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

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2022 Carbon Management Project Review Meeting

Capture from Power Generation

Lab/Bench-Scale Research

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Project Objective and Team

- **Objective is to develop a transformational sorbent based on a metal-organic framework (MOF)**
  - 90+% capture efficiency of CO_2
  - 95% purity recovered CO_2 purity
  - 30% lower costs than amine based systems with <$30 per tonne of CO_2
- **Main Project Tasks**

BP1	**- Demonstrate sorbent performance at the bench scale** **- Assess impact of flue gas contaminants (SO_2, NOx)** **- Develop cycle sequence** **- Preliminary TEA**
BP2	**- Scale-up sorbent production** **- Complete Life/Durability Tests** **- Optimize adsorption cycles and update TEA**
BP3	**- Slipstream field tests (6 months)** **- High Fidelity TEA and EH&S**

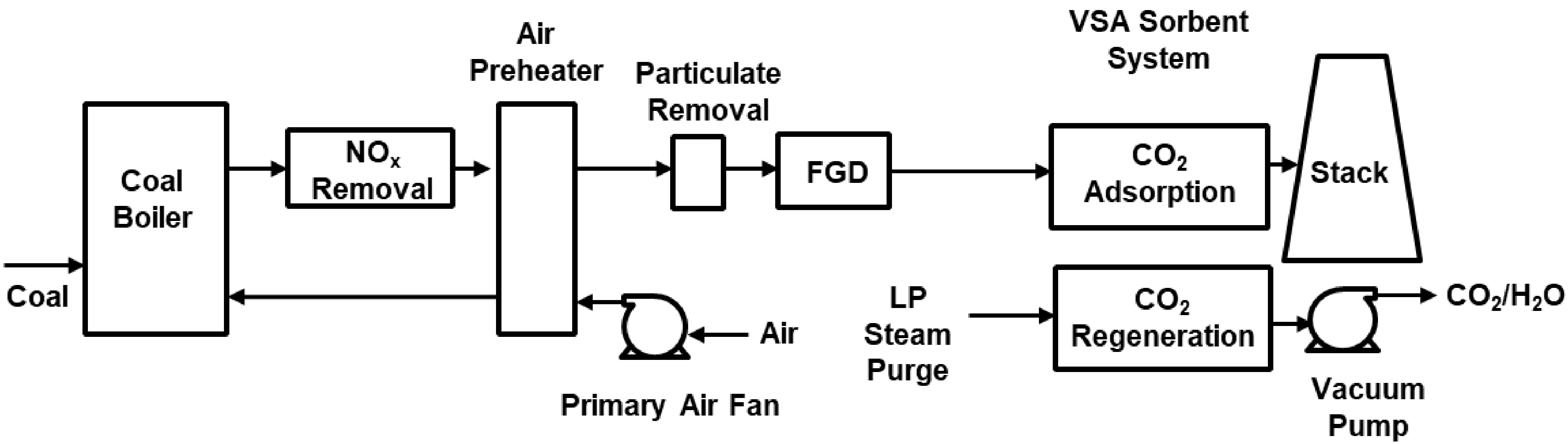
Overall Project Duration

- **Start Date = June 1, 2019**
- **End Date = May 31, 2024**

Budget

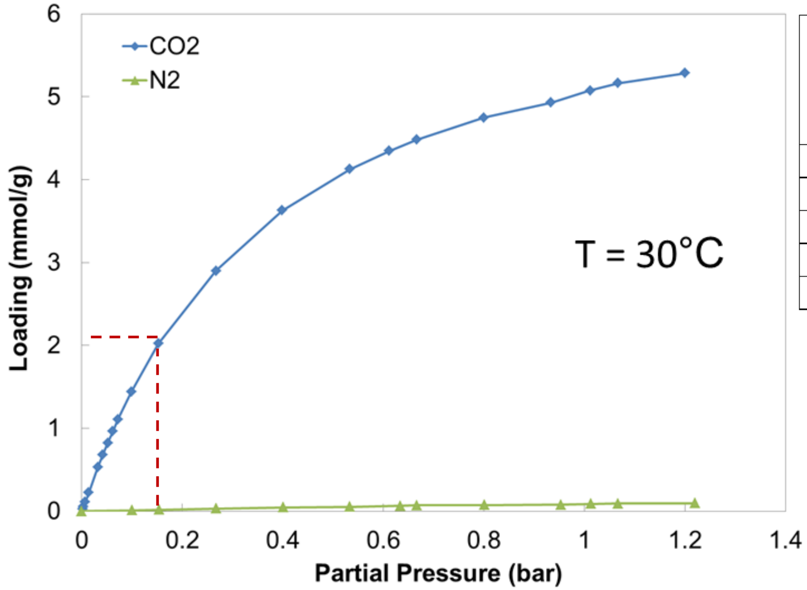
- **Project Cost = $3,750,000**
- **DOE Share = $3,000,000**
- **TDA and its partners = $750,000**

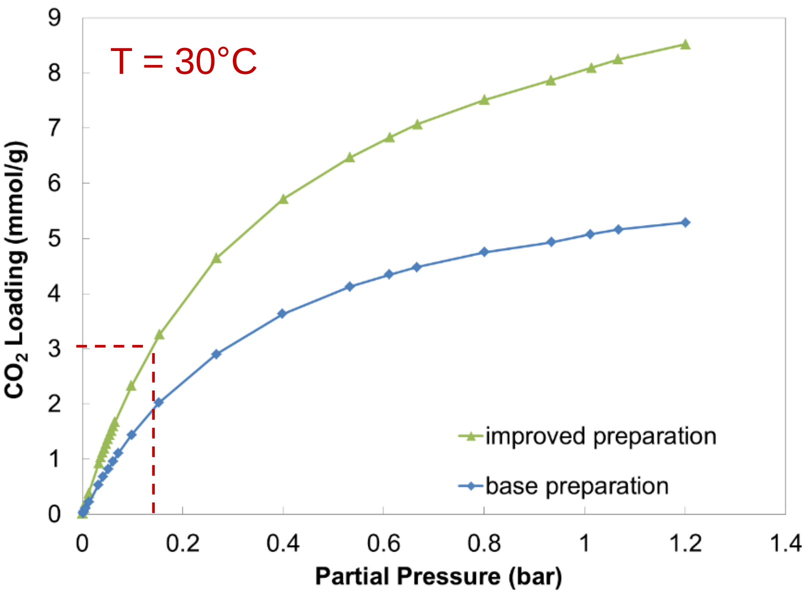
Process Schematic



- **Sorbent operates between 30-50ºC under vacuum (0.2-0.3 atm)**
  - Commercially available vacuum equipment
- **Capability to achieve 99% CO_2 removal efficiency**
- **High CO_2 selectivity results greater than 95% CO_2 product purity**
- **A new reactor design to ensure low pressure drop and reduced parasitic load**
- **Similar technology can also be applied to NGCC applications, with higher steam purge/energy penalty**

CO_2/N_2 Adsorption Isotherms



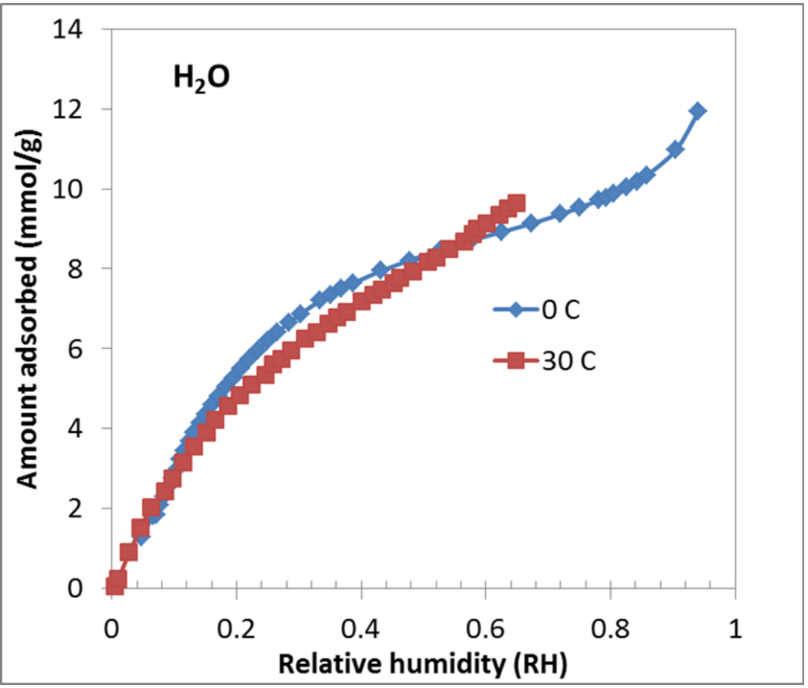


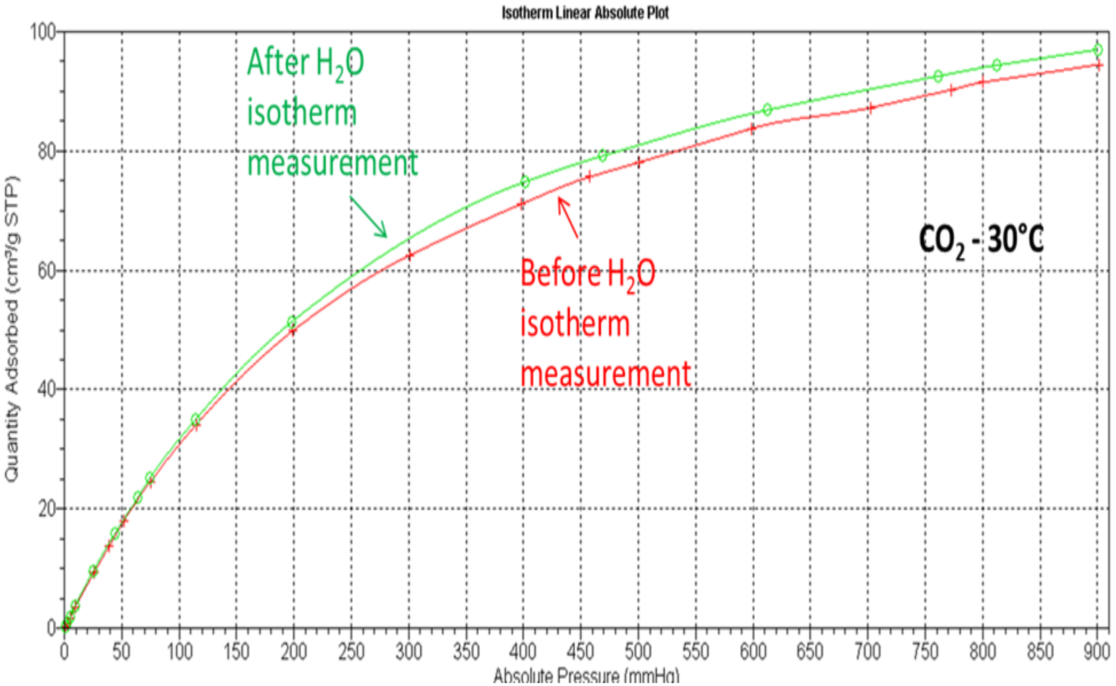
Physical Parameter	Units	TDA's MOF Adsorbent	
		Base preparation	Improved preparation
BET Surface Area	m^2/g	200.8	526.6
Langmuir Surface Area	m^2/g	246.4	618.2
Nanoparticle Size	nm	29.9	113.9
Pore Volume	cm^3/g	0.134	0.342
Median Pore Width	Å	17.0	14.4

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

- **High CO_2 uptake**
  - >2 mmol/g at 0.15 bar
  - ~3 mmol/g for the modified version
- **Very high selectivity towards CO_2 over N_2, which ensures a very high product purity**
  - Over 95% without any downstream purification needs
- **Heat of adsorption of CO_2 is measured as 11 kcal/mol at low surface coverage and 8 kcal/mol at higher coverages**
- **Improvements in linker synthesis results in very high CO_2 uptake**

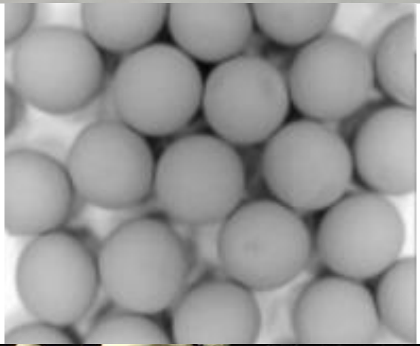
Water Adsorption Isotherms

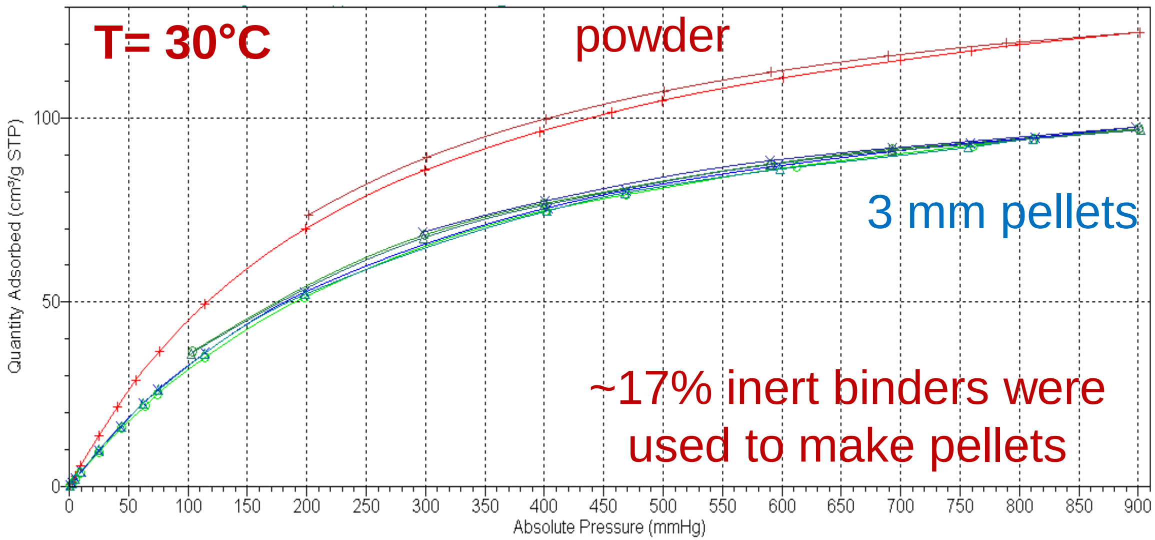




- **Low pressure water isotherms are linear indicating that water easily desorbs from the sorbent surface**
- **No change in low pressure isotherm before and after water isotherm measurements**

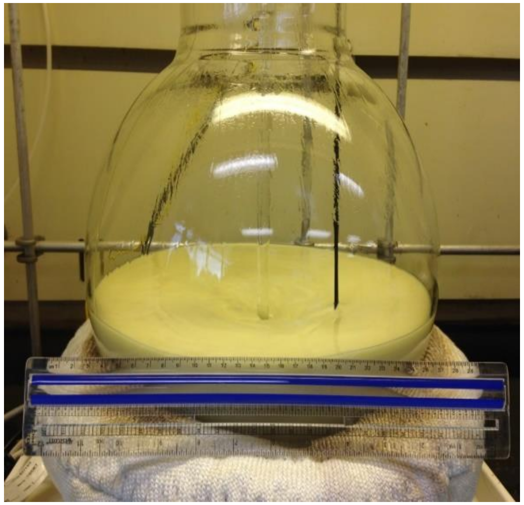
Pelletization of the MOF Sorbent





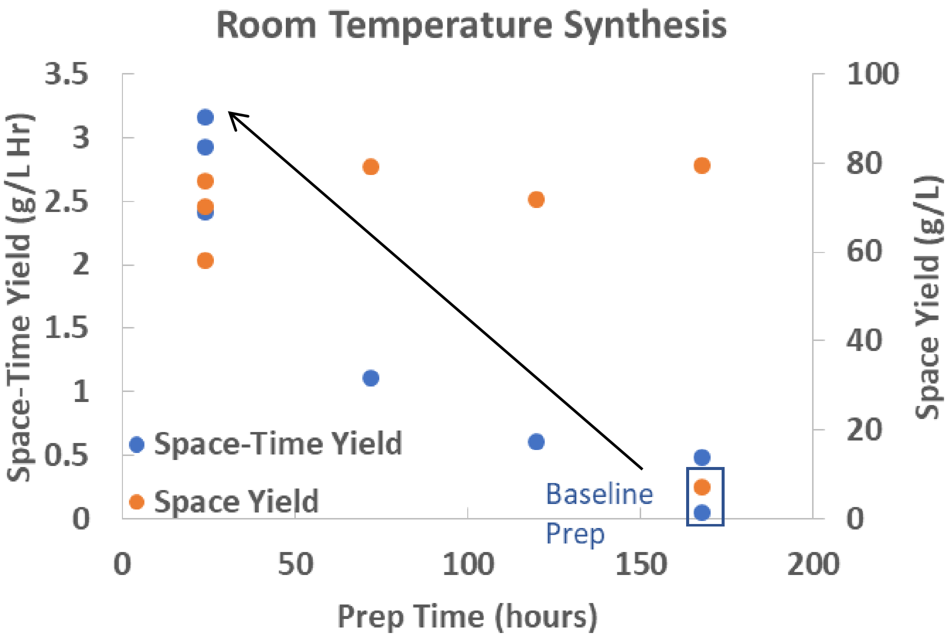
- **MOFs are difficult to pelletize or granulate**
- **Conventional powder compaction techniques could potentially damage the MOF structure**
- **TDA developed a pill-pressing method that results in pelletized sorbent to retain >95% of their capacity when normalized based on active MOF weight**

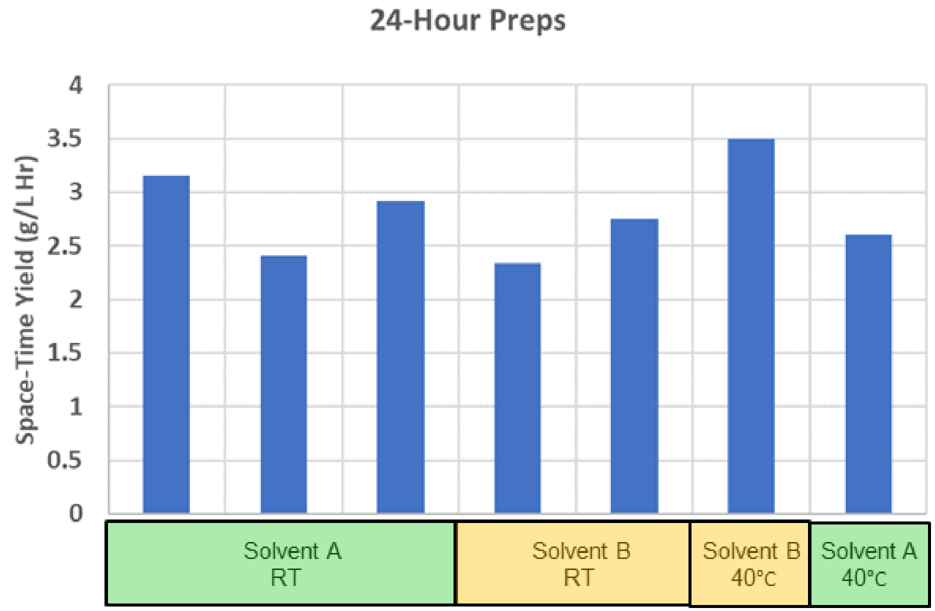
Scale-up of MOF Production



- **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 (via recycle)**
  - Space yield improvements of 10-15X
  - Time yield improvements of 5-8X
- **MOF synthesis, Filtration/Rinsing, Drying/Devolatilization are all sequentially carried out in the same reactor**
- **A classified area is designed and built to handle the equipment and solvents required for MOF processing**

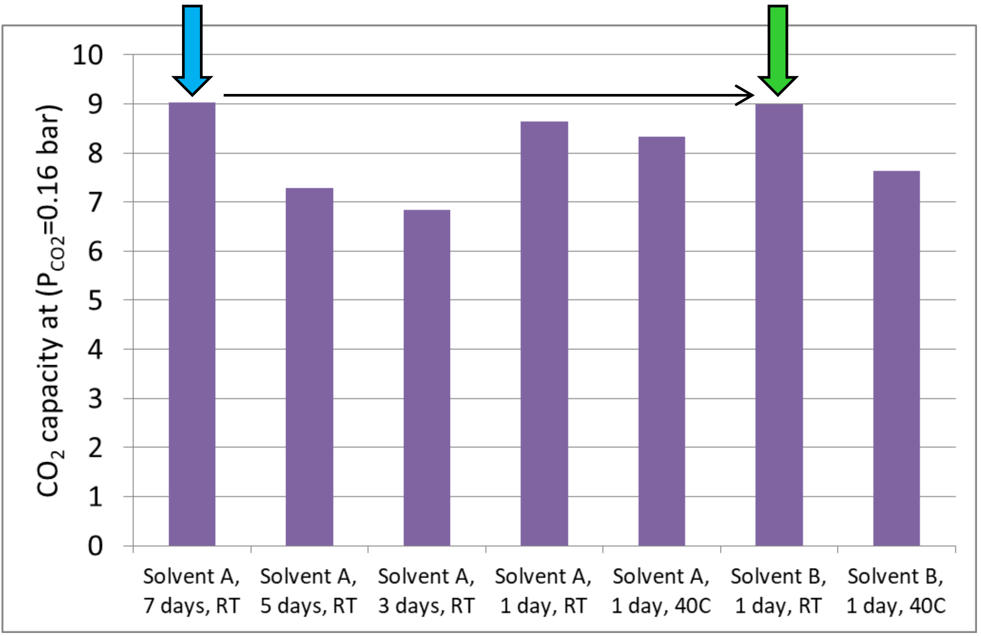
Optimization of Space Time Yield

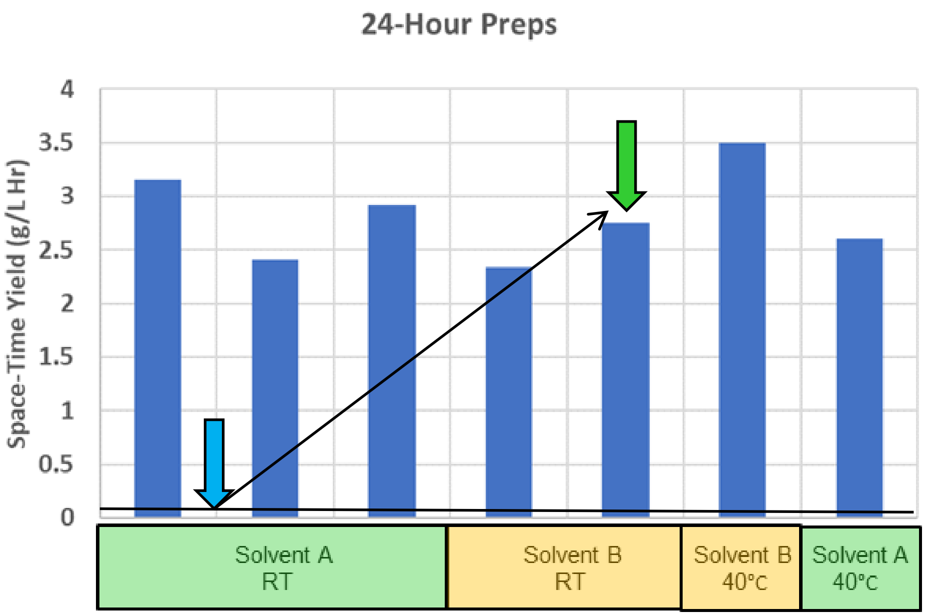




- **Space Yield was increased from <10 g/L to 75-80 g/L**
- **Synthesis time was reduced from 7 days to 1 day (24 h)**
- **We were able to increase the space time yield from <0.1 g/L/hr to >3.0 g/L/hr**

Sorbent Performance – Optimized Preparation



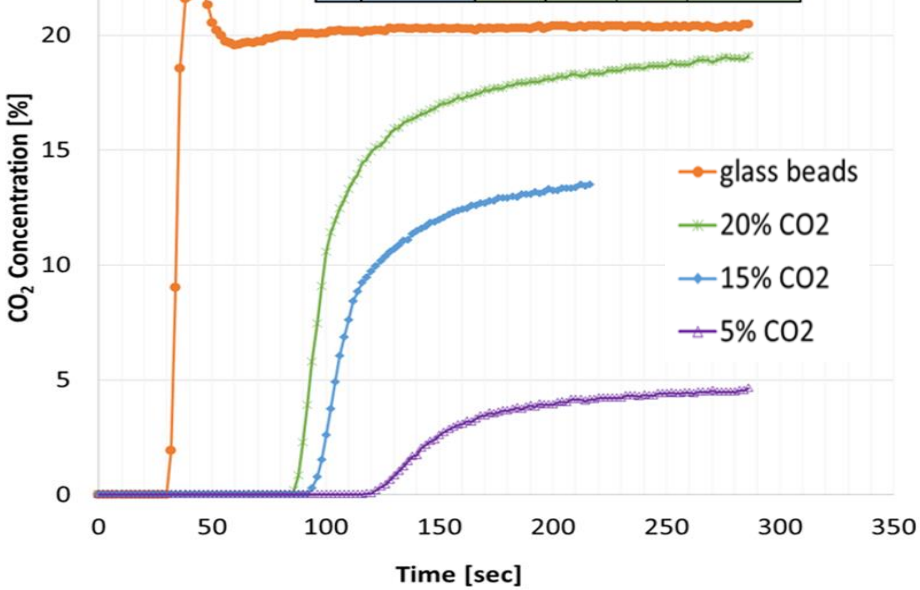


- **Reduced Preparation time of 24 hours was still able to provide a high yield while retaining the CO_2 adsorption capacity (Sorbent performance)**

Performance in Flow Experiments

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

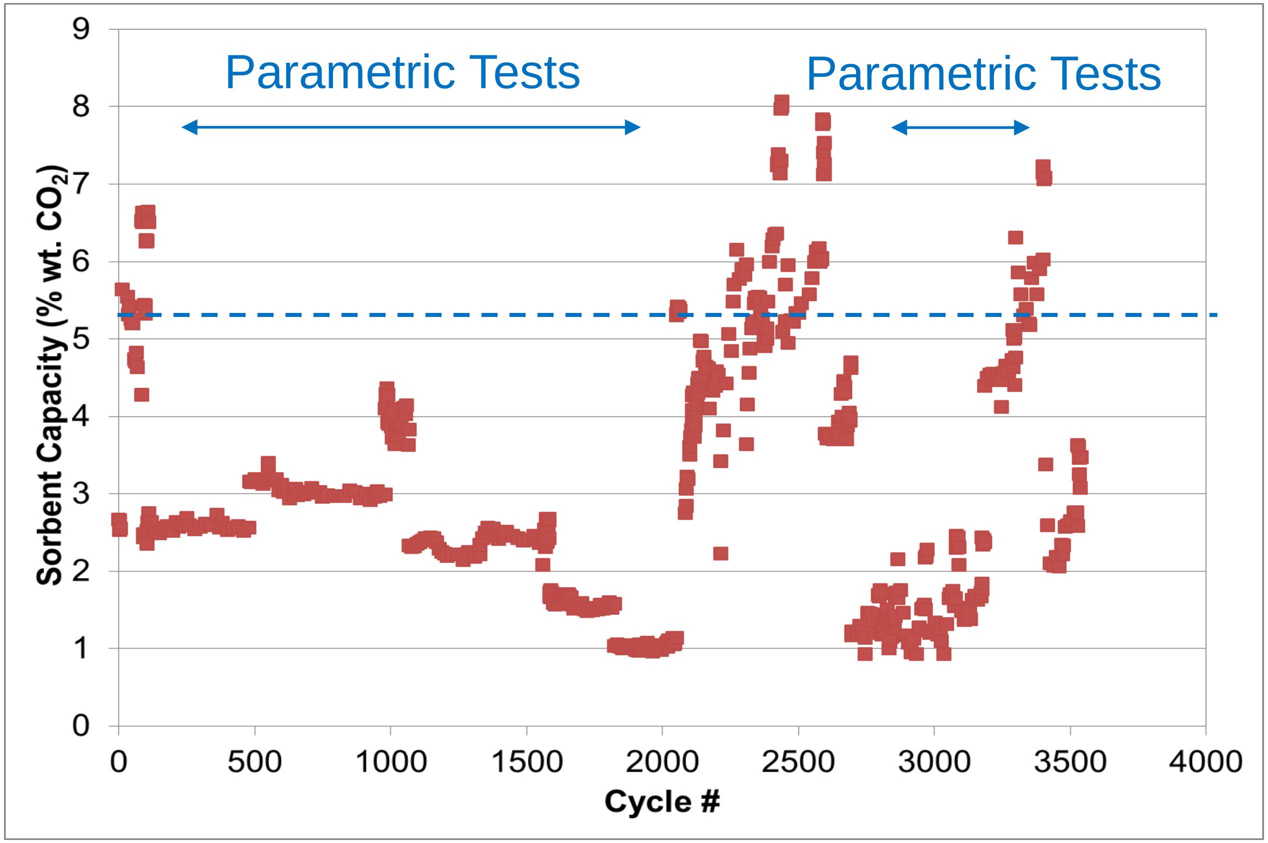
	T_{ads}=30°C	Fluegas CO2 (%) 20	15	5	
RH (%)	30	6.5	5.5	2.6	CO2 loading (% wt.)
	50	6.3	5.4	2.5	
	65	5.4	5.6	2.4	



- **A working capacity of 5+% wt. CO_2 at ~15% vol. CO_2 was demonstrated**
  - ~2.5% wt. CO_2 at 4% vol. CO_2
- **Temperature and humidity have limited impact on working capacity**
  - Higher temperatures lowered the working capacity
  - No significant impact of humidity up to 65%

Evaluation of Sorbent Life

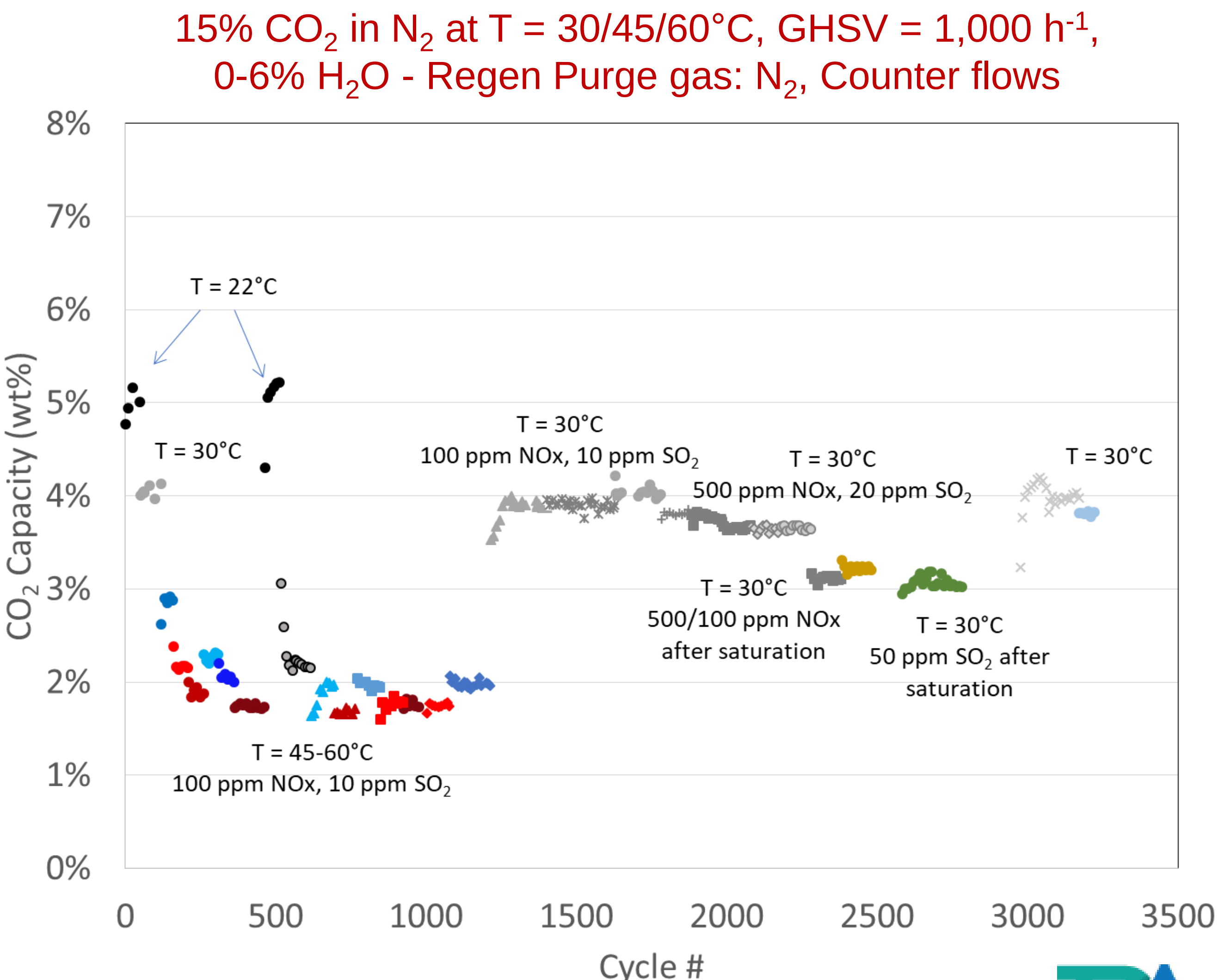
5/15/20% CO_2 in N_2 at T = 30°C, GHSV = 2,400 h^{-1}, 30/50/65% RH
Regen Purge gas: N_2, Counter flows



- **A stable working capacity of 5.5% wt. CO_2 was demonstrated in counter flow desorption under simulated coal flue gas conditions**

Life Tests in Presence of Contaminants

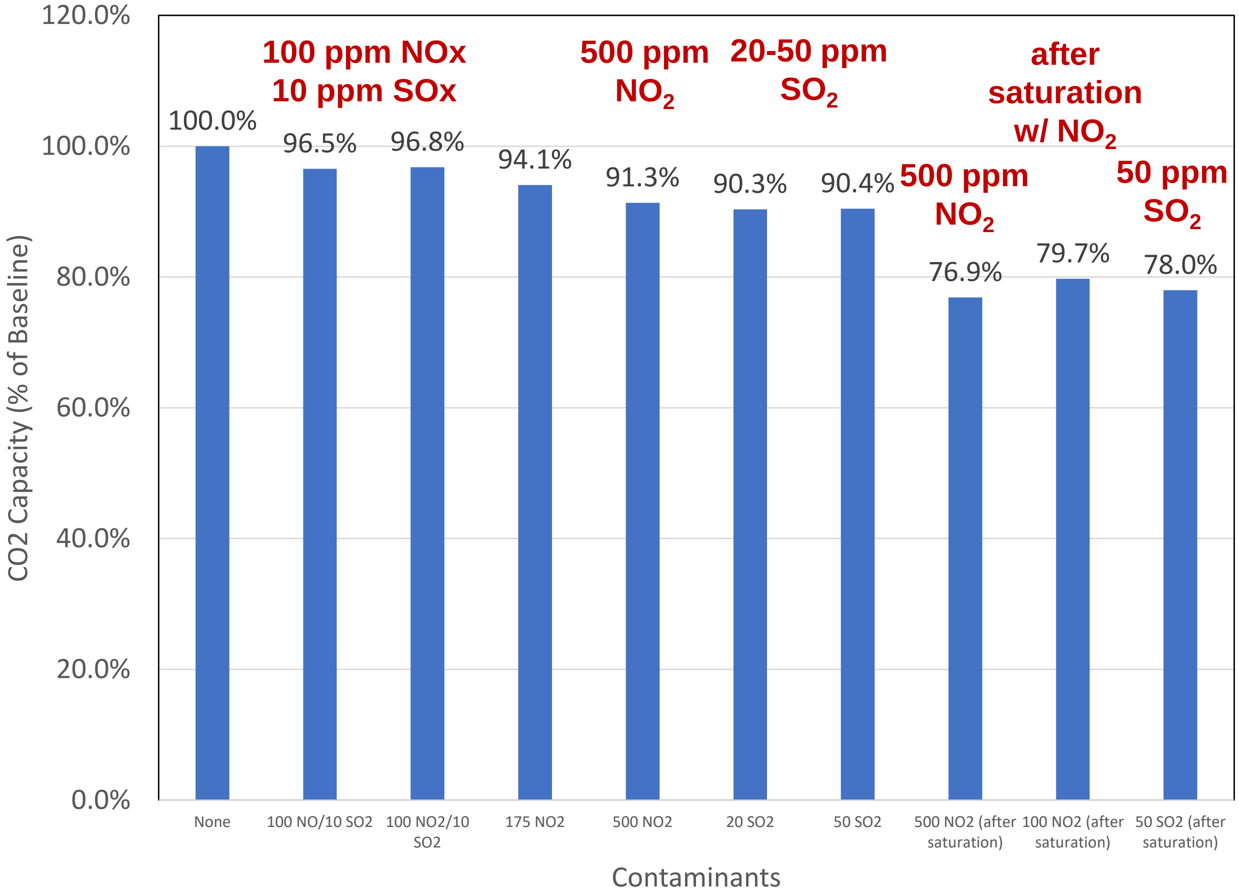
- Stable working capacity in the presence of flue gas contaminants such as humidity, NOx and SOx
- High stability up to 65% RH, 500 ppm NOx, 50 ppm SOx
- Maximum ~20% drop in capacity under high SOx and NOx concentrations



Impact of Contaminants

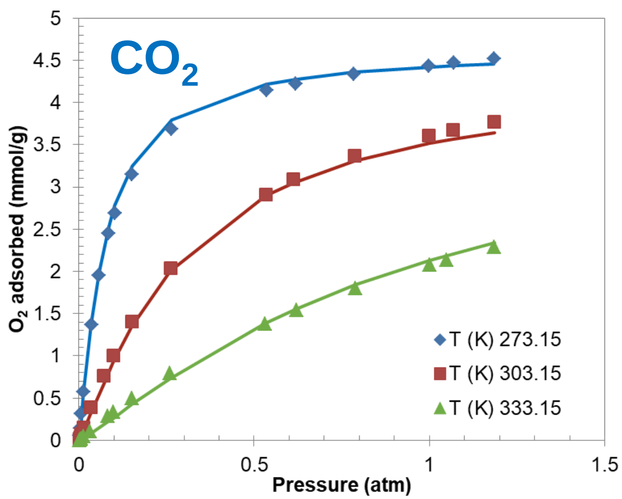
- **Only <5% drop in working capacity was observed at 100 ppm NOx and 10 ppm SOx**
- **At 500 ppm NOx and 50 ppm SOx the working capacity dropped by 10%**
- **After saturating the sorbent with 500 ppm NOx or 50 ppm SOx the sorbent working capacity dropped by ~ 20%**

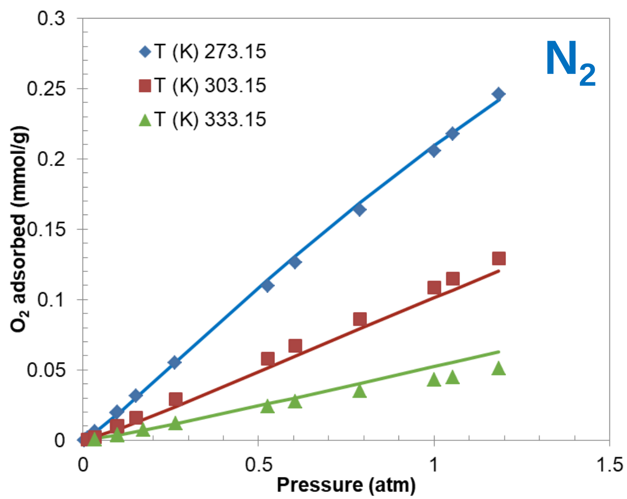
15% CO_2 in N_2 at T = 30/45/60°C, GHSV = 1,000 h^{-1}, 0-6% H_2O - Regen Purge gas: N_2, Counter flows

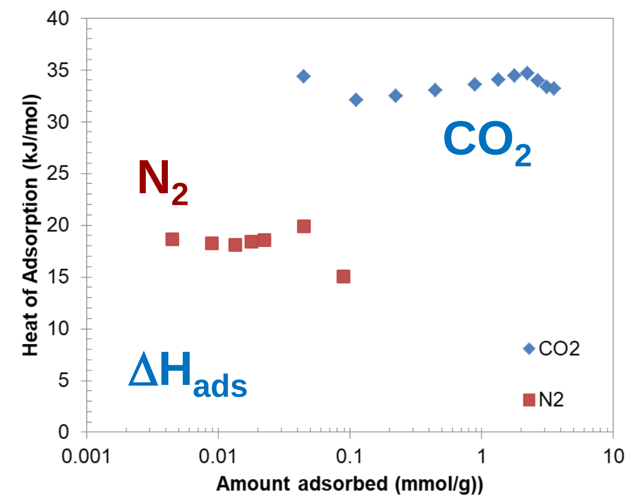


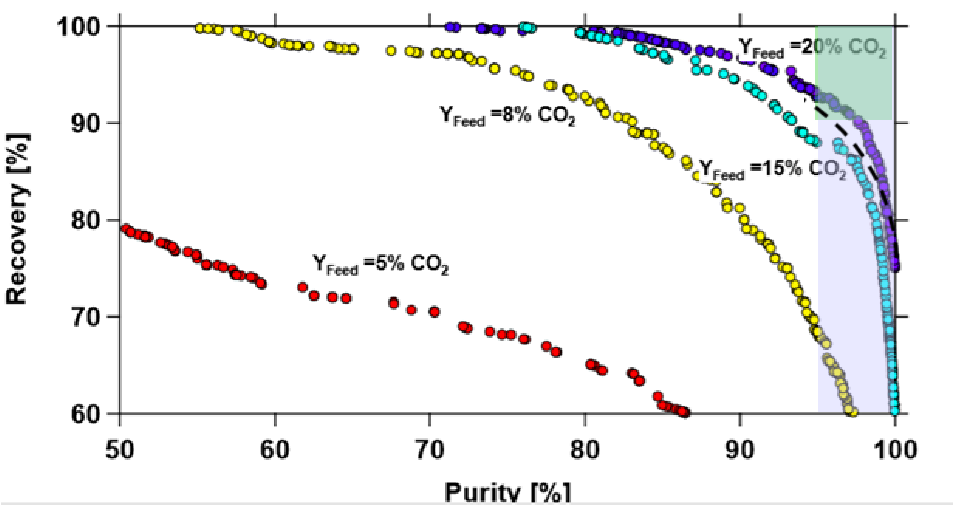
TDA RESEARCH

Adsorption Cycle Modeling









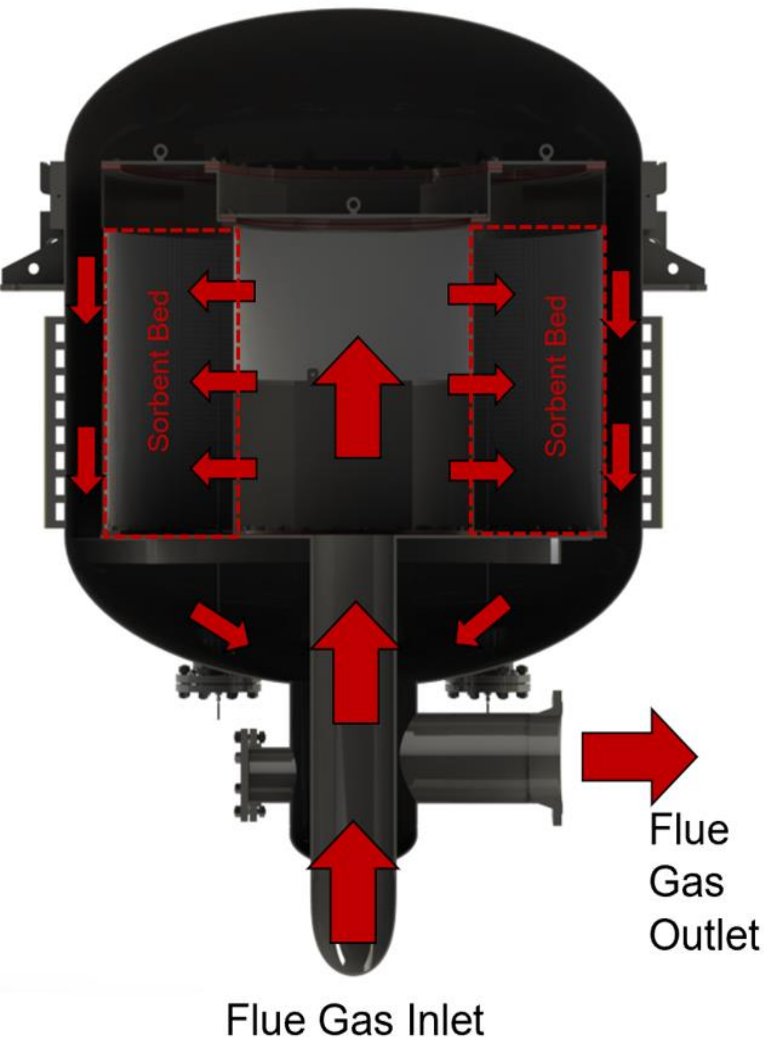
- Initial modeling results from University of Alberta shows simple cycle schemes without addition of steam purge can get close to DOE targets
- More advanced cycle schemes with steam assisted VSA results in 95% CO_2 purity with a CO_2 levels in flue gas as low as 4% (NGCC simulation)

Process Simulation (Rev. 4 basis)

Capture Technology	Sorbent Only	Amine	No Capture
Case Studies	**Case 1**	**B12B**	**B12A**
Gross Power, kWe	**795,063**	**770,000**	**685,000**
CO_2 Capture/Removal, kWe	47,679	29,530	-
CO_2 Purification, kWe	-	-	-
CO_2 Compression, kWe	58,141	44,380	-
Balance of Plant, kWe	39,243	46,050	35,040
Total Auxiliaries, kWe	**145,063**	**119,960**	**35,040**
Net Power, kWe	**650,000**	**650,040**	**649,960**
Net Plant Efficiency, % HHV	**33.4**	**31.5**	**40.3**
Carbon Capture, %	90	90	0
Coal Feed Rate, kg/h	258,208	273,628	214,112

- Energy for CO_2 capture is 26% lower compared to amine scrubbing

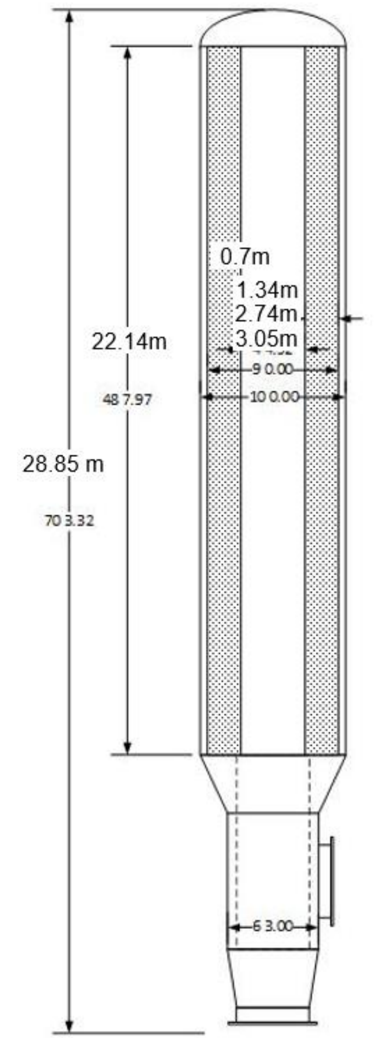
Reactor Vessel Design and Costing



Total ΔP (across the entire system) =105 mbar

Module Size:	137.5 MW
No. of Trains:	4
Beds/Train:	4
Total Beds:	16
Flue Gas Flow:	116.5 m^3/s
CO_2 Flow:	1.96 tonne/min
Capacity:	3.6% Wt%
Cycle Time:	1 min
Sorbent Inventory:	54.5 tonne/m^3
Sorbent Density:	0.55 tonne/m^3
Bed Volume:	99.5 m^3
Bed Area:	7.3 m^2

- Four radial beds per train (total of 16 beds)
- SA516-70 carbon steel, 0.5” thickness
- 120 in OD x 872 in T/T

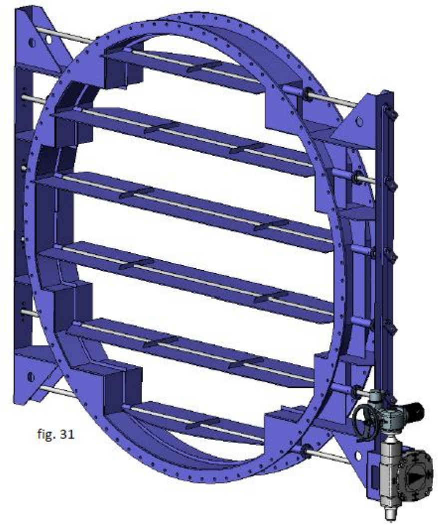


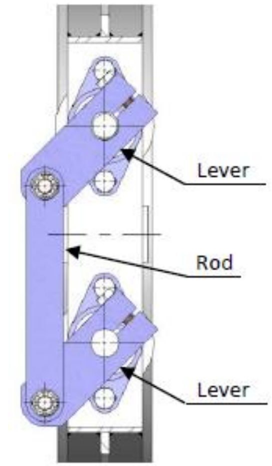
Reactor Vessel Design and Costing

Sorbent Only System

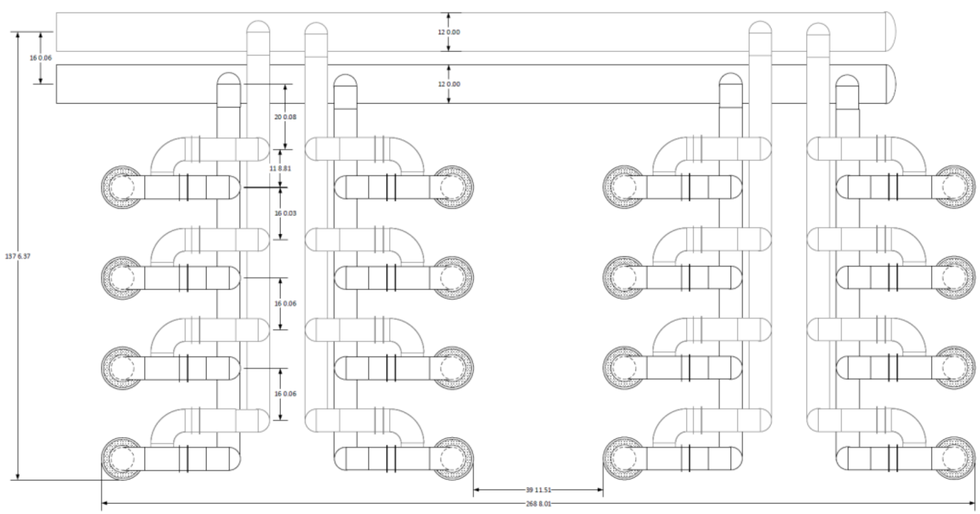
	Stage I		Stage II		Stage III		Stage IV	
Bed 1	Adsorption - Flue gas flow		Cocurrent Blowdown		Desorption - CO2 Product Out		Desorption - Air Purge flow	
Bed 2	Desorption - Air Purge flow		Adsorption - Flue gas flow		Cocurrent Blowdown		Desorption - CO2 Product Out	
Bed 3	Desorption - CO2 Product Out		Desorption - Air Purge flow		Adsorption - Flue gas flow		Cocurrent Blowdown	
Bed 4	Cocurrent Blowdown		Desorption - CO2 Product Out		Desorption - Air Purge flow		Adsorption - Flue gas flow	
336s	21s	21s	21s	21s	21s	21s	21s	21s

Adsorption - Flue gas flow | Cocurrent Blowdown | Desorption - CO2 Product Out | Desorption - Air Purge flow



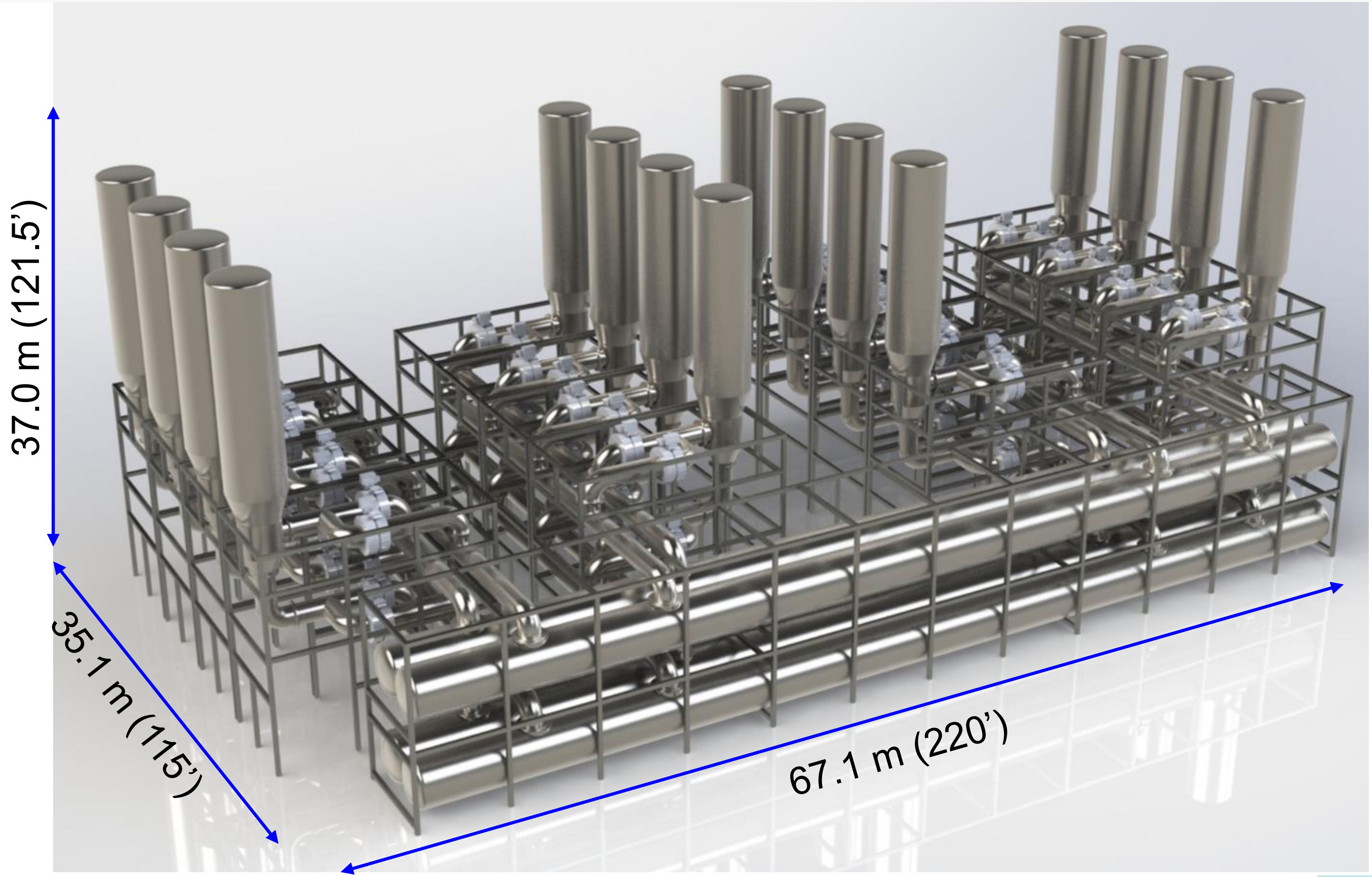


Damper valves
Price basis is 72” size



- 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

3-D Layout of the Sorbent System

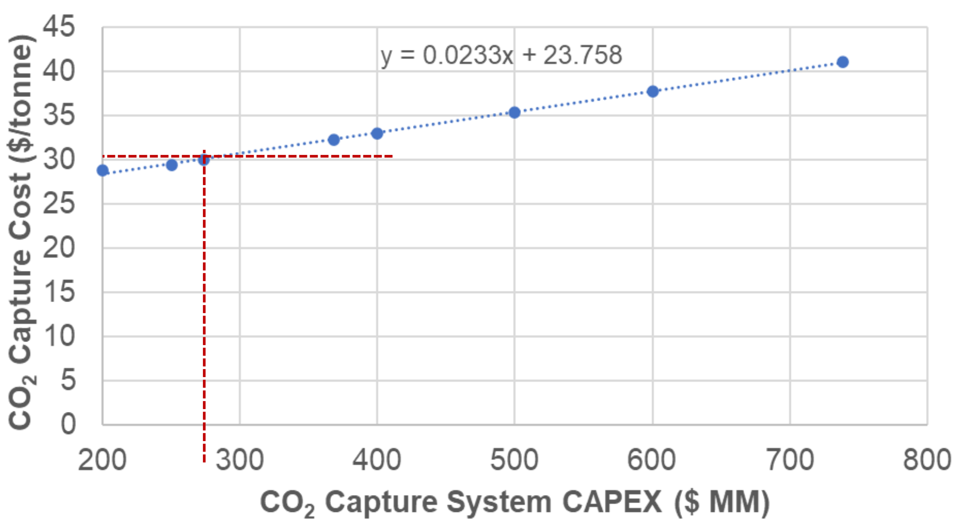


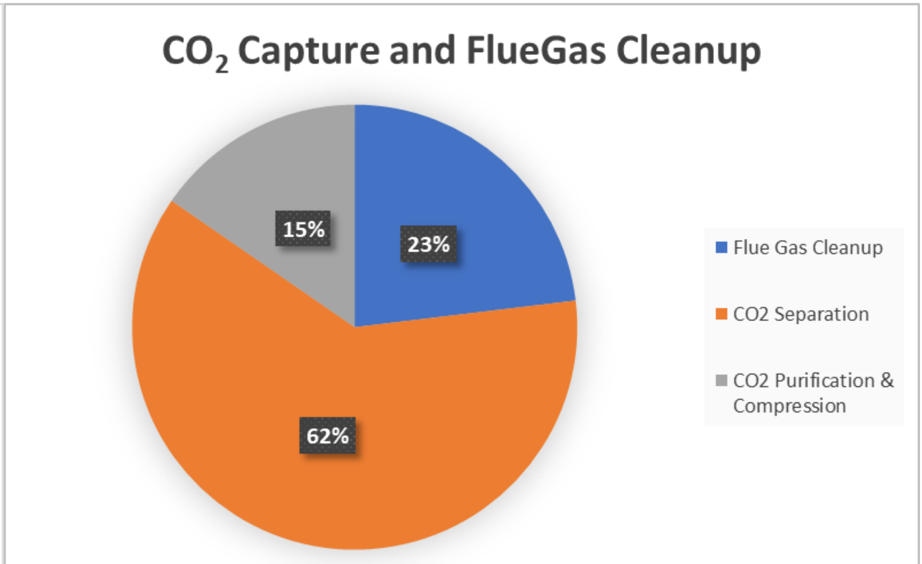
Cost of Capture Summary (Rev. 4 basis)

Capture Technology	Sorbent Only	Amine	No Capture
Case Studies	**Case 1**	**B12B**	**B12A**
Basis for Cost Estimates (Year)	2018	2018	2018
Net power, MW	650	650	650
Capacity factor (CF), %	85	85	85
Total plant cost (TPC), $	2,053,929,454	2,468,373,000	1,364,033,000
Total overnight cost (TOC), $	2,553,134,556	3,023,049,325	1,678,411,825
Total as spent capital (TASC), $	2,946,317,278	3,488,598,921	1,937,578,752
LCOE	**$/MWh**	**$/MWh**	**$/MWh**
Capital Charge (0.0707 X TASC)	43.04	50.96	28.30
Fixed Charges	13.73	16.13	9.48
Variable Costs	12.15	14.00	7.72
Fuel Costs	22.75	24.08	18.87
Byproducts (Credit)	0.00	0.00	0.00
Total (Excluding T&S)	**91.67**	**105.18**	**64.37**
CO2 T&S Costs	8.45	8.96	0.00
Total (Including T&S)	**100.12**	**114.14**	**64.37**
Cost of Capture	**$/tonne**	**$/tonne**	**$/tonne**
Breakeven CO2 Sales Price (compared to SCPC W/O capture)	32.25	45.52	-
Breakeven CO2 emissions penalty (compared to SCPC W/O capture)	52.29	73.40	-

- Cost of CO_2 capture with VLP steam purge is ~$32.25/tonne
- Cost of CO_2 captured is considerably lower for TDA's CO_2 capture system about 29.2% lower the reference Amine Case

Sensitivity Analysis – CAPEX (Rev. 4 basis)





- Total cost of CO_2 Capture System including flue gas treatment and compression is $368 MM
  - Cost of CO_2 capture ~$32.25/tonne
- CAPEX for CO_2 capture needs to go below $274 MM to meet transformational CO_2 capture targets (<$30/tonne)

Acknowledgments

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