Transformational Molecular Layer Deposition Tailor-Made Size-Sieving Sorbents for Post-Combustion CO_2 Capture

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Project Overview

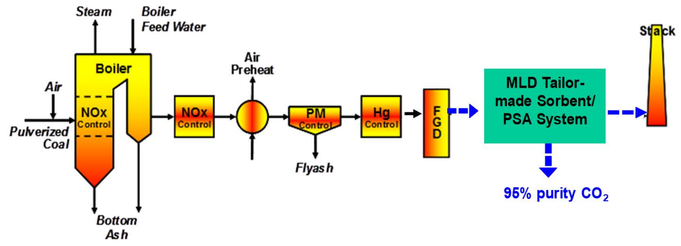
Funding: $3,000,000 from DOE; $759,206 Cost Share **Overall Project Performance Dates**:10/1/2019-12/31/2025

Overall Project Objectives:

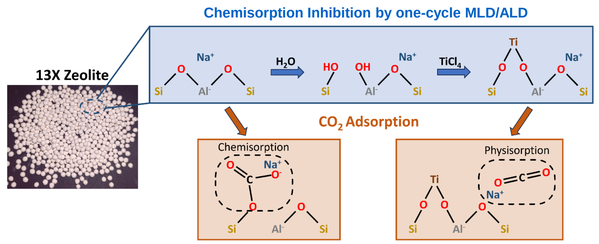
Develop a transformational molecular layer deposition tailor-made sorbent/PSA process (MLD-T-S/PSA) that can be installed in new or retrofitted into existing pulverized coal (PC) power plants for CO_2 capture with 95% CO_2 purity and a cost of approximately $30 per tonne of CO_2 captured; it will be ready for demonstration by 2030.

Background & Motivation:

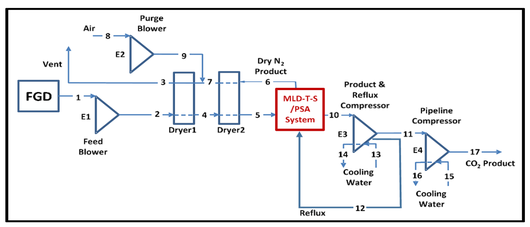
Integration with coal-fired power plants: installed downstream of FGD



UB's MLD-T-S for optimized CO_2 capture performance



USC's unique PSA process flow sheet from FGD to CO_2 compression



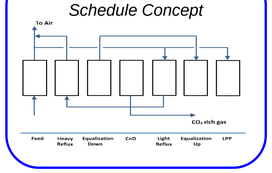
Technical and economic advantages

Advanced Sorbent Fabrication Procedure to Reduce Manufacturing Cost
- MLD/ALD for uniform internal modification from vapor phase
- Low cost MLD/ALD precursors
- Successful commercial roll-to-roll production

Ease of Scale-Up
- Pellets/beads of commercial sorbents can be directly used
- One-cycle deposition

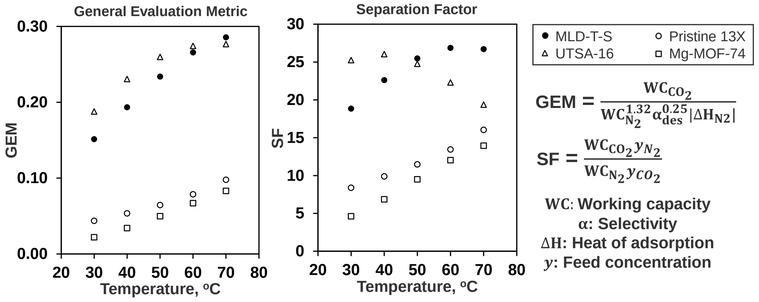
Long-Term Stability and Ease of Regeneration
- MLD/ALD modification introduces inorganic materials (e.g., TiO_2)
- Stable base sorbent materials, such as zeolites
- Lower temperature for regeneration

USC proprietary PSA Cycle Schedule Concept



MLD-T-S: Desired PSA Performance, Contaminant Tolerance, and Scale-up

MLD-T-S Compares Favorably to 13X & UTSA-16

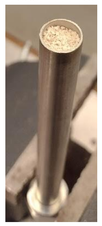


$$GEM = \frac{WC_{CO_2}}{WC_{N_2}^{1.32}\alpha_{des}^{0.25}|\Delta H_{N2}|}$$

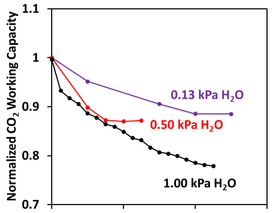
$$SF = \frac{WC_{CO_2}y_{N_2}}{WC_{N_2}y_{CO_2}}$$

WC: Working capacity
α: Selectivity
ΔH: Heat of adsorption
y: Feed concentration

Contaminant Tolerable Level



Small adsorbent bed for flue gas contaminant testing



- Realistic P/VSA schedule was emulated on a small bed of MLD-T-S
- CO_2/N_2 with 0.13, 0.50, & 1.00 kPa H_2O were explored
- Reversible adsorption of H_2O mitigated declined in CO_2 working capacity

0.13 kPa H_2O: 0.054 mmol $H_2O/(g_{MLD13X}\cdot cycle)$
0.50 kPa H_2O: 0.208 mmol $H_2O/(g_{MLD13X}\cdot cycle)$
1.00 kPa H_2O: 0.415 mmol $H_2O/(g_{MLD13X}\cdot cycle)$
Saturation capacity is ~14 mmol/g

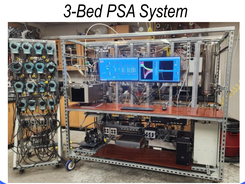
Note: MLD-T-S can be fully regenerated at 200°C.

MLD-T-S Scale-up

A) 3-liter ALD reactor; B) 200g MLD-T-S batch fabricated in a single batch; C) 1kg of accumulated MLD-T-S.

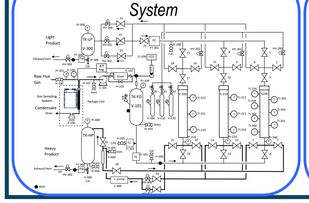
PSA for CO_2 Capture: PSA Skid Construction

Front View Photograph of the USC 3-Bed PSA System

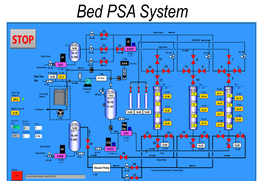


Back View Photograph of the USC 3-Bed PSA System

Schematic of the USC 3-Bed PSA System



LabVIEW Schematic of the USC 3-Bed PSA System



Status of the USC 3-Bed PSA System
- Construction 100 % complete
- Start-up and troubleshooting complete
- Testing at USC underway with 13X zeolite
- Testing at USC with MLD2 zeolite will follow
- Working out details to test at the NCCC
- NCCC testing with MLD2 zeolite forthcoming

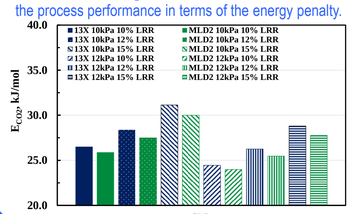
PSA for CO_2 Capture: DAPS Simulation and 1-bed PSA testing

Simulations of a VSA System with 8 Units, 3 Feed Beds, 6 Light Reflux Beds, R_{LD} = 1.0, D_p = 9 mm and T = 40 °C.

USC patented multi-feed step and multi-light reflux step PSA cycle schedule

Bed 1-3	F_1 to F_3	
Bed 4	HR	
Bed 5	EqD	CnD
Bed 6 to 5+n_{LR}	LR_1 to n_{LR}	
Bed 6+n_{LR}	EqU	LPP
Time	t_1	t_2
200 s	20 s	180 s

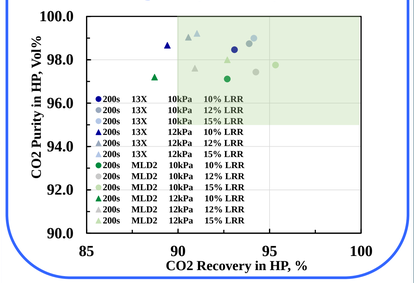
Comparison of MLD-T-S and 13X VSA process performances via DAPS simulations: Effect of the low vacuum pressure (P_L) and the light reflux ratio (LRR) on the process performance in terms of the energy penalty.



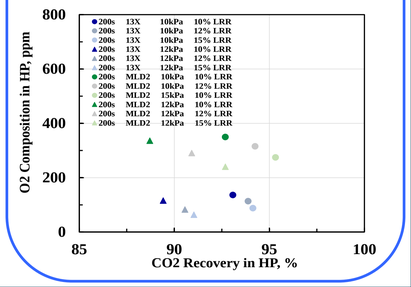
Photograph of the USC 1-Bed PSA System Used for Testing Scaled Up MLD-T-S

MLD-T-S Generally Performs Better Than 13X

Comparison of MLD2 and 13X VSA process performances via DAPS simulations: Effect of the low vacuum pressure (P_L) and the light reflux ratio (LRR) on the process performance in terms of the CO_2 purity and CO_2 recovery in the heavy.



Comparison of MLD2 and 13X VSA process performances via DAPS simulations: Effect of the low vacuum pressure (P_L) and the light reflux ratio (LRR) on the process performance in terms of the O_2 concentration in the heavy product.



Summary

- Optimized MLD-T-S shows improved CO_2 working capacity and CO_2/N_2 SF compared to 13X
- When exposed to CO_2/N_2 containing H_2O under an emulated P/VSA schedule, MLD-T-S showed stabilized loss in CO_2 working capacity ≤ 0.5 kPa H_2O.
- MLD-T-S was fabricated at kg-scale and sent to collaborators for P/VSA testing
- 3-bed PSA skid testing underway at USC; testing to begin soon at NCCC
- Large scale PSA process simulations continuing for process optimization
- 1-bed PSA testing with MLD2 at USC starting soon

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