWJ RPL	**Translation of best performing powder MIL-101(Cr)-amine sorbents to fiber and monolith forms**									
9.1		Synthesis and testing of best powder sorbent samples into fiber form								09/01/21	03/31/22
9.2		Synthesis and testing of best powder sorbent samples into monolith form	M4							09/01/21	03/31/22
10	MJR	**Estimate DAC system performance metrics**									
10.1		Determine estimated swing capacity and productivity of adsorbents								10/01/21	03/31/22
10.2		Determine estimated energy consumption per ton CO_2								10/01/21	03/31/22
10.3		Determine the system cost and life cycle energy inventory for 1 Mton of CO_2 scale system	M5							10/01/21	03/31/22

M indicates milestone.

- Work in progress; - To be completed (original schedule); - To be completed (extended schedule)