InnoCO2Sepra

Transformational Sorbent Materials for a Substantial Reduction in the Energy Requirement for Direct Air Capture (DE-FE0031953)

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U.S. Department of Energy
National Energy Technology Laboratory
Carbon Management Project Review Meeting
August 15 - 19, 2022

Executive Summary

- InnoSepra's direct air capture project utilizes physical sorbents with low heat of adsorption (~0.8 GJ/MT)
  - High CO_2 capacities at a CO_2 concentration of 400-ppm (>4-wt%)
  - Very long-sorbent life (>5 years)
  - Regenerable at low temperatures (<125^oC)
  - Can be quickly scaled up to very large quantities for commercial scale direct air capture
  - Potential for up to 50% reduction in the energy needed for Direct Air Capture, <4 GJ/MT
  - Potential for up to 50% reduction in the capture cost, <$200/MT
  - This DOE Project will
    - Optimize the physical sorbents for direct air capture through Monte Carlo simulations
    - Prepare and characterize the best materials both in beaded as well as structured forms
    - Perform a high level technical analysis to enable future TEA and LCA evaluations

The DOE Project (FE0031953)

- Objectives:
  - Develop and characterize materials that have the potential to reduce the energy required for direct air capture compared to current state-of-the-art technologies by up to 50%
  - Identify means to scale up the materials to thousands of tons/year needed for commercial scale up of direct air capture
  - Determine projected energy requirement based on lab testing and process simulation
- The total project budget is U.S. $1 million ($800K DOE, $200K match), During the project InnoSepra will
  - Develop the sorbents based on prior experience and Monte Carlo simulations and prepare downselected materials for lab testing
  - Carry out microbalance and lab experiments for further downselction
  - Prepare materials in structured forms for lab testing, perform high level TEA and LCA

Project Participants

DOE/NETL

- Project oversight, feedback, funding (Project Manager: Nicole Shamitko-Klingensmith/Naomi O'neil

InnoSepra

- Technology development at lab and bench scale, coordinate with partners, project management and reporting

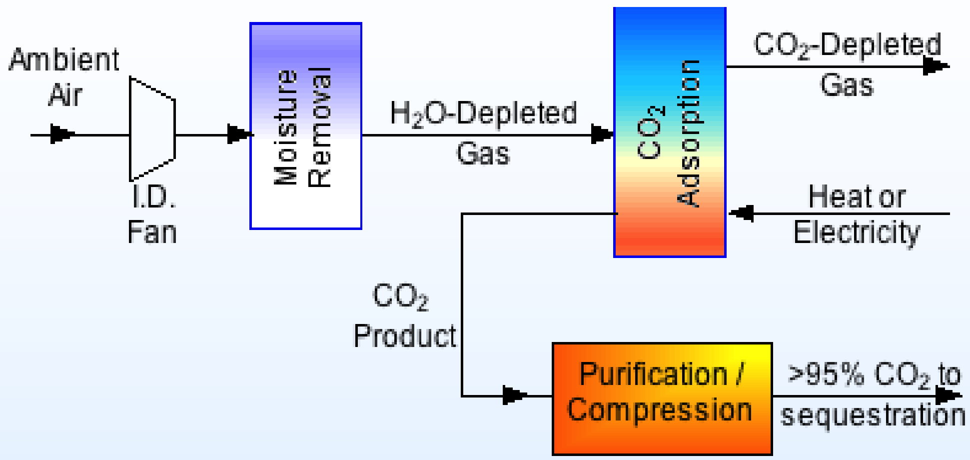
Adroitech

- Monte Carlo Simulation, fabrication of structured sorbents

Current Approaches for DAC

- Carbon Engineering uses an absorption system: reaction with NaOH, followed by regeneration with $Ca(OH)_2$ and reactivation of $CaCO_3$ to CaO, hydration of CaO to produce $Ca(OH)_2$ (Liu et al., Sust. Energy Fuels, 2020)
- Global Thermostat and Climeworks use amine-impregnated sorbents with either indirect regeneration or direct steam regeneration (Eisenberger, U.S. patents 8,500,855 & 10,413,866)
    - A very significant amount of energy needed for physisorbed water
- Both approaches need upwards of 8 GJ/tonne of CO_2 in thermal energy, a significant amount of this energy is needed at >900^{o}C for the Carbon Engineering Process
- Amine-based sorbents in dry form are not stable, sorbents in wet form can degrade irreversibly, short sorbent life

Technology Background



- Based on physical sorbents in structured form
- Base materials with high CO_2 capacity (>4-wt% at p_{CO2} = 0.04 kPa), low heats of adsorption (40-44 kJ/mol of CO_2)
- Chemical modification of base materials to improve capacity and selectivity during this project
- Materials are low cost, easily scalable to quantities needed for commercial use (thousands of tons), very stable (>5 year life)
- Challenges include fabrication of large quantities in structured form, process demonstration at a commercially relevant scale

Improvement in CO_2 Capacity with Chemical Modifications

Material	Capacity at P_{CO2} = 0.04 kPa, wt%	Capacity at P_{CO2} = 15 kPa, wt%
Starting Material	**1.6**	17.0
Chemical Modification 1	**3.3**	18.0
Chemical Modification 2	**6.2**	18.5

Technical Approach/Project Scope

Work Plan

- Literature review, procurement of base materials
- Optimization of base materials through Monte Carlo Simulations and lab experiments at a p_{CO2} of 0.04 kPa
- Measurement of CO_2 sorption/desorption isotherms and kinetics (0 to 125^{o}C)
- Preparation, testing and characterization of selected materials in beaded and structured forms; lab testing of structured matls
- High level process design incorporating the best materials in a DAC system; research results to enable future TEA and LCA

Key Milestones

- Sorbent down-selection based on capacity / energy requirements
- Preliminary technical design and analysis

Success Criteria and Potential Risks

The success criteria include

- Completion of materials characterization with results showing a CO_2 capacity >3.5-wt% for 400-ppm CO_2 in air
- Fabrication and testing of structured sorbents and a preliminary technical analysis showing that the materials have at least 50% lower energy requirements compared to current state of the art technologies

The key risks include

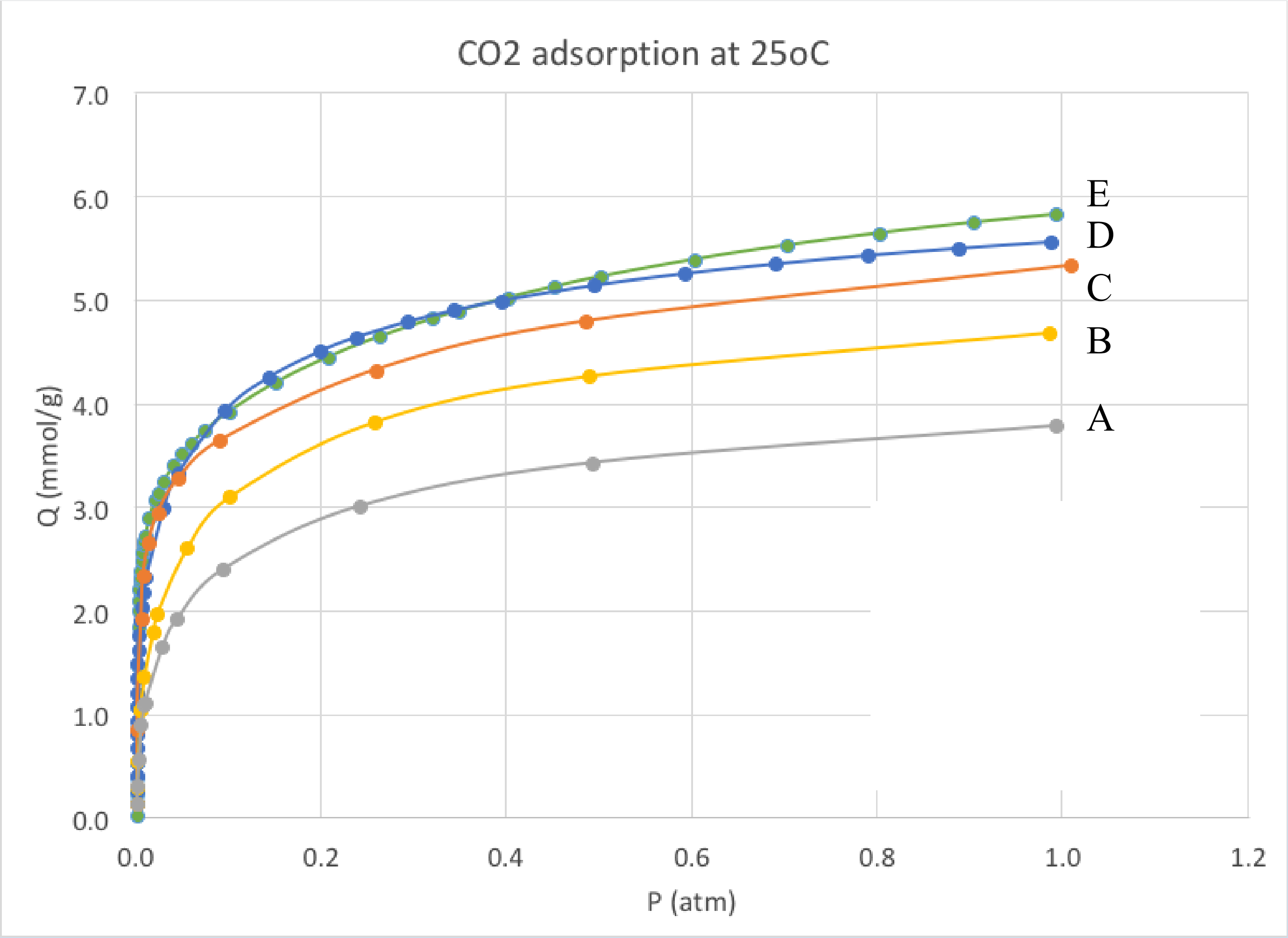
- Resource & management risks (availability and suitability of resources)
- Technical risks (CO_2 capture & regeneration)
- Cost & schedule risks (cost and schedule overruns)

Key Activities for BP1

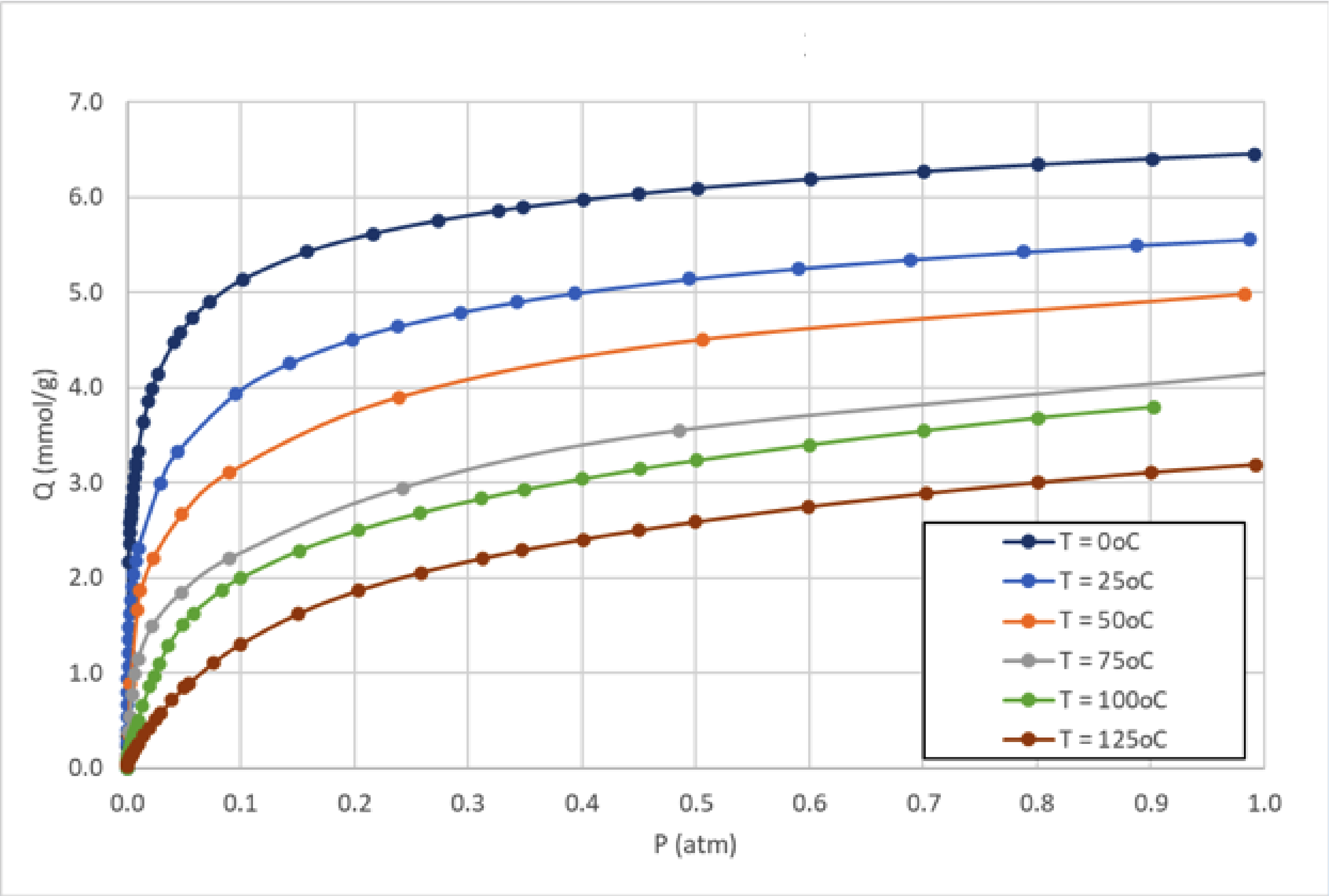
Budget Period I – Materials Development & Lab testing

- Monte Carlo Simulations, Prepare Materials for Isotherm Measurements
- Select up to 4 materials based on isotherms and kinetic measurements, prepare in beaded form
- Breakthrough testing in the lab unit
- Preparation and characterization of materials in structured forms
- Lab scale testing of structured materials
- High level process design/analysis
- Technical approach incorporating results for future TEA and LCA

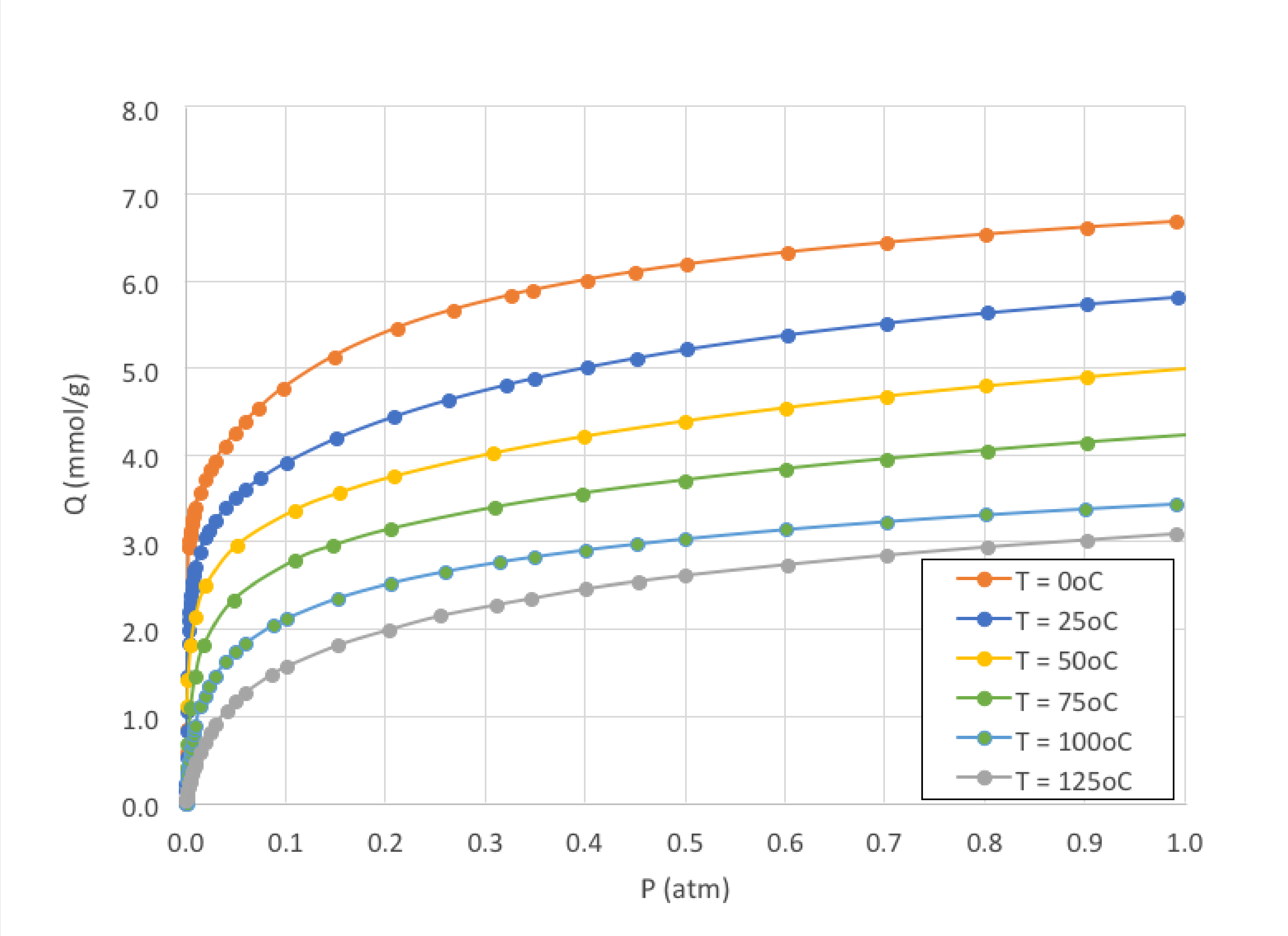
Sorption Isotherms at 25ºC



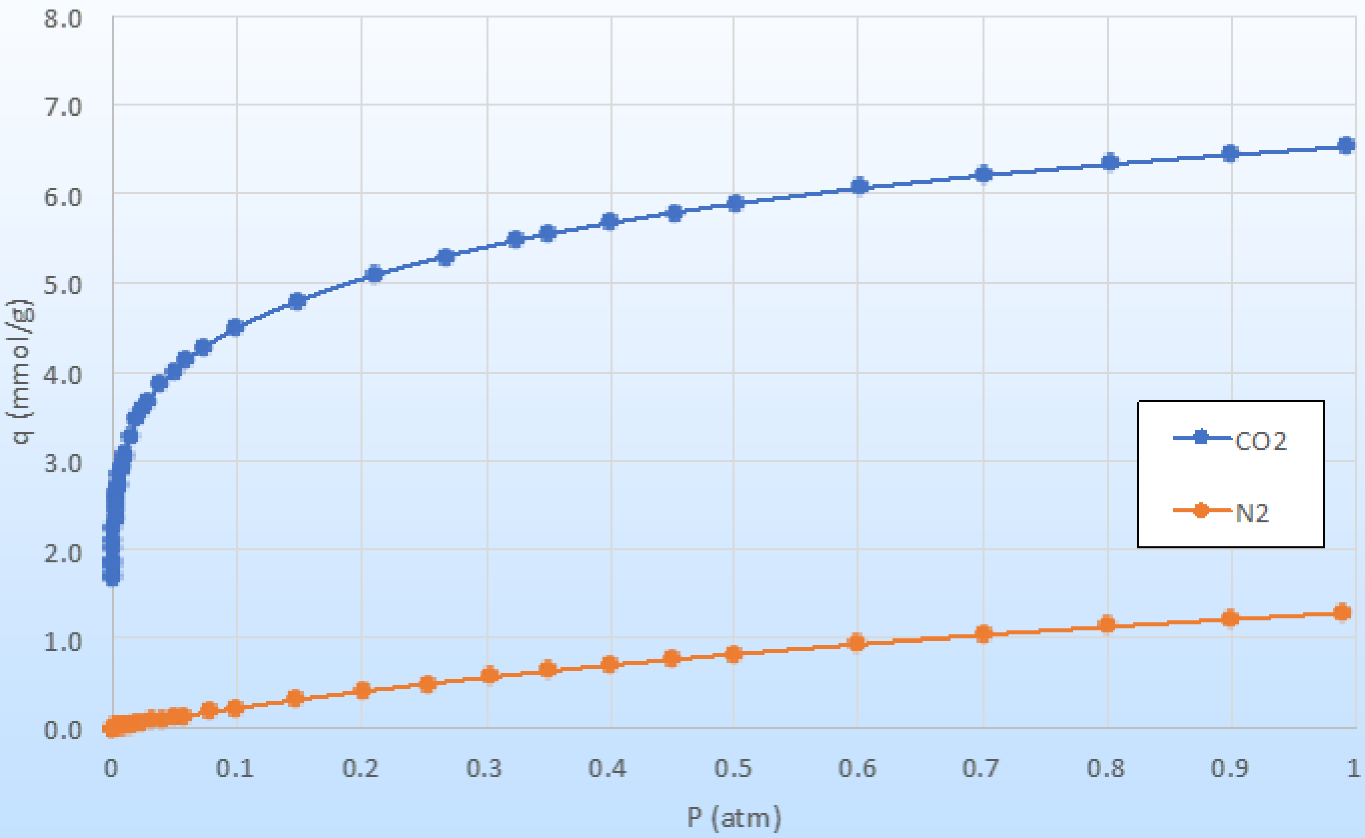
Sorption Isotherms for Material D



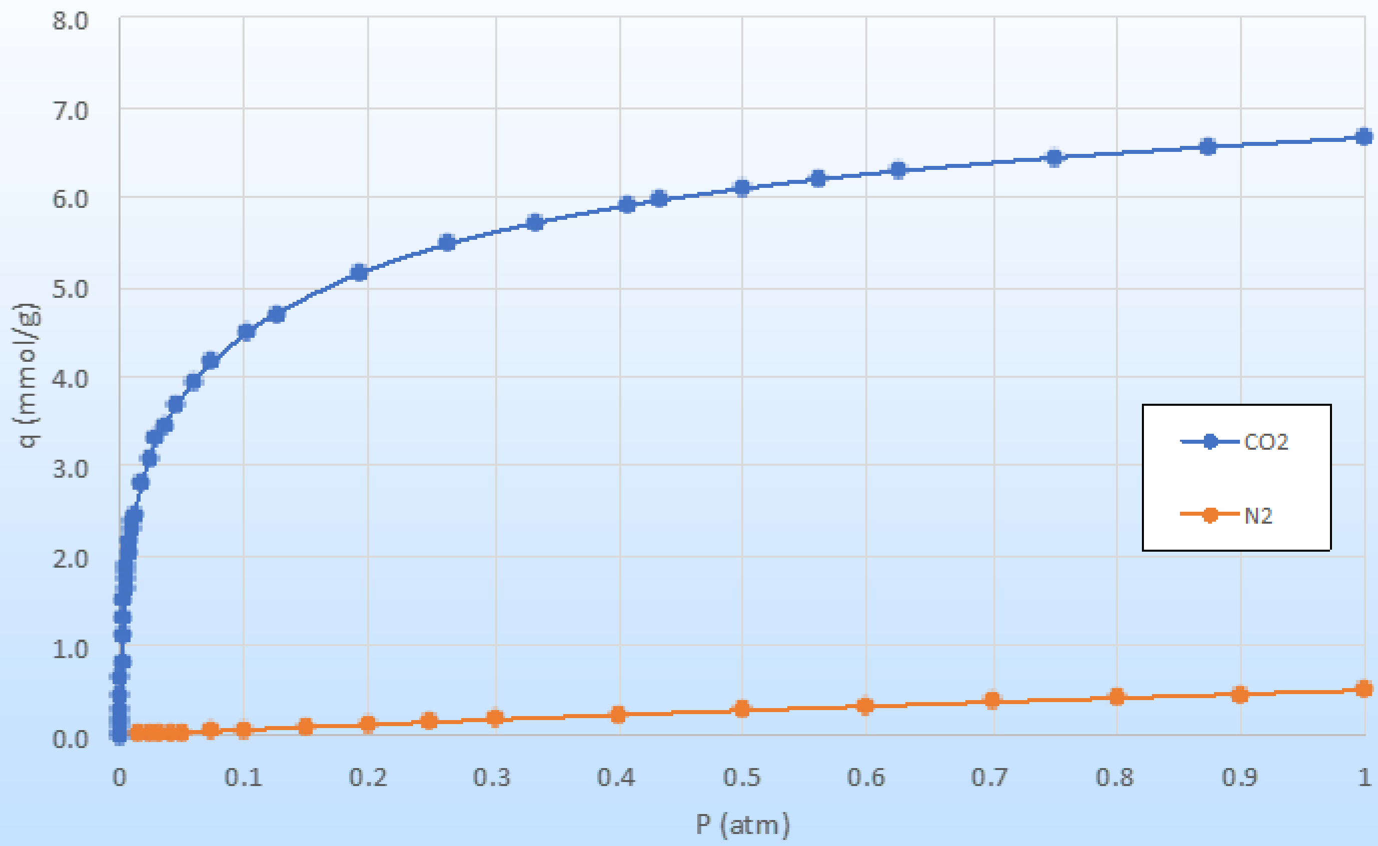
Sorption Isotherms for Material E



Base Material with High N_2 and High CO_2 Adsorption

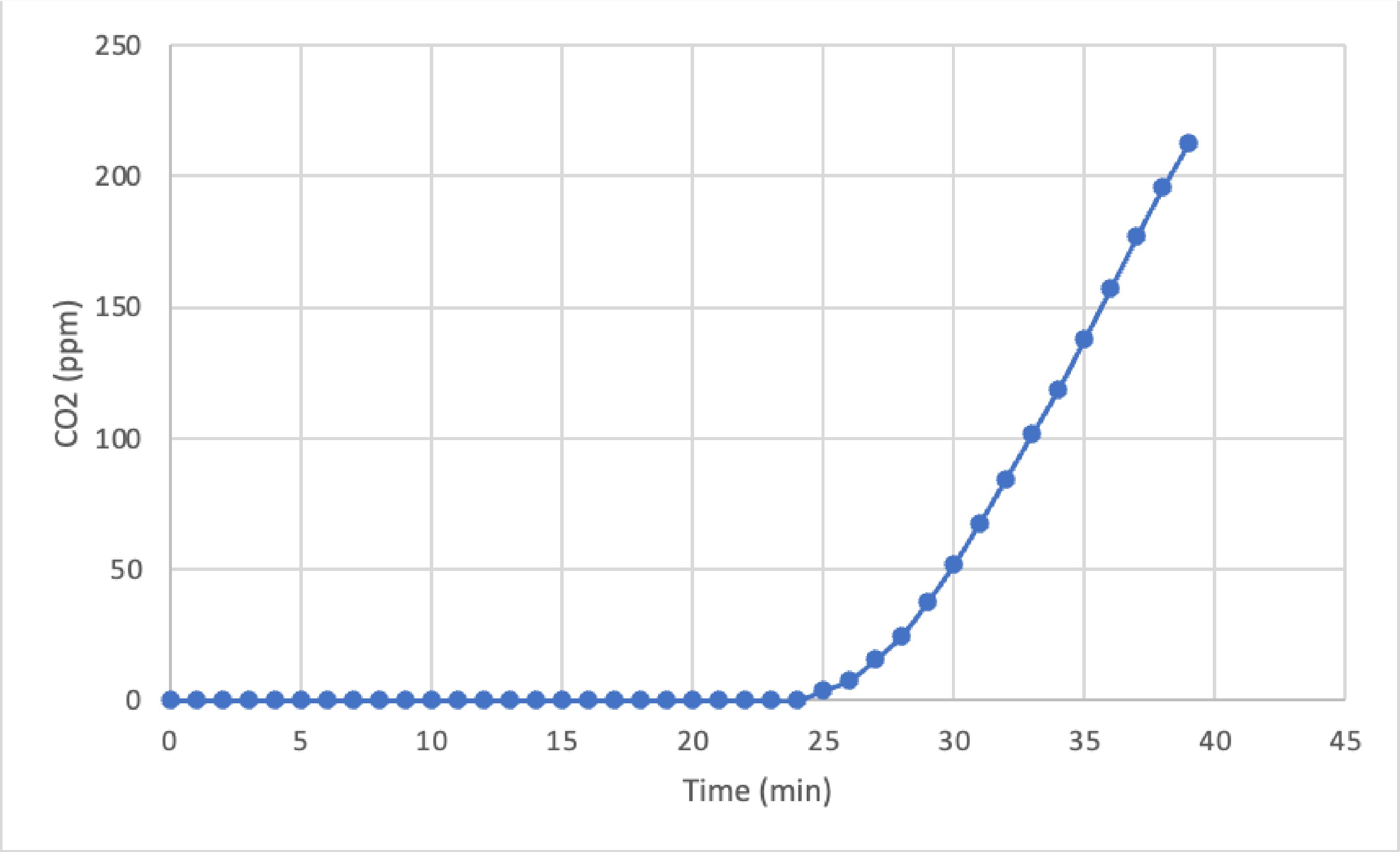


Modified Material with Lower N_2 and High CO_2 Adsorption



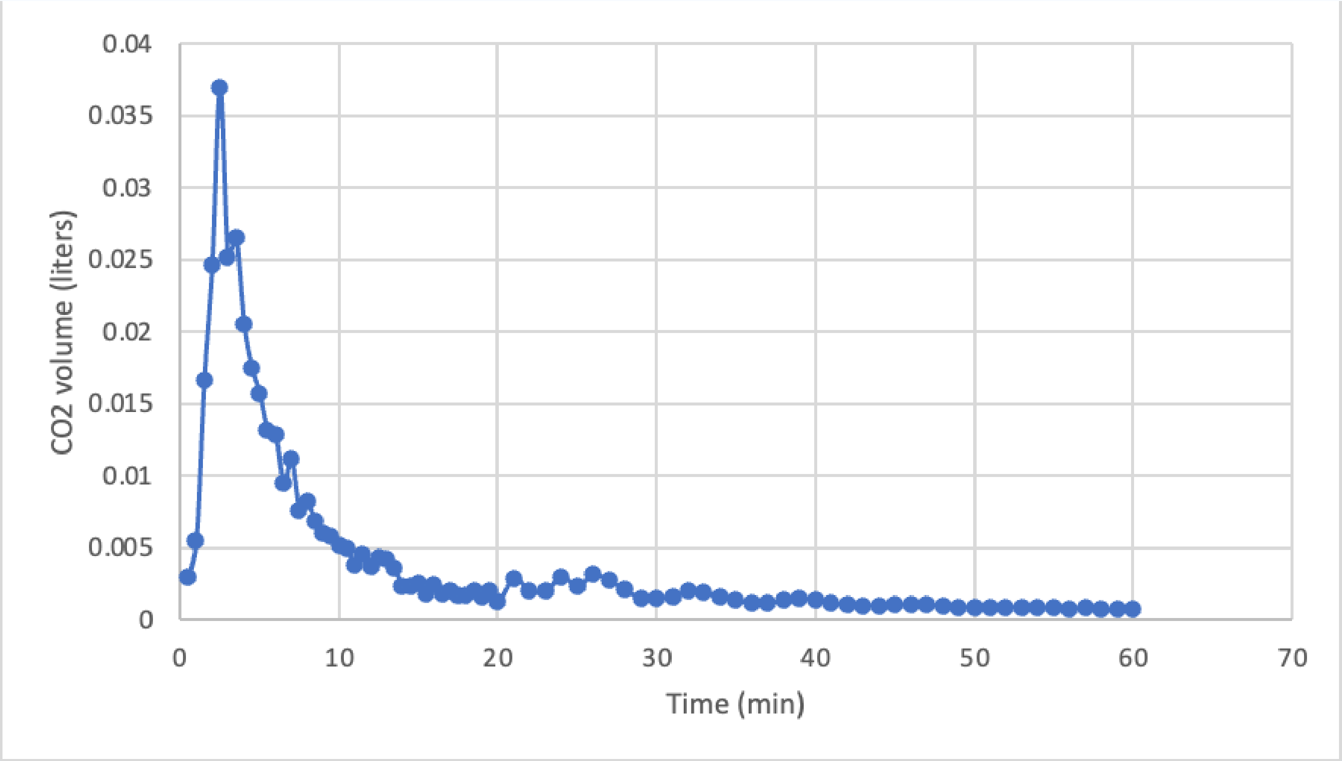
Breakthrough Test with Modified Sorbent

Operating conditions: 400 ppm CO_2 in N_2, 25 l/min, T = 20^oC



Regeneration Stage with a Modified Sorbent

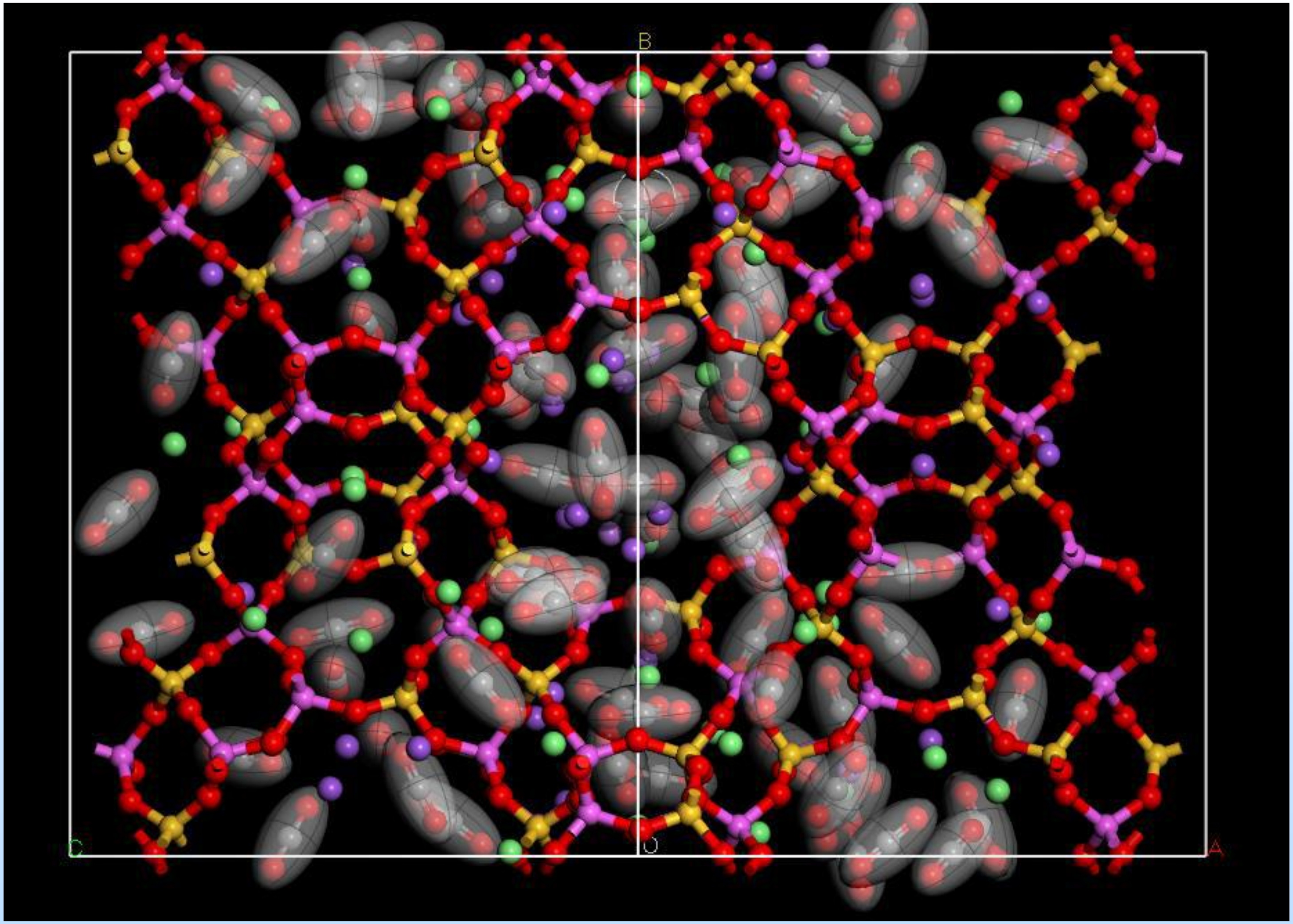
Operating conditions: N_2, 2 l/min, vacuum, T = 125^{o}C



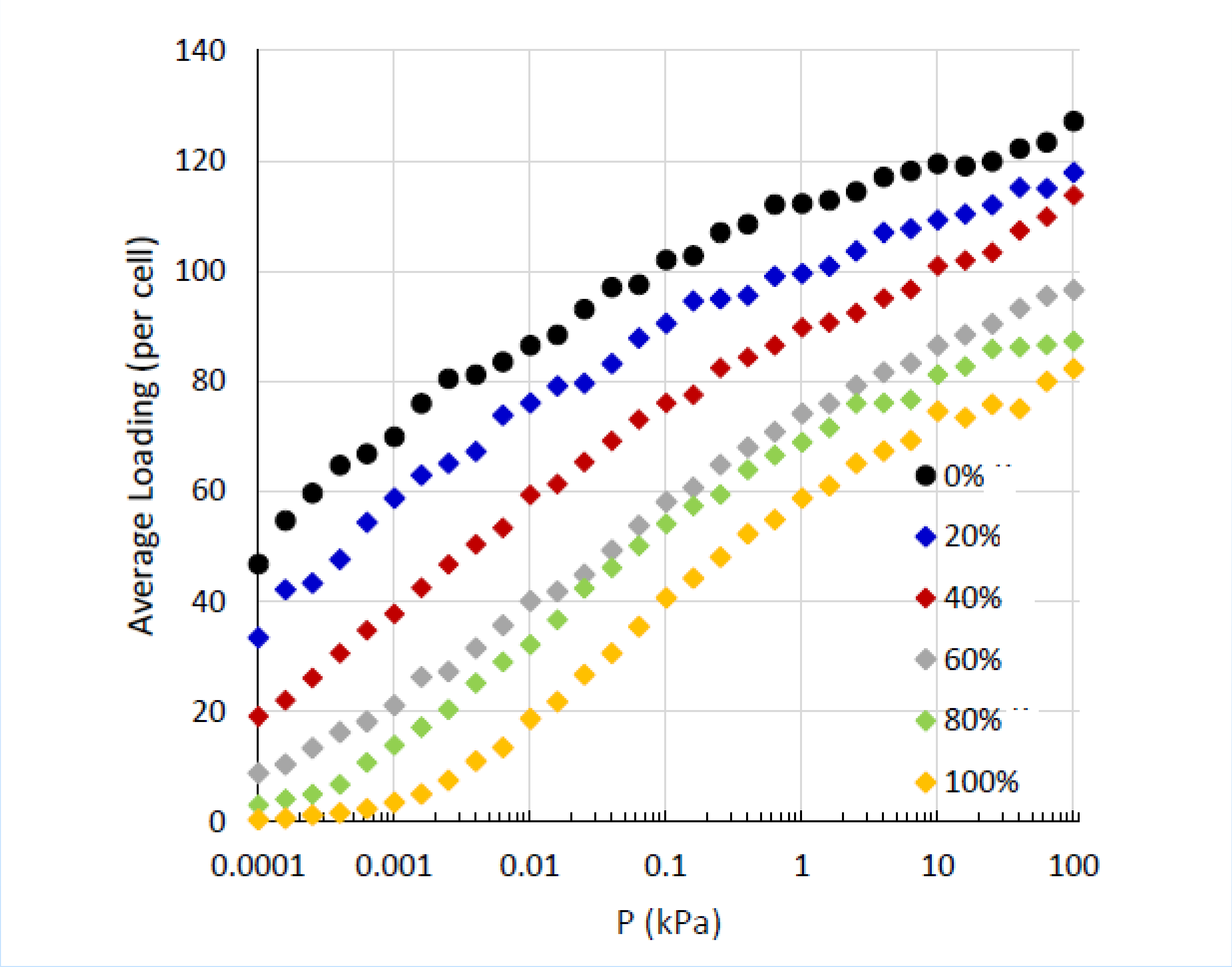
Summary of Isotherm Measurements and Breakthrough Testing

- CO_2 isotherm capacities between 3.5 and 4.5-wt% for a p_{CO2} of 0.04 kPa (400-ppm CO_2 in air) at 25°C
- Breakthrough capacities between 2.5 and 3.0-wt%
  - The materials with the highest isotherm capacities do not necessarily have the highest breakthrough capacities
  - N_2 coadsorption can be significant and needs to be considered
- Modeling of mixture isotherms to better understand N_2 coadsorption, IAST and other approaches
- Modification of materials to decrease N_2 adsorption while maintaining high CO_2 capacities

Monte Carlo Simulations for Improving Performance

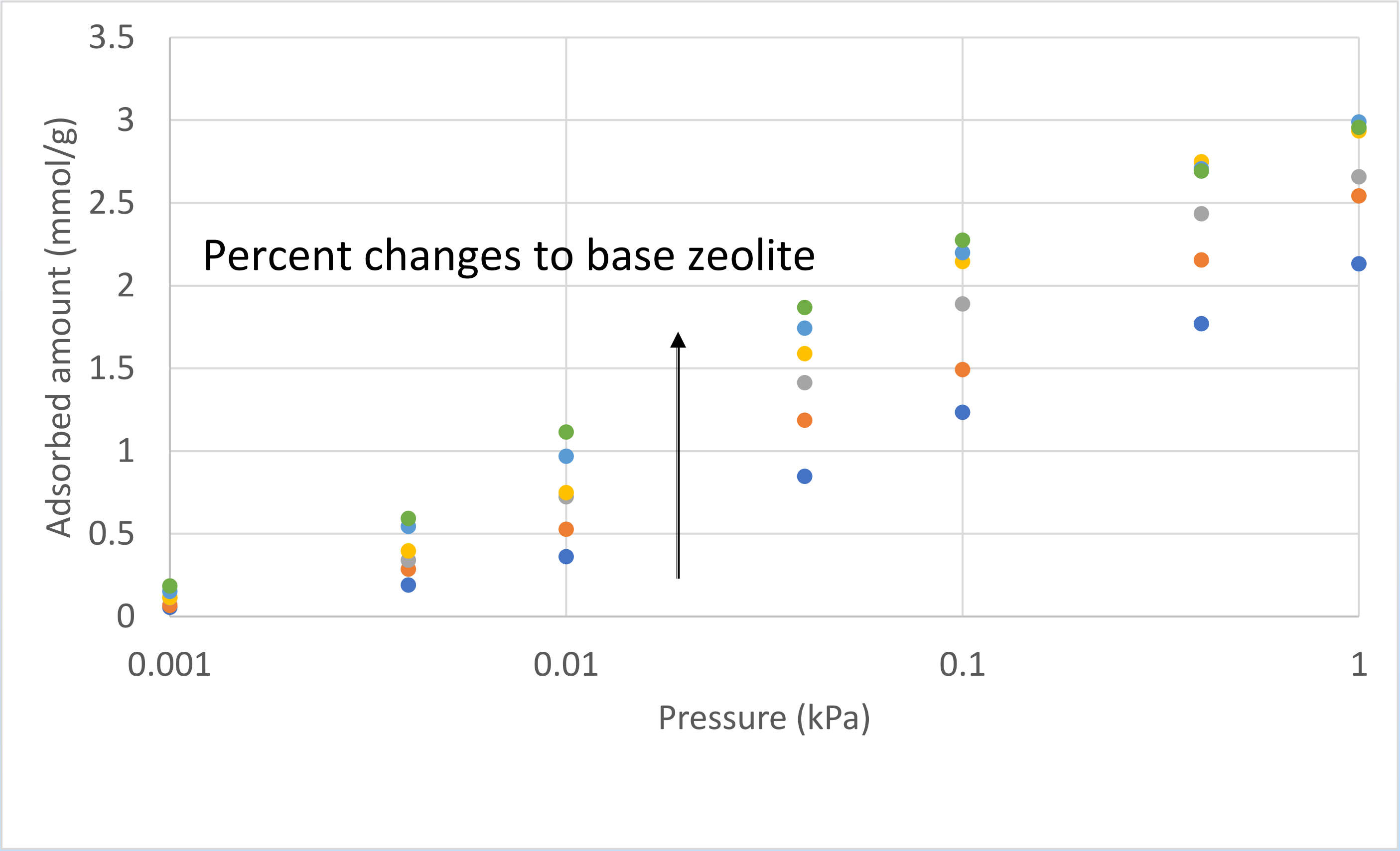


Effect of Sorbent Modification on CO_2 Adsorption



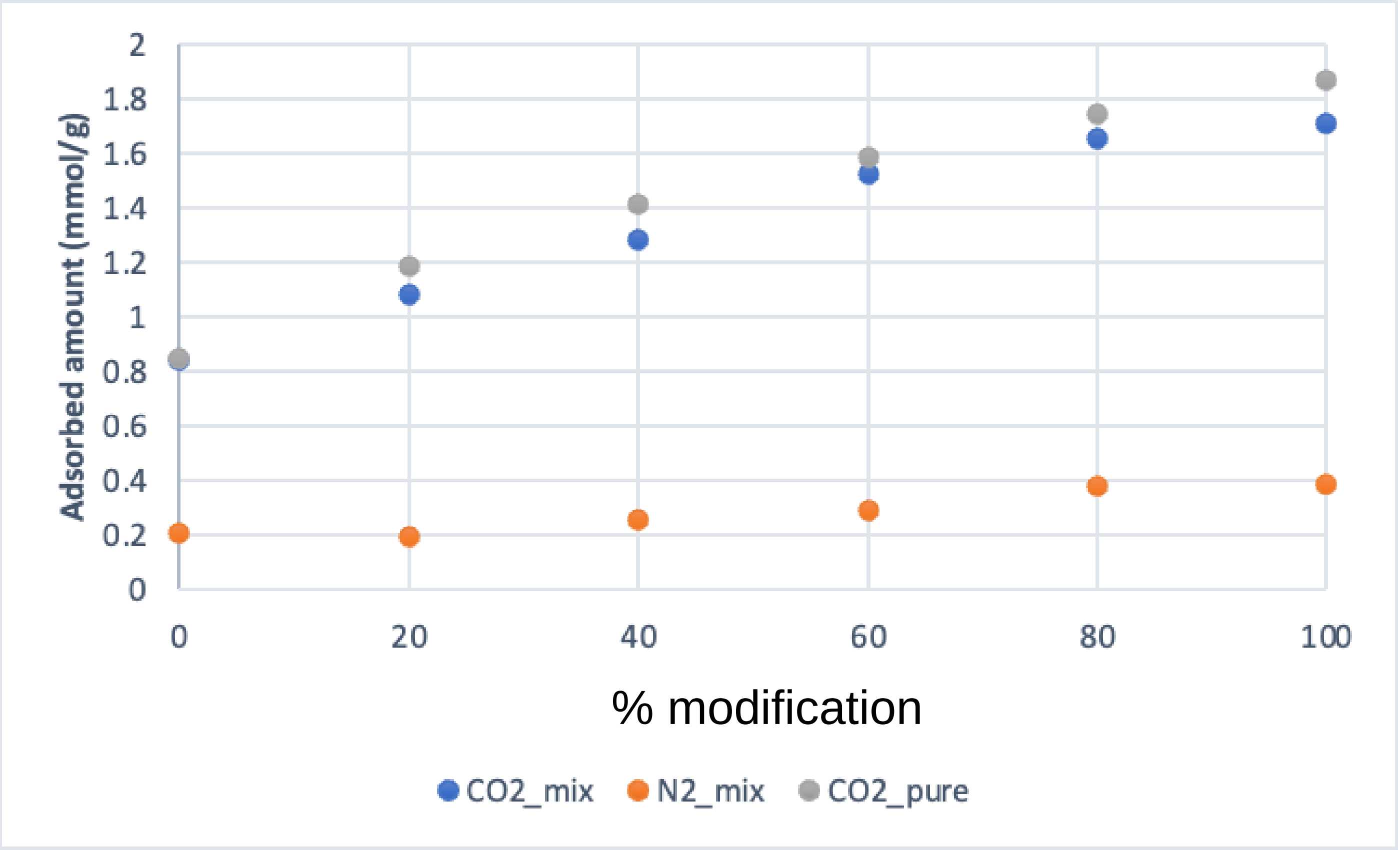
GCMC simulation of CO_2 adsorption on a Modified Sorbent

T = 25^{o}C



GCMC Simulation of CO_2 Adsorption on Modified Sorbent

CO_2 = 400 ppm, P = 100 kPa



Rotating Wheel Dehumidification Unit

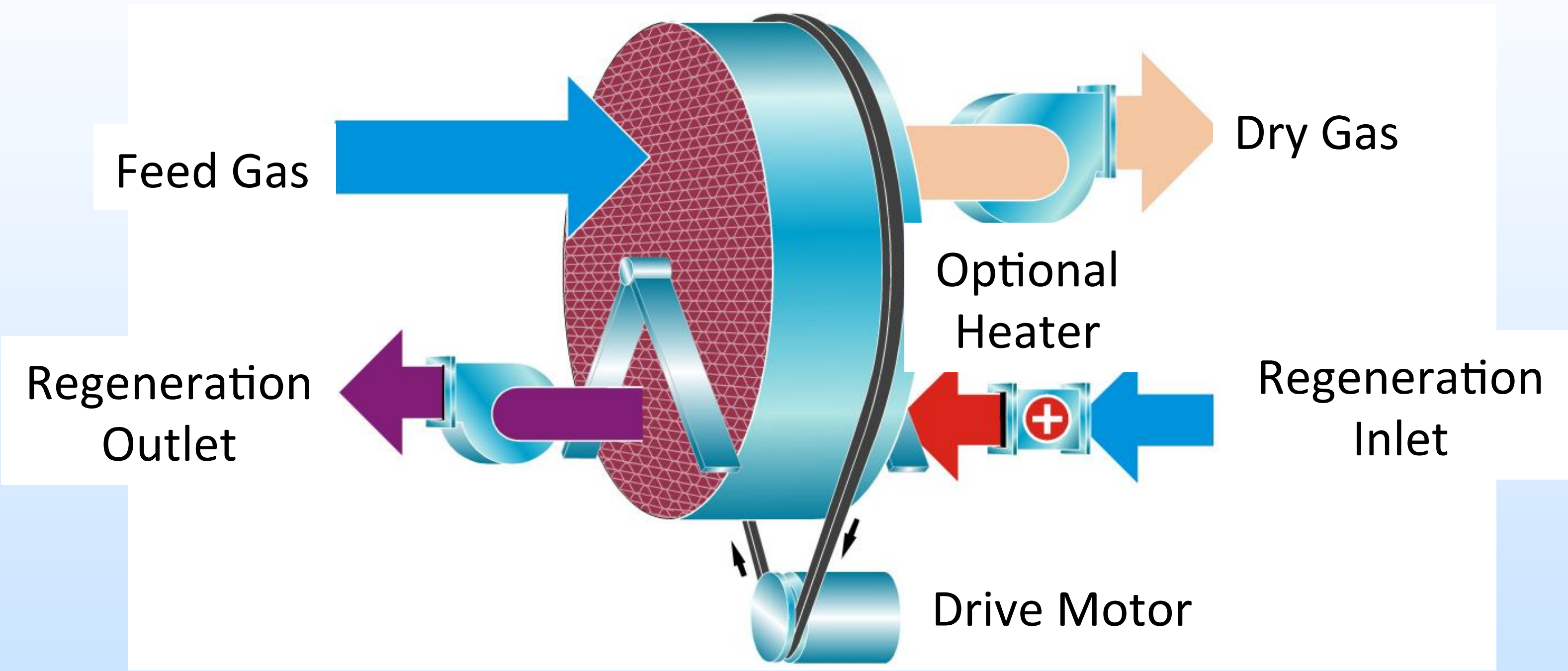
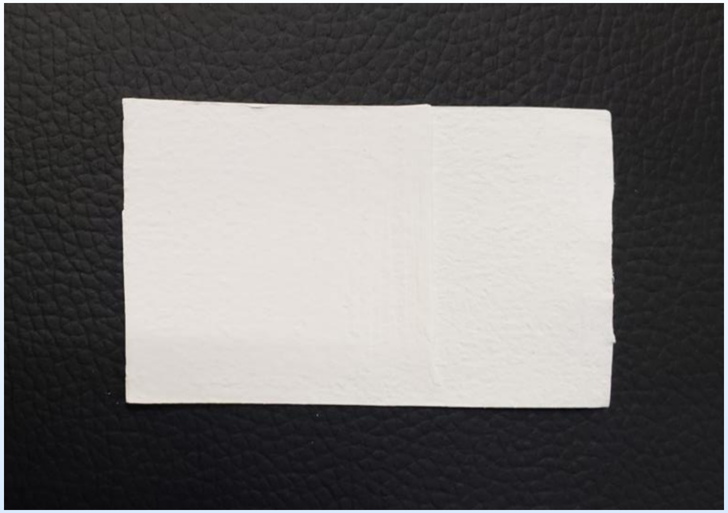


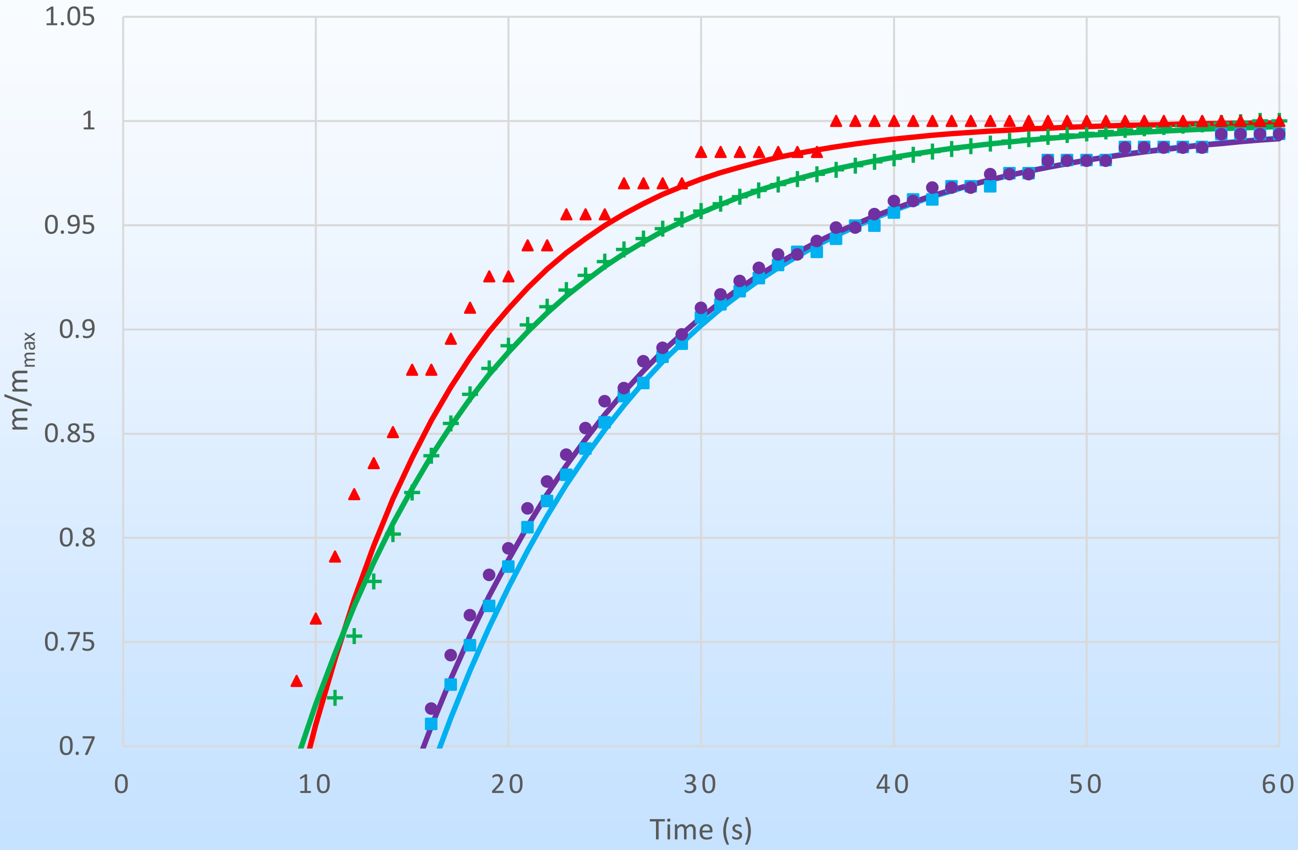
Figure 2: Rotating wheel dryer for feed dehumidification

Laminate Sorbents

- Both in house development and work with external partners



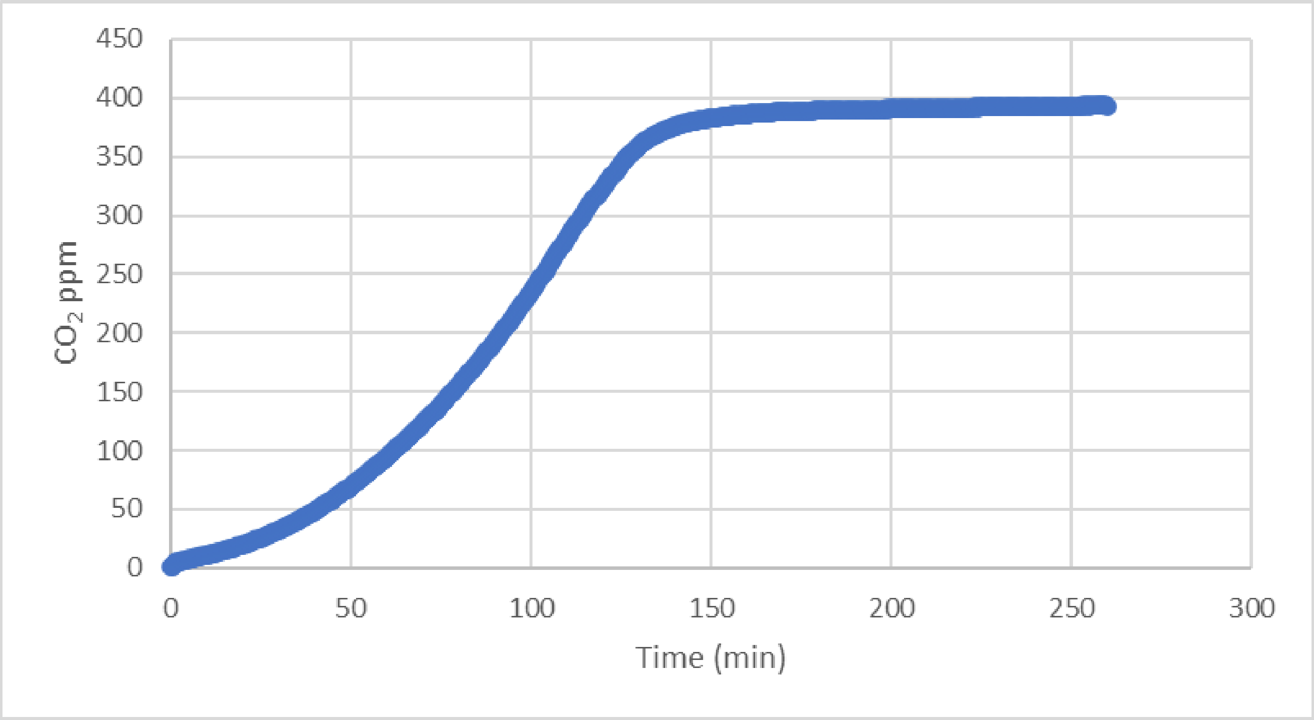
Uptake of CO_2 on the Laminate at 400 ppm



$$1 - \frac{m_t}{m_\infty} = \frac{6}{\pi^2} exp\left(\frac{-\pi^2 D_c t}{r_c{}^2}\right)$$

Breakthrough Test in Laminate Sorbent

Feed: 400 ppm CO_2 in N_2, 0.2 l/min, T = 20°C



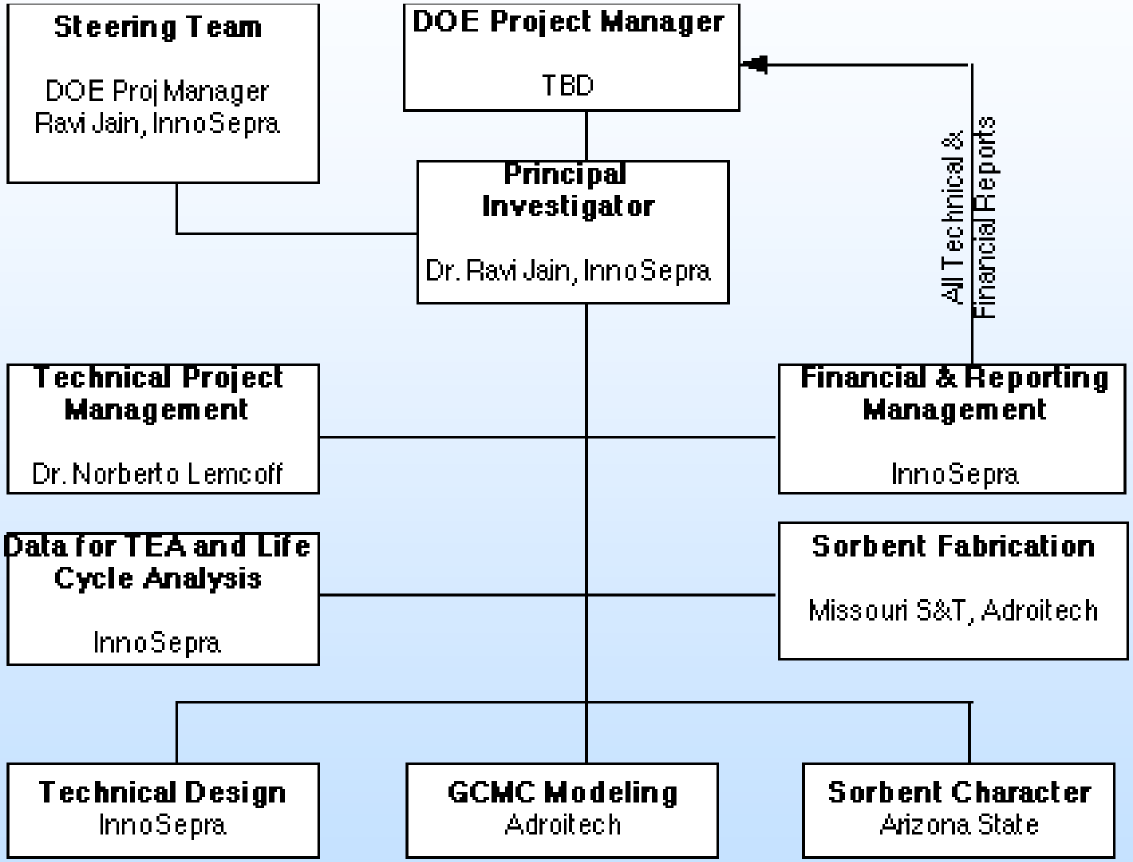
Plan for Future Testing / Commercializations

- Fabricate the optimized materials identified during the project in structured forms
- Test at NCCC under a DOE SBIR, Phase II Project (SC20740) at semi-bench scale
- Further scale up depending on NCCC test results

Summary

- The InnoSepra DAC materials have the potential for a significant reduction in the energy required for direct air capture
- It is possible to obtain high purity CO_2 (>95% purity) with physical sorbents while meeting the pipeline transport specifications
- Potential to reduce the energy required by more than 50% over current DAC processes (<4 GJ/MT)
- The materials are low cost and can be produced in very large quantities fairly quickly
- Potential for a significant reduction in the CO_2 removal cost with the ability for quick deployment after pilot scale validation

Project Organization Chart



Project GANTT Chart

ID	Task Name	Start	End	Q4-20	Q1-21	Q2-21	Q3-21	Q4-21	Q1-22	Q2-22	Q3-22	Q4-22	Q1-23
1	**Project Management & Planning**	10/1/20	3/31/23										
	1.1 Project Management Plan	10/1/20	3/31/22										
	1.2 Technology Maturation Plan	10/1/20	8/31/21										
	Milestone 1: Update Proj Mgmt Plan		9/10/21										
	Milestone 2: Project Kickoff Meeting		9/21/21										
	Milestone 3: Technology Maturation		8/20/21										
2	**Lit Review, Matls Procurement**	10/1/20	12/31/21										
3	**GCMC simulations, matls procure**	10/1/20	11/31/21										
4	**Isotherm/kinetic measurements**	1/1/21	11/15/21										
	Milestone 4: Identify suitable materials		11/15/21										
5	**Lab unit construction & testing**	2/1/21	12/31/21										
	Milestone 5: Update Proj Mgmt Plan		12/31/21										
6	**Prepn/Charac of structured matls**	1/1/22	9/30/22										
	6.1 Materials for indirect regen	1/1/22	5/31/22										
	6.2 Materails for direct regen	2/1/22	6/30/22										
	6.3 Isotherm/kinetic measurements	4/1/22	7/31/22										
	6.4 Flow characterization of matls	5/1/22	8/31/22										
7	**Lab testing of structured matls**	6/1/22	10/31/22										
8	**Tech approach utilizing DAC matls**	5/1/22	11/30/22										
	Milestone 6: Prelim Technical Design		11/30/22										
9	**Research results for TEA/LCA**	10/1/22	1/31/23										
10	**EH&S Risk Assessment**	10/1/22	1/1/23										
	Milestone 7: EH&S Risk Assessment		1/1/23										
11	**Final Project Report**	1/1/23	3/31/23										
	Milestone 8: Present Closeout Report		3/31/23										