Direct Air Capture Work at NIST: Reference Materials to Advance DAC Technologies

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NIST Climate Program

NIST addresses climate change in impactful ways, from measurements and modeling of greenhouse gas (GHG) emissions to research and tools to build more resilient communities and alternative energy infrastructure. NIST programs advance research and measurements for energy efficiency and sustainability, as well as standards, frameworks and other resources for enabling metrology.

Climate Measurements and Monitoring

- Traceability of GHG measurements
- GHG measurement technology
- Ensuring climate data quality and standardization

Decarbonization of the Economy

- Built environment
- Energy infrastructure
- Carbon Dioxide Removal (CDR), Carbon Capture Utilization and Sequestration (CCUS)
- Manufacturing

Adaptation and Resilience

- Disaster and failure studies
- Wildland-Urban Interface fires
- Community resilience
- Connected systems resilience

Life Cycle Analysis, Carbon Accounting

NIST provides key tools to mitigate and adapt to climate change in the form of:

- Measurement methods, calibrations and performance metrics,
- Reference materials and data,
- Unique facilities and testbeds, and
- Technical guidance and resources for communities and researchers.

Benchmark Materials

Develop critical measurement science to accelerate innovation and enable timely, effective, and scalable direct air capture

NIST is developing a series of DAC benchmark materials as Research Grade Test Materials (RGTMs)

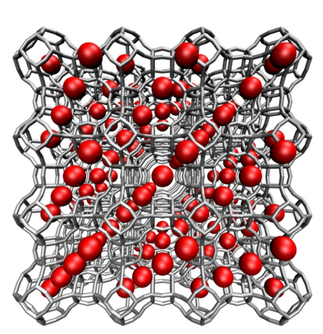
✓ Seeking industry feedback on measurements and prioritizing materials of interest through workshop

✓ Coordinating with DOE's DAC facilities to support measurement needs

✓ Collaborating with large-scale manufacturers in RGTM process

Key questions

- How much CO_2 is adsorbed and desorbed?
- How fast does it happen?
- How much energy does it take?
- How does it perform in real-world conditions?
- How long will it last?



Benchmark Measurements

Anticipated Range of Performance Conditions

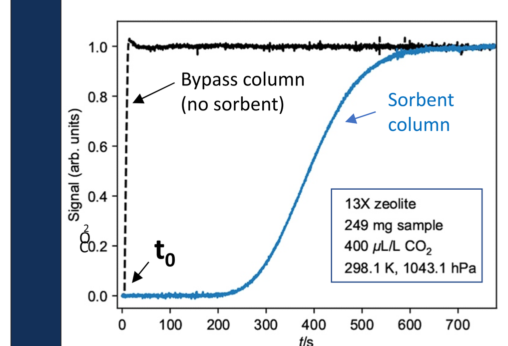
Figure of Merit	Range	Units
Temperature	-233.1 to 323.1	K
Pressure	300 -1050	hPa
Relative Humidity	0 - 80	%
CO_2 Concentration	400	mL/L

The following methods were identified as top priority for the NIST DAC Benchmark Materials:

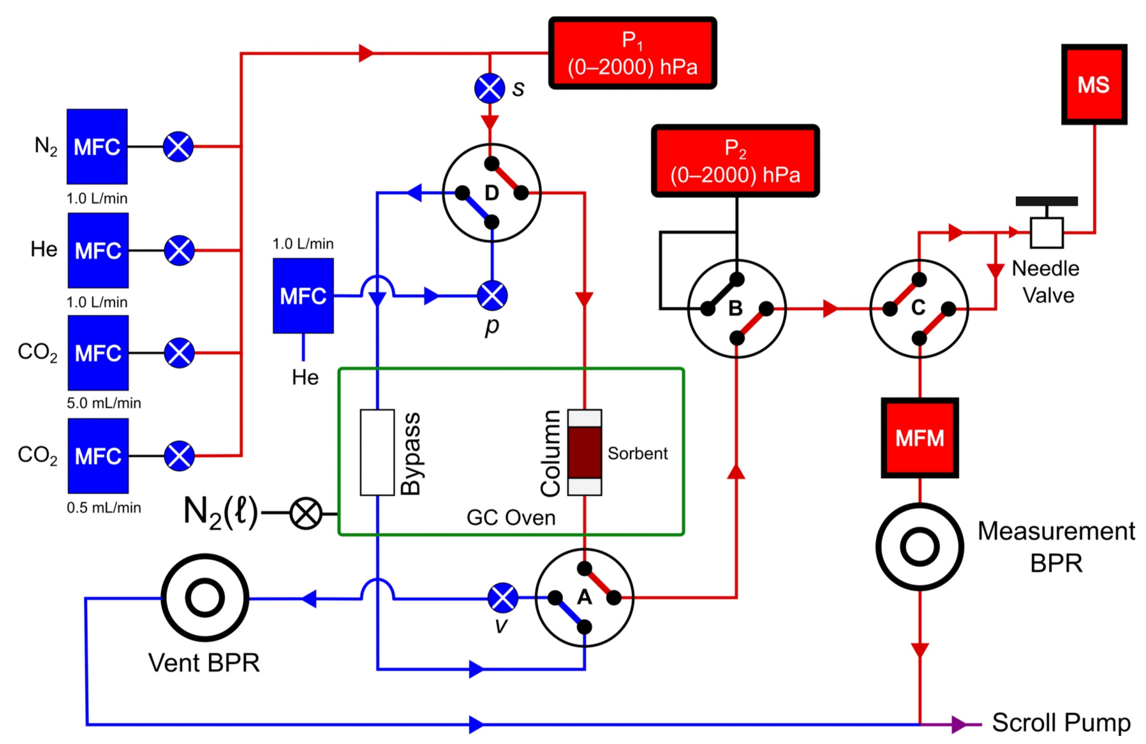
- Breakthrough
- Adsorption Isotherms
- Density/Porosity
- Microstructure Characterization (SEM)
- Heat Capacity

Dynamic Column Breakthrough

NIST has developed instrumentation and measurement methods to characterize the adsorption of gaseous species



Example Data. DCB curves for CO_2 on 13X zeolite exposed to 400 μL/L CO_2 in He at 500 cm^3/min. Shown are the respective mass spectral *m/z* 44 signals (CO_2 parent peak) for the empty bypass column (black dashed curve) and the sorbent column (blue solid curve). t_0 indicates the initiation time of each experiment. The measured capacity under these conditions is 0.23 mol/kg; static adsorption isotherm measurements yield 0.22 mol/kg.



Schematic of the NIST DCB apparatus. Valve orientations and gas flow paths (red for the sample and blue for the purge) correspond to those at the initiation of a sorbent column adsorption experiment (i.e., t0). Bold letters identify two-way, four-port rotary valves, and crossed circles are on−off valves, with some labeled for reference in the text. MFC indicates a mass flow controller, and MFM is a mass flowmeter. MS is the mass spectrometer, P1 and P2 indicate manometers of the total system pressure, and BPR refers to a back pressure regulator.

References

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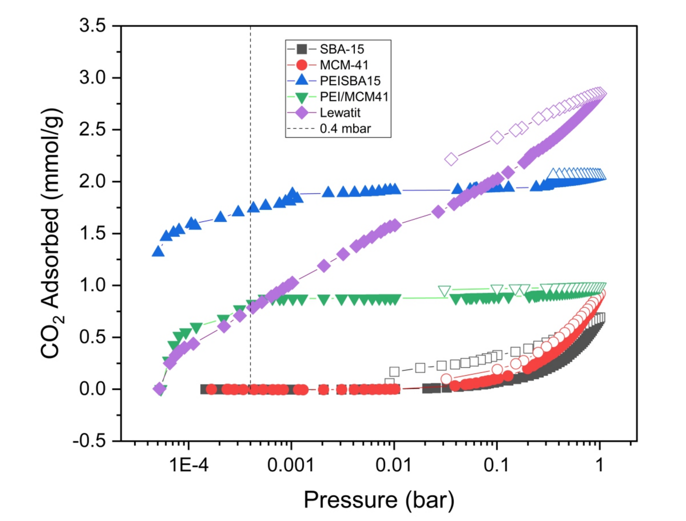
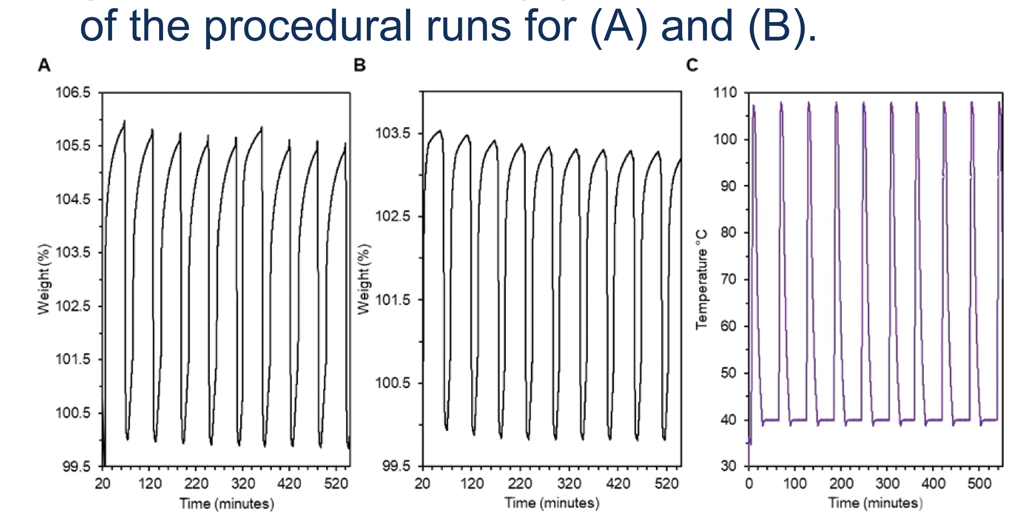
Adsorption and Temperature Effects



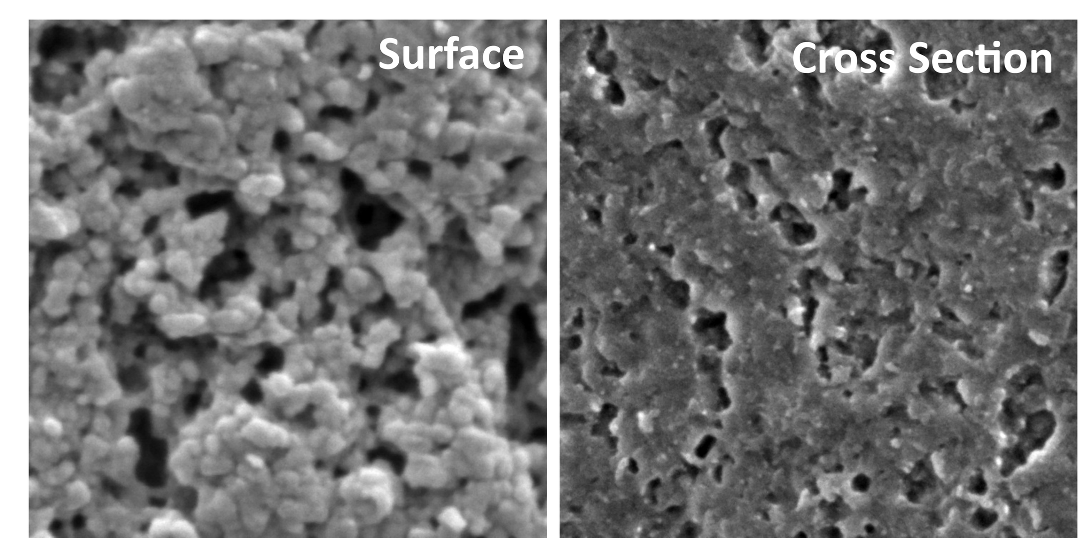
Representative excess pure CO_2 sorption isotherms at 25 °C (298 K) for various DAC materials. The dotted line marks CO_2 uptake at 0.4 mbar (equivalent partial pressure to 400 ppm). Filled symbols are for adsorption; open symbols are for desorption. Uptake is given as mmol of CO_2 per g of dry sample.

Cyclic TGA adsorption and desorption study of (A) PEI impregnated MCM-41, (B) DAS grafted MCM-41, and (C) temperature profile of the procedural runs for (A) and (B).



Cross instrument temperature cycling via TGA and DCB have been used to probe stability and viability of DAC materials.

Microstructural and Heat Capacity



Preliminary data and analysis revealed similar porosity between the surface and internal structure of the candidate RGTM.

Through image analysis, the % porous area can be calculated for the material.

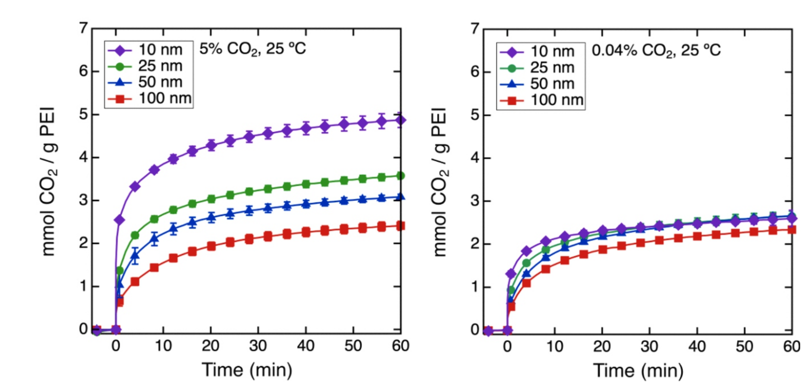
Sample	% Porous Area
Surface	5.682
Cross Section	4.636

The heat capacity of the RGTM candidate was determined using 2 methods: (a) the MDSC mode (reversing heat capacity), and (b) the Direct/Standard DSC mode (total heat capacity).

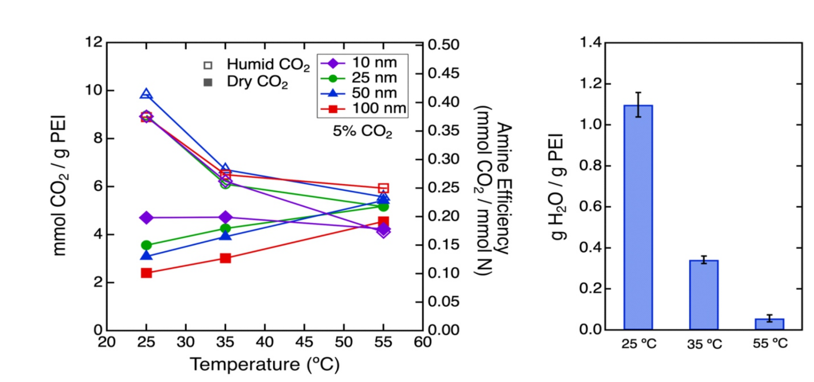
Temperature [°C]	MDSC - C_p [J/(g.°C)]	Standard DSC - C_p [J/(g.°C)]
10	1.292	1.349
25	1.395	1.453
50	1.542	1.732
100	1.702	3.189
180	1.957	2.046

CO_2 Sorption in Thin Films

Dry and humid CO_2 sorption in PEI thin films species in polyethyleneimine films



- Thinner films exhibit greater CO_2 capture capacity per g of PEI, suggesting more amine sites are accessible due to lower diffusional resistance.
- This effect is less pronounced, but still true, when capturing 400 ppm CO_2.



- Humidity enhances the CO_2 capacity and amine efficiency of the PEI, due to increased mobility and facilitated carbamate formation.
- Enhancement due to humidity decreases with temperature due to decrease in overall water sorption.

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