Bench-Scale Development and Testing of Rapid PSA for CO_2 Capture

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UNIVERSITY OF SOUTH CAROLINA

catacel™
Driving Reaction Technology

JM
Johnson Matthey
Process Technologies

Battelle
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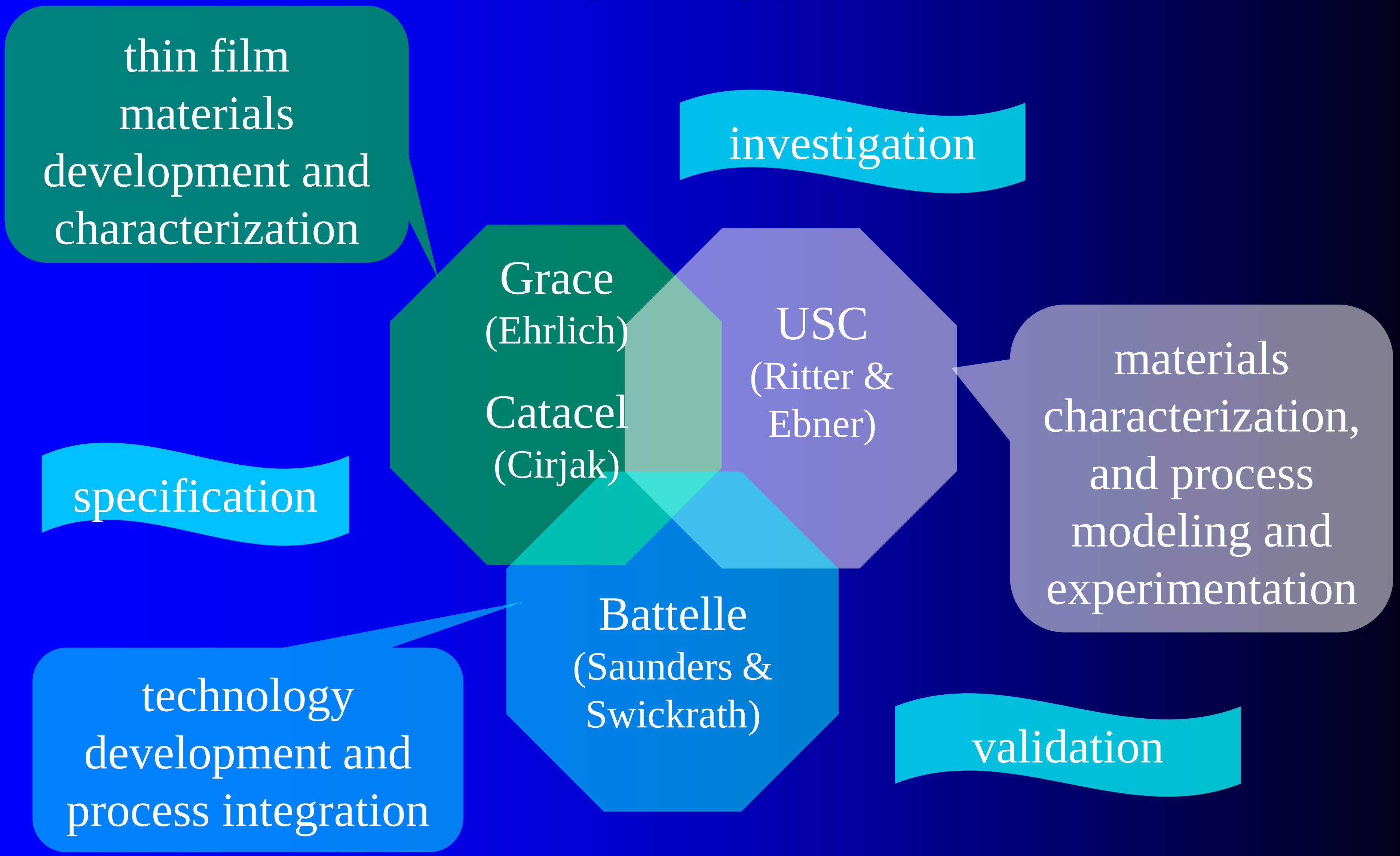
2015 NETL CO_2 Capture Technology Meeting
Pittsburgh, PA, June 25, 2015

Overall Project Objectives

- design, develop and demonstrate a bench-scale process for the efficient and cost effective separation of CO_2 from flue gas using Pressure Swing Adsorption (PSA)
- goal to reduce energy consumption, capital costs, and environmental burdens with novel PSA cycle/flow sheet designs
- applicable to both large (500-1000 MW) and small (5-50 MW) capacity power plants, and industries with 10 to 100 times less CO_2 production

Process simulations and experiments; structured adsorbent material development, CFDs and experiments; and complete flow sheet analyses being used for demonstrating and validating the concepts.

The Team

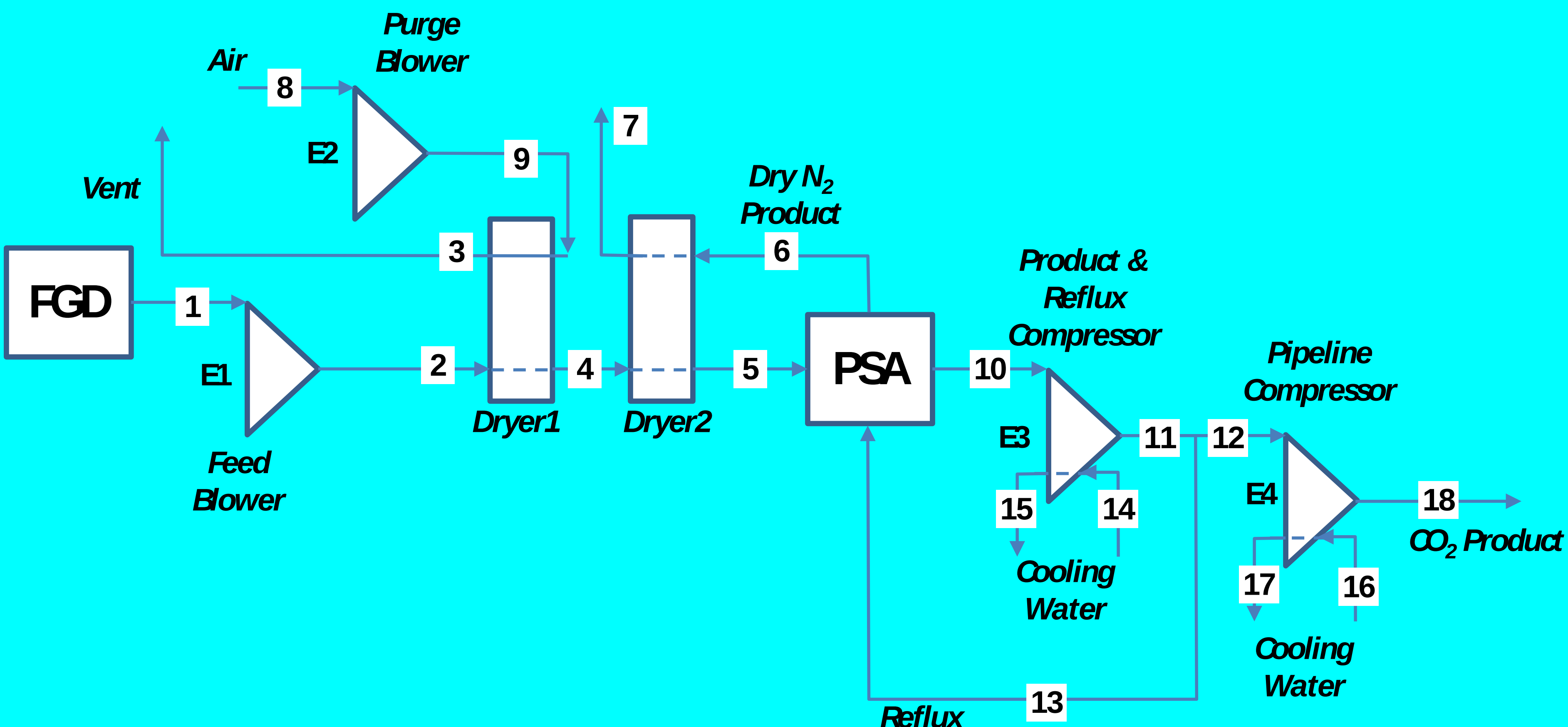

thin film materials development and characterization
investigation
Grace (Ehrlich)
Catacel (Cirjak)
USC (Ritter & Ebner)
materials characterization, and process modeling and experimentation
specification
Battelle (Saunders & Swickrath)
technology development and process integration
validation

Key PSA Technology Challenge

….to develop a structured adsorbent around an efficient PSA cycle that exhibits a high enough packing density to allow the fastest possible cycling rate (→ smallest possible beds), while improving pressure drop and mass transfer and eliminating attrition issues….

Where have we been?

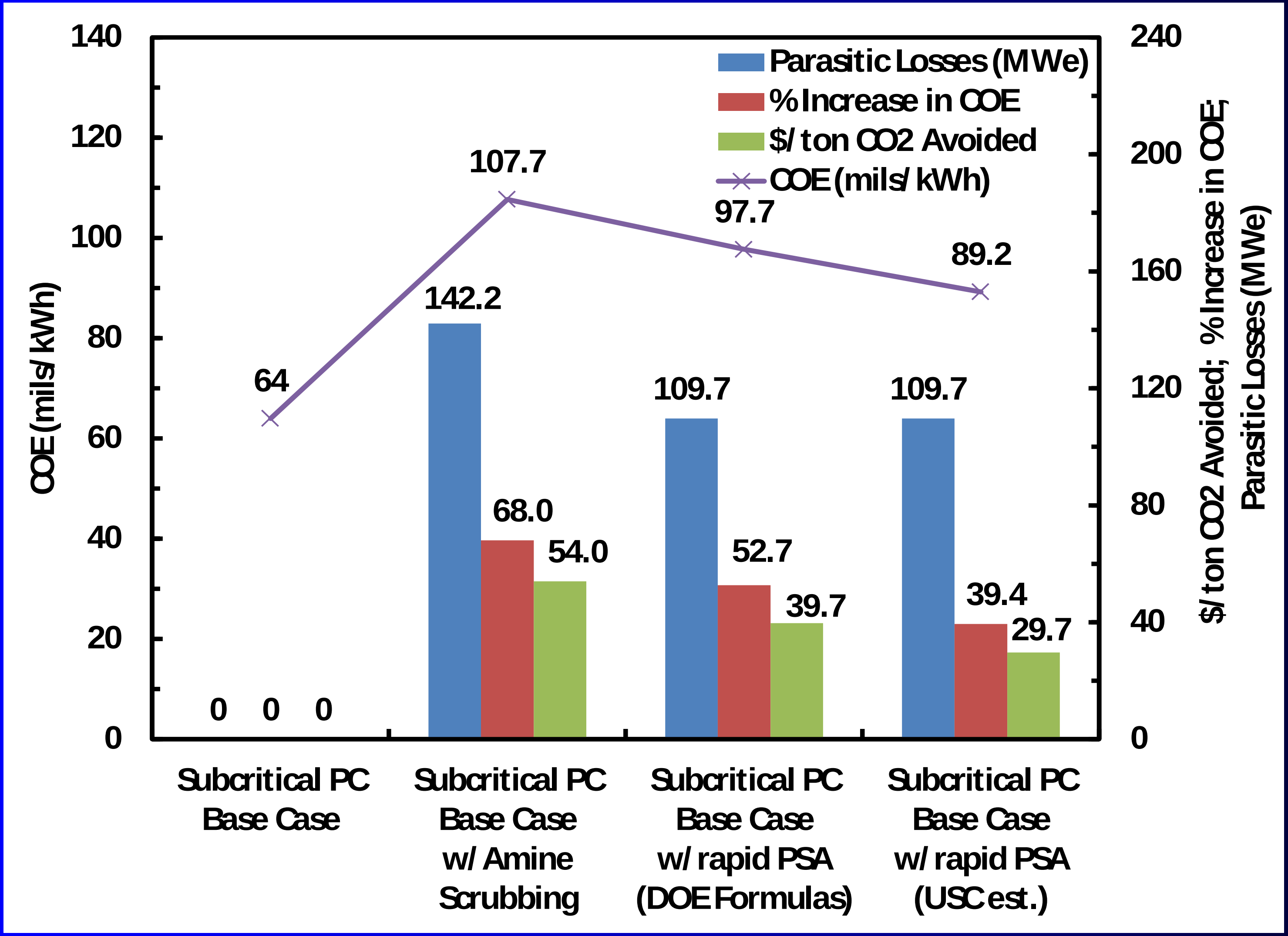
USC Rapid PSA Process Flow Sheet*



* USC Provisional Patent Filed

Preliminary Technical and Economic Feasibility Study

Overall Outcome



Where are we now in Budget Period (BP) 2?

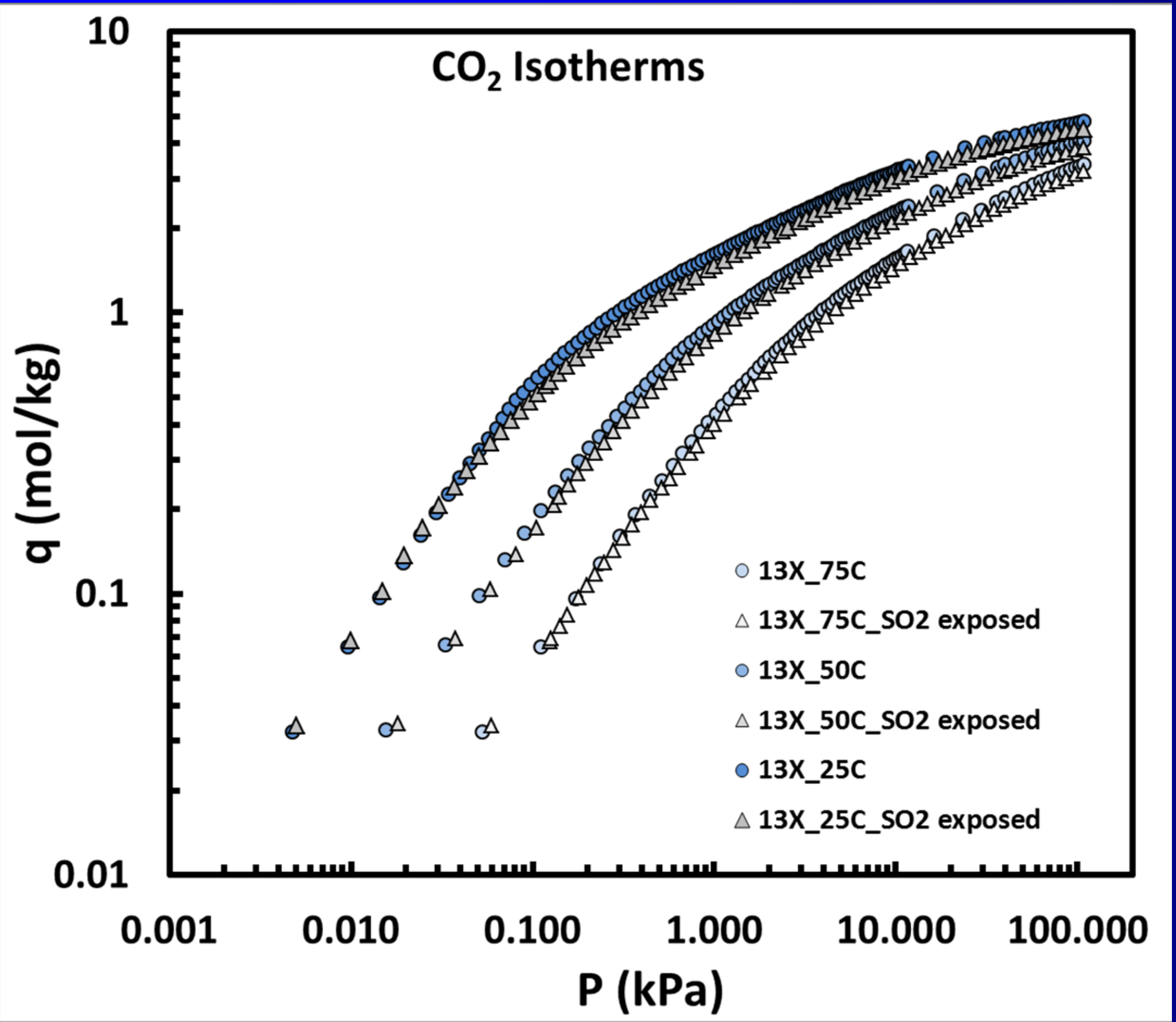
Significant Outcomes so far in BP 2

- developed test procedures for measuring effects of trace levels of both SO_x and NO_x on zeolites and silica gels; some *preliminary* results have been obtained
- completed start-up and trouble-shooting of 1-bed bench scale PSA apparatus; system now capable of mimicking all cycle steps of multi-bed PSA process
- completed *preliminary* CO_2-N_2 cycling with 3 mm zeolite beads in larger 1-bed bench scale PSA apparatus; results showing very good separation/recovery at reasonable throughput
- fabricated three, 6 inch Catacel cores coated with 50 μm thick layers of zeolite crystals, achieving 240 kg/m^3 bed density; awaiting testing in larger 1-bed bench scale PSA system
- fabricated two, 6 inch Catacel cores, one uncoated and one coated with 50 μm thick layers of zeolite crystals; awaiting testing in VFR apparatus to determine mass transfer rates

Significant Outcomes so far in BP 2

- completed construction of multi-bed bench scale PSA apparatus; currently undergoing start-up, troubleshooting and testing with 3 mm zeolite beads
- developed parallel channel structured adsorbent pressure drop correlation (PD) for use in DAPS; currently being used with DAPS to simulate full scale PSA process
- completed CFD modeling showing when plug flow (packed bed) conditions prevail in parallel channel structured adsorbent (PCSA); simpler 1-D packed bed models can now be used to study PCSAs in DAPS with modified PD correlation
- completed first phase of CFD modeling, revealing use of slower 2-D and 3-D models to train much faster 1-D models; currently being used to determine optimum Catacel core structure

Equilibrium Adsorption Isotherms for CO_2 on 13X Zeolite



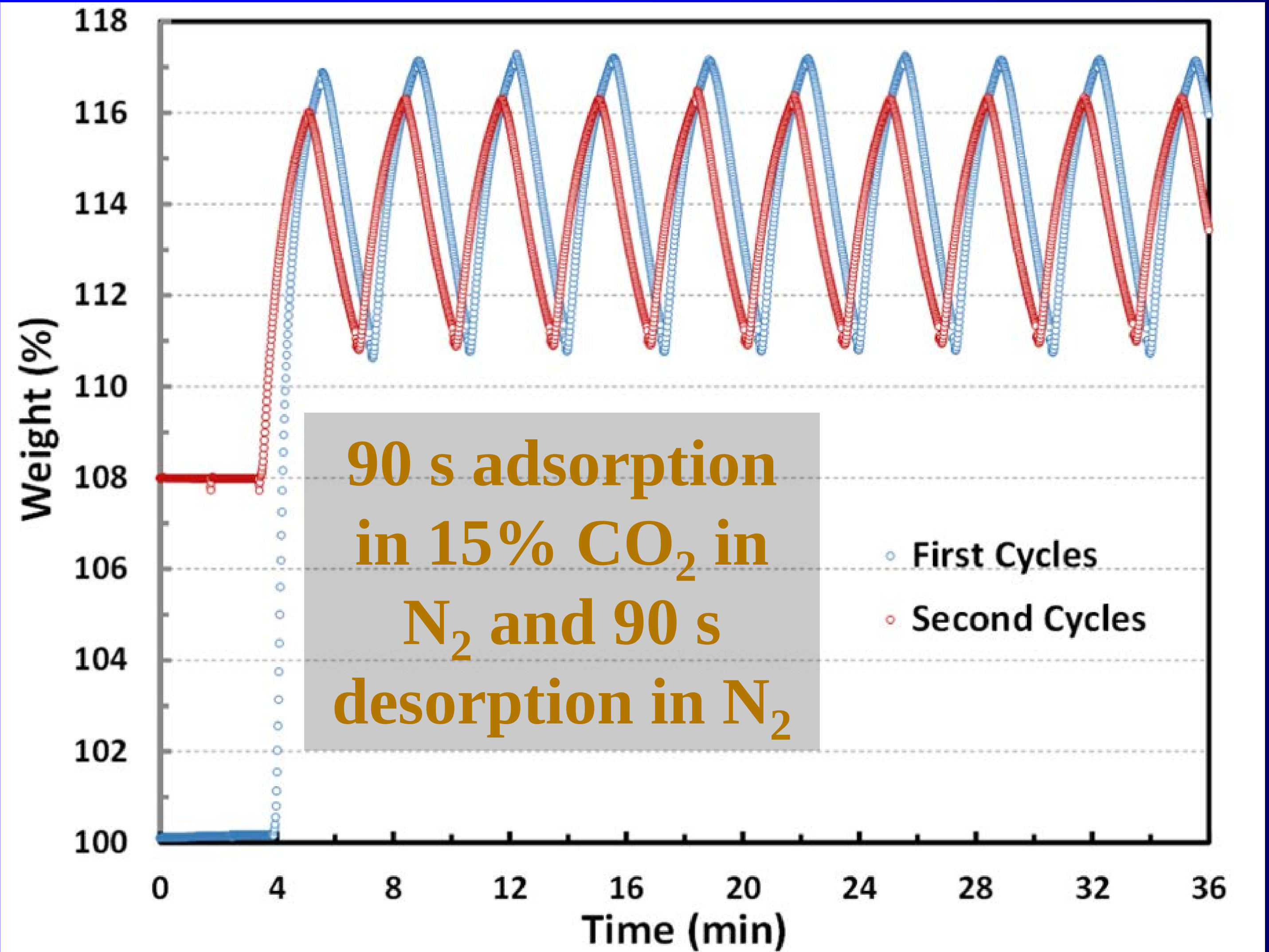
Effect of Exposure to 500 ppm of SO_2 in N_2 with Subsequent T Regeneration

5% to 10% Decrease in Capacity Realized Especially at High Loadings

Working Capacity (wt%) of CO_2 on 13X Zeolite

Effect of SO_2 and NO_x Exposure

TGA CO_2 Cycling Tests at 70 ºC and 1 atm



sample exposed to 2.5 hr of 42 ppm of SO_2 in N_2 between sets of cycling tests – no regeneration

Working Capacity (wt%) of CO_2 on 13X Zeolite

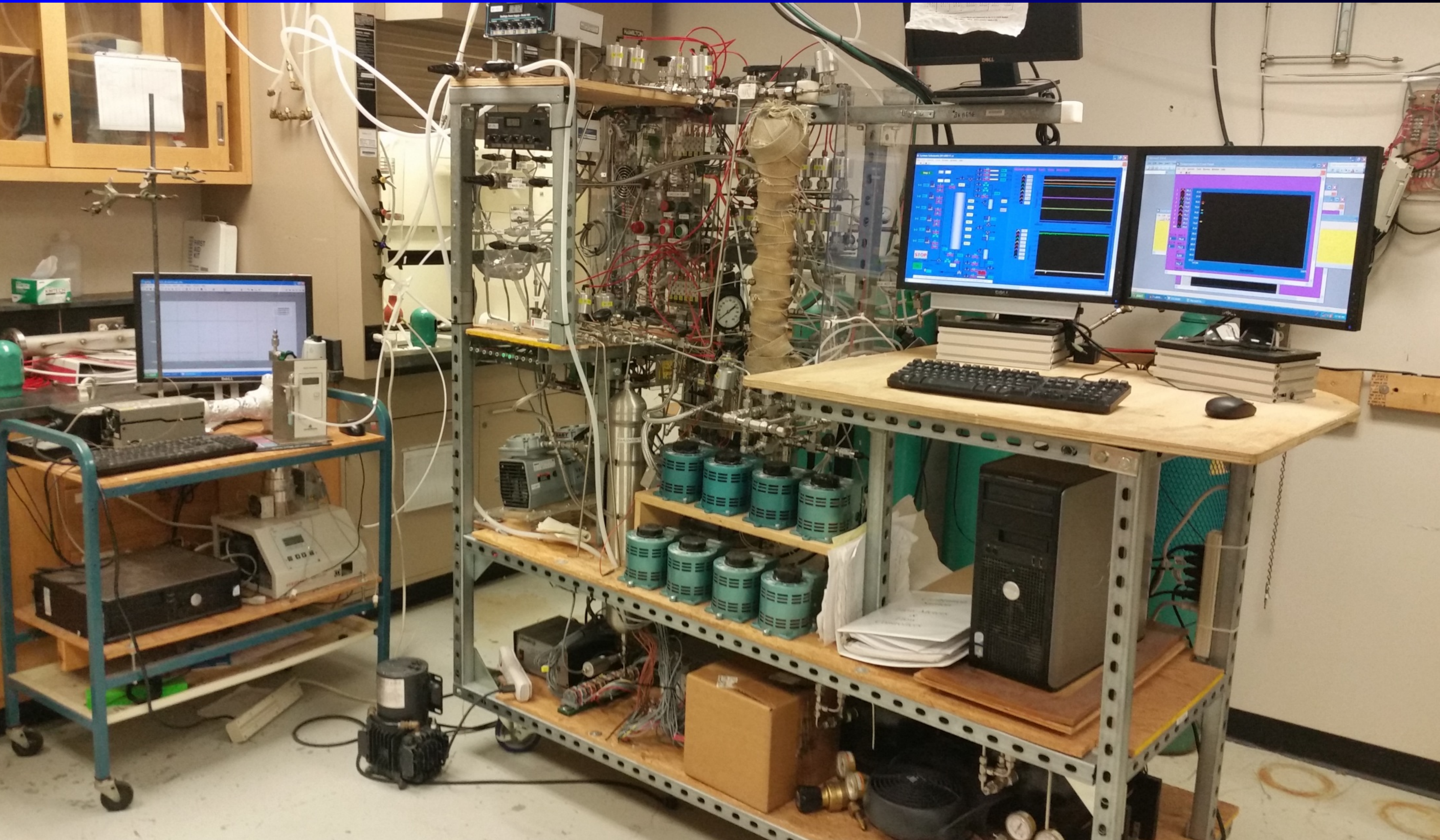
Effect of SO_2 and NO_x Exposure

Gas	Before Exposure	After Exposure	% Decrease
He*	7.05	5.87	16.7
SO_2 (42 ppm)	6.56	5.18	21.0
SO_2 (500 ppm)	6.88	5.66	17.7
NO_2 (74 ppm)	6.44	5.43	15.7

* only helium run, so sample not exposed to any SO_2 or NO_x – implies decrease in all cases, since similar, most likely due to trace H_2O vapor leaking into TGA

1-Bed PSA System

Rapid Complex PSA Cycle Schedule Analysis



1-Bed PSA System

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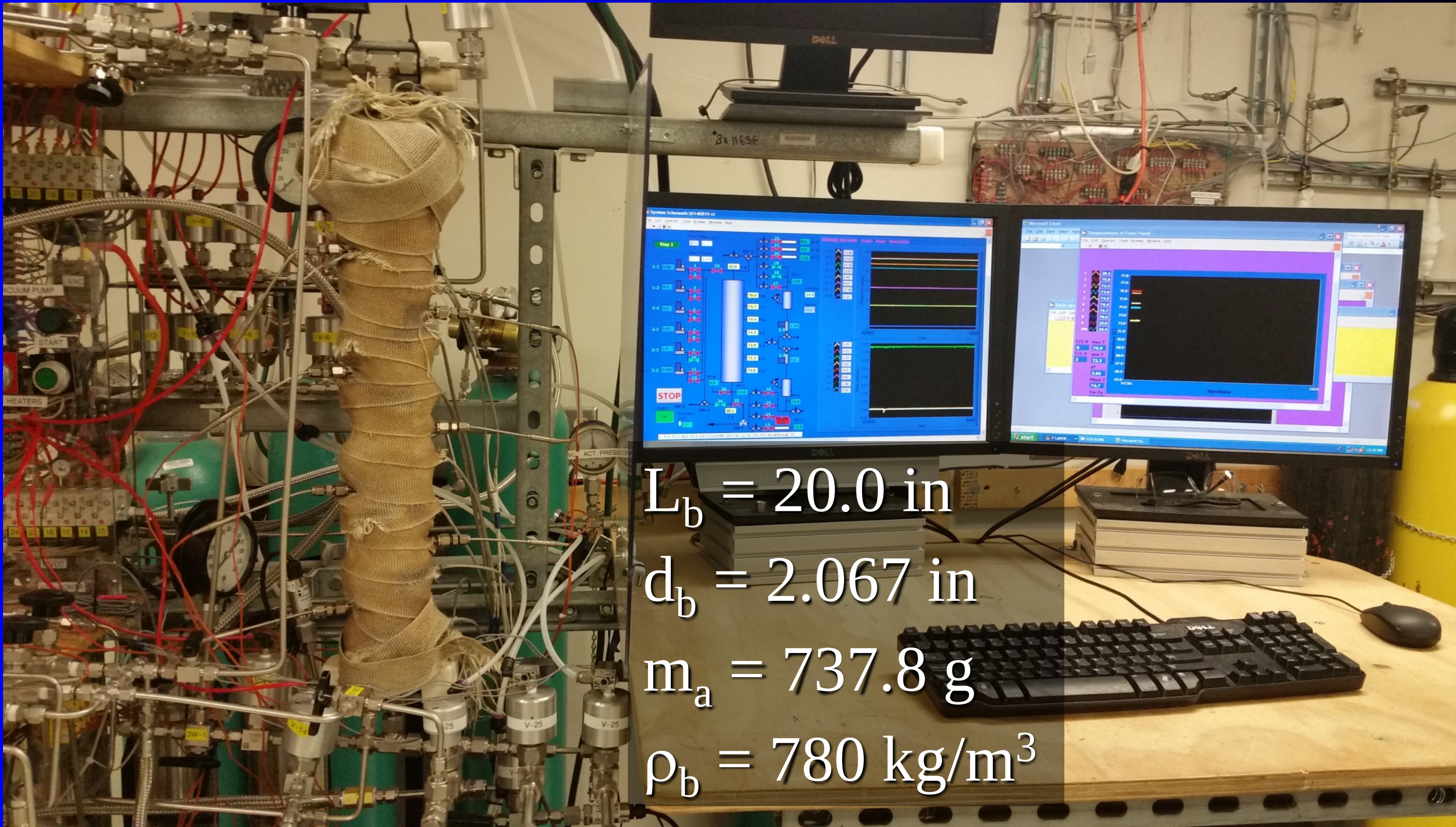


L_b = 20.0 in

d_b = 2.067 in

m_a = 737.8 g

ρ_b = 780 kg/m^3

1-Bed PSA System

Preliminary Results with Zeolite Beads

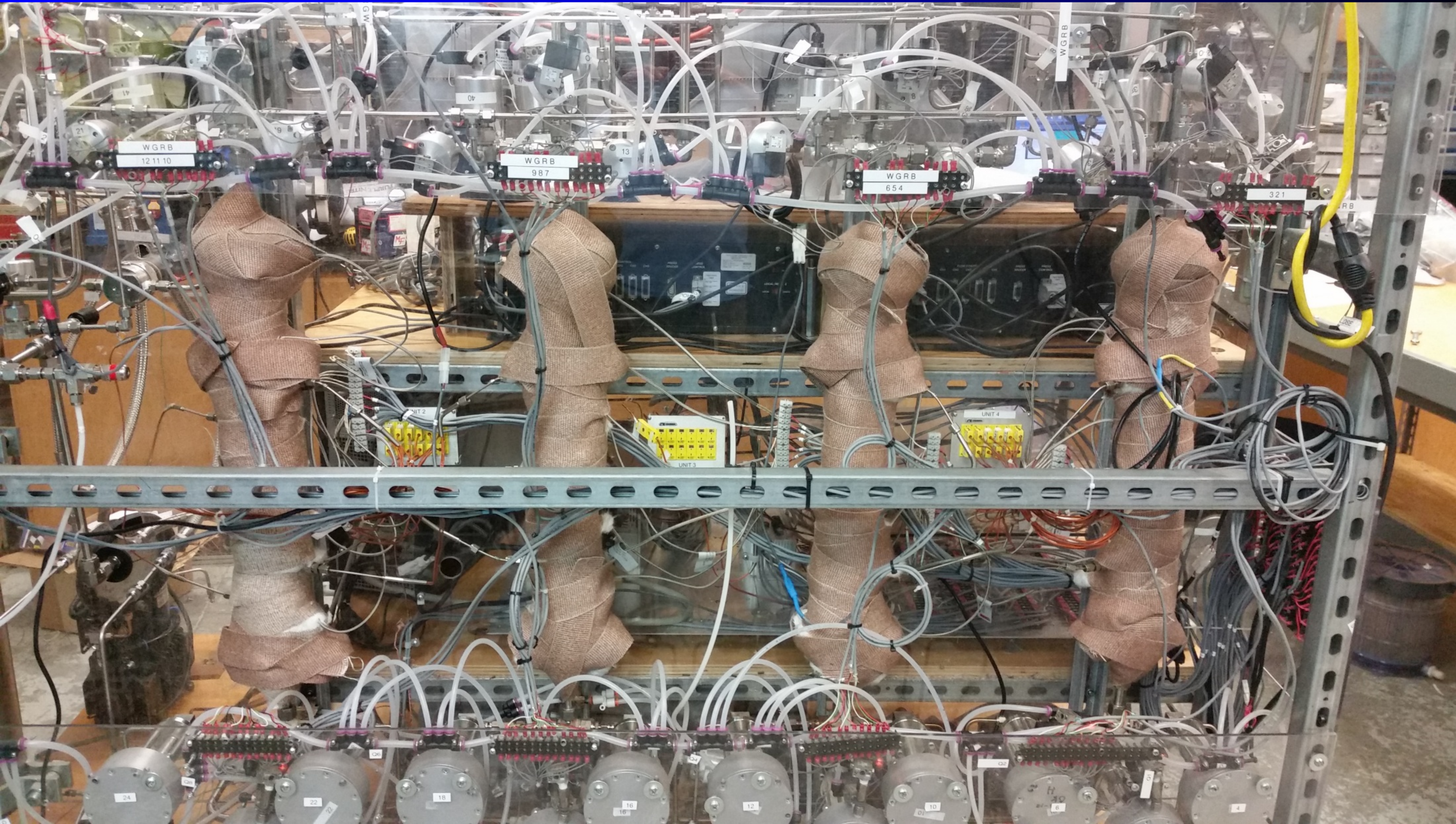
Exp No.	Feed Flow Rate [SLPM]	Cycle Time [sec]	Feed Throughput [L(STP)/hr/kg]
1	12.97	720	351.60
2	14.26	720	386.55
3	7.13	1440	193.32
4	7.85	1440	212.67

15 vol% CO_2 in N_2 Fed at 120 kPa with Column at 70 °C and Regeneration by Vacuum with P_{low} = 5 kPa

Exp No.	HP CO_2 Pur (%)	HP CO_2 Rec (%)	LP N_2 Pur (%)	LP N_2 Rec (%)
1	88.31	92.16	98.18	96.53
2	89.82	89.98	97.40	97.42
3	88.50	94.50	98.46	97.50
4	89.37	93.08	98.18	97.35

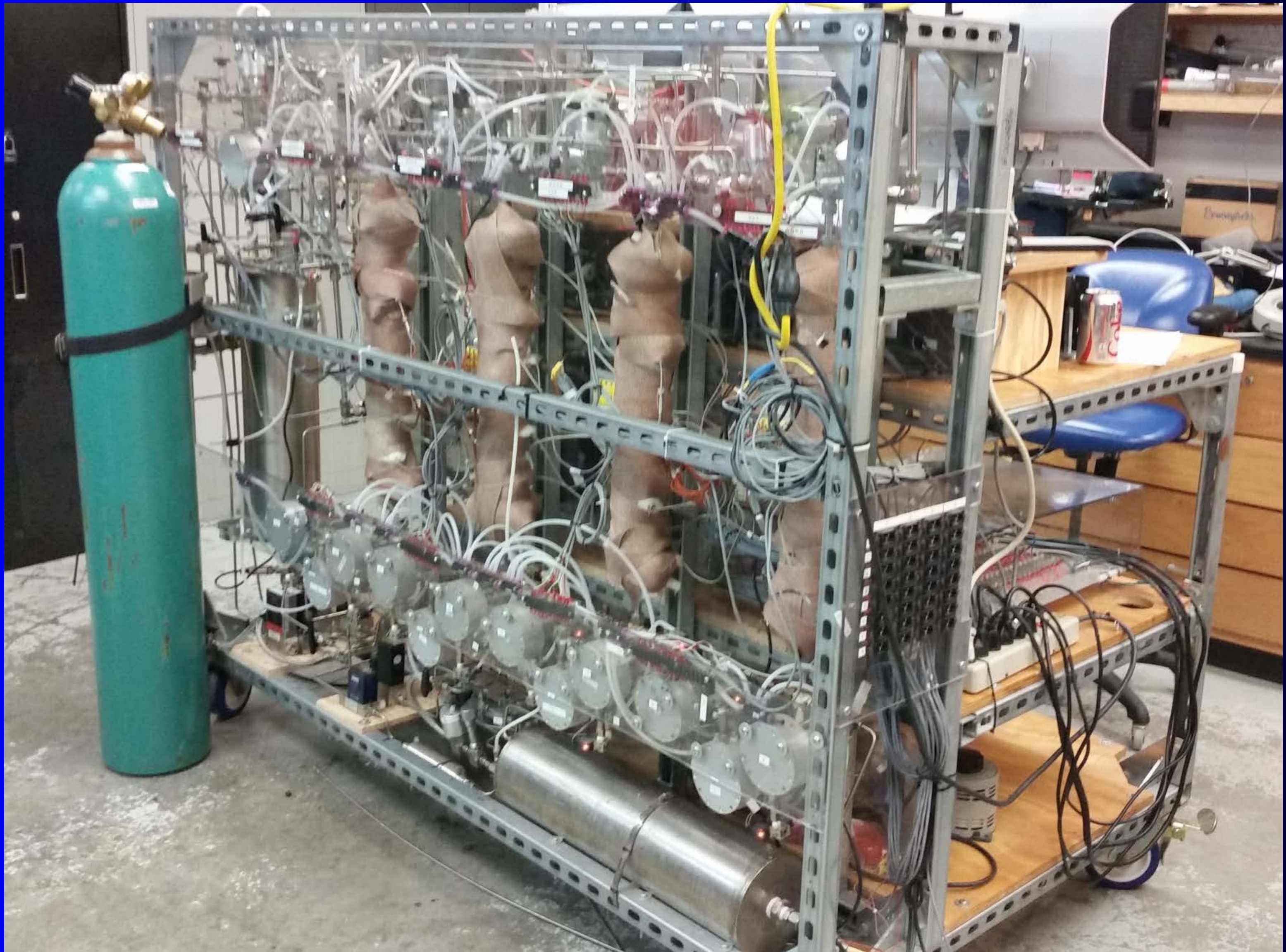
4-Bed PSA System

Suitable for Power Plant Demonstration



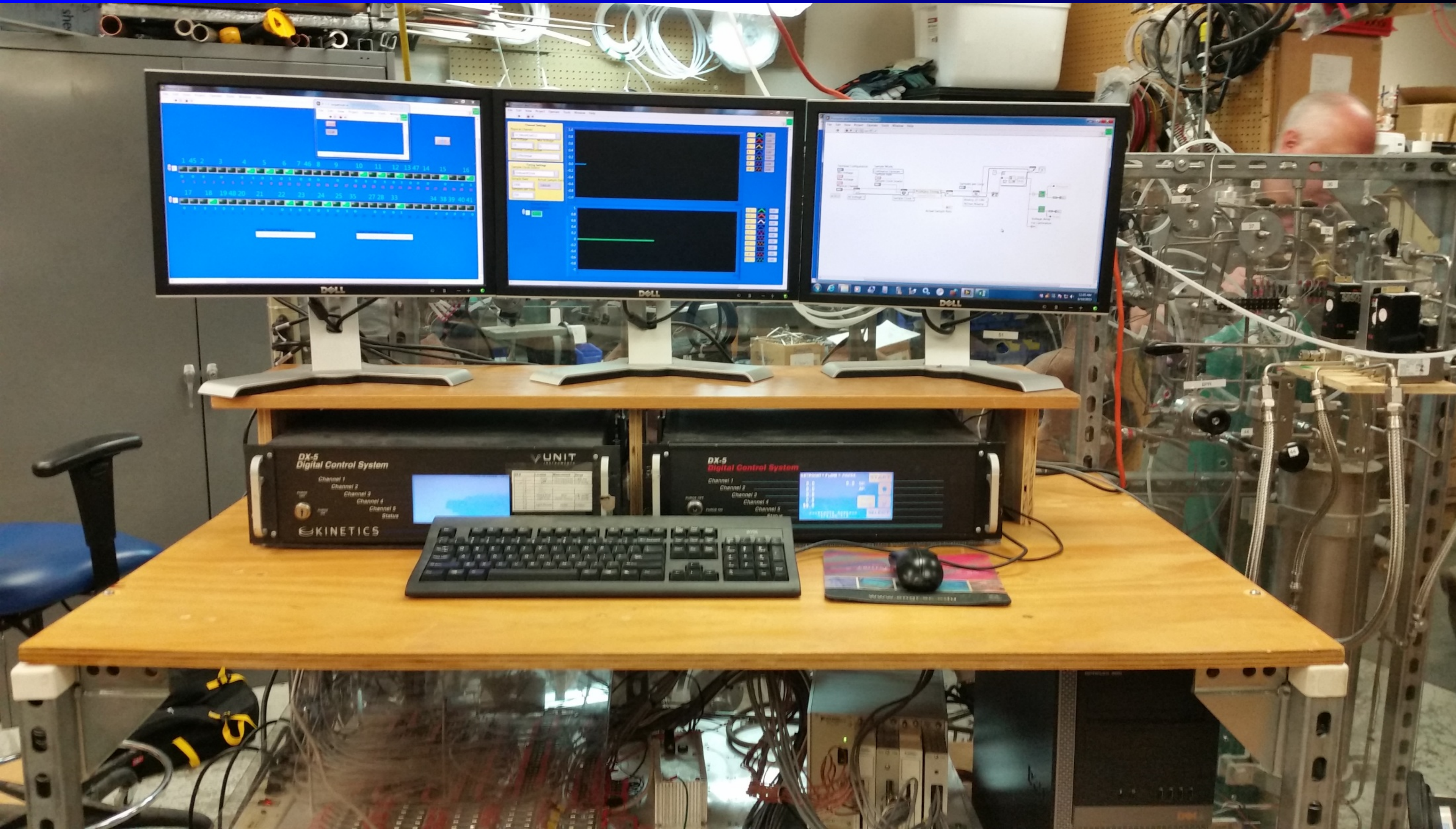
4-Bed PSA System

Suitable for Power Plant Demonstration

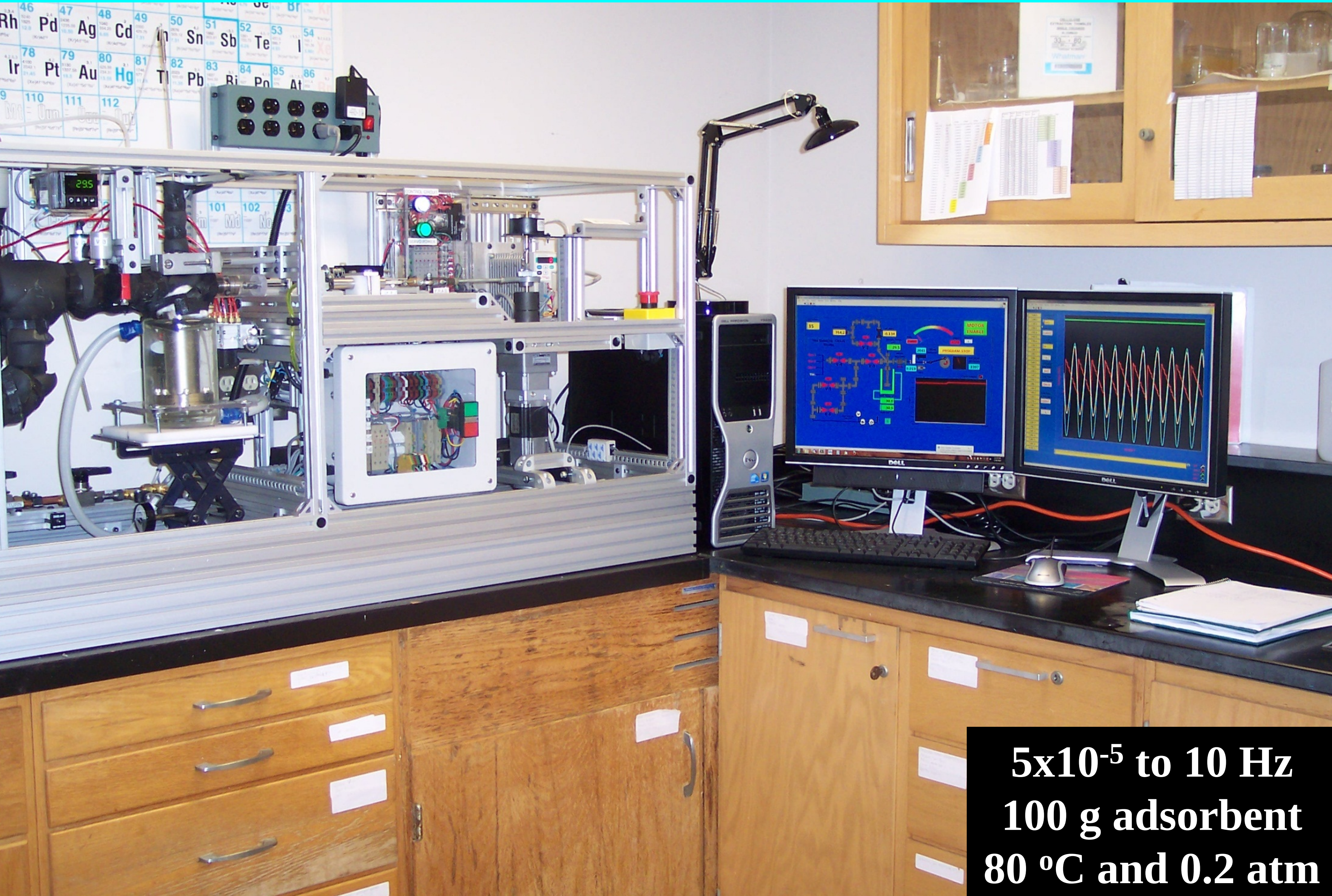


4-Bed PSA System

Suitable for Power Plant Demonstration



Volumetric Frequency Response Apparatus



$5x10^{-5}$ to 10 Hz
100 g adsorbent
80 ºC and 0.2 atm

Comparison of Mass Transfer Coefficients

N_2 and CO_2 on 13X Zeolite Beads at 25 °C

	k s^{-1}	
	VFR	**1-Bed RPSA**
CO_2	**3.3**	**7.5**
N_2	**5.1**	**4.6**

- VFR: volumetric frequency response
- 1-Bed rapid PSA experiments

Higher values are expected in the structured adsorbent!

Uncoated and Zeolite Coated Catacel Cores

Specially Designed for Use in VFR Apparatus

CPSI = 741

$\varepsilon_b = 0.64$

$w_{foil} = 52\ \mu$

$w_{coating} = 51\ \mu$

$\rho_b = 241.93\ \mathrm{kg/m^3}$

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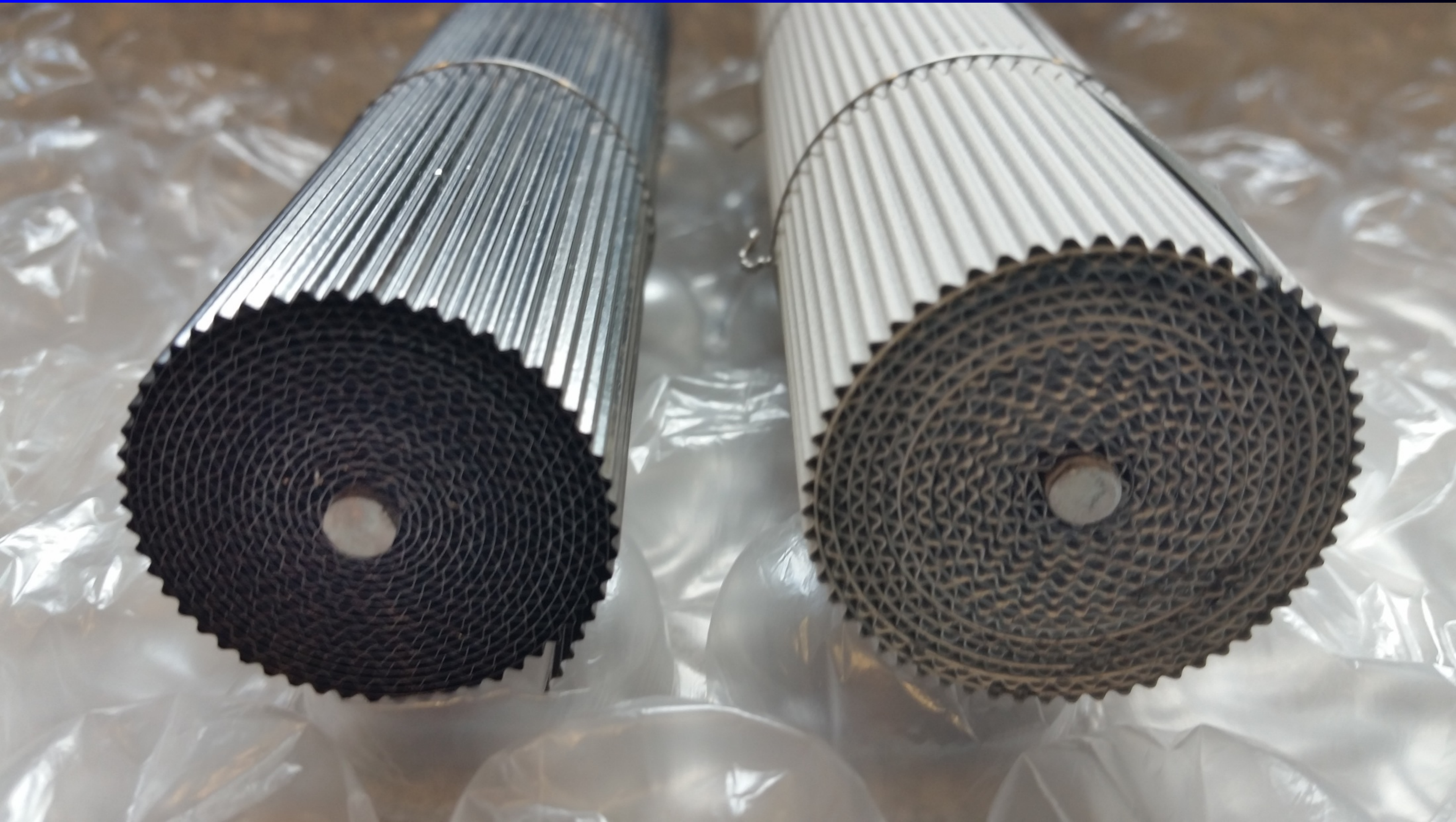
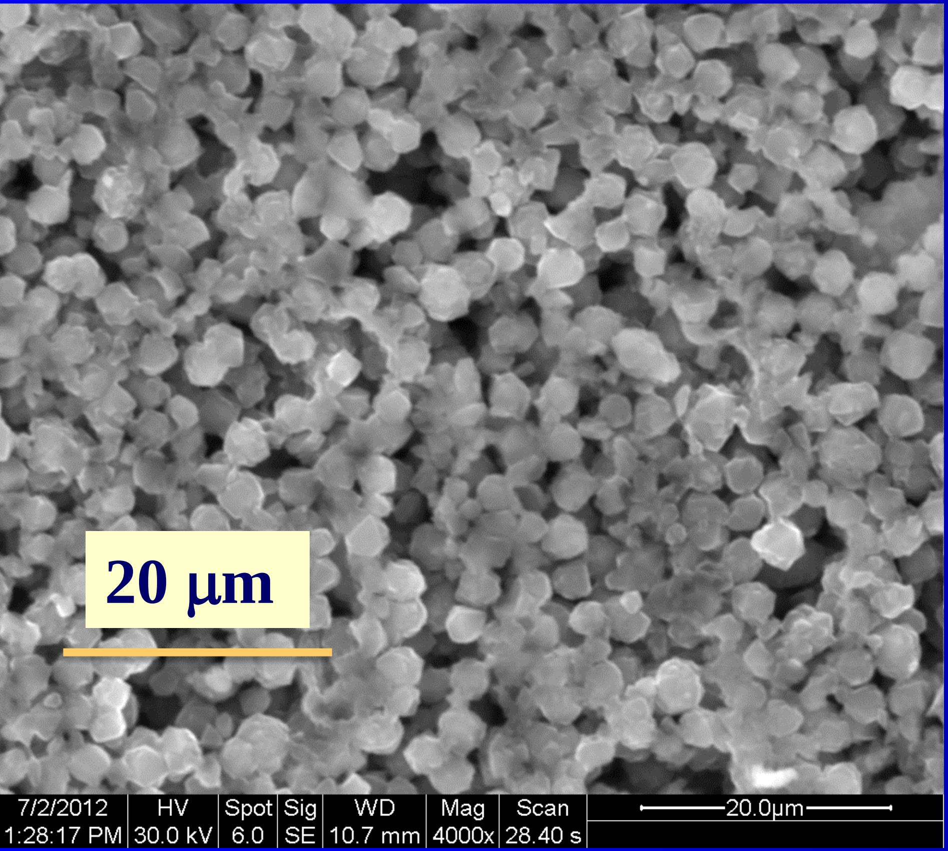
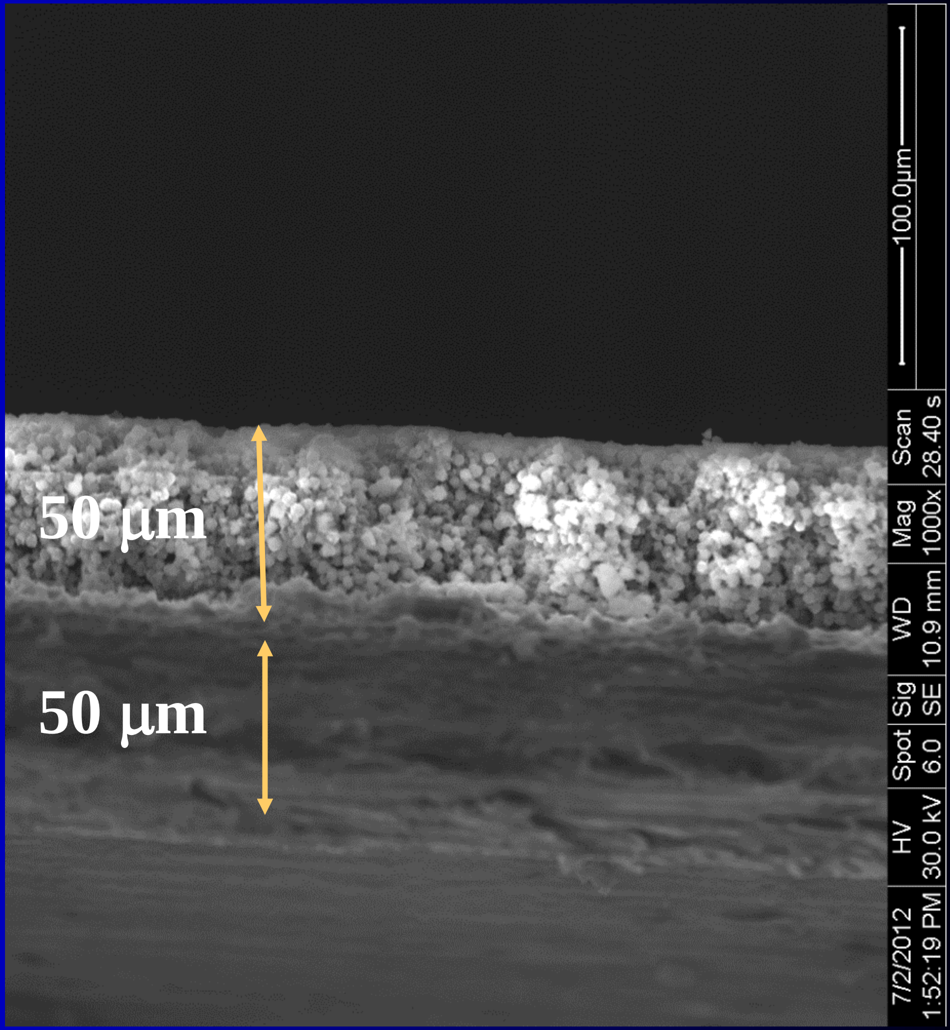


Zeolite Coated Catacel Metal Foil





Parallel Channel Structured Adsorbent Column Containing Three 6” Zeolite Coated Catacel Cores

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Structured Adsorbent Pressure Drop

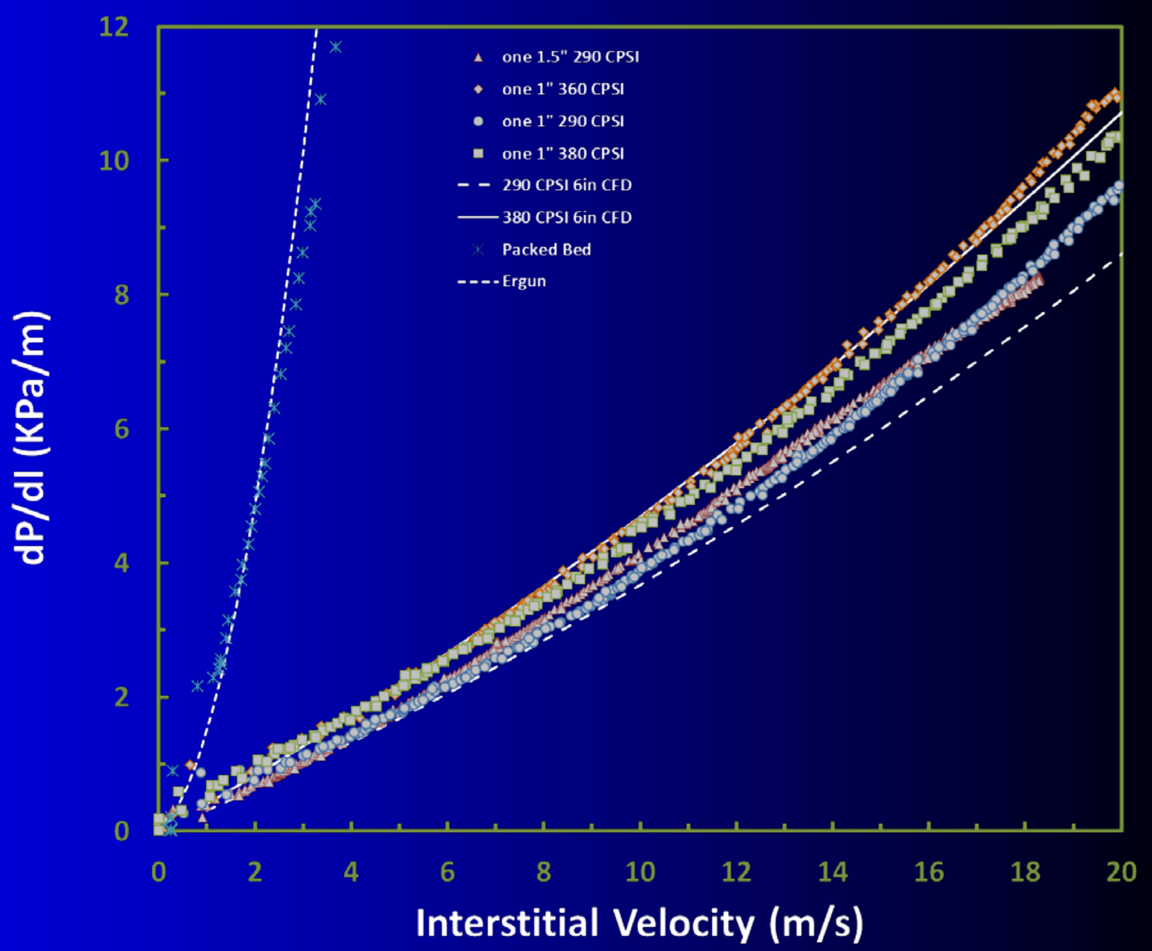
Open Cell Corrugated Structure and Beaded Media

Pressure Drop Apparatus

Q_{max} = 1000 SLPM

ΔP_{max} = 30, 70 or 140 in H_2O

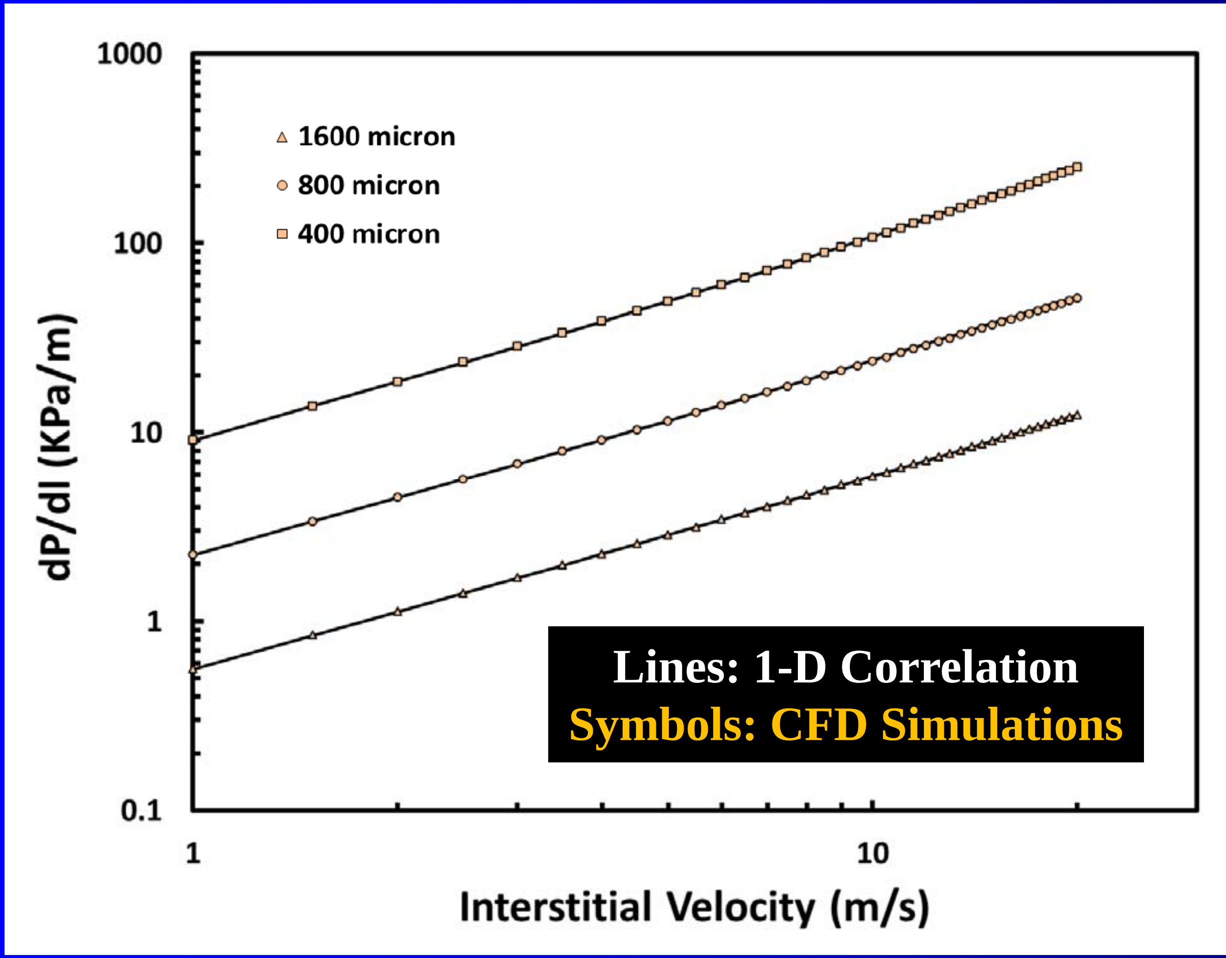
goal: ΔP_{max} < 20 kPa/m at design velocity of 20 m/s



3-D CFD

Compressible Navier-Stokes Equations

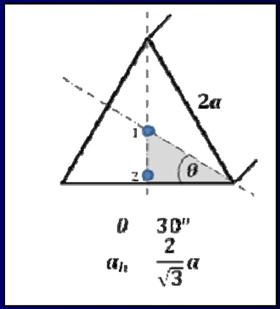
New 1-D Pressure Drop Correlation for Parallel Channel Structured Adsorbent and Use in DAPS

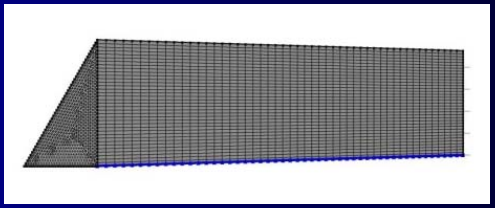


$$f(Re) = f_1 + \frac{f_2}{Re}$$

$$Re = \frac{2\rho V_Z a_h}{\mu}$$

$$f_1 = 2.5\text{x}10^{-3}$$
$$f_2 = 25.42$$



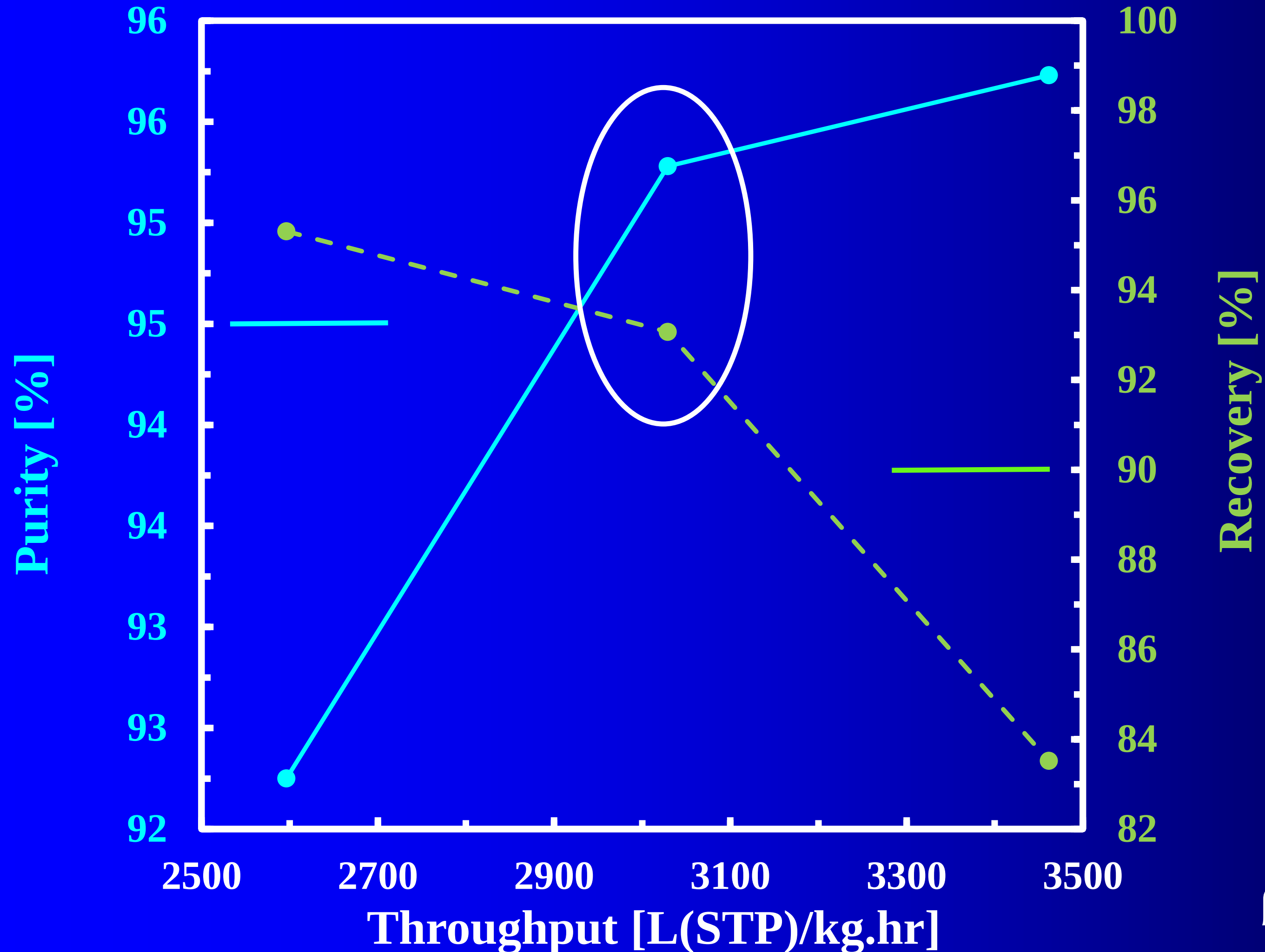


Developed from 3-D CFD Simulations

DAPS of Bench Scale PSA Processes

Zeolite Coated Catacel Structured Core

y_F = 0.1592 CO_2, 0.8029 N_2 and 0.0379 O_2



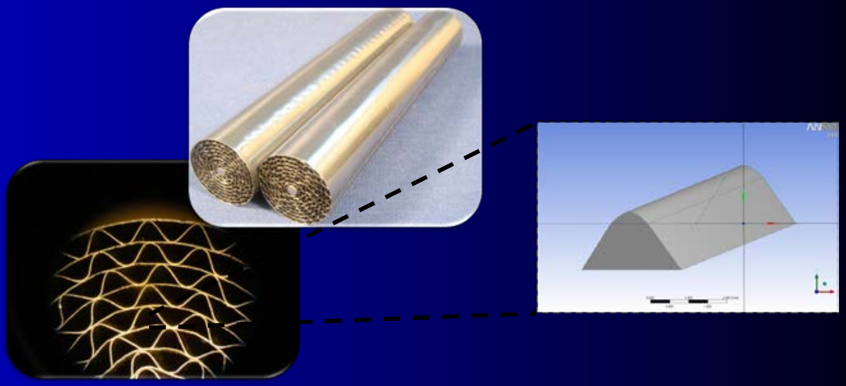
P_H= 103.3 kPa
P_L= 5 kPa
t_c = 120 s
T = 75 ^oC
L_b= 0.125 m
d_b = 0.098 m
k_{LDF} = 1 s^{-1}

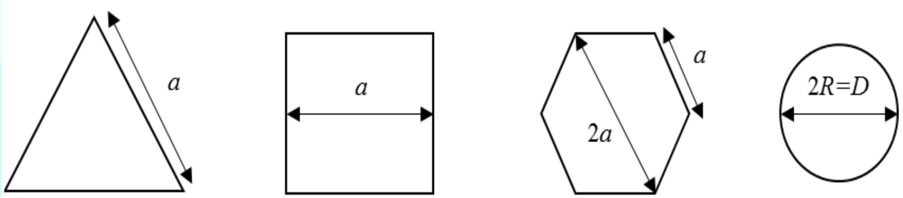
CPSI = 741
ε_b = 0.64
w_{foil} = 52 μ
$w_{coating}$ = 51 μ
ρ_b = 241.93 kg/m^3

Determination of Optimal Channel Shape

- use 1-D models with friction factors and mass transfer parameters determined by 3-D CFD
- match performance to predictions from DAPS, then find minimum parasitic energy over key parts of cycle

Shape (sides)	Hydraulic Diameter, D_h	Friction Factor, f
Triangle (*n*=3)	$D_h = \frac{\sqrt{3}}{3}a$	$f = \frac{53.3}{Re}$
Square (*n*=4)	$D_h = a$	$f = \frac{56.9}{Re}$
Hexagon (*n*=6)	$D_h = \sqrt{3}a$	$f = \frac{60.2}{Re}$
Circle (*n*=∞)	$D_h = 2R$	$f = \frac{64}{Re}$

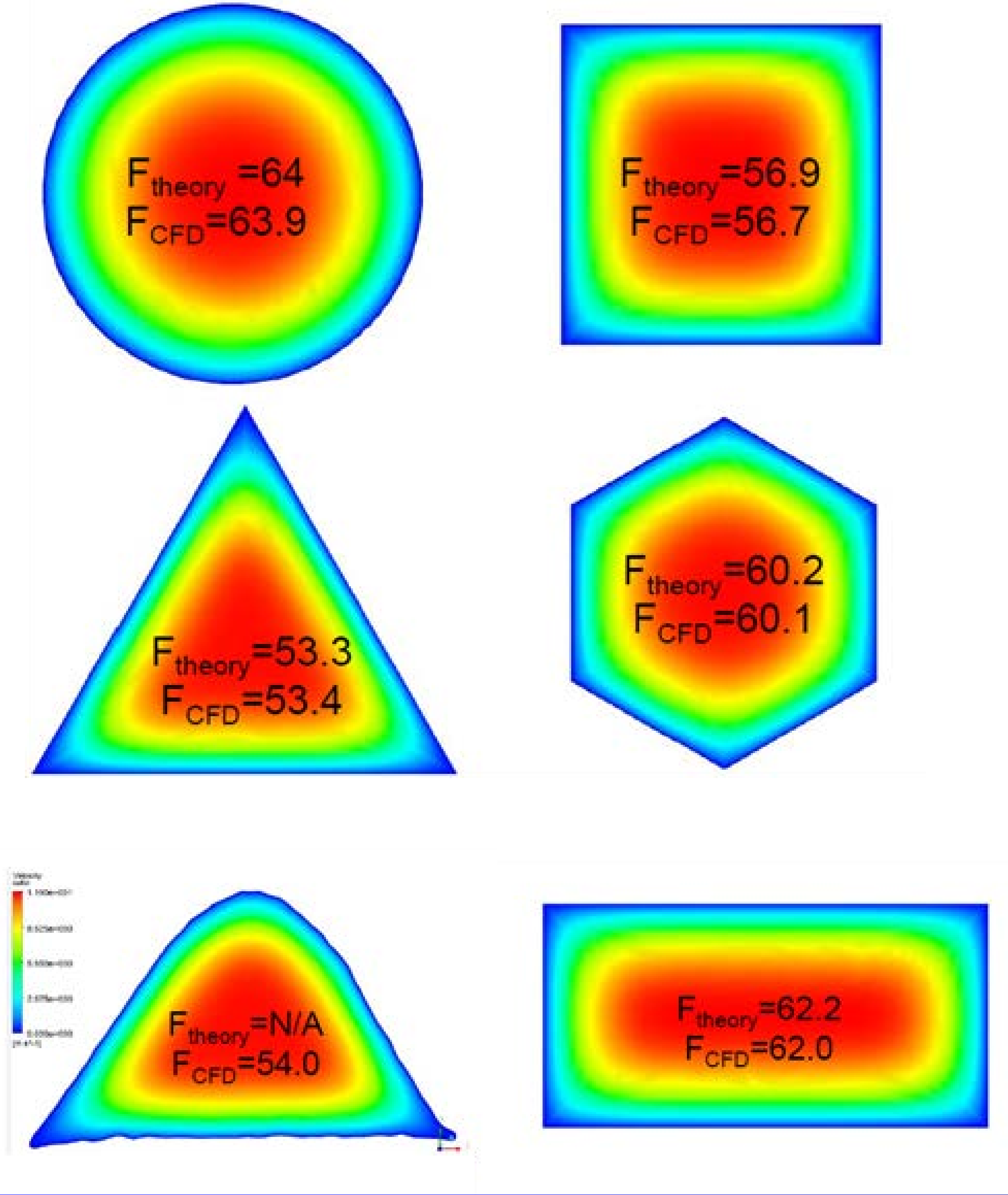




Best Shape Estimates from Rapid 1D Model

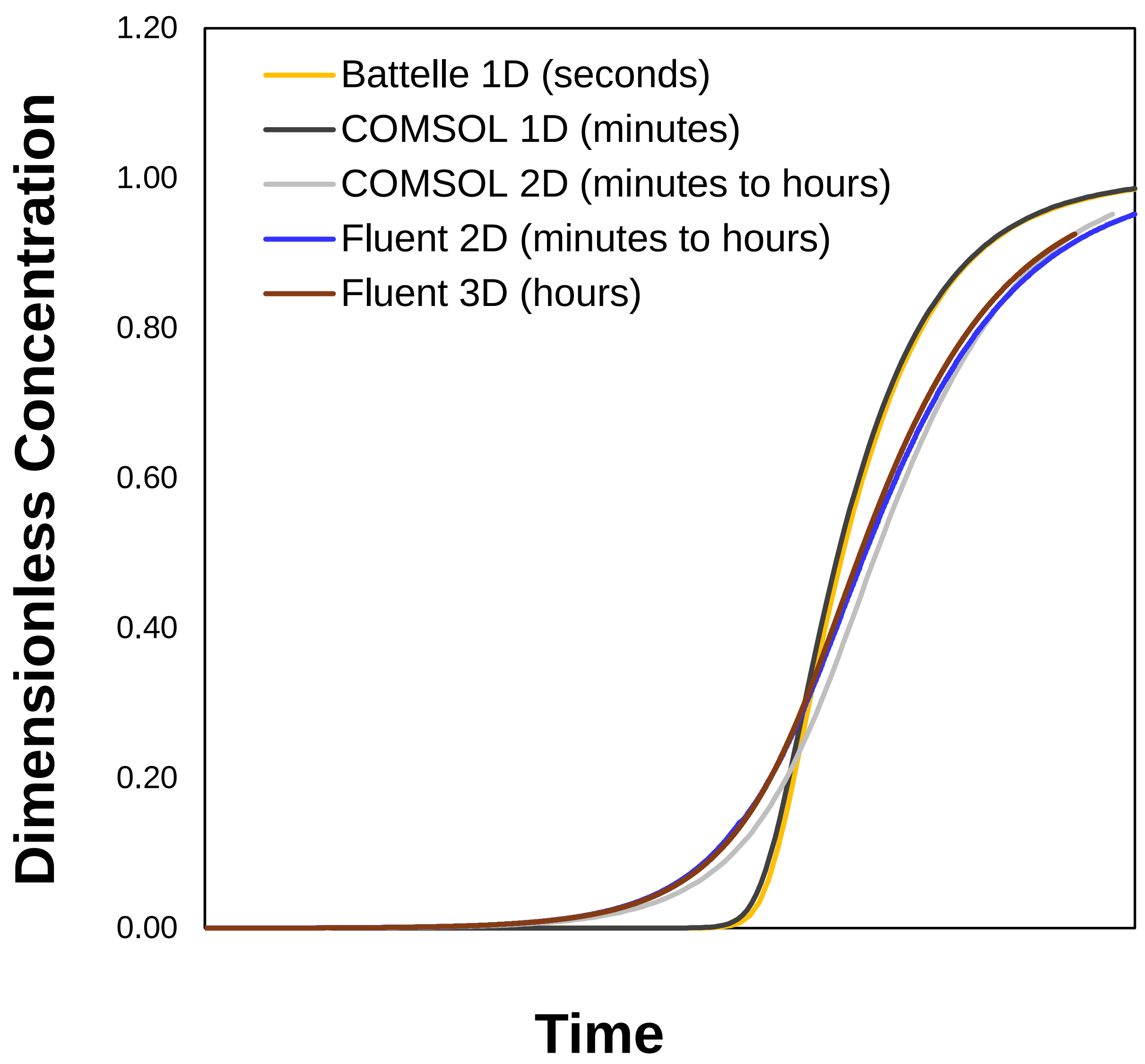
Based on Parameters from 3-D CFD Models

Comparison of Friction Factors from CFD and Theory



Best Shape Estimates from Rapid 1-D Model

Based on Parameters from 3-D CFD Models



Comparison of Breakthrough Times from Different Mass Transfer Models


Where are we headed?

On-Going Tasks to Complete in BP 2

- test breakthrough and cycling behavior of zeolite coated Catacel cores with CO_2-N_2 in 1-bed PSA apparatus
- test cycling behavior of multi-bed PSA apparatus with CO_2-N_2 using 3 mm zeolite beads
- validate DAPS with results from bench scale PSA systems utilizing zeolite beads and zeolite coated Catacel cores
- measure pressure drop through zeolite coated Catacel cores
- characterize thermodynamic and mass transfer properties of zeolite coated Catacel cores and refine PSA cycle schedule via modeling with DAPS
- study adsorbent (zeolite crystals and silica gel) stability in presence of trace levels of NO_x and SO_2
- validate 1-D, 2-D and 3-D CFD models by comparison to DAPS
- investigate friction factor and mass transfer assumptions during dynamic adsorption and desorption to refine 1-D models
- use 1-D models to optimize Catacel channel shape

Budget

Project Team Member	Budget Period 1		Budget Period 2		Budget Period 3		Total
	Gov. Share	Cost Share	Gov. Share	Cost Share	Gov. Share	Cost Share	
Grace	139441	34860	75084	18772	145089	36272	449518
USC	670000	167500	490000	122500	490000	122500	2062500
Battelle	239115	59978	191791	47930	159744	39998	738556
Catacel	125592	31398	172187	43047	100662	25166	498052
TOTAL	1174148	293736	929062	232249	895495	223936	3748626

Breakdown in % of Total Budget

USC	55.0%
Battelle	19.7%
Catacel	13.3%
Grace	12.0%

Acknowledgements

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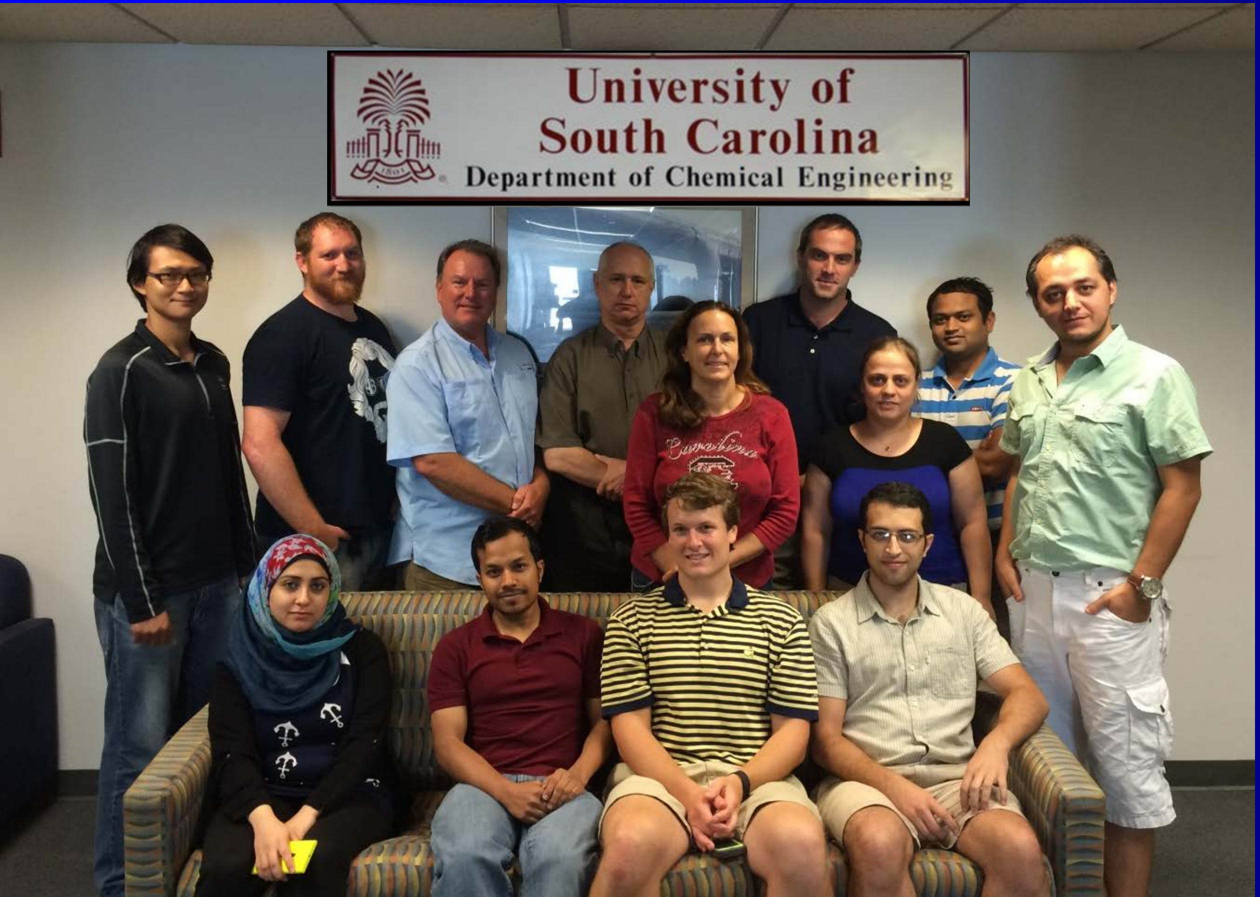
DOE/NETL and
SAGE is greatly appreciated!



Thank You!

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