Transformational Sorbent System for Post-Combustion Carbon Capture (DE-FE0031734)

Gökhan Alptekin, PhD
Ambal Jayaraman, PhD
Matthew Schaefer
Sarah Devoss
Ewa Muteba
Michael Ware
Nathan Roszel

Carbon Management/Oil and Gas Research Project Review Meeting Point Source Capture — Lab, Bench, and Pilot-Scale Research

August 17, 2021

TDA Research Inc. • Wheat Ridge, CO 80033 • www.tda.com

Project Objective

- **Objective is to develop a transformational metal-organic framework (MOF) based sorbent system that can:**
  - Capture more than 90% of CO_2 emissions from a coal power plant
  - Recover CO_2 at 95% purity
  - Cost of electricity at least 30% lower than amine based capture systems with the capture cost less that $30 per tonne of CO_2
- **TDA will develop a highly stable high capacity physical adsorbent to remove CO_2 from the flue gas using a novel adsorption cycle scheme**
- **Main Project Tasks**

BP1	**- Demonstrate sorbent performance in lab scale**
	- Assess impact of flue gas contaminants (SO_2, NOx, HCl)
	- Develop adsorption cycle sequence
	- Preliminary Techno-economic analysis (TEA)
BP2	**- Scale-up sorbent production**
	- Complete Life Tests
	- Optimize adsorption cycles and update TEA
BP3	**- Complete field tests (6 months duration)**
	- High Fidelity TEA and EH&S assessment

TDA RESEARCH

Project Team

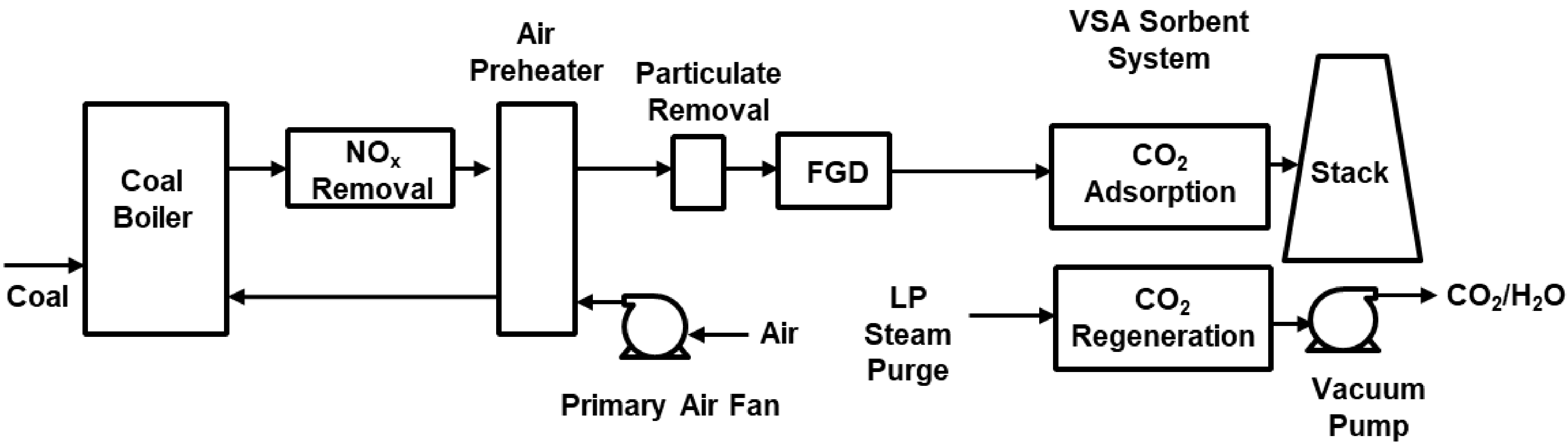
<u>Overall Project Duration</u>

- **Start Date = June 1, 2019**
- **End Date = May 31, 2022**

<u>Budget</u>

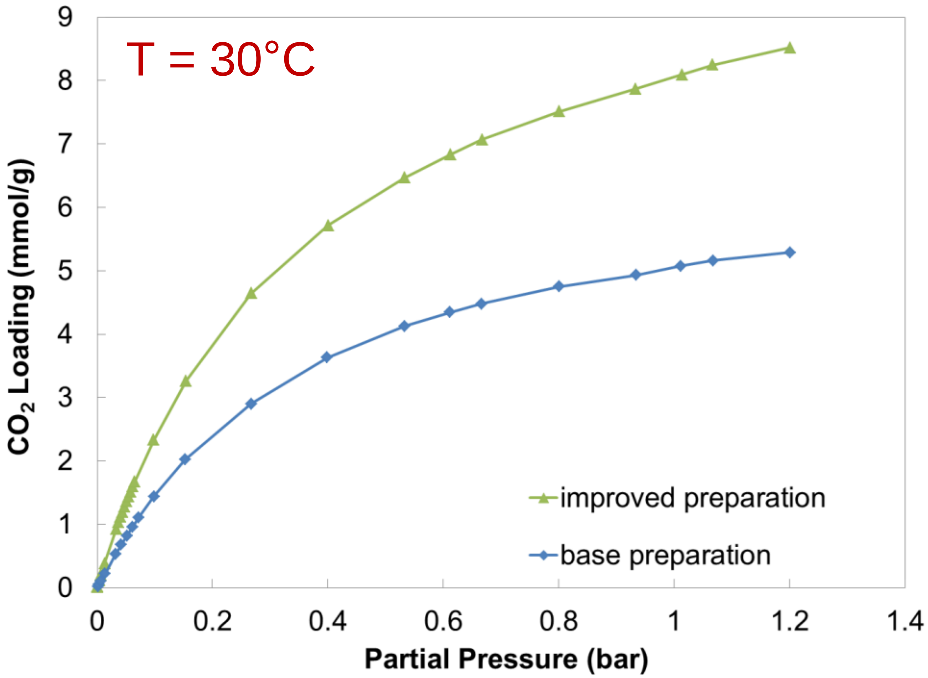
- **Project Cost = $3,750,000**
- **DOE Share = $3,000,000**
- **TDA and its partners = $750,000**

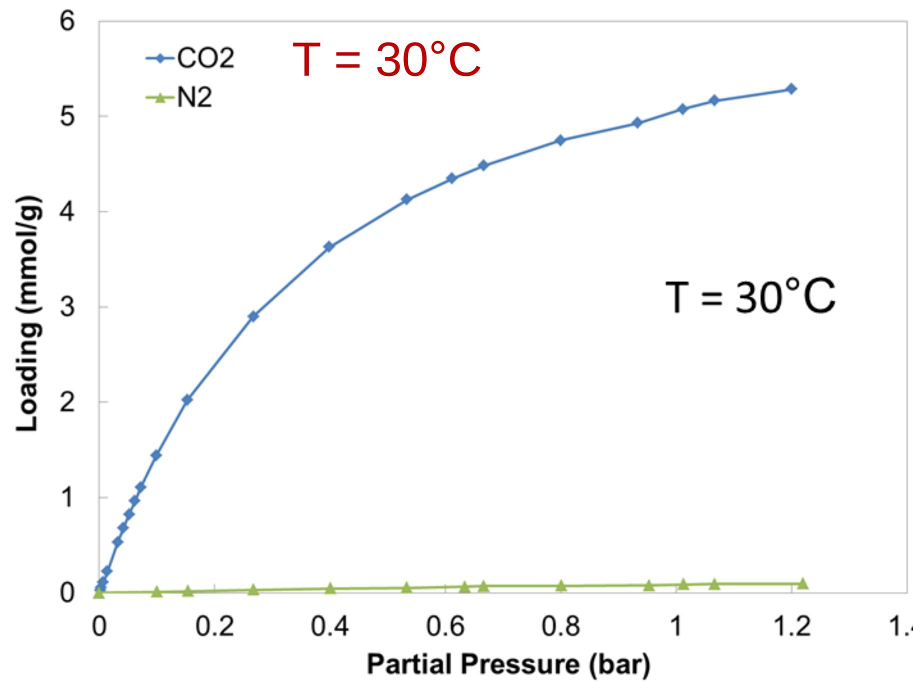
Process Schematic



- **Sorbent operates between 30-50°C under vacuum, (0.2-0.3 atm) with steam purge removes ≈99% of CO_2 (requires more steam purge than Case 1)**
  - Low pressure drop, reduced parasitic load
  - High CO_2 selectivity resulting in greater than 95% CO_2 purity
- **Similar technology can also be applied to NGCC applications, with higher steam purge/energy penalty**

TDA's MOF Sorbent

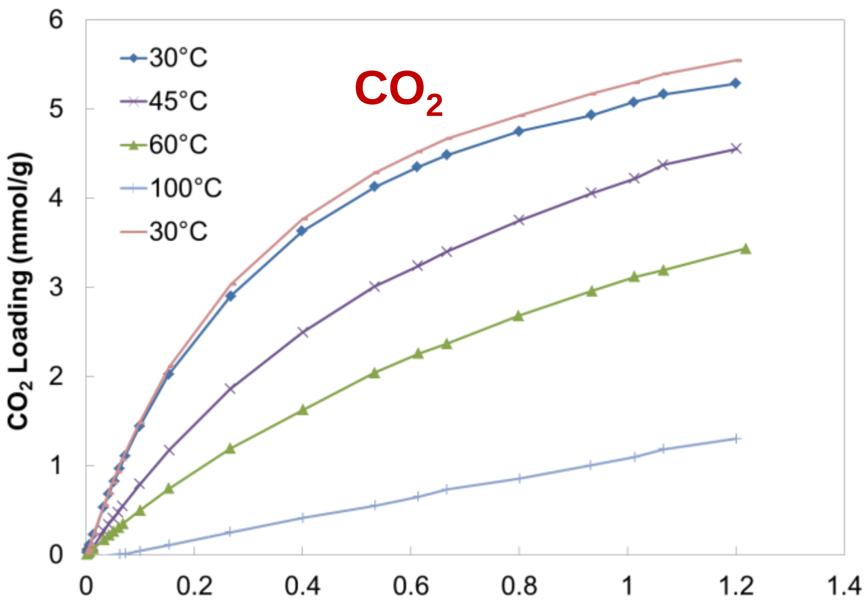


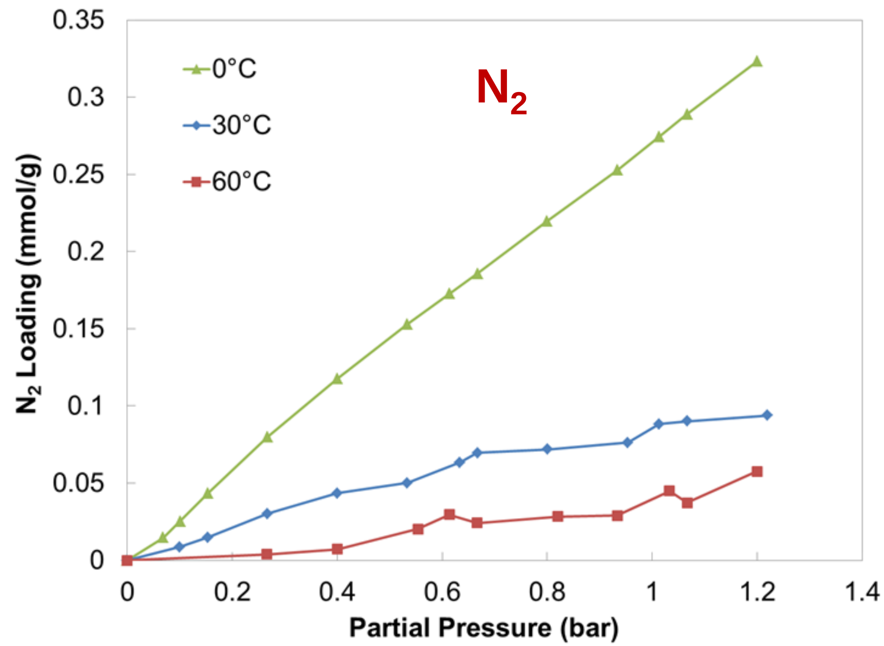


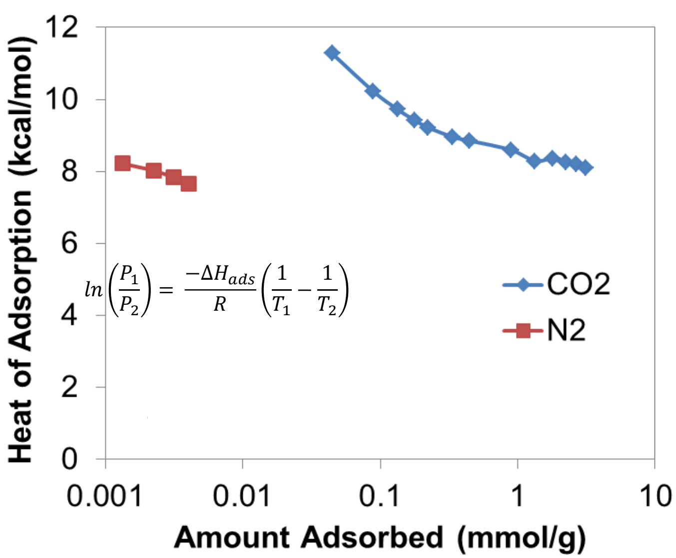
Physical Parameter	Units	TDA's MOF Adsorbent	
		Base preparation	Improved preparation
BET Surface Area	m^2/g	200.8	526.6
Langmuir Surface Area	m^2/g	246.4	618.2
Nanoparticle Size	nm	29.9	113.9
Pore Volume	cm^3/g	0.134	0.342
Median Pore Width	Å	17.0	14.4

TDA MOF	Selectivity
P_{CO2} (bar)	CO_2/N_2
0.05	9.32
0.1	16.29
0.15	22.92
1	57.52

Heat of Adsorption

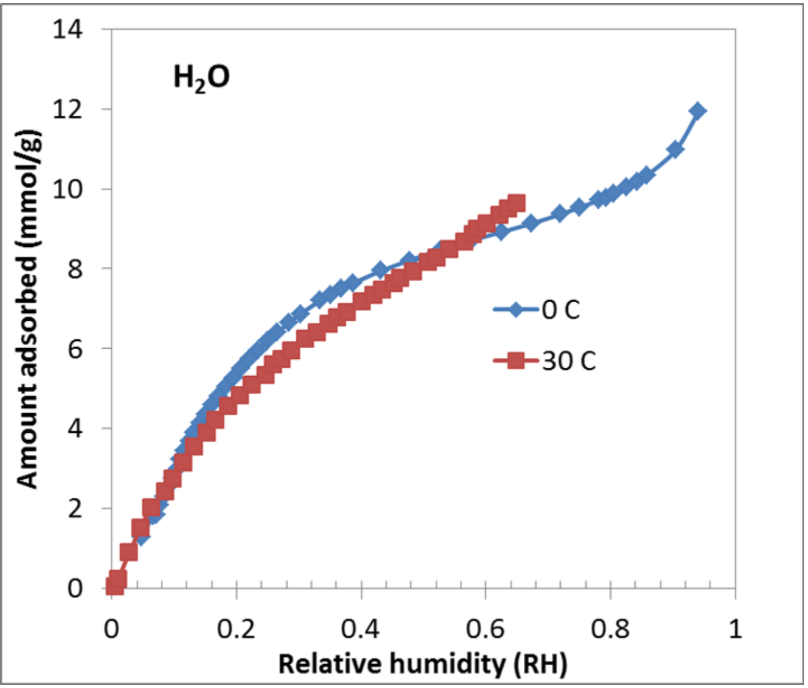


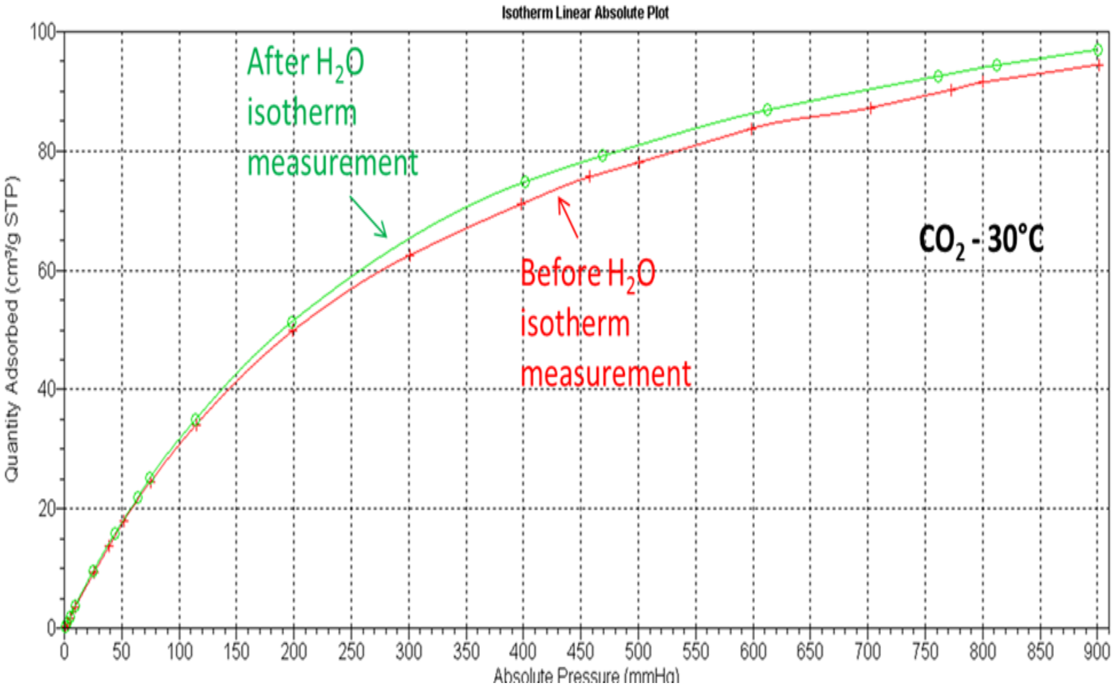




- Heat of adsorption of CO_2 has strong dependence on surface coverage (11 kcal/mol at low surface coverage and 8 kcal/mol at higher coverages)
- Heat of adsorption for N_2 is 8 kcal/mol and had very minimal changes due to surface coverage

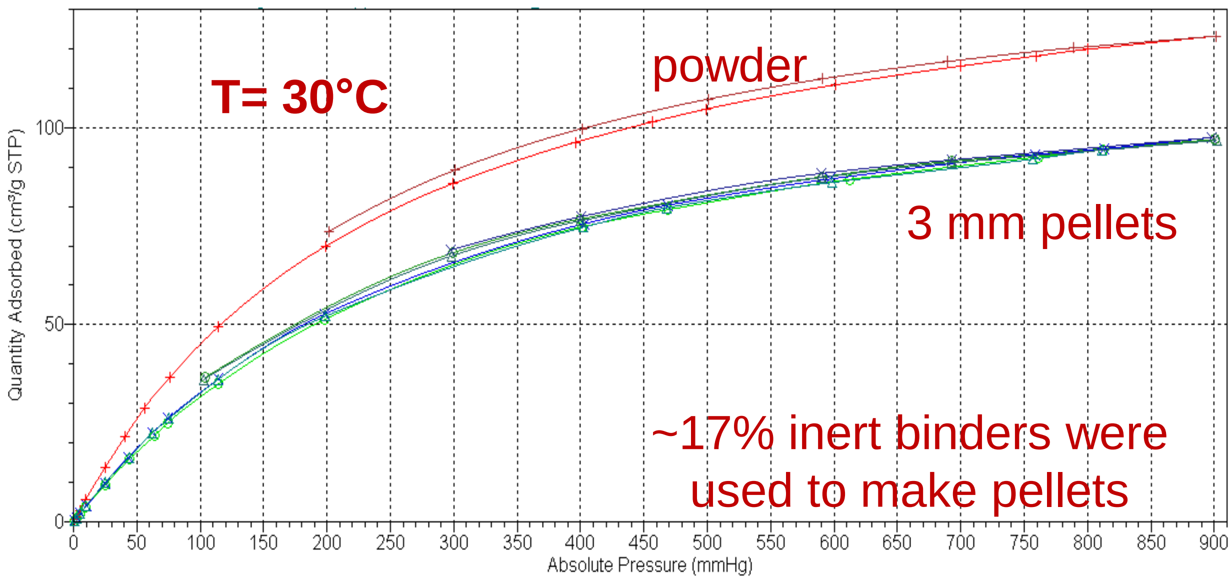
Water Adsorption Isotherms





- Low pressure water isotherms are linear indicating that water easily desorbs from the sorbent surface
- No change in low pressure isotherm before and after water isotherm measurements

Pelletization of the MOF Sorbent



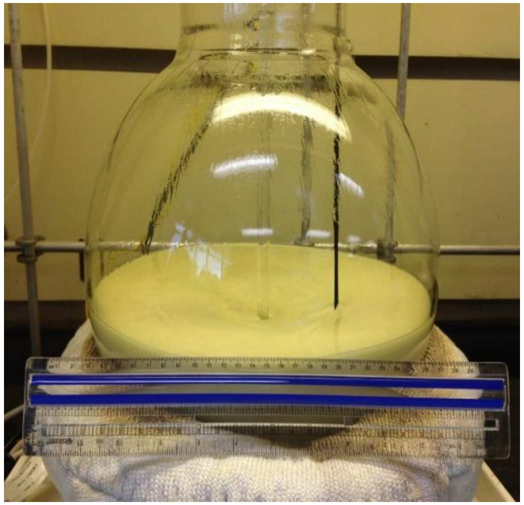
Powder Material

Pelletized Materials

Pelletized sorbent retained >95% of their capacity when normalized based on active MOF weight

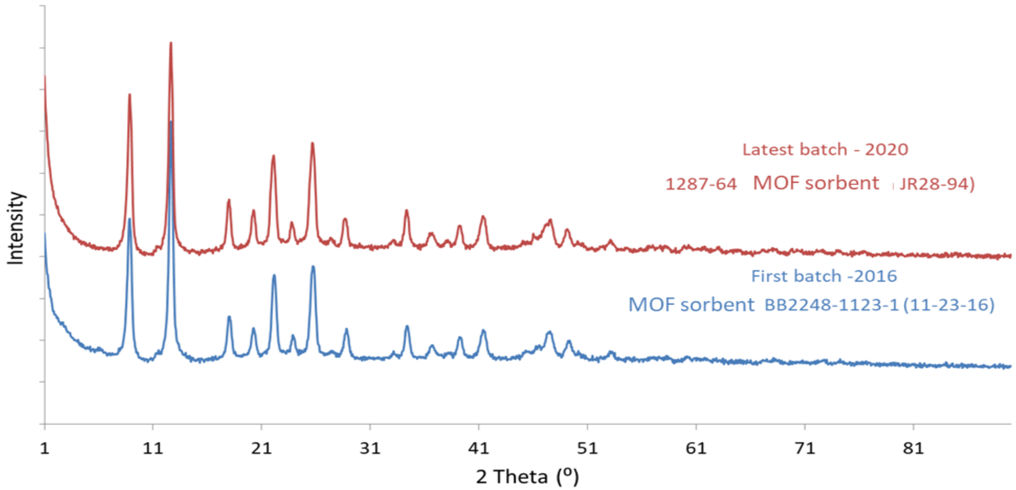
Physical Parameter	Units	SIFSIX-2-TDA MOF 2016 base preparation	SIFSIX-2-TDA MOF 2020 improved preparation
BET Surface Area	m^2/g	200.8	526.6
Langmuir Surface Area	m^2/g	246.4	618.2
Nanoparticle Size	nm	29.9	113.9
Pore Volume	cm^3/g	0.134	0.342
Median Pore Width	Å	17.0	14.4

MOF Scale-up: Bench Scale – Complete



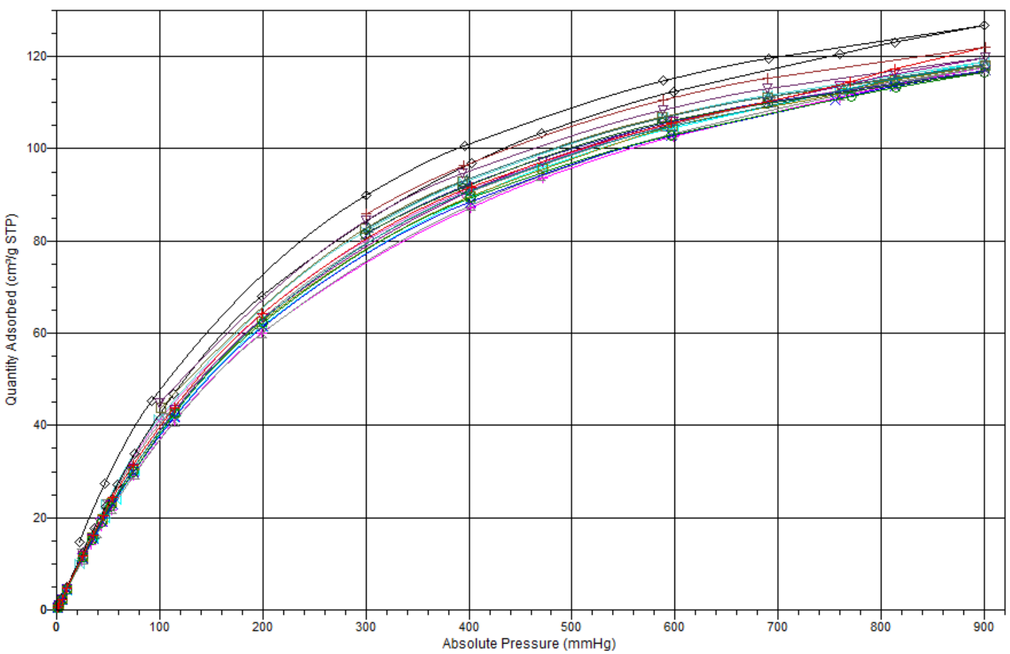
- **Scale-up from 1L to 22L flask and to 180L Hastelloy reactor in BP2**
- **BP1 evaluations have focused on improving synthesis parameters and space-time yields while conserving raw materials**
    - Synthesis improvements have produced space yield improvements of 10-15X, and time yield improvements of 5-8X
- **The reactor is equipped to perform MOF synthesis, Filtration/Rinsing, Drying/Devolatilization all sequentially in the same reactor**
- **A classified area is designed and built to handle the equipment and solvents required for MOF processing**

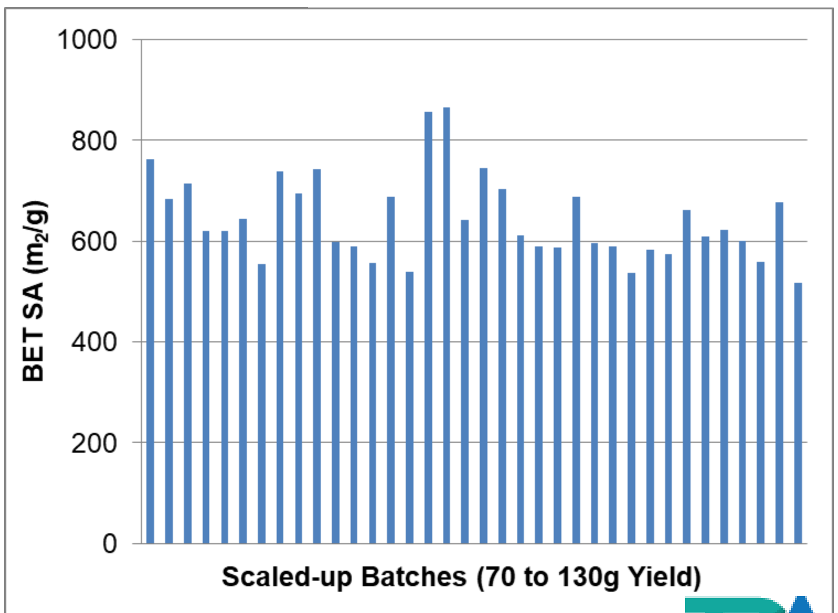
Synthesis Variation: Scale Up Batches



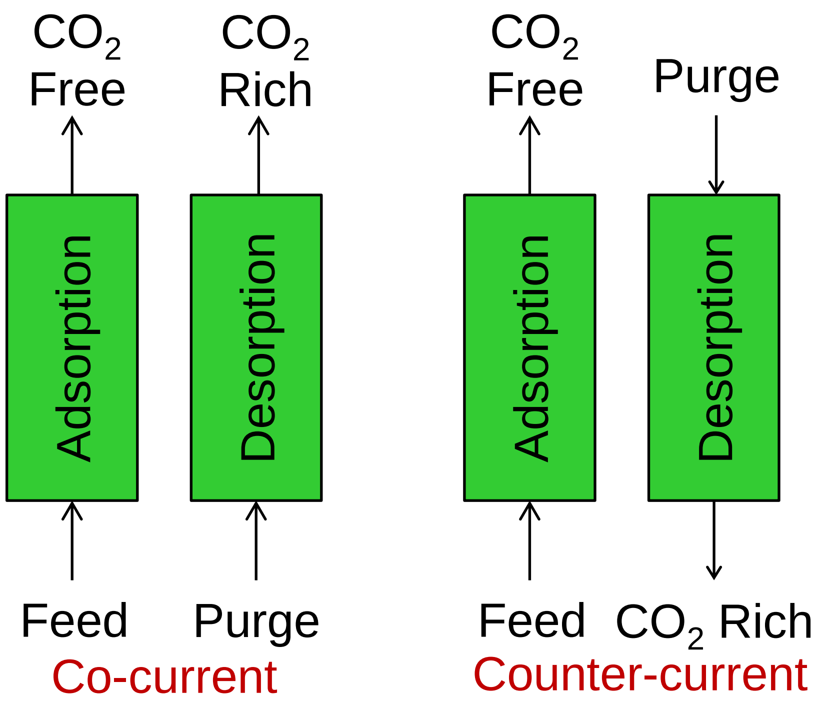
Minimal batch to batch variations

		Wt% Loading
		CO2 Pressure (torr)
Description	**Test**	**122**
1334-10	CO2@30C	8.98
1334-8	CO2@30C	8.69
1334-15	CO2@30C	8.54
1334-9	CO2@30C	8.78
1334-7	CO2@30C	8.81
1334-3	CO2 @30C	8.73
1287-99	CO2@30C	9.59
1287-100	CO2 @30C	8.34
1287-98	CO2 @30C	8.56
1287-96	CO2 @30C	8.36





Fixed Bed Adsorption Tests



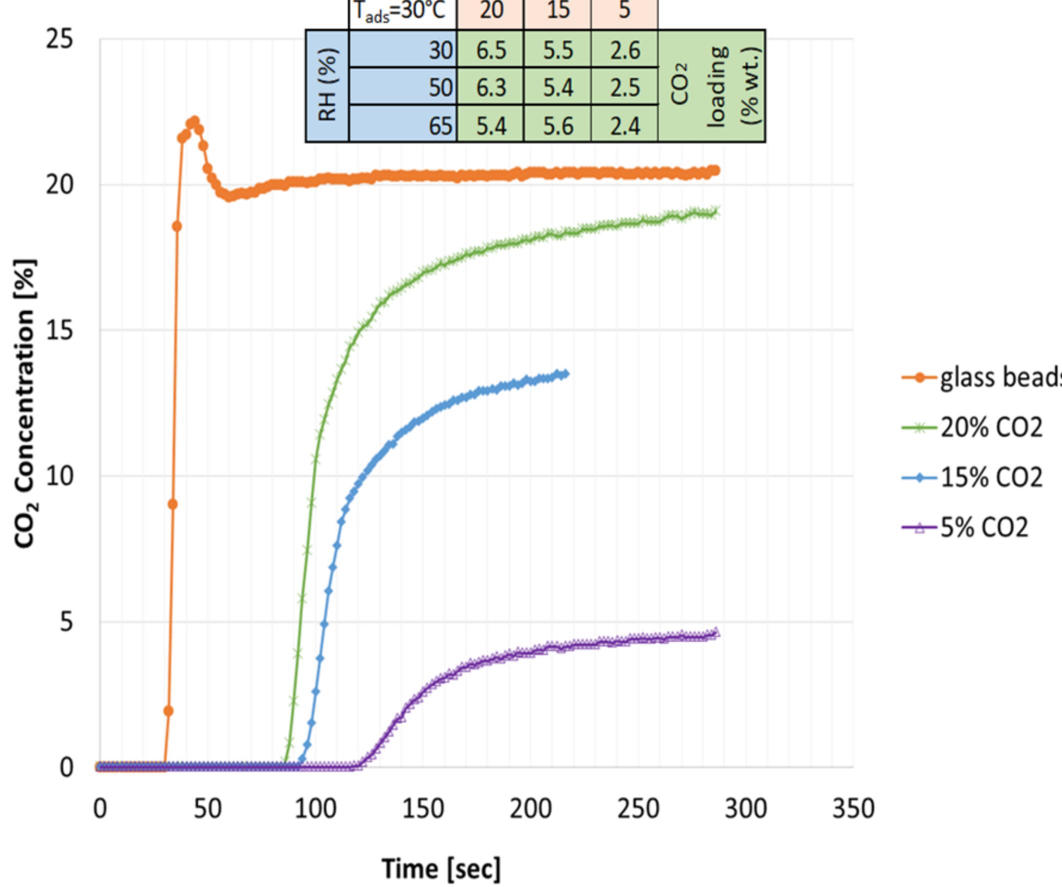
- **TDA employed multiple fixed-bed adsorption system to carry out adsorption breakthrough and adsorption/desorption cycle tests**
  - Adsorption Breakthrough Tests
  - Counter current adsorption/ desorption cycles
  - Cycle Tests in the presence of contaminants (NOx, SOx)

TDA MOF Performance

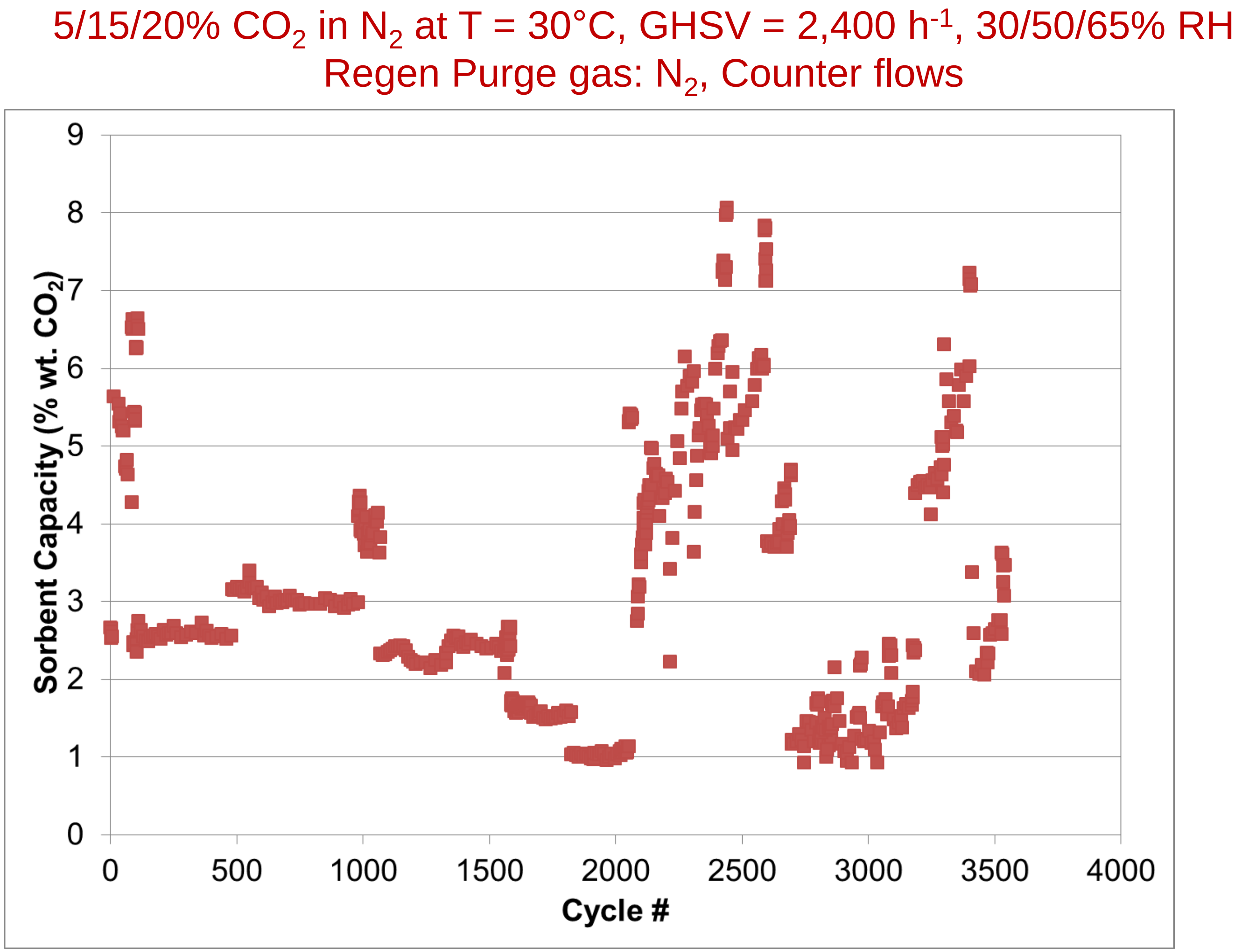
5/15/20% CO_2 in N_2 at T = 30°C, GHSV = 2,400 h^{-1}, 30/50/65% RH
Regen Purge gas: N_2, Counter flows

- We demonstrated a high working capacity in excess of 5% wt. CO_2 at ~15% vol. CO_2
- ~2.5% wt. CO_2 at 4% vol. CO_2
- We also showed that the temperature and humidity levels have limited impact on sorbent's working capacity
- Higher temperatures resulted in lower working capacity
- No significant impact in the presence of humidity up to 65%
- Higher temperatures resulted in lower working capacity

	T_{ads}=30°C	Fluegas CO2 (%)			
		20	15	5	
RH (%)	30	6.5	5.5	2.6	CO2 loading (% wt.)
	50	6.3	5.4	2.5	
	65	5.4	5.6	2.4	



Life Tests

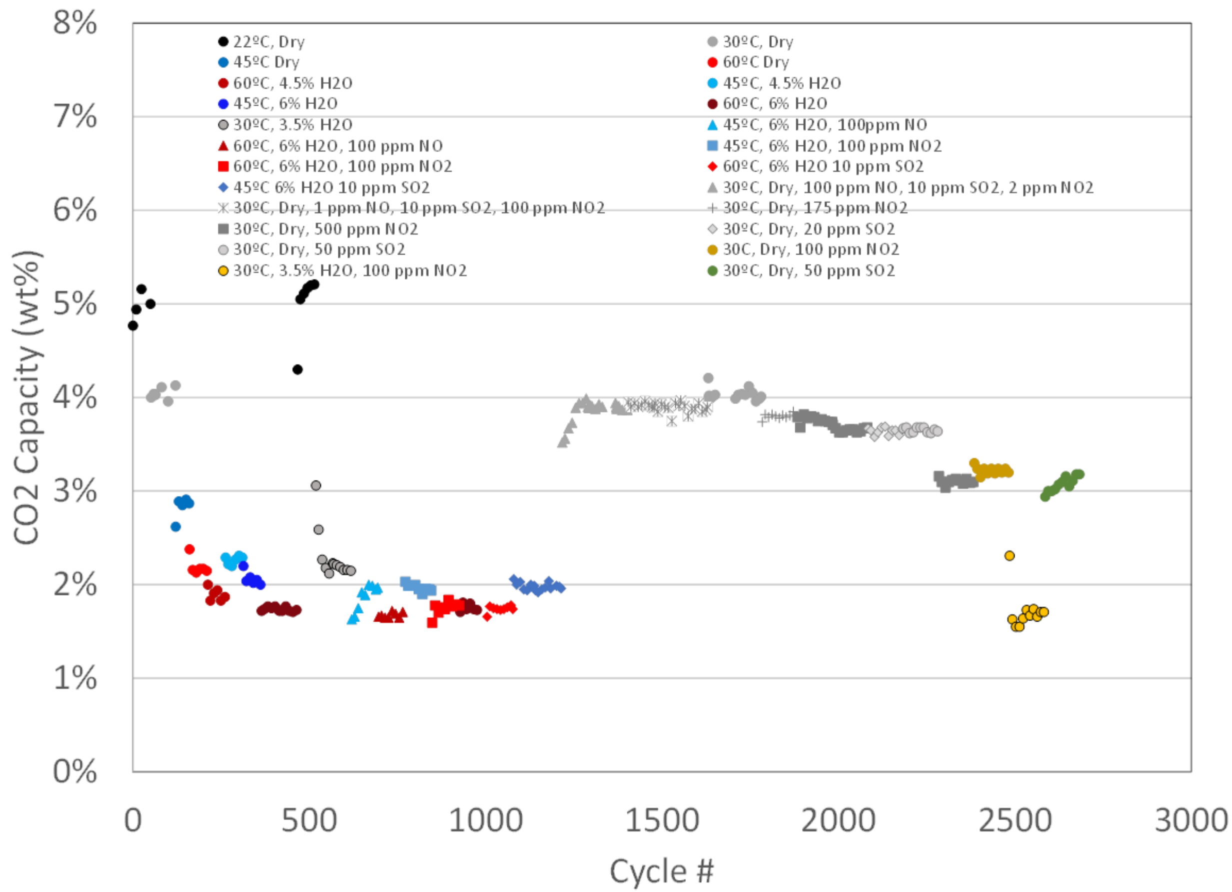


- **A stable working capacity was demonstrated in counter flow desorption**

Life Tests in Presence of Contaminants

- We demonstrated stable working capacity in the presence of flue gas contaminants such as humidity, NOx and SOx
- Up to 65% RH, 500 ppm NOx, 50 ppm SOx
- Maximum ~ 20% drop in capacity under high SOx and NOx concentrations

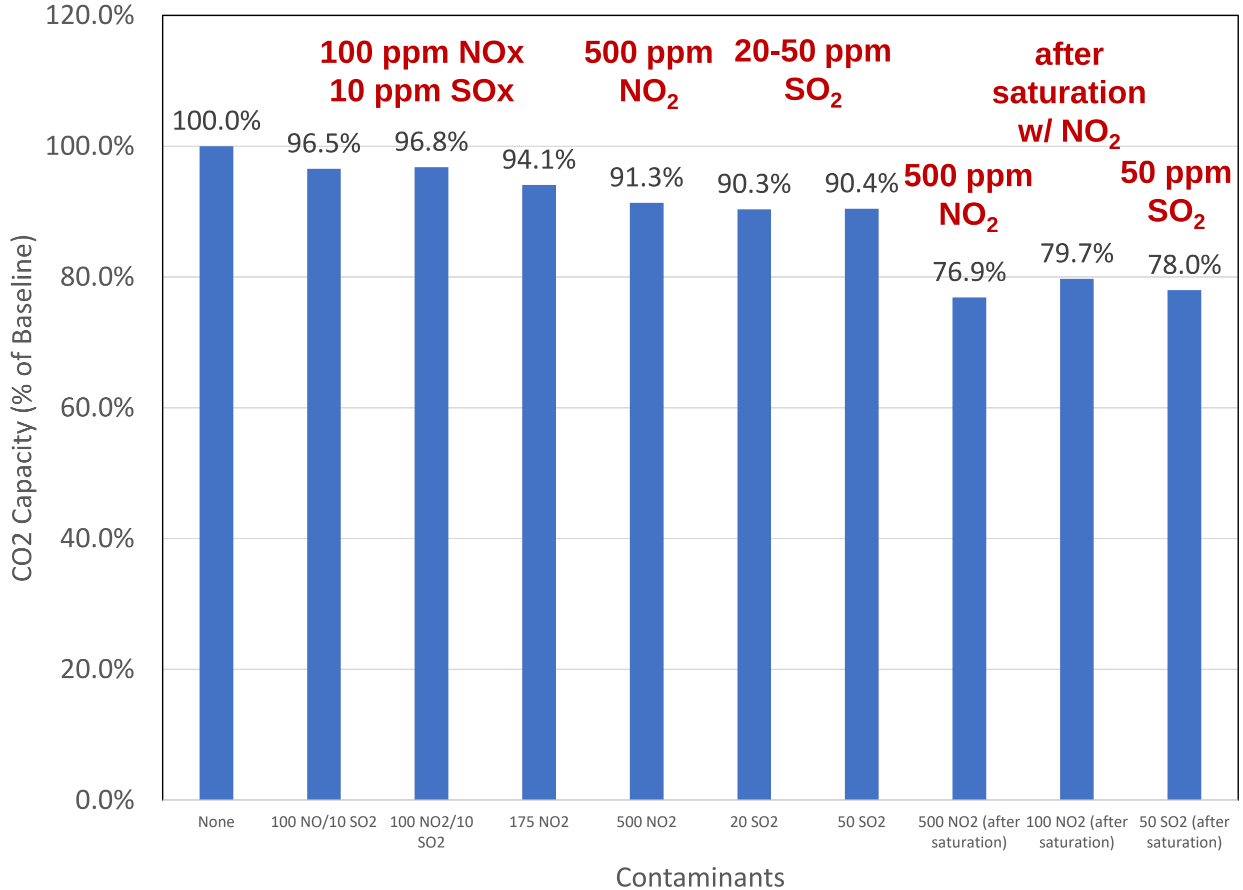
15% CO_2 in N_2 at T = 30/45/60°C, GHSV = 1,000 h^{-1}, 0-6% H_2O
Regen Purge gas: N_2, Counter flows



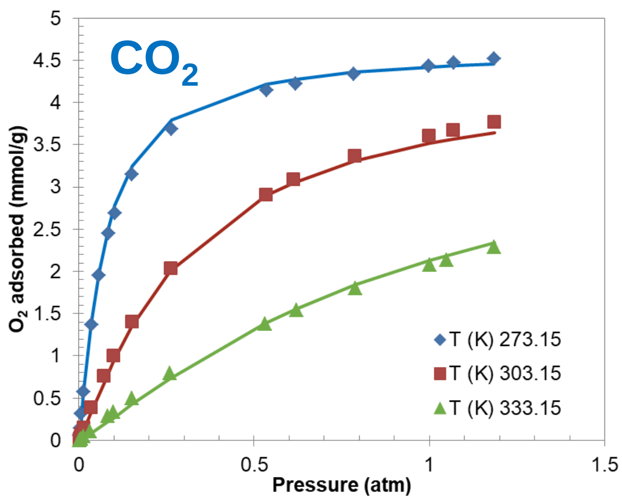
Impact of Contaminants

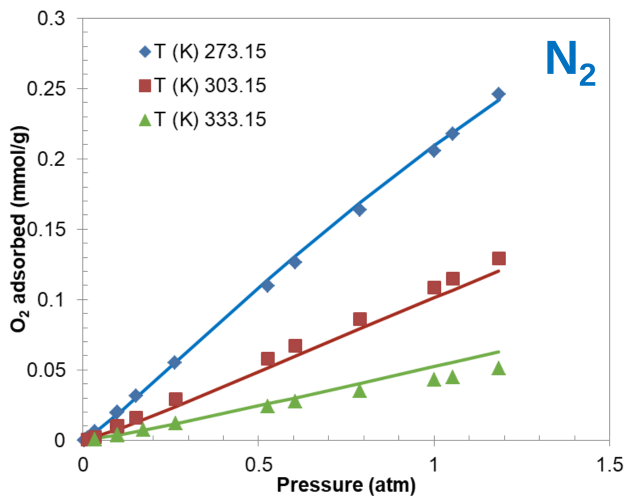
- We observed <5% drop in working capacity at 100 ppm NOx and 10 ppm SOx
- At 500 ppm NOx and 50 ppm SOx the working capacity dropped by 10%
- After saturating the sorbent with 500 ppm NOx or 50 ppm SOx the sorbent working capacity dropped by ~ 20%

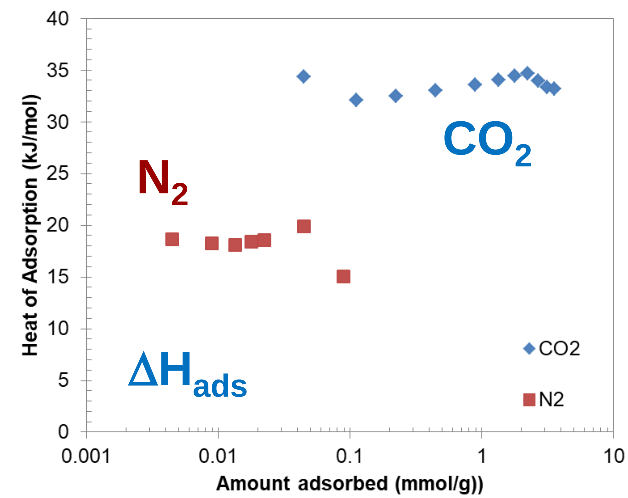
15% CO_2 in N_2 at T = 30/45/60°C, GHSV = 1,000 h^{-1}, 0-6% H_2O
Regen Purge gas: N_2, Counter flows

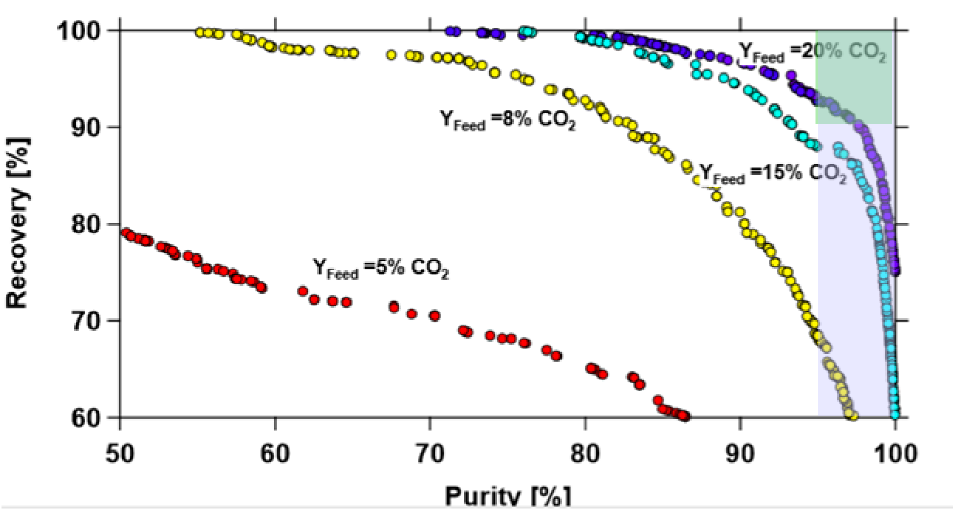


Adsorption Cycle Modeling









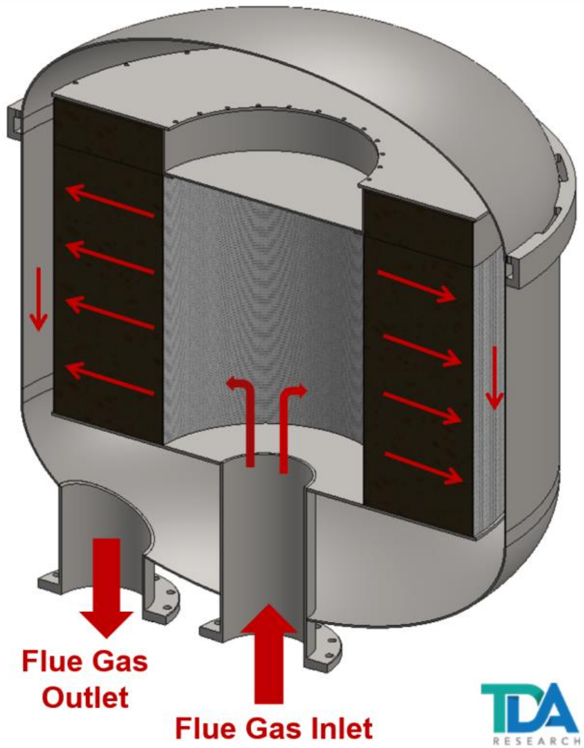
- Initial modeling results from University of Alberta shows we are able to use simple cycle schemes without addition of steam purge is shown
- When having a more advanced cycle schemes with steam assisted VSA we can achieve 95% CO_2 purity with a CO_2 levels in flue gas as low as 8%

Process Simulation

CASE NO.	UNITs	DoE 11	DoE 12	Case 1B	Case 2	Case 3
CO_2 capture technology		**No Capture**	**Amine**	**Recirculation - regen@ 0.2 bar Steam purge**	**Recirculation - regen@ 0.1 bar NO Steam Purge**	**No Recirculation - regen@ 0.2 bar Steam Purge**
Steam turbine power	kWe	580,400	662,800	709,618	709,805	677,749
Total auxiliary consumption	kWe	30,410	112,830	159,618	159,805	127,749
Net power output	**kWe**	**549,990**	**549,970**	**550,000**	**550,000**	**550,000**
Auxiliary load summary						
Flue gas booster + CO_2 removal	kWe	0	20,600	11,958	11,798	8,552
VSA Vacuum pump	kWe	0	0	53,829	54,876	32,524
CO_2 compression	kWe	0	44,890	48,877	48,205	45,842
CO_2 cryogenic purification	kWe	0	0	0	0	0
Common Auxiliaries	kWe	30,410	47,340	45,588	44,907	40,832
% Net plant efficiency	**% HHV**	**39.3**	**28.4**	**30.52**	**30.94**	**32.66**
Net heat rate	kJ/kWh	9,165	12,663	11,794	11,636	11,062
Condenser cooling duty	10^6 kJ/h	2,298	1,737	2,774	2,879	2,534
Consumables						
Thermal input , Coal	kWt HHV	1,400,162	1,934,519	1,801,849	1,777,736	1,684,206
Carbon captured	**%**	**0**	**90**	**90**	**0**	**90**
Energy for carbon capture	kWh/tonne		305	216	201	140
including compression	kWh/tonne		388	313	299	237

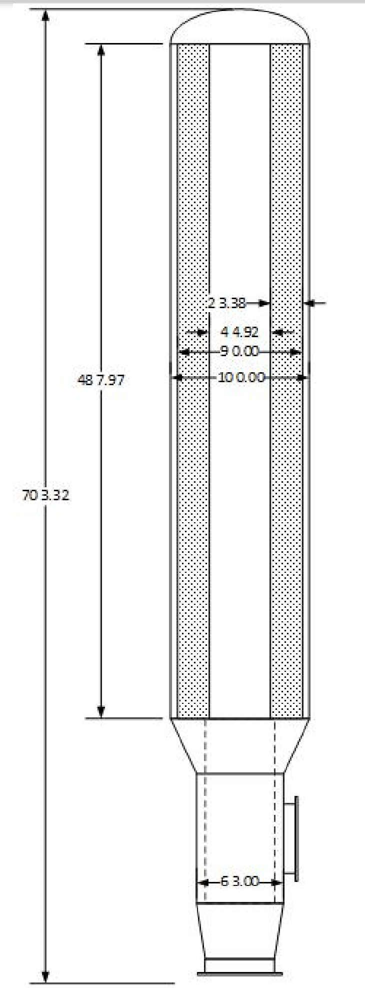
- Energy for CO_2 capture is 54.2% lower for TDA's sorbent based CO_2 capture systems than amine scrubbing

Reactor Vessel Design and Costing



ΔP=105 mbar

Module Size	137.5 MW
No. of trains	4
No. of bed per train	4
Total no. of beds	16
Flue gas flow	161.2 m^3/s
CO_2 flow	4.5 tonne/min
Capacity	7.0% wt. CO_2
Bed online	1 min
Sorbent needed	64.0 tonne
density	0.55 $tonne/m^3$
Bed vol.	116.4 m^3
Bed CSA	11.4 m^2



SORBENT VESSEL DIMENSIONS

- Four radial beds per train (total of 16 beds)
- SA516-70 carbon steel, 0.5” thickness
- 120 in OD x 565 in T/T
- Cost per bed $587,504 FOB
- Total reactor cost $9,400,068

Reactor Vessel Design and Costing

Sorbent Only System

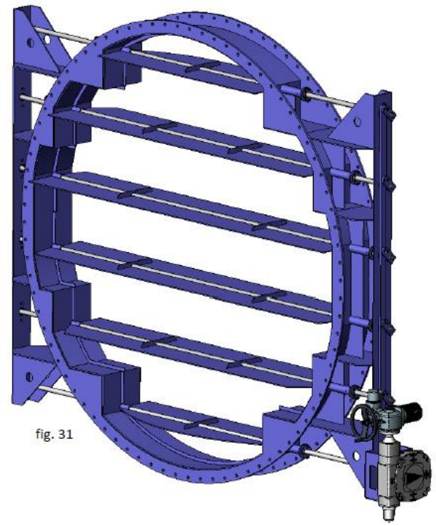
	Stage I		Stage II		Stage III		Stage IV	
Bed 1								
Bed 2								
Bed 3								
Bed 4								
336s	21s	21s	21s	21s	21s	21s	21s	21s

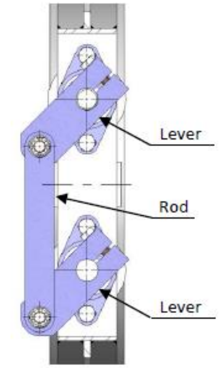
Adsorption - Flue gas flow

Cocurrent Blowdown

Desorption - CO2 Product Out

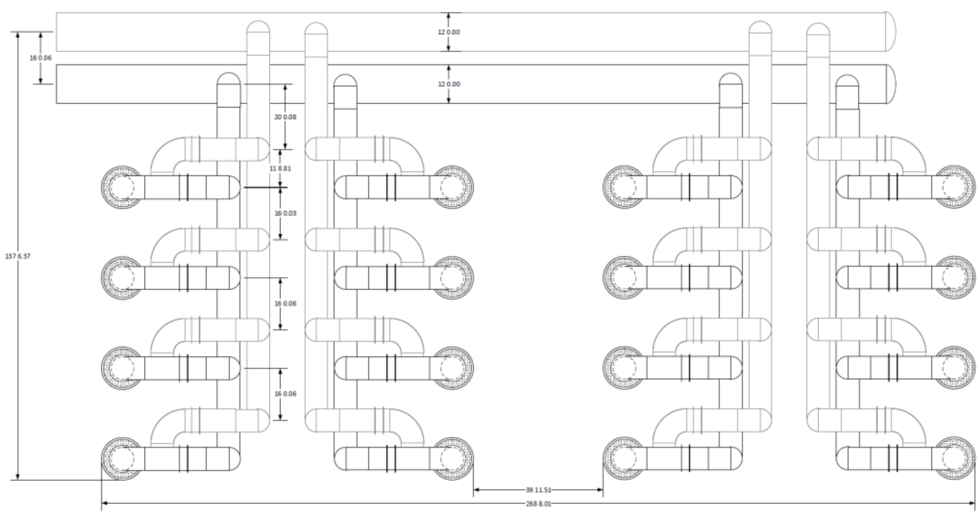
Desorption - Air Purge flow





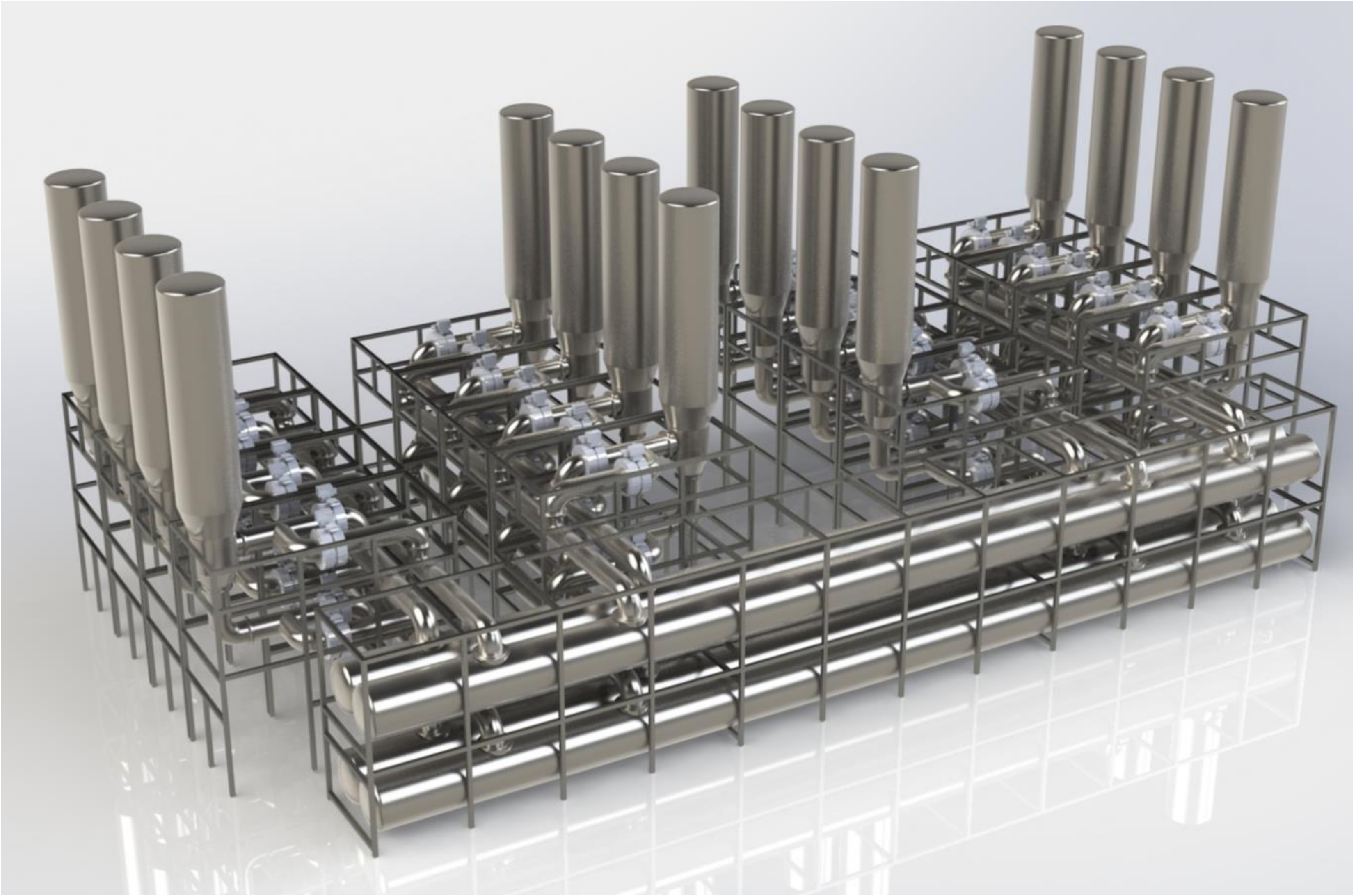
LR series damper valves

Price basis is 72” size

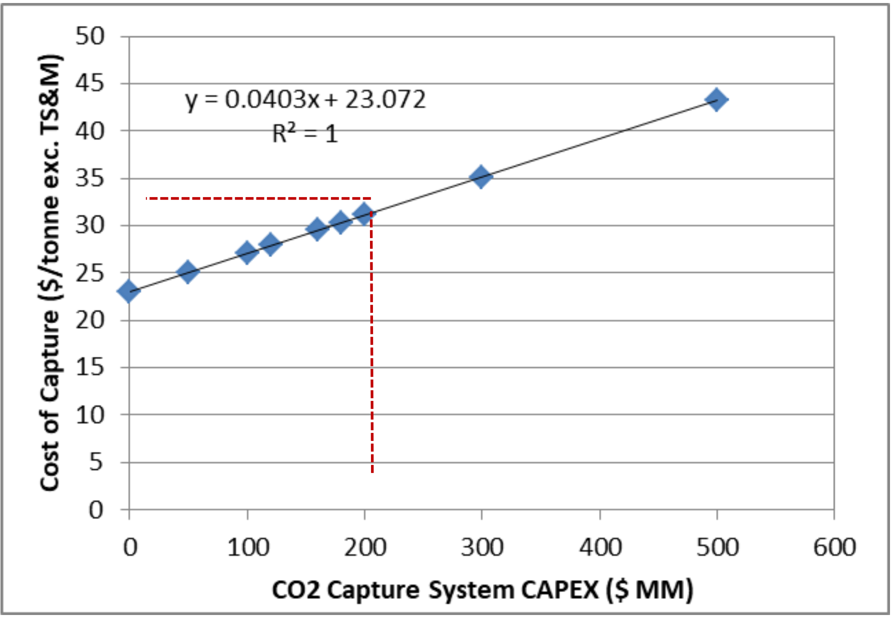


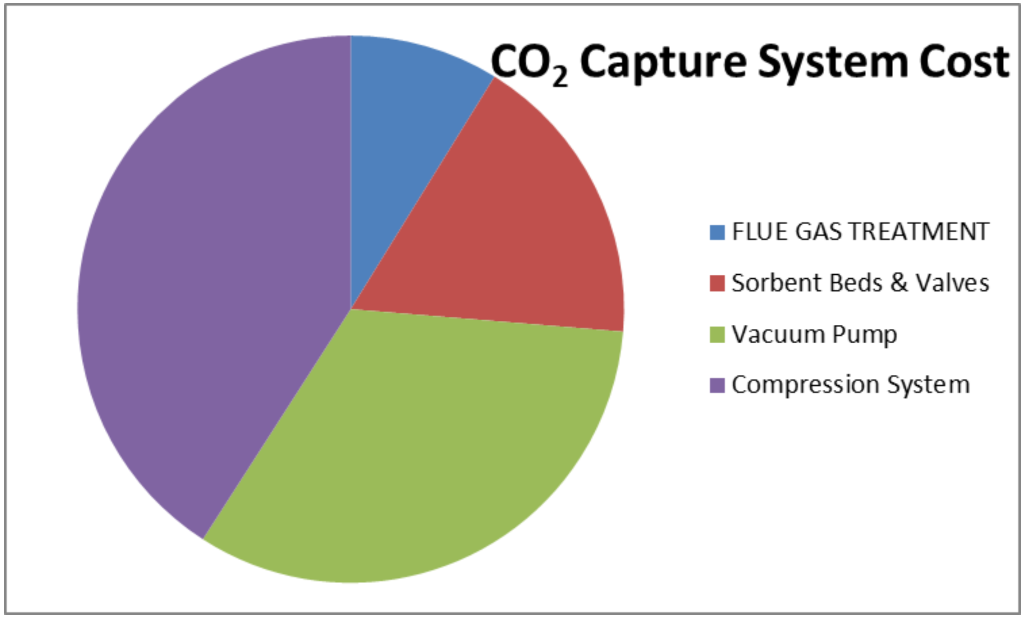
- Rapidly actuating valves are identified to change the bed position in a few seconds
- 60 in NPS, 0.375 in thickness (standard schedule) process piping for flue gas and air regeneration lines
- Two (2) 12 ft OD flue gas distribution and return manifolds)
- 2,000 linear feet, estimated from concept layout

3-D Layout of the Sorbent System



Sorbent Only Steam Purge - CAPEX





- Total cost of CO_2 Capture System including flue gas treatment is \$207.8 MM (\$378/kW)
  - Cost of CO_2 capture ~\$37/tonne
  - This meets DOE's current target of < \$40/tonne at <\$450 MM
- CAPEX for CO_2 capture needs to go below \$180 MM to meet transformational CO_2 capture targets (<\$30/tonne)

Cost of Capture Summary

CASE NO.	DOE Case 12	TDA Case 1B	TDA Case 2	TDA Case 3
CO_2 CAPTURE TECHNOLOGY	Reference Amine	CO_2 recirculation VSA: Regen at 0.2 bar & BFW Heating	CO_2 recirculation VSA: Dry Regen at 0.1 bar	NO CO_2 recirculation VSA: Regen at 0.2 bar VLP Steam
CO_2 Recirculation	-	yes	yes	-
VLP Steam Purge	-	yes	no	yes
Net power, MW	550	550	550	550
Capacity factor (CF), %	85	85	85	85
Total plant cost (TPC)	1,959,399,000	1,555,700,000	1,549,006,000	1,478,373,800
Total Plant Cost, $/kW	**3,563**	**2,829**	**2,816**	**2,688**
1st year cost of electricity (COE) w/o CO_2 TS&M, $/MWh	137.3	114.8	113.8	109.0
1st year cost of electricity (COE), $/MWh	147.3	123.0	122.0	117.3
1st year CO_2 captured costs w/o TS&M, $/tonne	**56.41**	**36.97**	**36.42**	**30.67**

- The cost of CO_2 capture is considerably lower for sorbent only CO_2 capture systems: 34.5% (for Case 1B); 35.4% (for Case 2); 45.6% (Case 3)

- Cost of CO_2 capture for Sorbent only system with re-circulation of flue gas CO_2 is ~ 36.4/tonne while for a Sorbent only System with VLP steam purge is ~$30.7/tonne

TDA RESEARCH