A New Thermal Swing Adsorption Process for Post-Combustion Carbon Capture from Natural Gas Plants—DE-FE0032151

Gökhan Alptekin
Ambal Jayaraman
David Gribble
Anthony Bosch
Ewa Muteba
Meredith Haanstad
Sarah DeVoss

TDA Research, Inc.
Wheat Ridge, CO

Carbon Management Review Meeting

August 29, 2023

Project Team and Objectives

Dr. Ashok Rao

Project Duration

- Start Date = September 23, 2022
- End Date = November 30, 2025

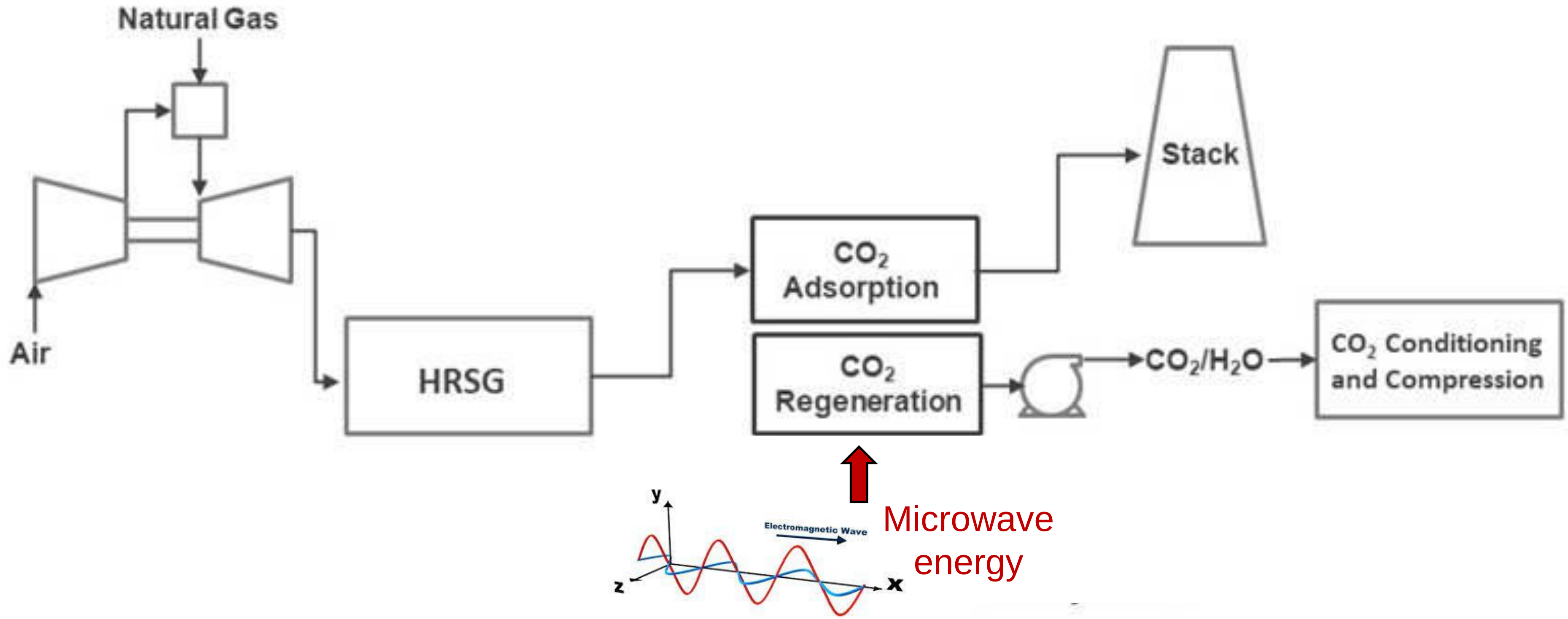
Budget

- Project Cost = $3,125,000
- DOE Share = $2,500,000
- TDA and Partners = $625,000

- **Demonstrate the viability of a transformational microwave-assisted thermal swing adsorption (MTSA) based process to efficiently capture CO_2**
  - **CO_2 capture efficiency target ≥ 95%**
  - **CO_2 product purity target ≥ 95% CO_2**
  - **CO_2 source is flue gas from a natural gas combined cycle power plant (simulated)**
- **Reduce the capture cost >25% against a reference NGCC plant with liquid amines (e.g., Cansolv®)**

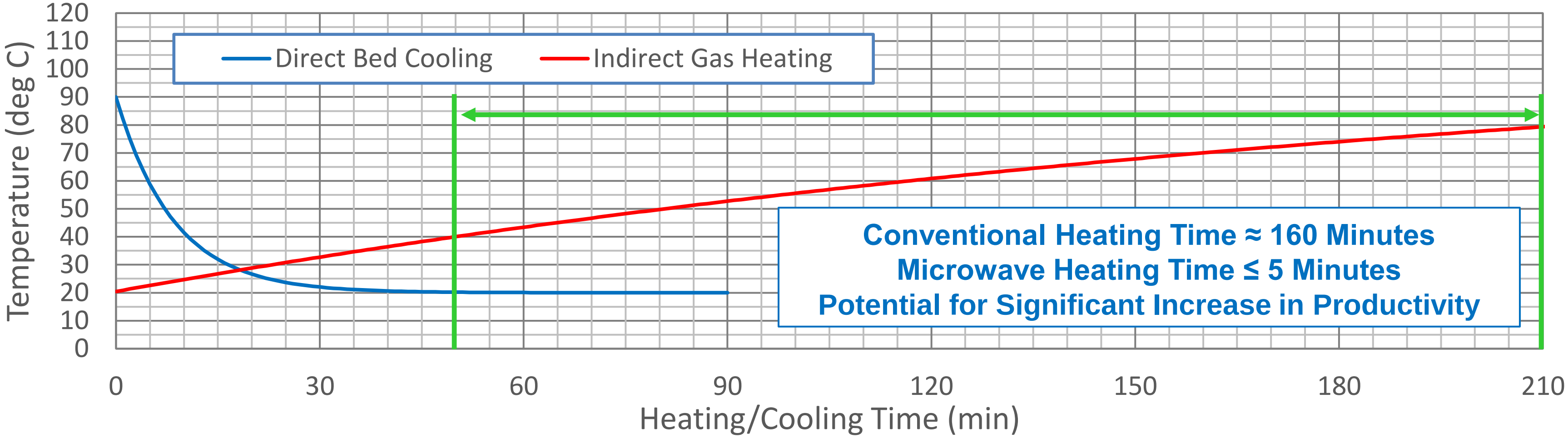
BP	Period	Main Activity
1	Year 1	Material synthesis Adsorption & CFD modeling Bench-scale system design Preliminary TEA
2	Year 2	Bench-scale system fabrication Commissioning/troubleshooting
3	Year 3	Bench-scale evaluations Techno-economic Assessment Life Cycle Analysis EH&S Analysis

2-Bed MTSA CCS Cycle

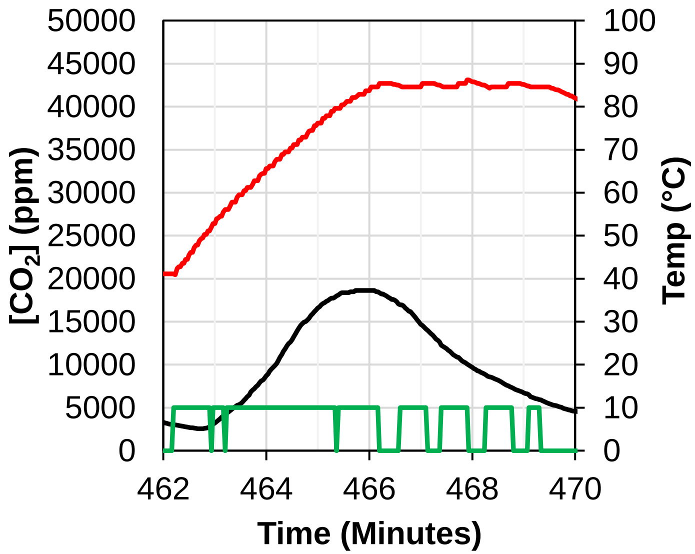


- CO_2 stripped from flue gas (>95% capture) by the system at 60°C
- Microwave heating increases the sorbent temperature to 90°C (30°C ΔT)
- Mild vacuum (10 psia or 0.68 bara) is applied to improve the CO_2 recovery
- Product stream (95% CO_2, dry basis) is conditioned and compressed
- The sorbent bed is repressurized and cooled using raw flue gas

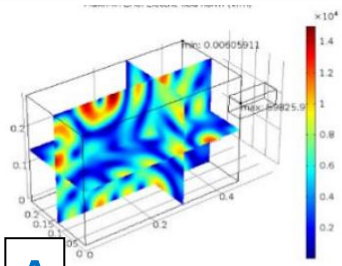
Why Use Microwave Heating?



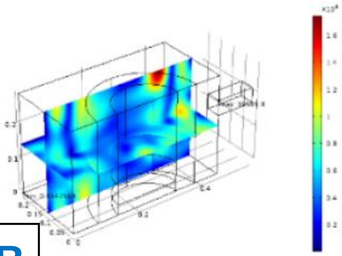
- **Conventional heating is slow with a large mismatch between heating and cooling time**
  - **Indirect gas circulation heat is used to prevent diluting CO_2**
  - **Sorbents are poor thermal conductors—resulting in slow heating and poor temperature uniformity**
  - **Direct cooling with CO_2-laden process gas is relatively fast**
- **Microwave heating is much faster**
  - **Microwave heating is common in several industrial settings**
  - **Microwave heating can be more uniform—the RF frequency, penetration depth and reactor geometry are matched**
  - **Sorbent packing can be increased by eliminating heat transfer elements from the bed—reducing vessel size/cost**
  - **Cavity/reactor integration can limit the heat delivered to vessel, reducing waste heat and improve efficiency**



How Does the Microwave Work?

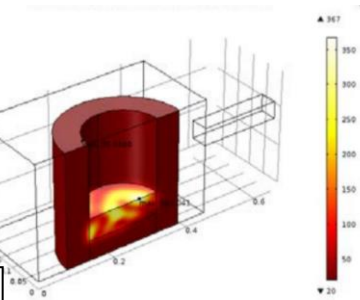


A



B

- Microwave radiation is generated in the magnetron
- Radiation is coupled to a cavity by a waveguide
- Materials interact with the electromagnetic field
- Electromagnetic power losses result in direct heating of the material
- Can heat sorbents directly or through susceptors

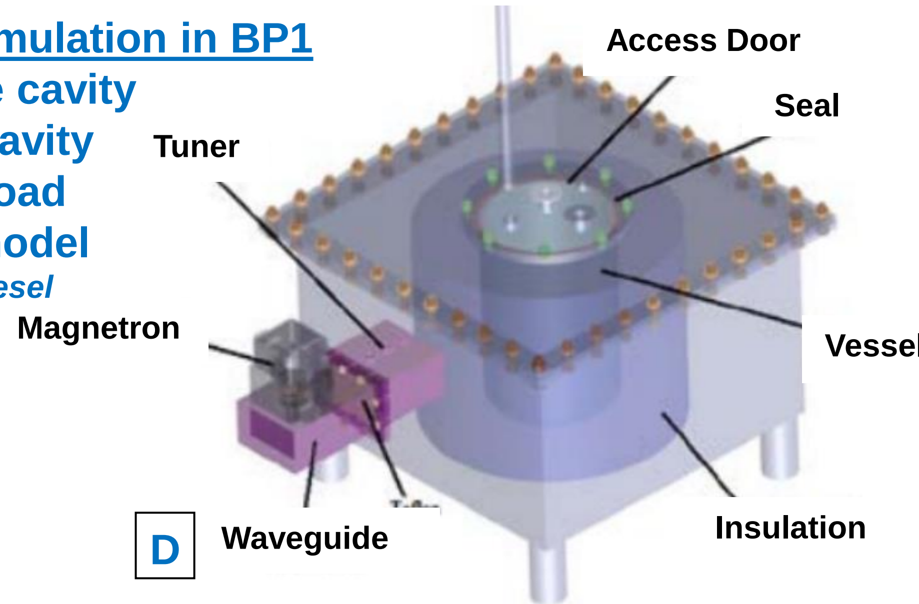


C

Detailed Modeling & Simulation in BP1

A. Unloaded microwave cavity
B. Loaded microwave cavity
C. Heat distribution in load
D. Microwave/reactor model

—COMSOL modeling for biodiesel



D

Design and Modeling of an Enhanced Microwave Reactor for Biodiesel Production: Ong & Nomanbhay; dx.doi.org/10.29322/IJSRP.8.12.2018.p8465

Electromagnetic Field Model Field (Maxwell)

$$\nabla \times (\mu_r{}^{-1} \nabla \times \boldsymbol{E}) - \frac{\omega^2}{c^2}(\varepsilon_r - j\sigma/\omega\varepsilon_0)\boldsymbol{E} = 0$$

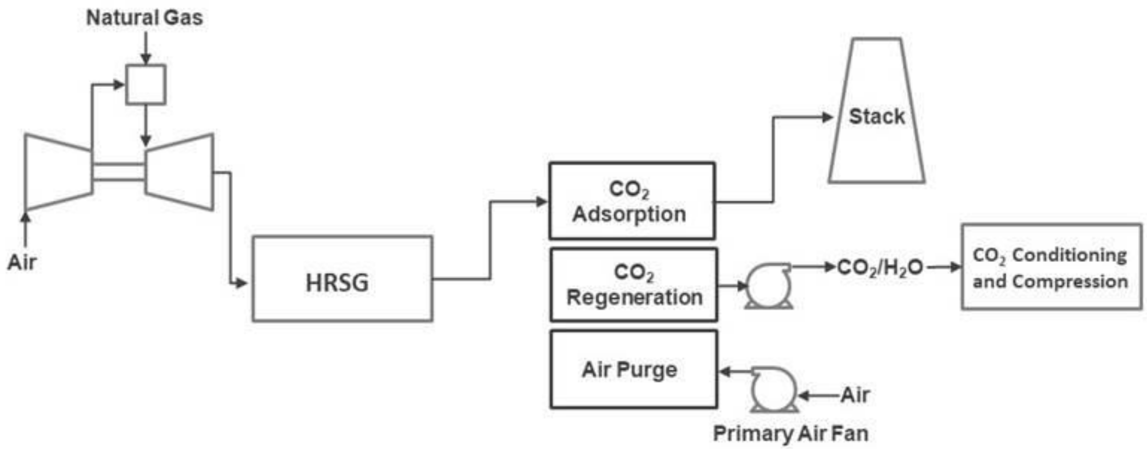
Heat Transfer Modeling (Fourier)

$$\rho C_p(\partial T/\partial t) + \nabla \cdot (-k\nabla T) = Q$$

Electromagnetic Losses (Poynting)

$$Q_{RMS} = 1/2\{\sigma \boldsymbol{E} \cdot \boldsymbol{E}^* + \omega\varepsilon'' \boldsymbol{E} \cdot \boldsymbol{E}^* + \omega\mu_r \boldsymbol{H} \cdot \boldsymbol{H}^*\}$$

2-Bed MTSA CCS Cycle

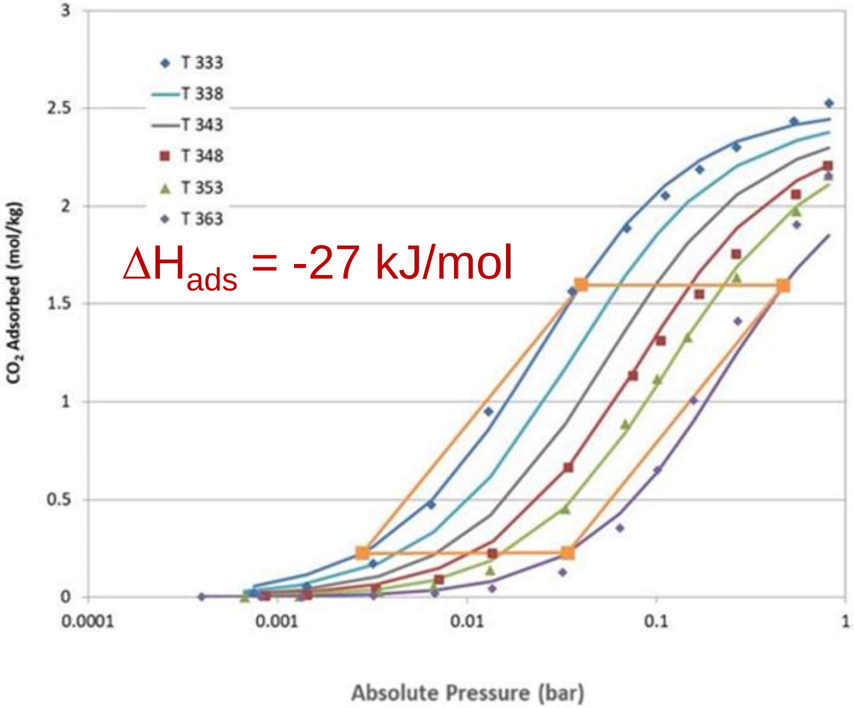


Time (min)	6	6	3	6	6	3
Bed 1	Adsorption (CO_2 stripped from FG) Cooling (90 → 60°C)			MW Heating 60 → 90°C	CO_2 Recovery 1.05 → 0.68 bara	Pressurize 0.68 → 1.05 bara
Bed 2	MW Heating 60 → 90°C	CO_2 Recovery 1.05 → 0.68 bara	Pressurize 0.68 → 1.05 bara	Adsorption (CO_2 stripped from FG) Cooling (90 → 60°C)		

- **2-bed MTSA cycle time is 30 minutes**
- **With conventional heating, the same ΔT would require ≥ 180 minutes**
- **Microwave heating is expected to yield up to a 6X increase in sorbent utilization**

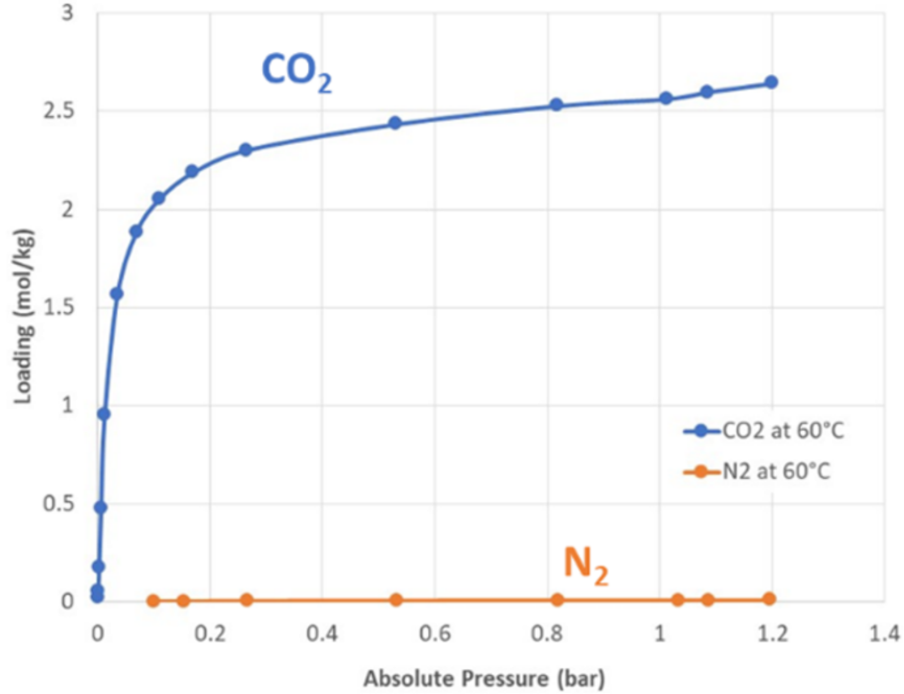
Adsorption Isotherm—Polymer Sorbent

CO_2 Uptake



CO_2 adsorption isotherms from 60–90°C showing working capacity of 6% wt. CO_2

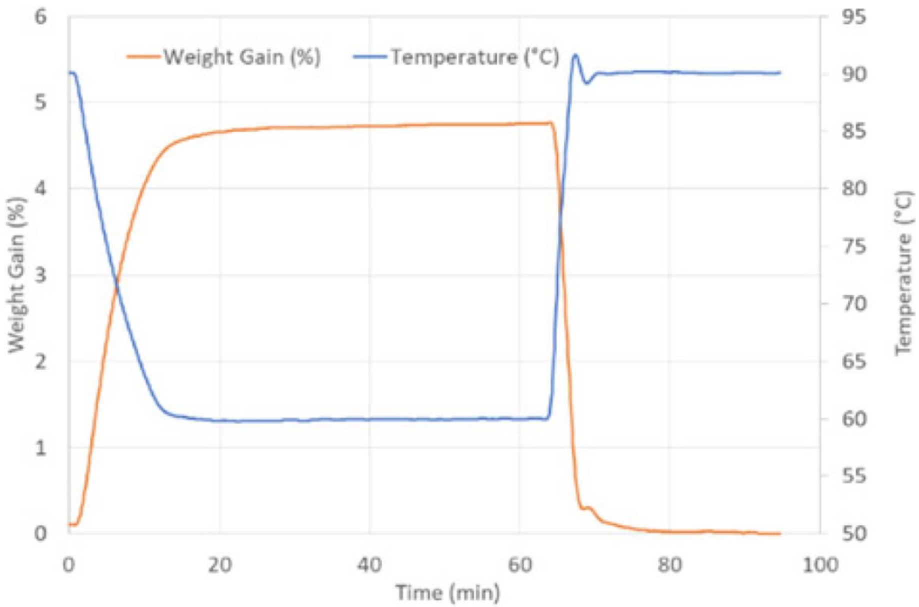
CO_2 Selectivity

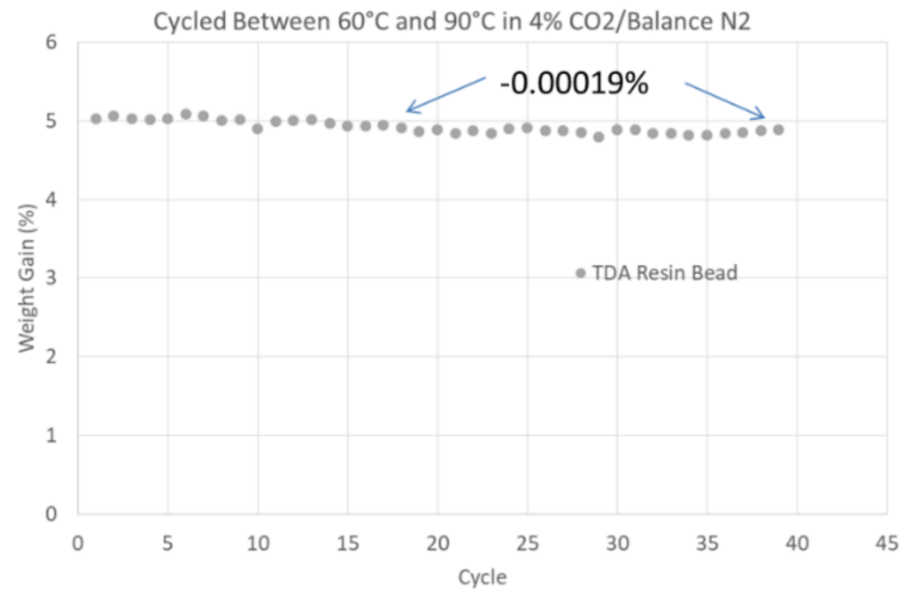


CO_2 and N_2 adsorption isotherms at 60°C showing selectivity >2,800

Thermogravimetric Cycling (Single-Cycle)

ΔT ≈ 30°C; ΔM = 4.75%

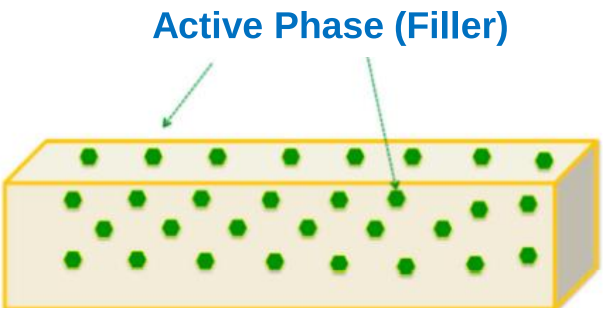


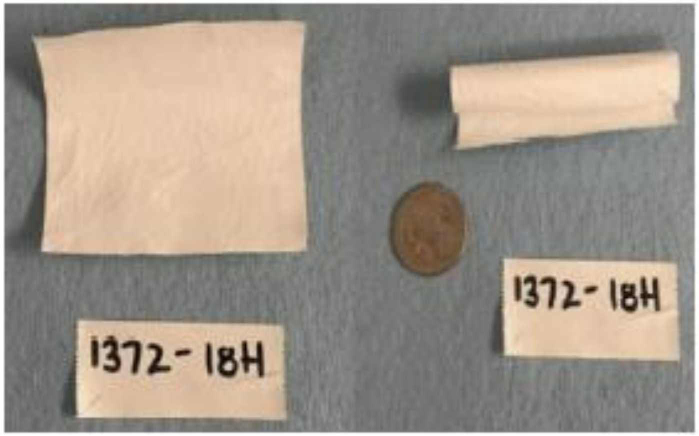


- **TGA tests (left) indicate that rapid CO_2 uptake and release**
- **CO_2 release appears to be more rapid, but in conventional TSA processes, release is the rate limiting step**
- **Adsorbed CO_2 is released in less than 7 minutes, when temperature is cycled from 60°C to 90°C**
- **TDA's sorbent maintained its stability; the apparent loss in capacity over the initial 40 cycles is lower than the cycle-to-cycle variation**

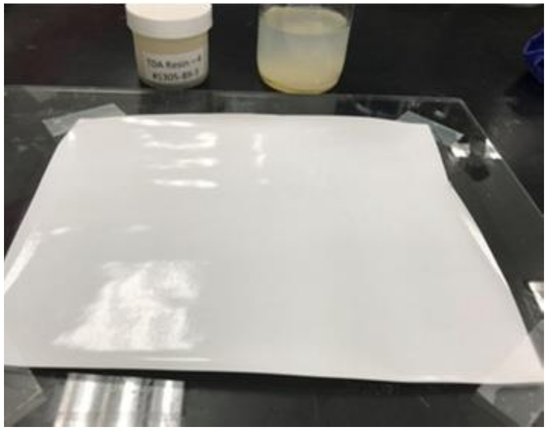
Mixed-Matrix Laminates

Laminate Concept

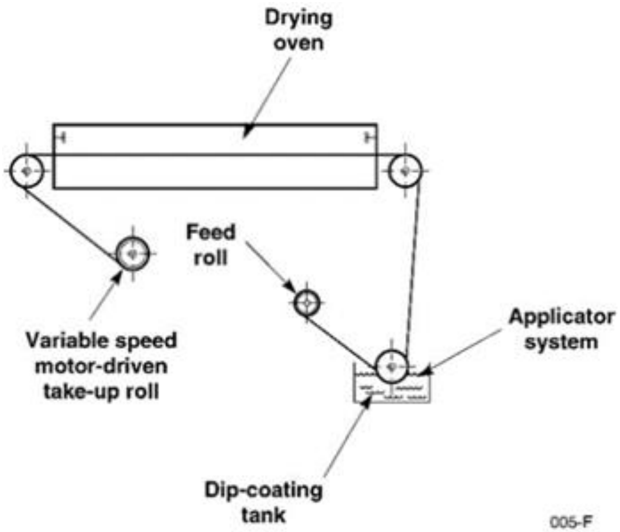




Small-Scale Production
(Screening Tests & Characterization)

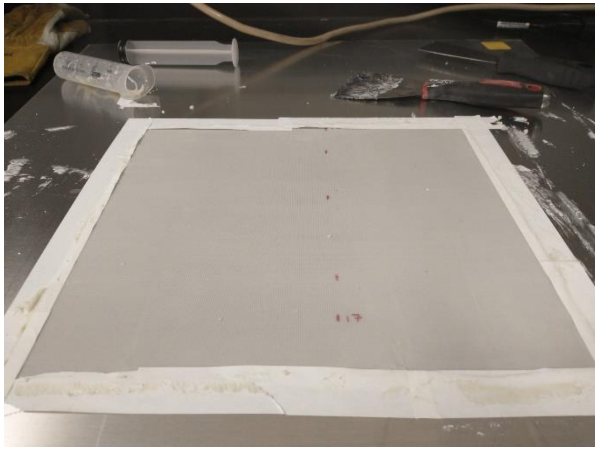


Bench-Scale Sheets
≈ 8' x 8"

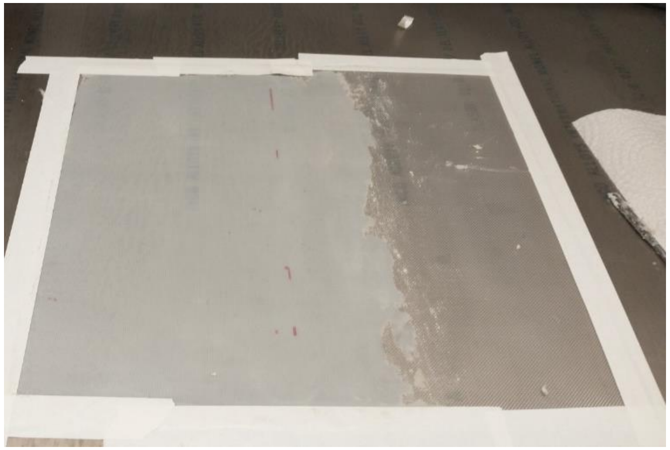


Scale-Up Equipment (MTR)

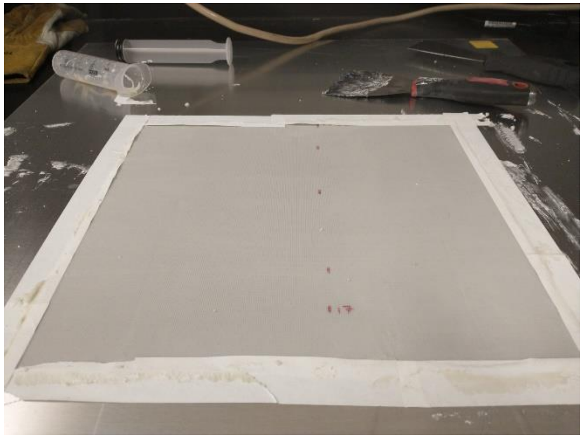
Bench-Scale Laminate Production (12”x 12”)



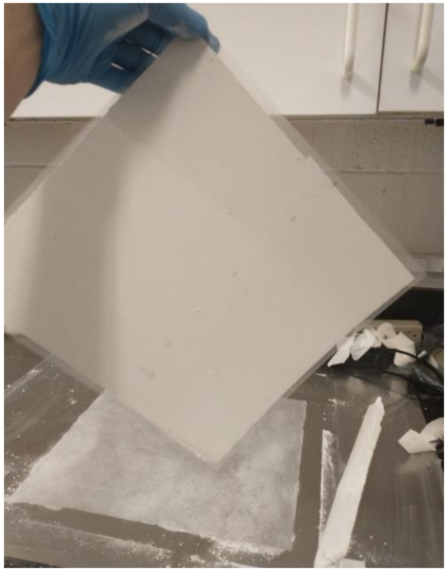
12” x 12” mesh support



Half coated support

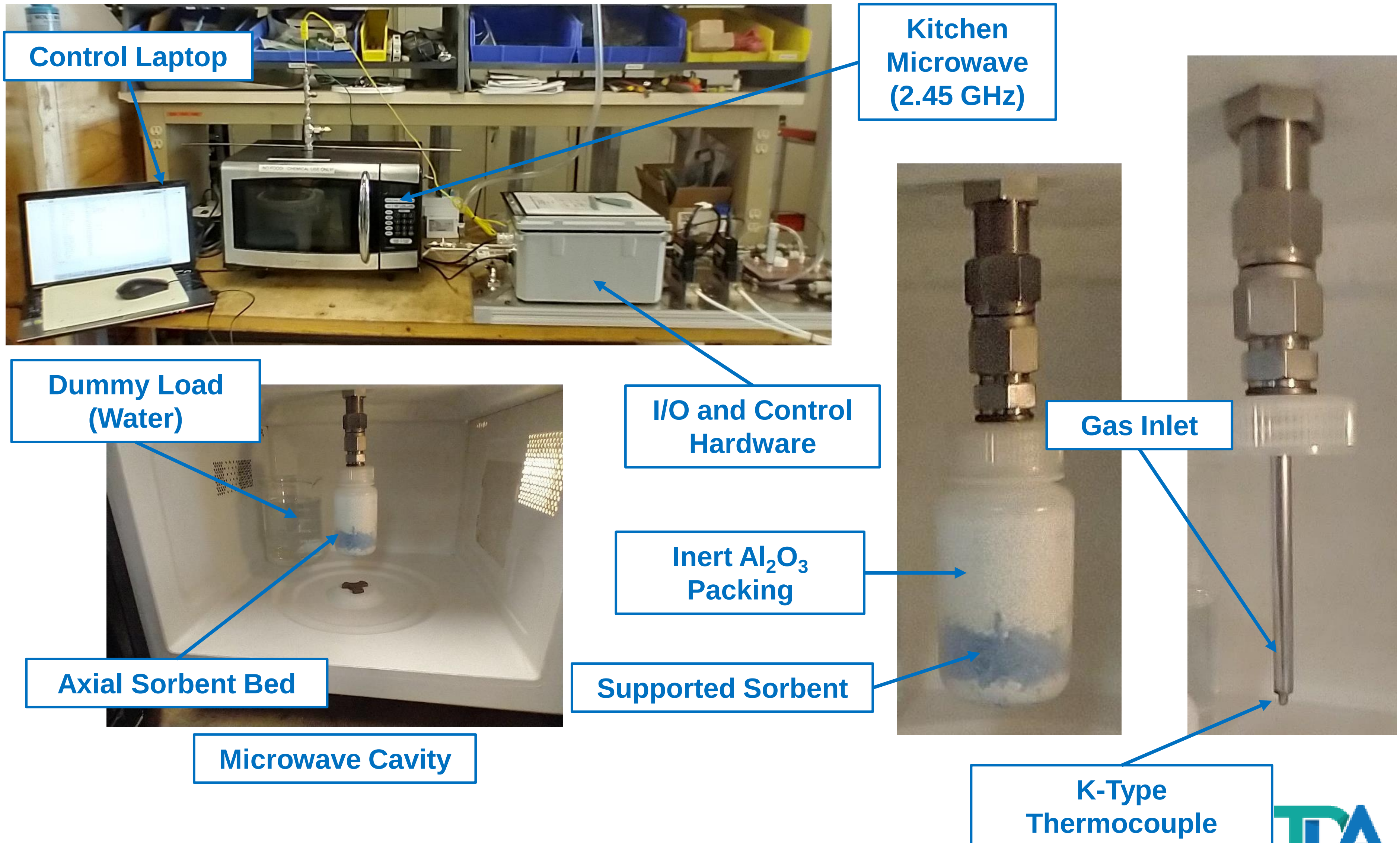


Fully coated support



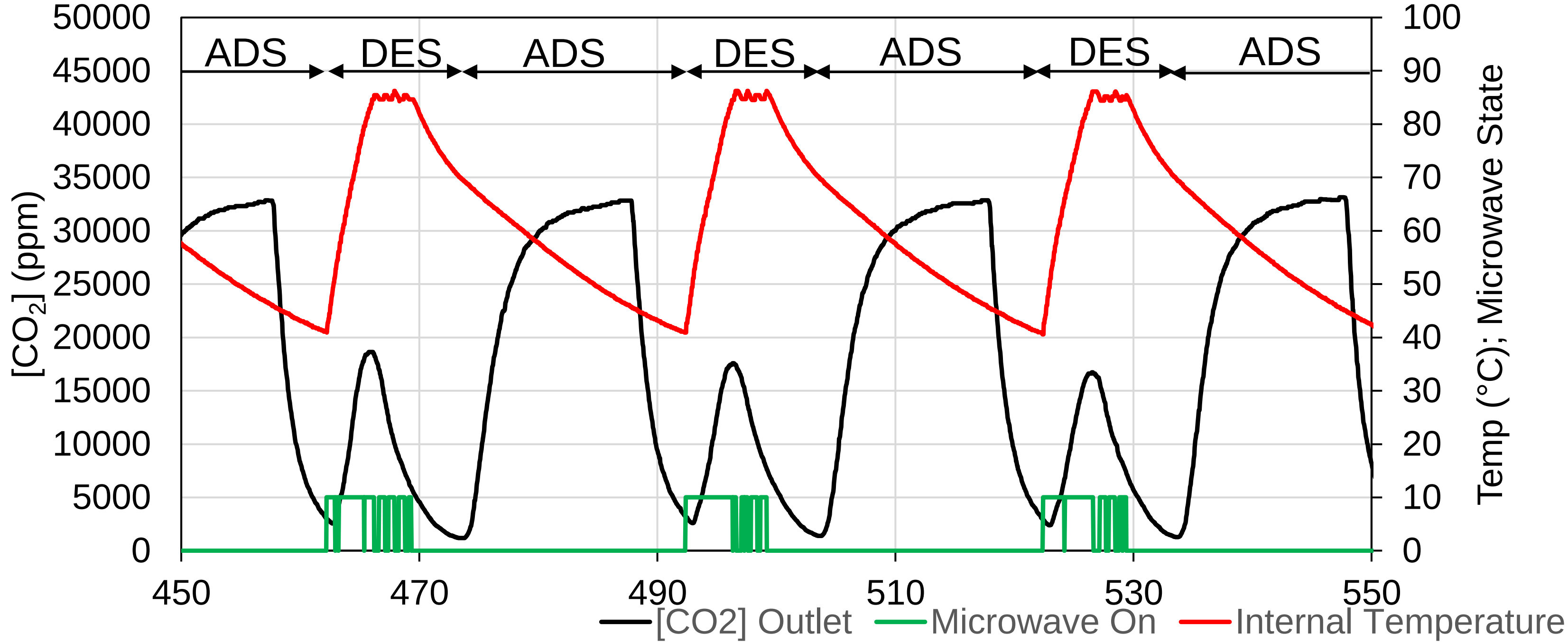
12” x 12” laminate after drying

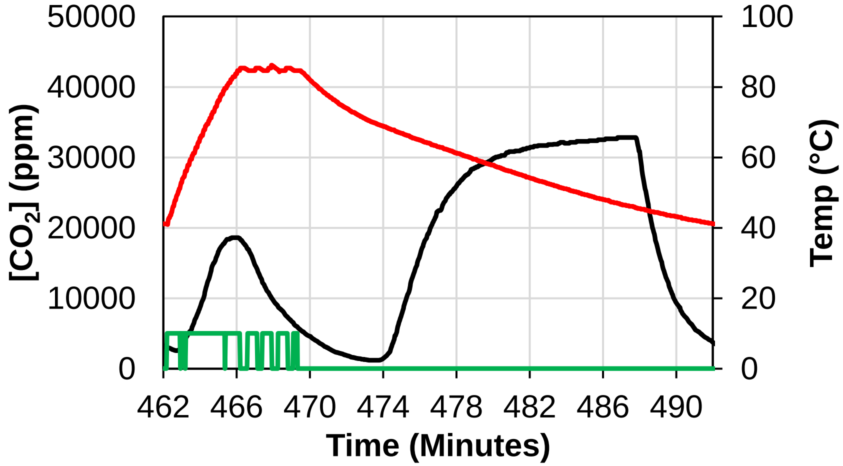
Early Experiments



Single Cycle; ADS ≈ 20 Minutes; Des ≈ 10 Minutes

Microwave-Assisted Regeneration



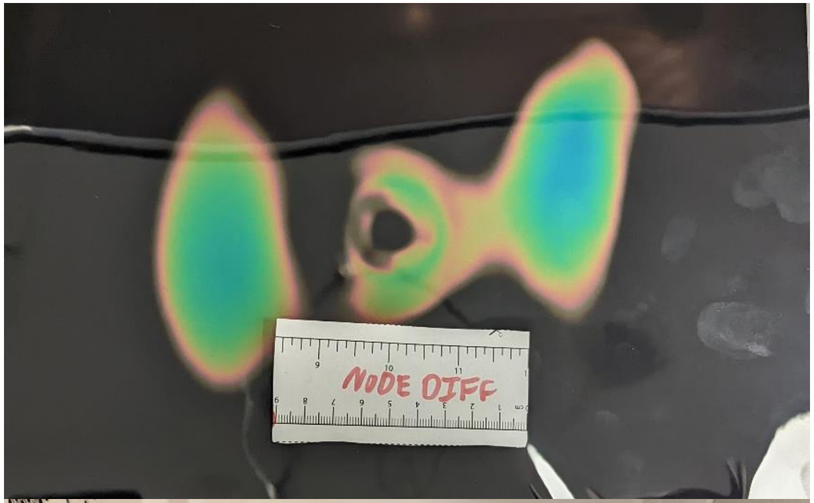


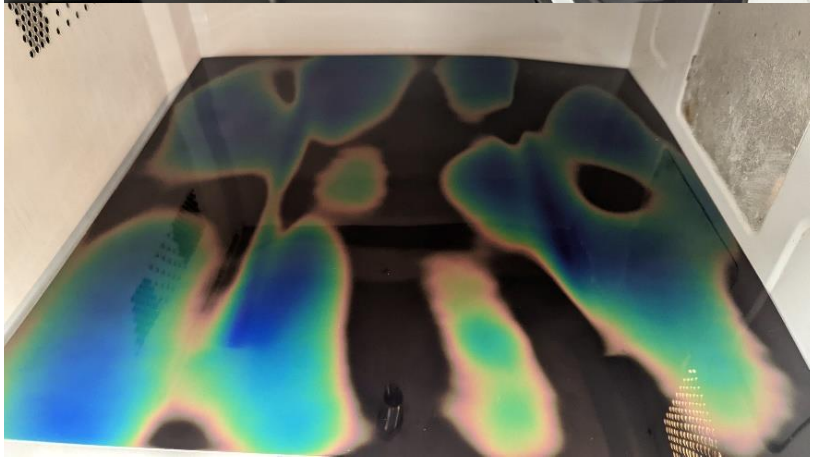
Single Cycle; ADS ≈ 20 Minutes; Des ≈ 10 Minutes

- **Heating and the subsequent CO_2 recovery are nearly instantaneous upon microwave energization—allowing for reduced regeneration cycle times while minimizing the heat transferred to the vessel**

Node Characterization

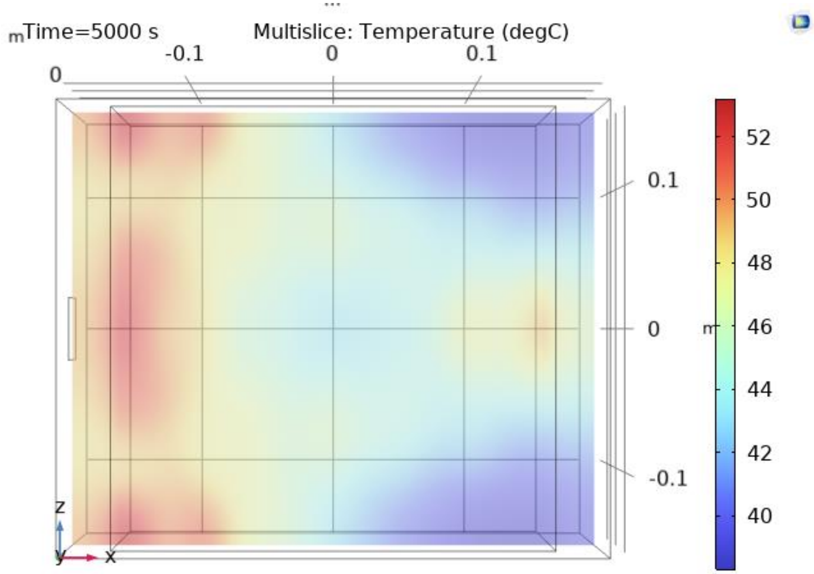
- Commercial Microwaves operate by creating a standing wave inside the microwave cavity
- This standing wave creates “hotspots” or nodes
- For a standing wave with fixed frequency, the spacing between nodes is calculated from $d = \lambda/2$
- For a kitchen microwave with a frequency of 2.45 GHz, d ≈ 6.1 cm
- For an industrial microwave operating at 915 MHz, d ≈ 16.4 cm
- Experimental verification of a typical kitchen microwave matches the expected (calculated) node spacing for a given plane
- Experimental images (right) show areas of color change (heating) within the microwave cavity



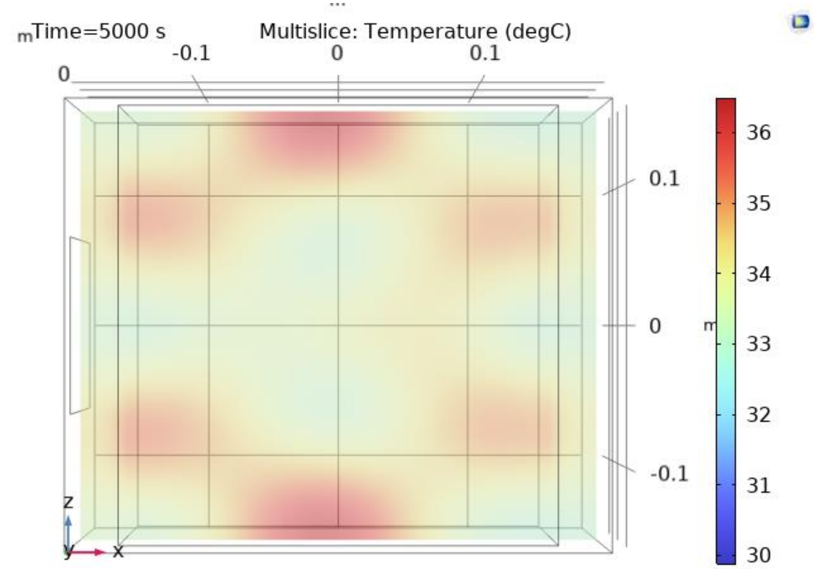


Sorbent Module Design—Microwave Frequency

Cavity Wavelength Optimization: 915 MHz Selected



2.45 GHz Block Heating Model 1kW



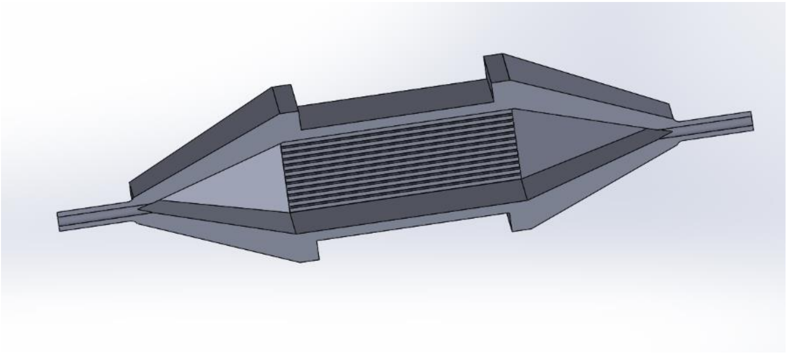
915 MHz Block Heating Model 1kW

Advantages

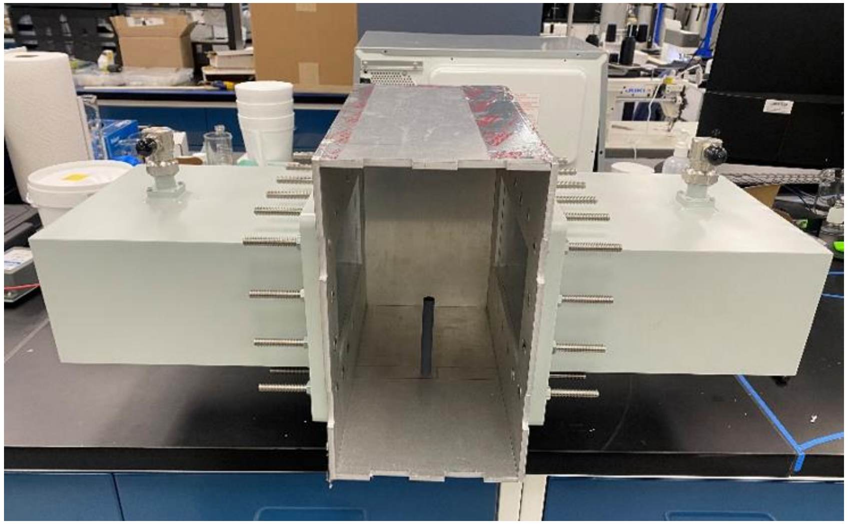
- The temperature variation is smaller for 915 MHz heating vs. 2.45 GHz heating
- High-power industrial microwaves are readily available at 915 MHz
- 915 MHz microwave generators can operate more efficiently
- At lower frequencies, the penetrating depth increases

Bench Scale System Design

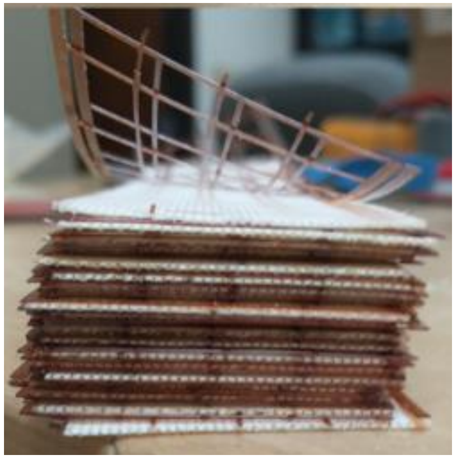
Sub-Scale Model Validation and Sorbent Material Capacity Demonstration



- 3D-printed contactor for a 16-layer, sub-scale sorbent module
- Module assembled using from 3” x 3” coupons production sheets
- S-parameters are measured with a vector network analyzer and compared with COMSOL models
- A 915 MHz source and amplifier are used to validate heating models
- CO_2 adsorption/desorption will be tested to validate adsorption models and demonstrate sorbent capacity

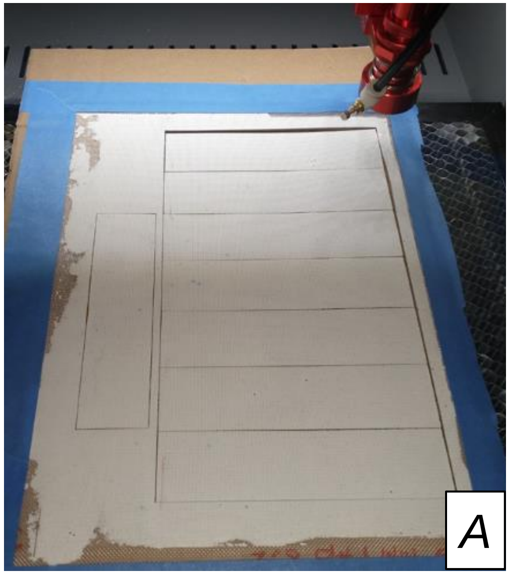


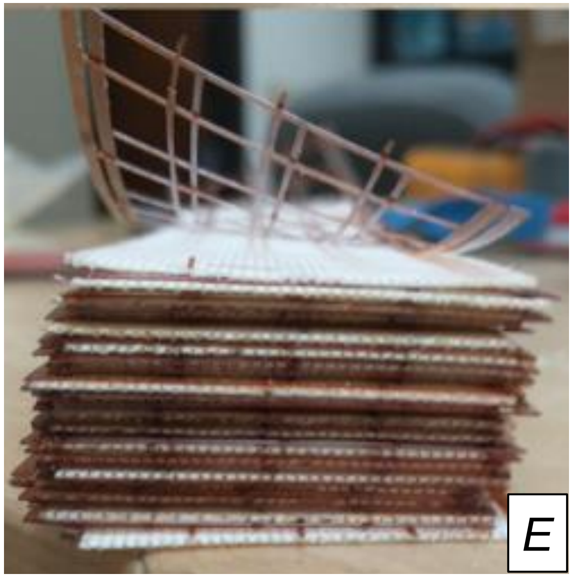
Custom-made validation cavity with dual 915 MHz waveguide-to-coax transitions

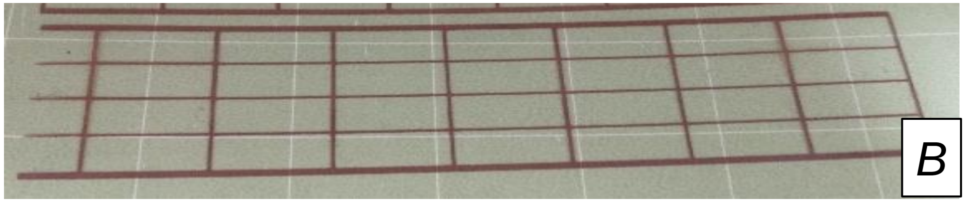


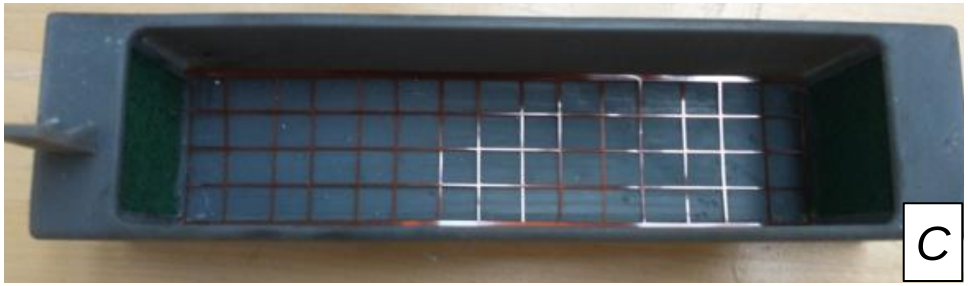
TDA RESEARCH

Structured Sorbent Preparation





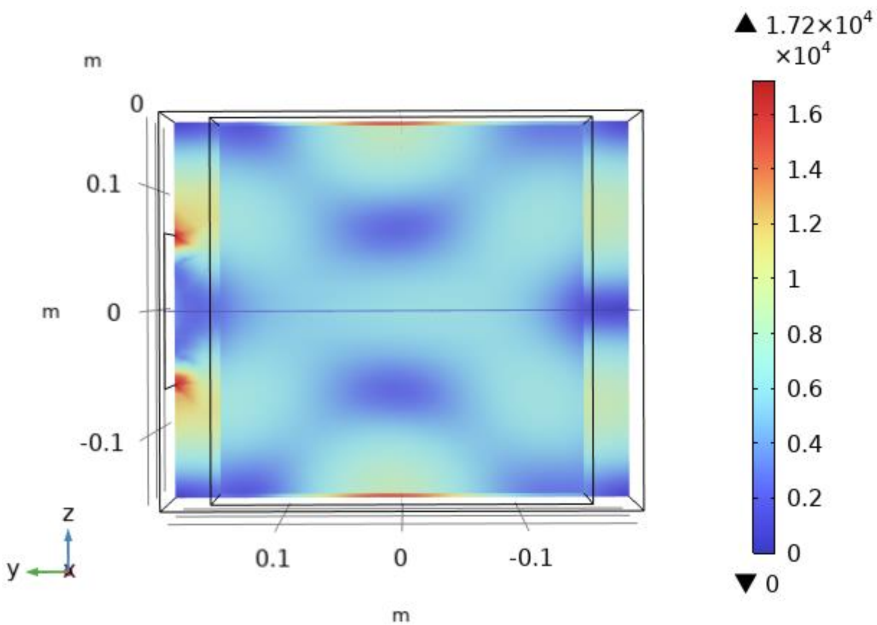




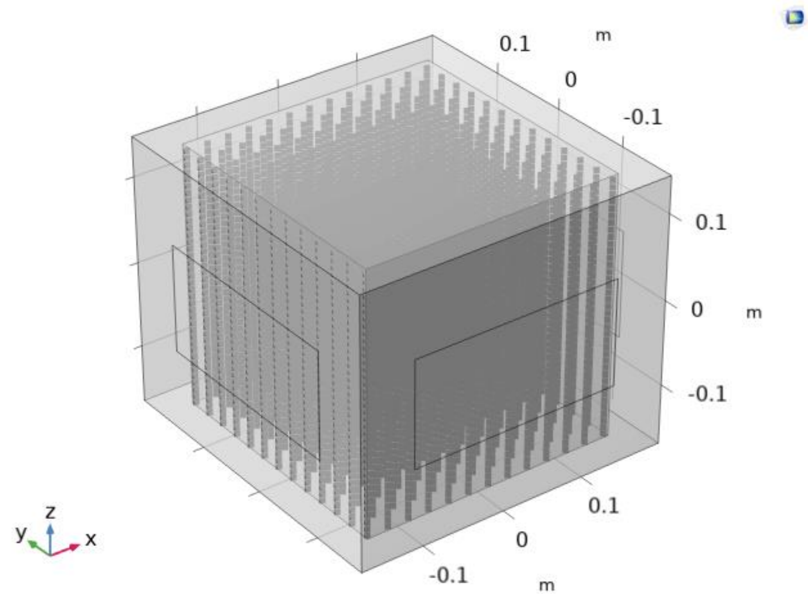
Sorbent films are laser cut (A and stacked alternating with spacer grids in a holder (C and D) to make a module or stack (E)

Sorbent Module Design—Cavity Modeling

Bench-scale microwave cavity and sorbent stack placement have been optimized for field uniformity at 915 MHz



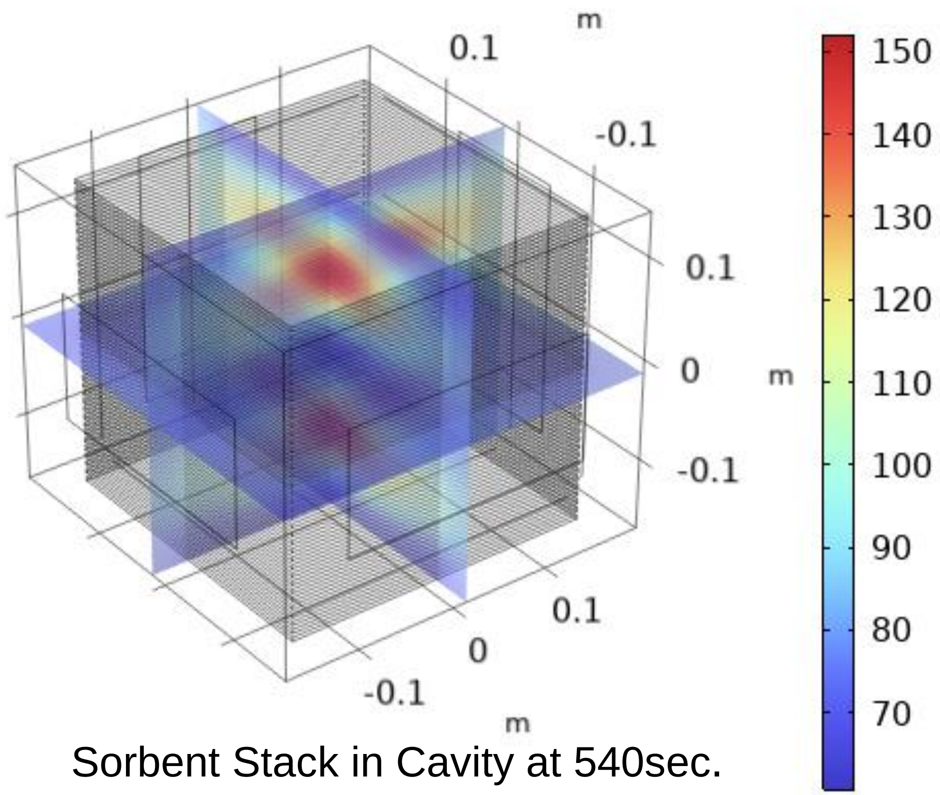
Optimized cavity & EM field distribution



Optimized cavity with discrete Analysis points

Numerical modeling calculates the temperature for a constant array of points—allowing for quantitative comparison of heating concepts

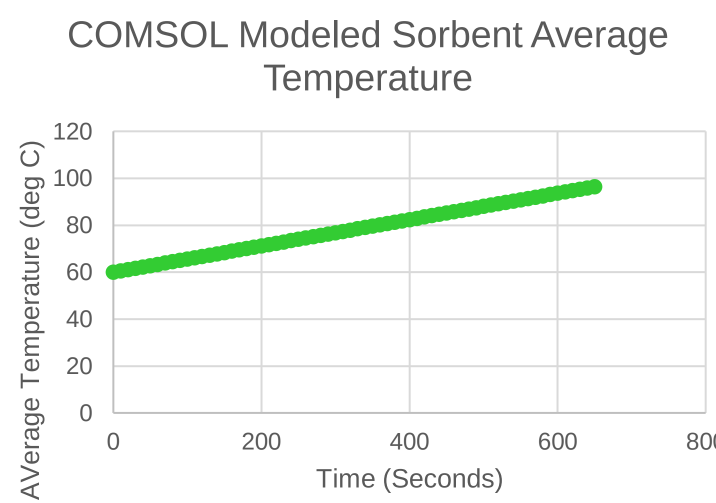
Sorbent Module Design—Modeling Assumptions



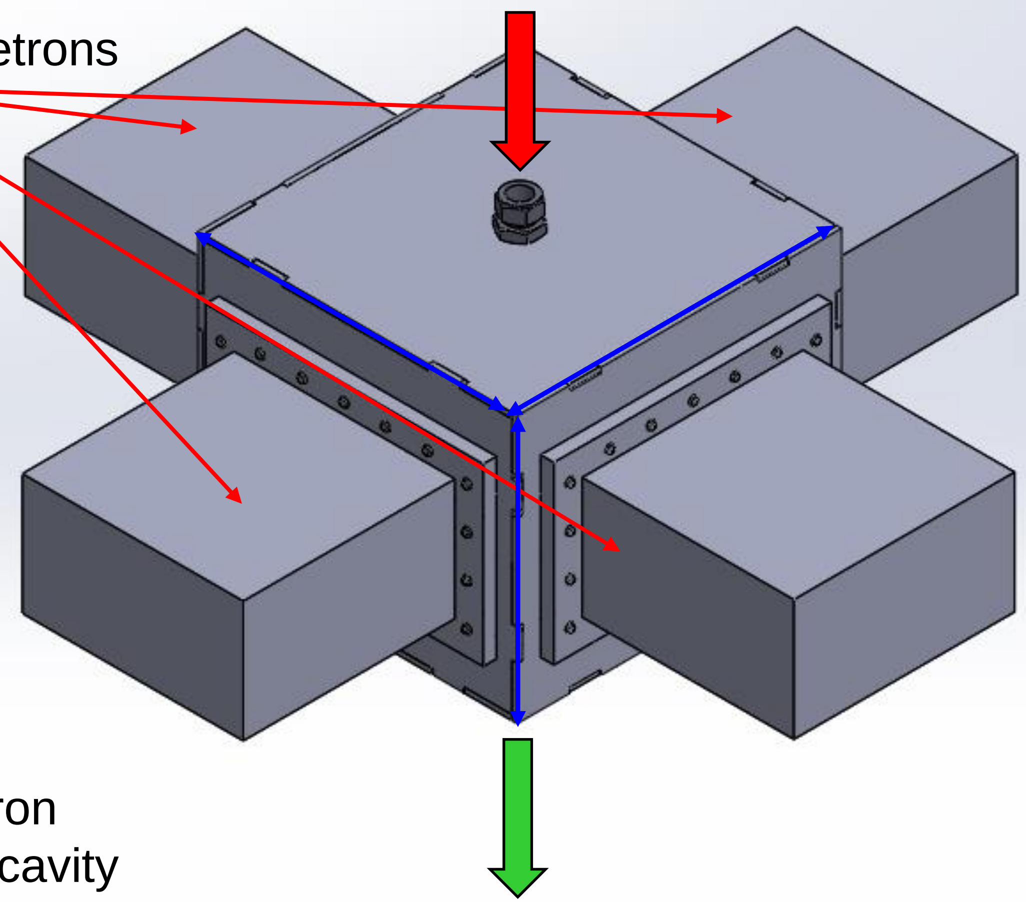
Sorbent Stack in Cavity at 540sec.
(average sorbent temp = 60°C)

	Property	Va	Value	Unit	Property group
☑	Relative permeability	m...	1	1	Basic
☑	Thermal conductivity	k...	9.225	W/(m·K)	Basic
☑	Density	r...	5258.3	kg/m^3	Basic
☑	Heat capacity at constant pressure	C...	1296	J/(kg·K)	Basic
☑	Loss tangent, dissipation factor	t...	0.0189	1	Loss tangent, dissipation fact...
☑	Relative permittivity (real part)	e...	1.737	1	Loss tangent, dissipation fact...
	Electrical conductivity	s...	1.45*10^-13	S/m	Basic

- 915 MHz microwave
- 9-minute heating cycle
- 38-layer sorbent stack
- Laminate thickness = 4mm
- Laminate spacing = 8mm
- Laminate area = 1 ft^3
  (12” x 12” x 12”)



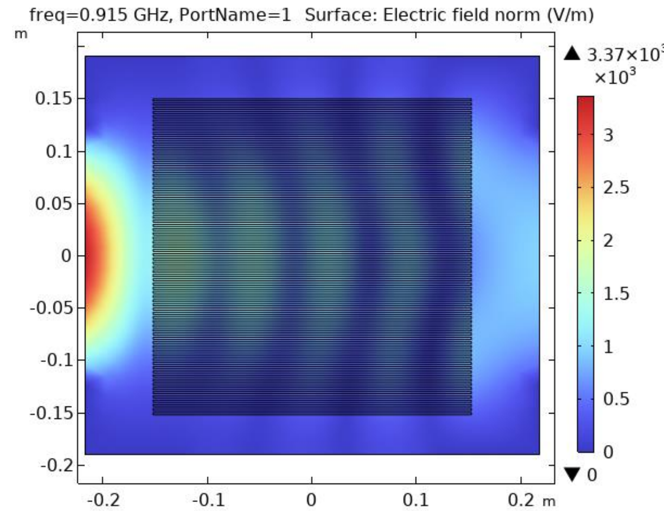
Sorbent Module Design—Cavity Design

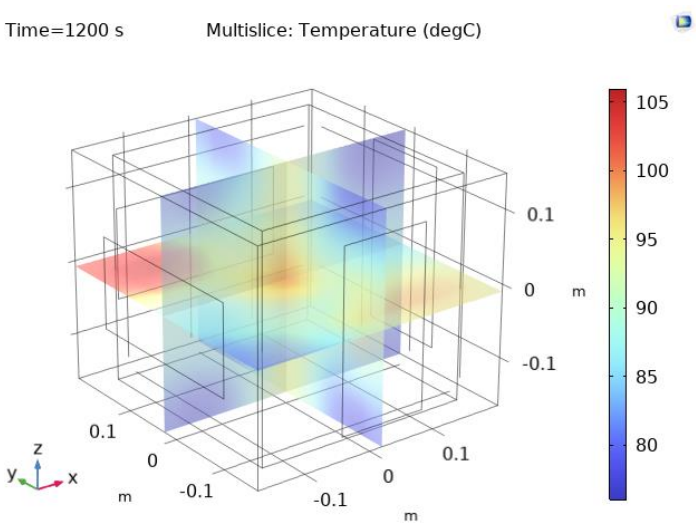


Several magnetron configurations and cavity shapes/sizes have been evaluated.

Sorbent Module Design Optimization

- Cavity is modeled with several waveguides/ports
- Electromagnetic field distribution is modeled using COMSOL for each combination
- A reinforcement learning algorithm is employed to determine the optimal combination/sequence for uniform heating

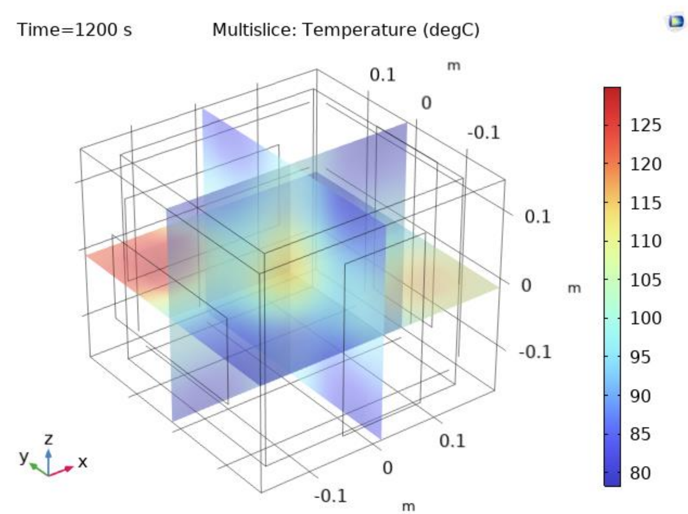




Optimized

Hotter "hot" spots →

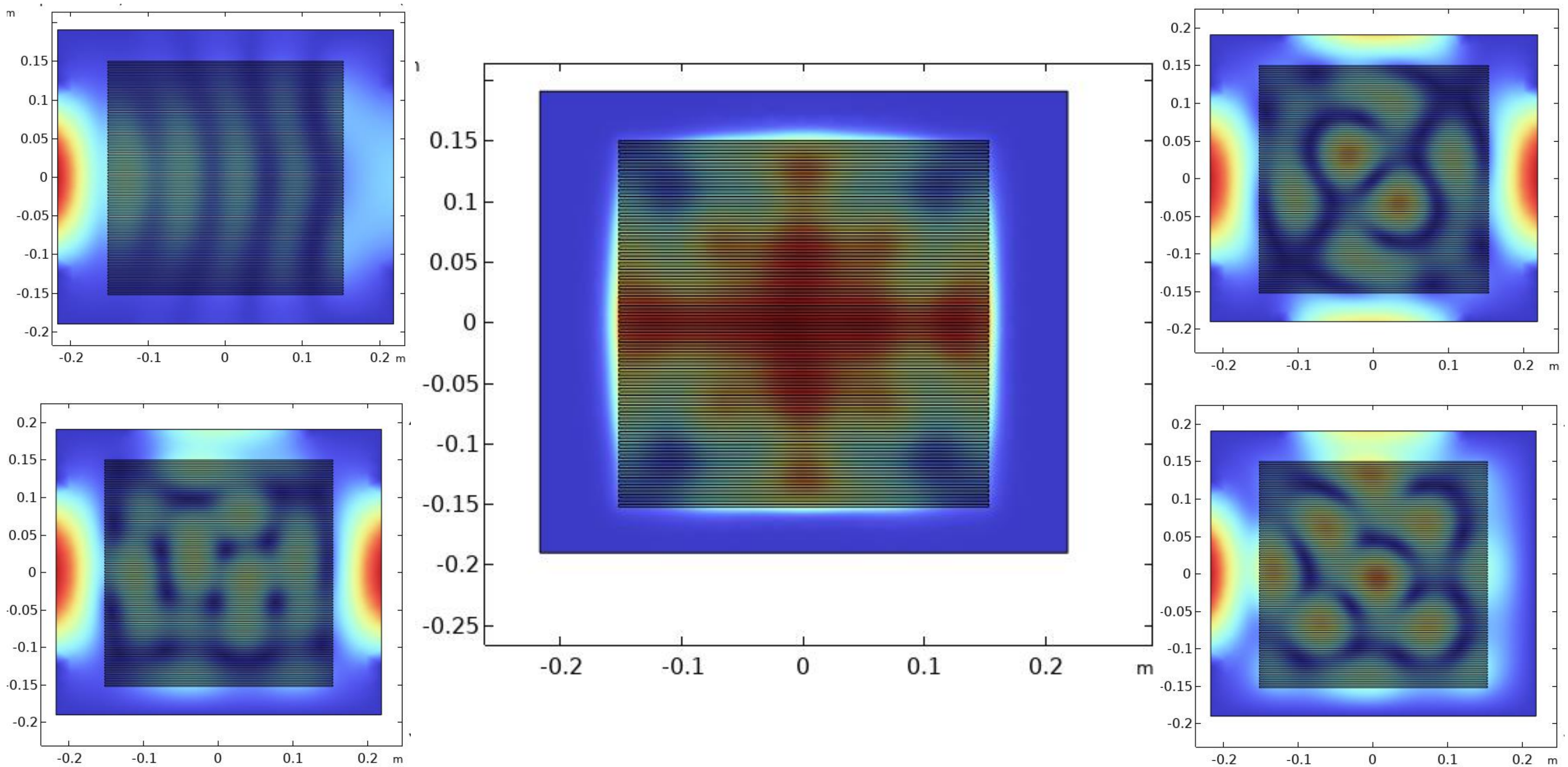
← Improved Uniformity



Standard

TDA RESEARCH

Sorbent Module Design—Waveguide Optimization



The field distribution from various waveguide configurations and the optimized combination (center)

Preliminary Process Design

Est. CO_2 Capture System Power

CO_2 Capture System Power		TDA 90%	TDA 95%
DCC Pump	kWe	311	311
Booster Blower	kWe	8,488	8,488
Vacuum Pump	kWe	8,548	9,012
Pre-Compressor	kWe	3,774	3,978
Microwave Power Input	kWe	22,367	25,699

Max Allowed Microwave Power

Microwave Power			TDA 90%	TDA 95%	
Theoretical MW Power			22,367	25,699	kWe
Sorbent Heating	%	100%	22,367	25,699	kWe
Laminate Heating	%	0%	0	0	kWe
Microwave Efficiency	%	100%	22,367	25,699	kWe

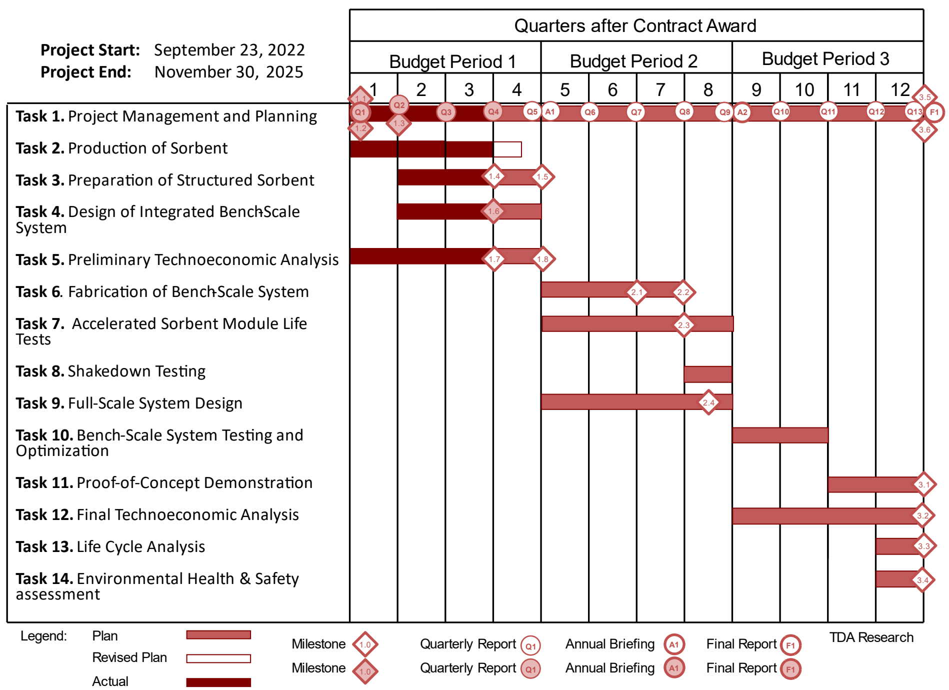
Theoretical energy requirement is being estimated from the experimental material capacity and the modeled energy required for a 1 ft^3 sorbent bed.

The max allowable microwave power for sorbent regeneration (upper limit) is 80% of the power Cansolv power requirement (energy basis)—i.e., the preliminary target is a 20% reduction.

- Threshold MW power ≈ 0.36 kJ/g CO_2 (90% capture efficiency)
- Threshold MW power ≈ 0.39 kJ/g CO_2 (95% capture efficiency)

Current Budget Period Work

Deadline	ID	Task	Title	Verification Method
10/23/2022	**M1.1**	**1.1**	**Update (PMP)**	**PMP File**
10/28/2022	**M1.2**	**1**	**Kickoff Meeting**	**Presentation**
12/12/2022	**M1.3**	**1.2**	**Complete Initial Technology Maturation**	**TMP File**
7/5/2023	**M1.4**	**3.0**	**Prepare multiple 12"x 12" in size sorbent laminates**	**Pictures**
9/22/2023	M1.5	3.1	Demonstrate sorbent capacity ≥ 0.9 mol CO_2 per kg at a ΔT=30°C with 12" x 12" sorbent laminates	State Point Table
7/5/2023	**M1.6**	**4.1**	**Complete the detailed design of the sorbent module integrated with heating and cooling for rapid cycling**	**3-D Layout in Annual Report #1**
7/5/2023	**M1.7**	**5.0**	**Complete Prelim process design to show TDA's system can achieve 20% reduction in CO_2 capture energy compared to Cansolv (95% capture)**	**Annual Report #1**
9/22/2023	M1.8	5.1	Complete Prelim TEA to show TDA's system can achieve 20% reduction in CO_2 capture costs compared to Cansolv (95% capture)	
7/5/2023			BP2 Continuation Application	Annual Report #1



Future Work

Budget Period 2:

- **Task 6. Fabrication of the Bench-scale System (**2–3 scfm of simulated flue gas)
  - Subtask 6.1. Sorbent Reactor Module Fabrication
  - Subtask 6.2. Modifications to Bench-Scale System
- **Task 7. Accelerated Sorbent Module Life Tests**

Budget Period 3:

- **Task 8. Shakedown Testing**
- **Task 9. Full-scale System Design**
- **Task 10. Bench Scale System Testing and Optimization**
- **Task 11. Proof-of-Concept Demonstration (min 1**,000 hours)
- **Task 12. Final Techno-economic Analysis**
- **Task 13. Life Cycle Analysis**
- **Task 14. Environmental Health & Safety Assessment**

TDA RESEARCH

Acknowledgments

- DOE Funding: Contract DE-FE0032151
- DOE Program Manager: Dustin M. Brown
- TDA Electrical Engineers: Josh Wewerka and David Long
- TDA Chemists: Ewa Muteba, Meredith Haanstad, and Sarah DeVoss
- MTR: Tim Merkel, Jay Kniep, and Jenny He
- Comsol Technical Support

TDA RESEARCH