Advanced Structured Adsorbent Architectures for Transformative Carbon Dioxide Capture Performance

Project Number: DE-FE0031732

August 18, 2022

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Project Overview

Cooperative Agreement No.: DE-FE0031732

- Award Period: 05/01/2019 through 12/30/2022

- Project Funding
  - Total Funding: $5,121,897.00
  - Federal Funding: $3,890,195.00
  - Cost Share Funding: $1,231,702.00

- Project Participants
  - Prime: Electricore, Inc.
  - Technology, Design and Operation / Cost Share Provider: Svante, Inc.
  - Techno-Economic Analysis (TEA): Susteon

- DOE-NETL Team
  - Project Manager: Carl P. Laird & Andrew Jones
  - Contracting Officer: Jacqulyn M. Wilson

Overall Project Objectives
Cooperative Agreement No.: DE-FE0031732

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The objective of this project is to:

- Evaluate Svante's (Mark-II) VeloxoTherm™ Technology via the development and bench-scale testing of an advanced structured adsorbent, including novel Bi-layer, laminated adsorbent structures and segmented beds.

- Select, synthesize, and characterize tailored solid adsorbents for
  - computational modeling,
  - advanced structured adsorbent development,
  - process simulations, and
  - dynamic bench-scale (~1-10 kg/day CO2 captured) testing

- Demonstrate key performance indicators (KPIs), such as recovery, product purity, regeneration energy, and the integrated system's productivity in lifetime analysis.

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Technology Background

Fundamental performance enablers:

- Low flow resistance of parallel channel structure.
- Low heat capacity relative to adsorption capacity.
- Very fast kinetics with contact time < 1s, 30-60s total cycle time
  - Transient conditions throughout the bed length (RH, temperature)
- Availability of different sorbents

Significant challenges:

- Sorbent lifetime needs to be multiple years (5+ yrs., < 0.01 kg sorbent/tone CO_2 capture)
- Cost of sorbent needs to be modest (20-30 $/kg)
- Regeneration energy of the process (mainly steam) needs to be minimized.

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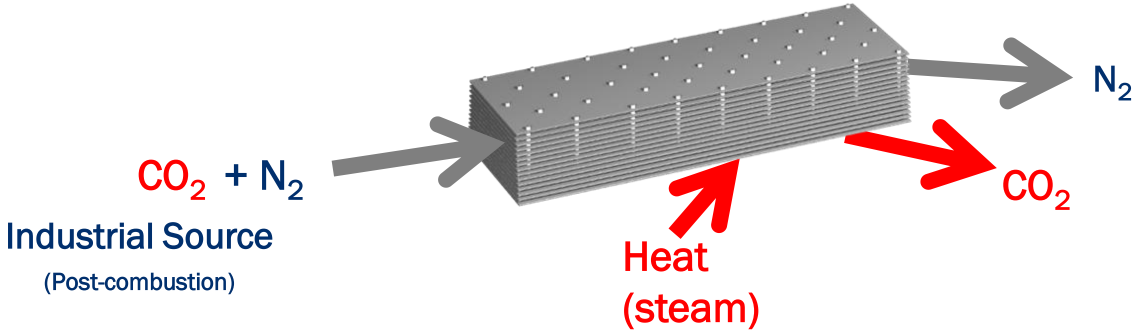
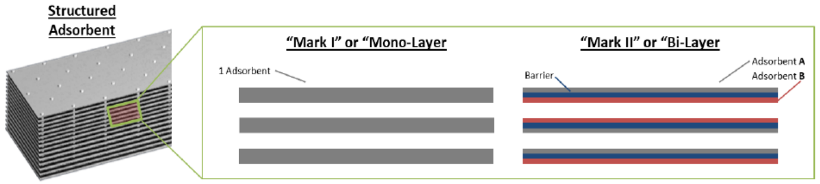
Program Phases

Exploring two configurations of laminates :

- Phase 1- Parallel layers => Bilayer
- Phase 2- Sequential layers => Segmented bed

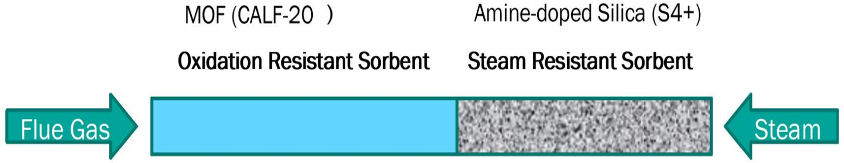


Phase 1- Bilayer Structure
05/01/2019 - 07/31/2021



- Absorbent B can use the heat generated by Absorbent A … Reduce steam
- Absorbent B doesn’t need to be steam resistant… better O_2 resistance.

Phase 2- Segmented Bed Structure
08/01/2021 – 12/30/2022



- Segmented bed concept matches the best sorbent to the position of the bed (based on RH and Temperature profile)

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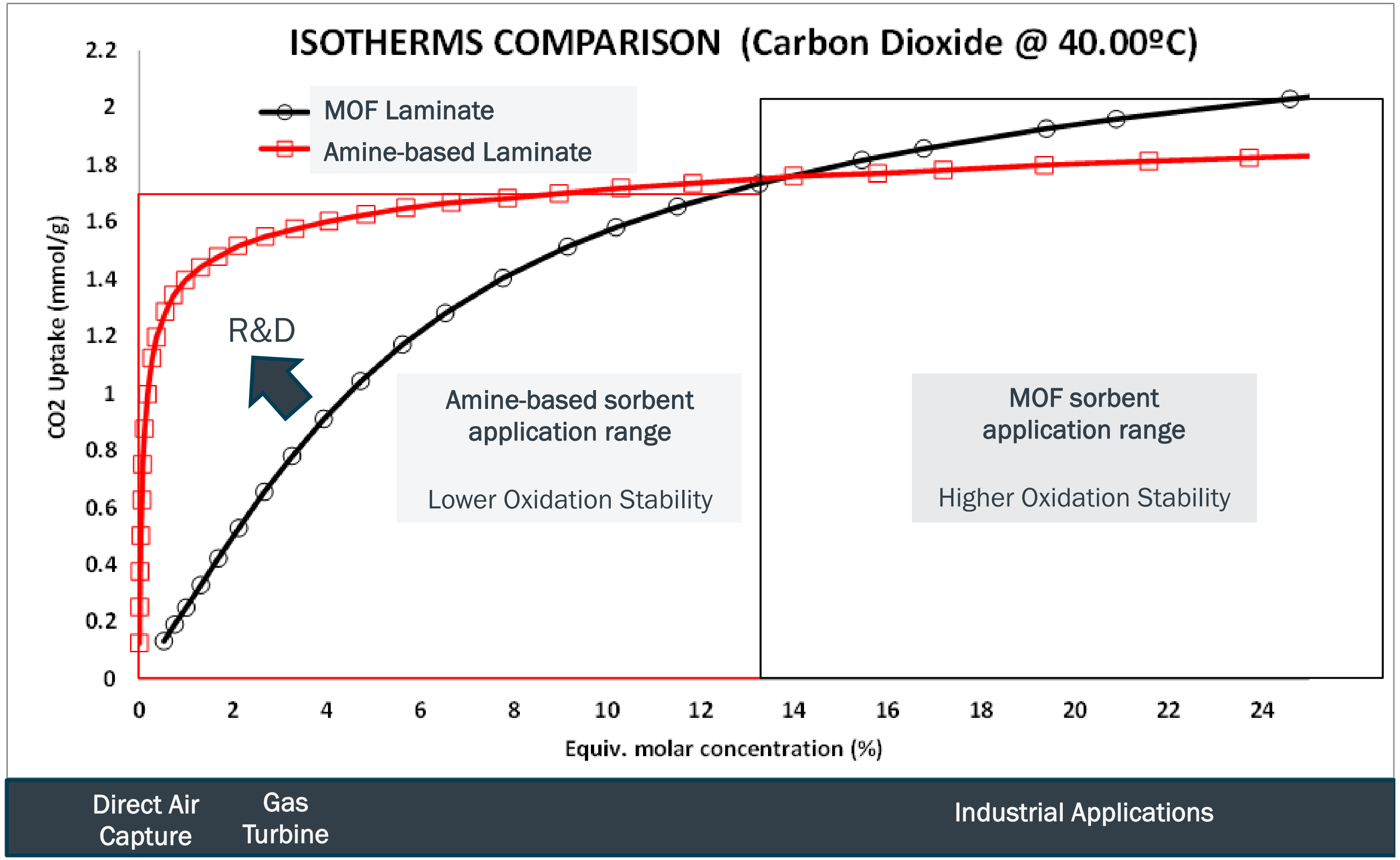
Application Domain of Svante's Adsorbent

Svante's Sorbents (Amines vs Metal Organic Framework)

- ✓ High volumetric & gravimetric capacity [All];
- ✓ 100% water & steam stability to perform direct heating/cooling [All];
- ✓ higher resistance to O_2 (up to 200^{0}C) and contaminants (SOx and NOx) [MOF];
- ❑ Higher capacity at flue gas lower CO_2 concentration [Amines];
- ❑ Higher CO_2/N_2 selectivity [Amines].



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Phase 1 / Bilayer Project - (05/01/2019- 07/31/2021)

Phase 1 / Bilayer Project Achievements

- Select, synthesize, and characterize tailored solid adsorbents for building Advanced structures development
- Scale up at tonnes scale of an amine base water and steam stable adsorbent and confirmed infield stability at FOAK 400 series
- Scale up at tonnes scale of an ultra-stable MOF material (BASF)
- Confirming the synergy between two sorbents, decreasing the demand on regen energy (steam) by ~36%

Phase 1 / Bilayer Project Challenges

- Bed assembly to combine the three layers is a challenge and could significantly increase bed cost
- Adding much higher complexity to the Rotary Adsorption Machine and balance of plant
- It was not possible to achieve the target productivity (10-15 TPD/m^3) with the available materials and design
- Techno-economic advantage of the bi-layered structure is still a challenge [higher complexity].

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Confirming Stability of Amines based Sorbent (Field Testing)

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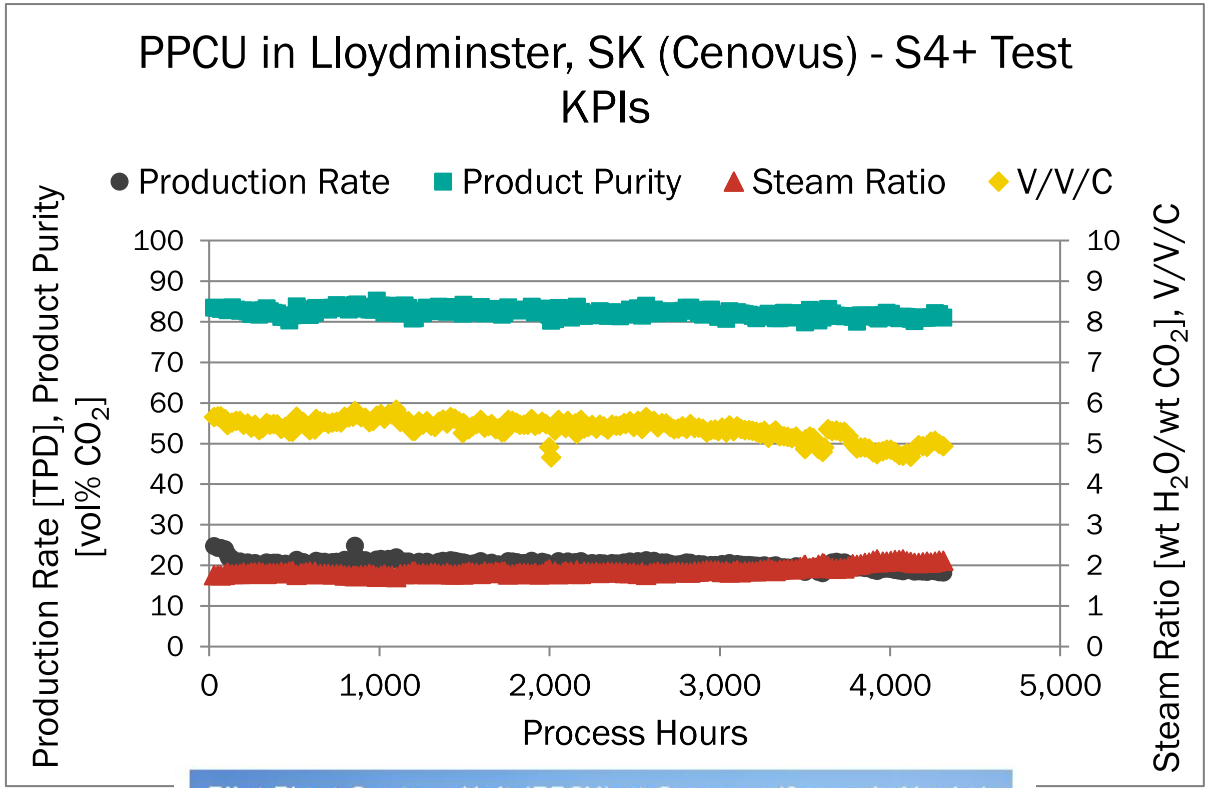
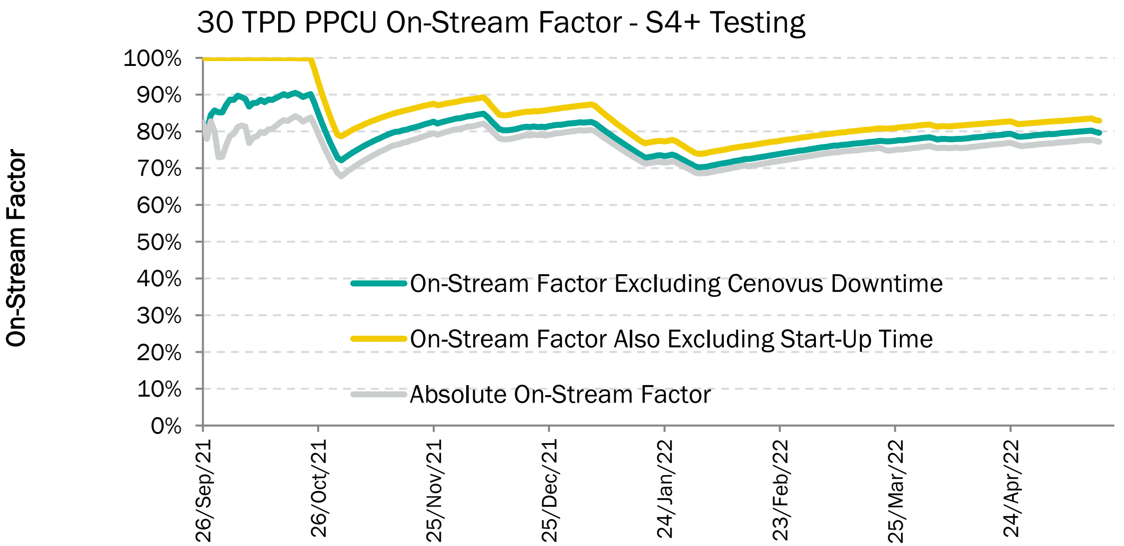
- ✓The FOAK 400 Series pilot plant in Saskatchewan has now achieved >9,000 process hours over 3 generations of SAB filter design
- ✓Current test is on S4+, amine-impregnated silica fully stable to water and steam, beds and has achieved >4,500 hours on test with strong stability performance KPIs
- ✓On-stream factor >80% (excluding plant shutdown and start-up time





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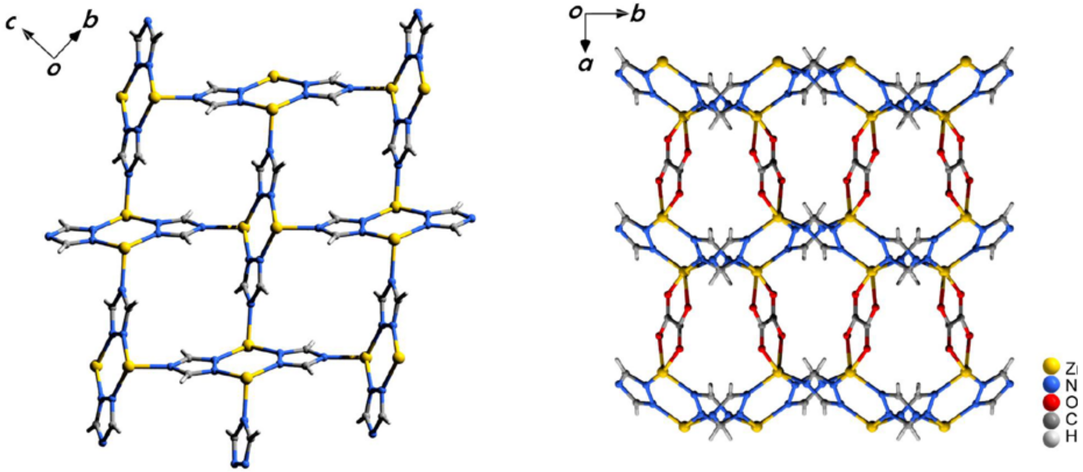
Scale-up of CALF-20 MOF

Metal Organic Framework (MOF)

CALF-20 – Zinc 1,2,4-Triazolate Oxalate



- Structure from Rietveld – crystals have never grown
- 3-D channels comprising 38% of the volume, ~500 m^2/gm surface area.
- pores (vdW radii) of 2.73 × 2.91, 1.94 × 3.11, 2.74 × 3.04 Å ([100], [011], [0-11]

Taylor, Vaidhyanathan, Lin, Mah, Dawson, Iremonger, Deakin, Shimizu
Patent awarded and licensed for post-combustion and air capture.

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-Metal framework (Zn)
-Organic Ligand (oxalte)
-Not amine based (physisorbtion)

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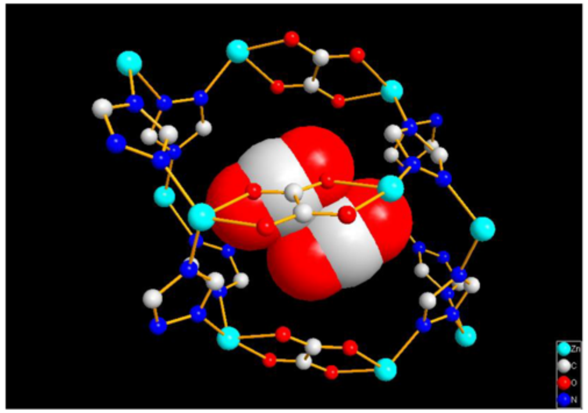

At 1.00 atm pressure, the main CO_2 binding site is between the oxalate groups.

This MOF has very special properties:
-High volumetric and gravimetric CO2 capacity
-Stable to water (liquid, steam)
-Stable to O2 up to 140C
-Easily scalable (low cost)
-Processeable in a laminate
-More stable to Nox and SOx

More than 7 tonnes of MOF manufactured so far at BASF

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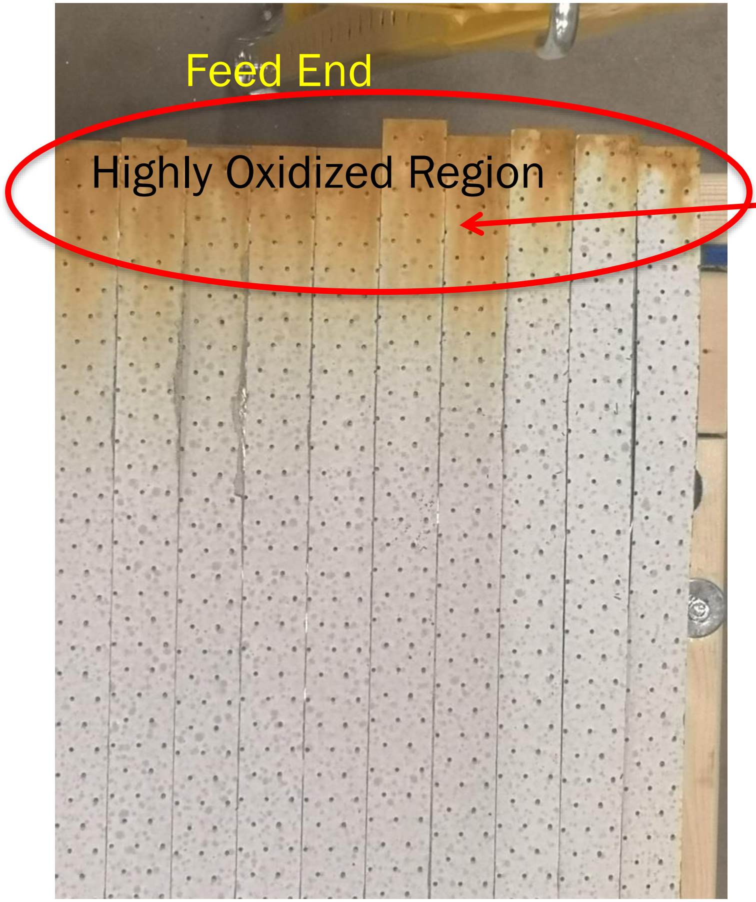
Phase 2 / Segmented Bed - New Advances Structure Adsorbent Idea

- Design a serial bed design using a multi-sorbent capable of achieving higher productivity and compatible with current RAM design, BoP and bed assembly at a larger scale
- Take advantage of the Rapid Cycling VeloxoTherm Technology with non-equilibrium conditions (RH, temperature) throughout the bed
- Use the appropriate sorbent at the right position

  - **Amines** => High capacity @ high RH, lower oxidation resistance at low RH and low CO_2
  - **MOF** => High O_2 stability, Low Capacity @ high RH

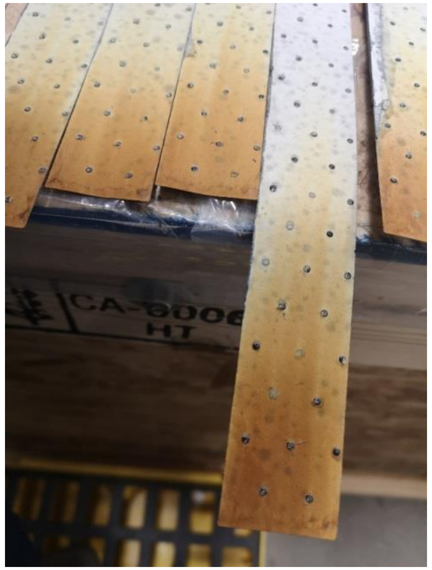
Some Experimental Observation of Non-Uniformed Degradation

S-Series Sorbent after PDU testing



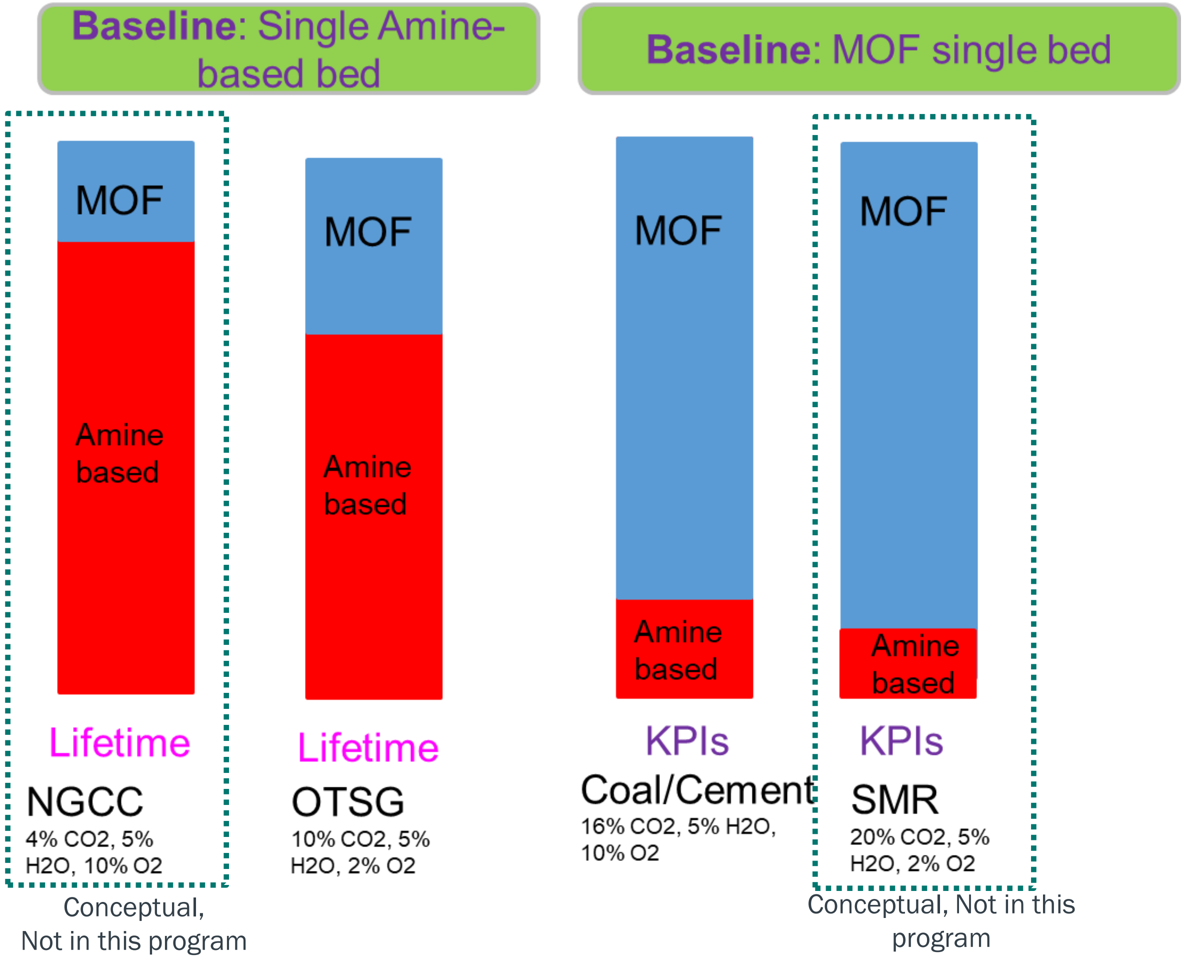
Top of the bed:

- ➢ Low average RH (detrimental for Amine-based sorbent)
- ➢ Decrease bed lifetime
- ➢ The best chemical environment for CALF-20 to perform (high temp, low RH)



Phase 2 / Segmented Bed Project – (08/01/2021 – 12/30/2022)

- Design a bed with a multi-sorbent in a serial configuration with compatibility with current manufacturing and plant design

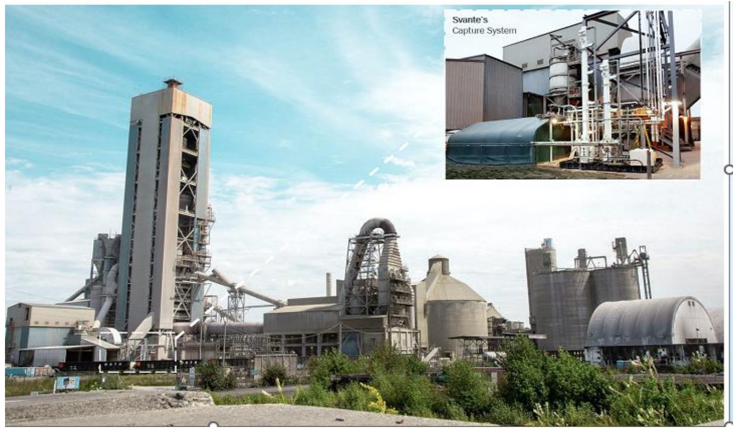


Project Steps, Work Plan and Key Milestones

- Structure sorbent optimization of the position, length, laminate thickness and density, and channel height, using
  - Modelling (CFD and UFD)
  - VTS testing data
- Cycle optimization for the optimized geometry
  - VTS Testing
- Bed packaging optimization
- Lifetime stability
  - PDU testing / In-House
- Field Testing
  - 1 TPD @ Lafarge Cement Plant

0.1 TPD Testing station- PDU at Svante

LafargeHolcim CO_2MENT Project, Vancouver, BC, Canada



Key Milestones (one-year period)

Budget Period	Task	Milestone Description	Planned Completion Date	Actual Completion Date
3	*17*	*Final Gen-1 Segmented bed design and process cycle condition for bench scale bed testing on OTSG applications (Cat. 1)*	*12/30/2021*	***01/20/2022***
3	*17*	*Final Gen-1 Segmented bed design and process cycle condition for bench scale bed testing on Coal, Cement & SMR applications (Category 2)*	*06/01/2022*	***06/01/2022***
3	*17*	*Segmented bed model verification and development for sensitivity analysis.*	*06/01/2022*	***06/01/2022***

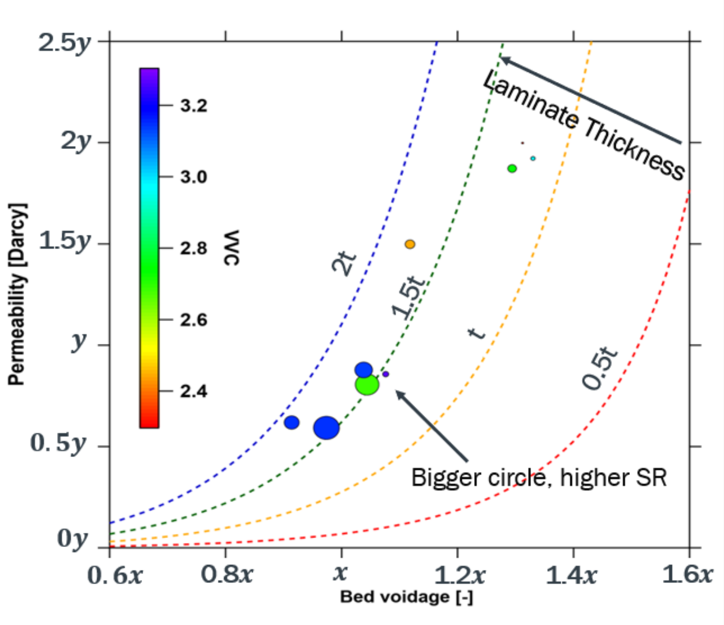
Laminate Optimization

MOF Laminate Thickness and Density Optimization vs VTS KPIs

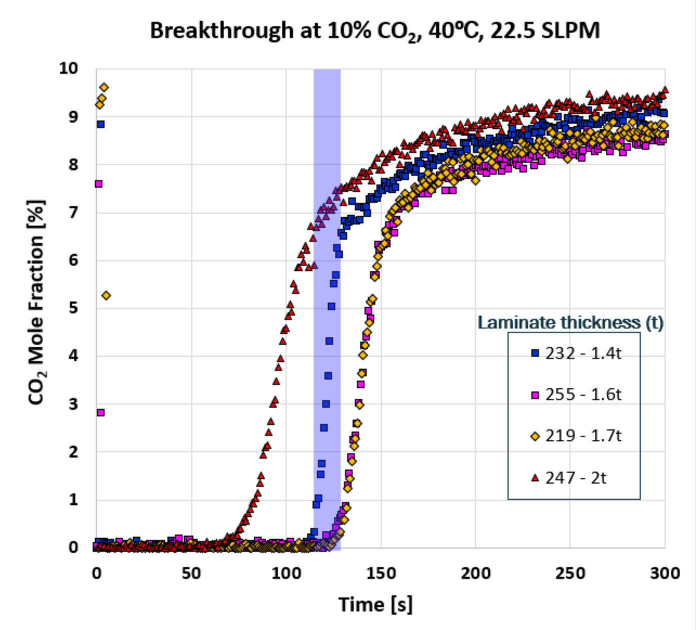
MOF laminate thickness sensitivity was evaluated using VTS beds from the following three main thickness groups:

- $1.4t \pm 0.1t$
- $1.6t \pm 0.1t$
- $1.9t \pm 0.1t$

MOF Laminate Thickness Optimization KPIs Mapping



MOF laminate thickness sensitivity



At $1.4t$ -$1.8t$ thickness, higher productivity (VVC) was observed, and a lower steam ratio was recorded at ~$1.5t$ thickness.

Note:

- x: Bed voidage
- y: Permeability
- t: Laminate thickness

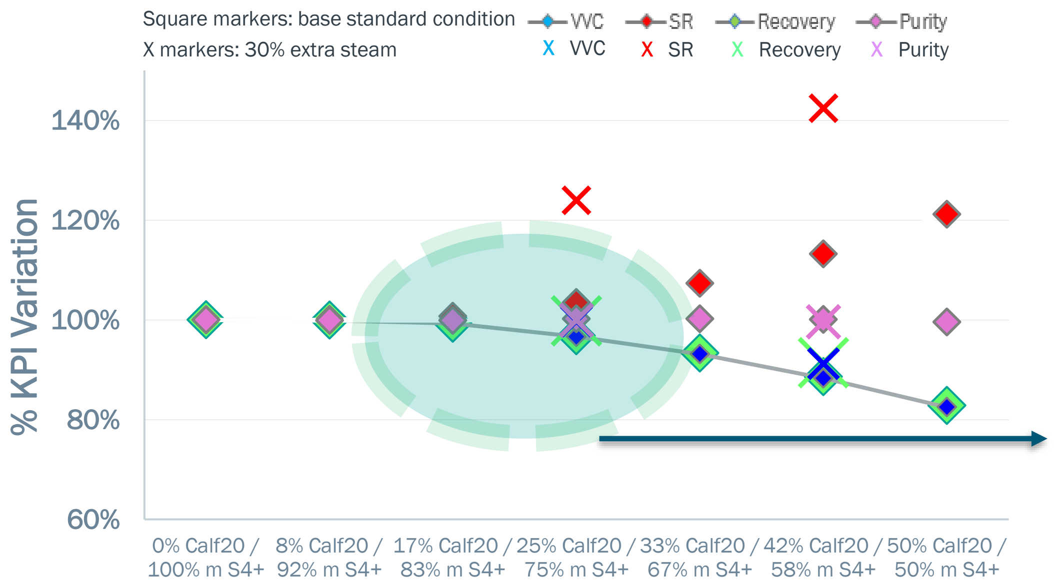
Category 1
Low Concentration CO_2
OTSG Application

Segment’s Length Optimization

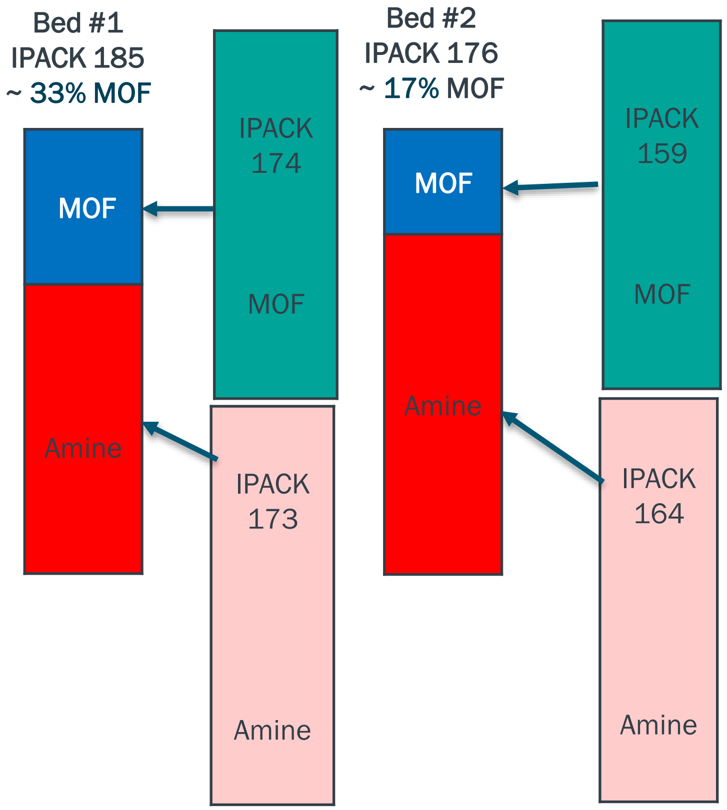
(Category 1- OTSG Application)

Two VTS beds with different MOF segment lengths were built for the proof of concept in category 1 [Low CO_2 concentration]

VTS results for these beds show potential replacement of Amine with MOF on top 17% cm without much impact on KPIs



Category 1- Segment Length Sensitivity Analysis (ADSIM model results)



Based on this optimization and under this modelling condition, incorporating a 17%-25% MOF segment in a segmented bed is recommended for the final VTS bed structure for Category 1

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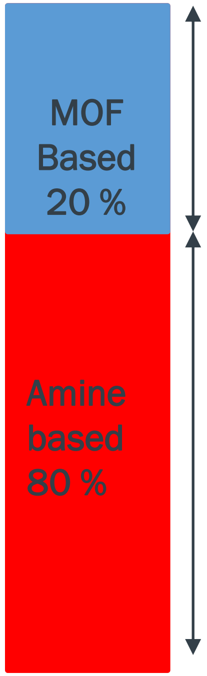
Segmented Bed Final VTS Bed-IPACK274 OTSG application(Category-1)



OTSG application(Category-1) Feed: 10% CO_2, 4.8-5.0% H_2O in feed			
KPI	Amine bed Std. configuration	Final Segmented Bed (20% MOF/80% Amine)	Program Target KPI
Productivity [TPD/M^3]	12.2	12.3	>11.0
Recovery [%]	84	>95	>90
Prod. Purity [%]	93.3	95.5	95
Steam Ratio	2.1	2.1 ± 0.2	< 2

These VTS results allow confirming that the model and test results were aligned. **The PDU bed geometry was finalized at this stage and the next step will be PDU testing to study the bed lifetime of the Segmented bed on the OTSG application.**

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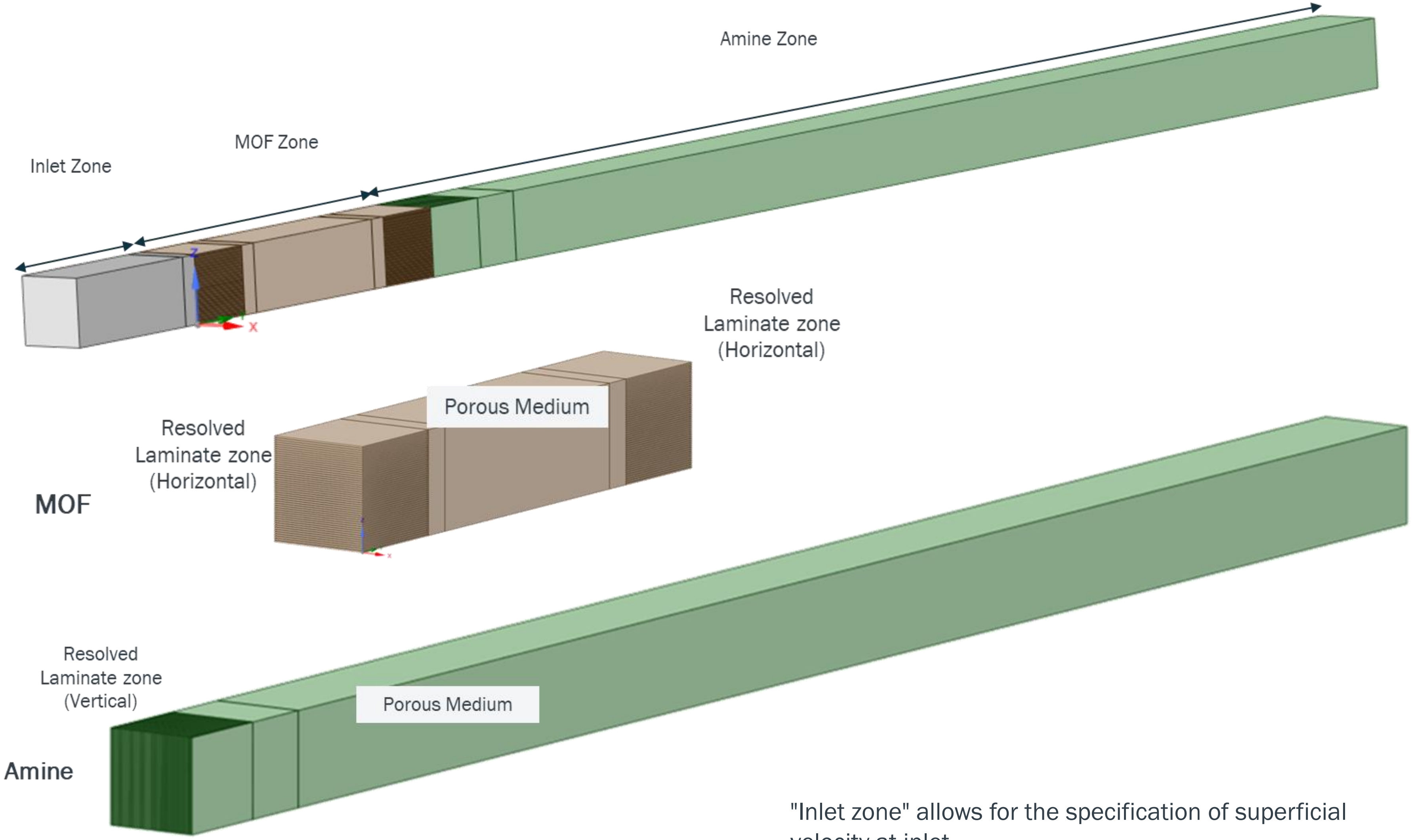
CFD Modelling

Full Solid CAD Model

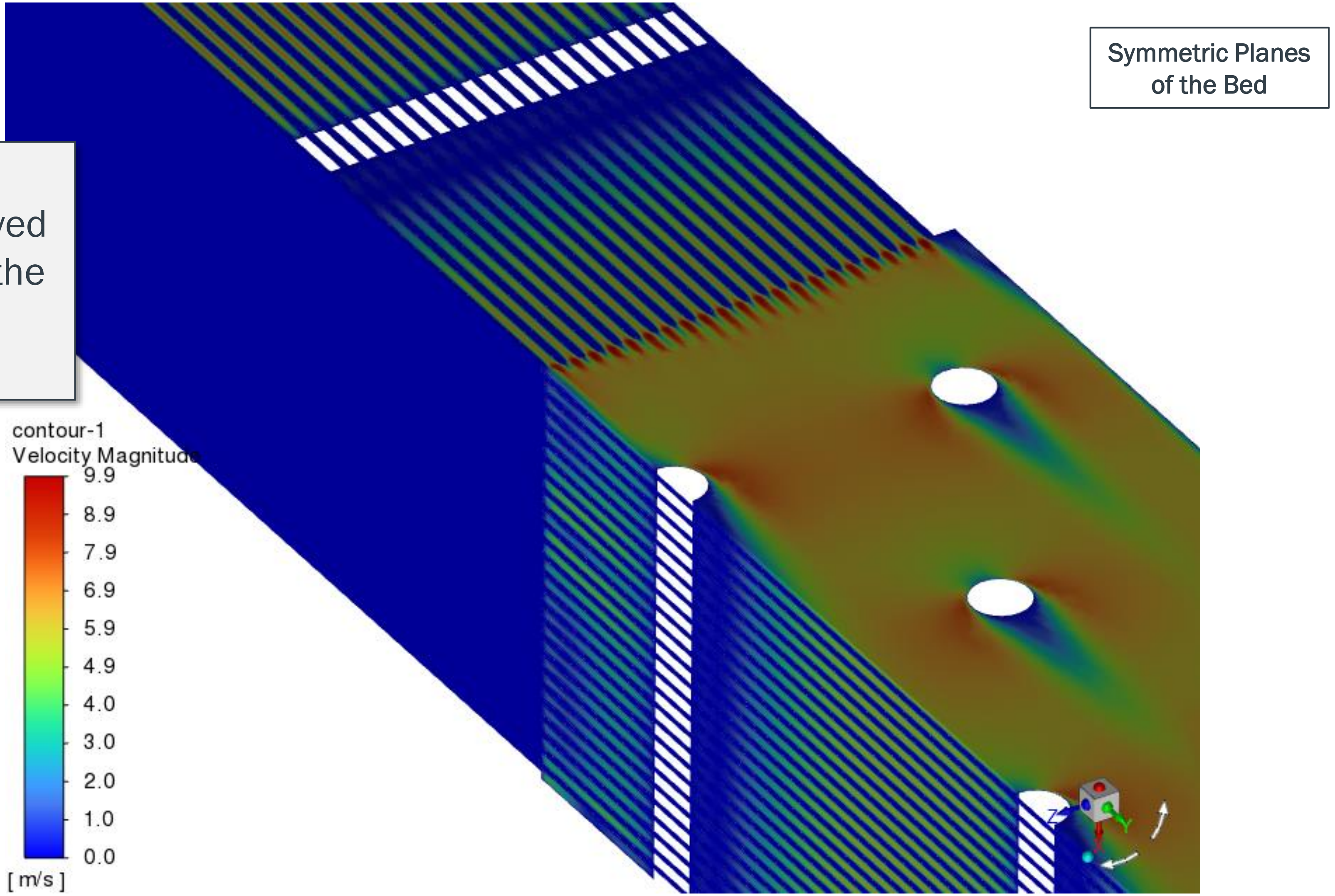
The goal is to develop a model that will accurately represent the pressure drop and velocity at the interface and throughout the length of the bed, among other factors.



"Inlet zone" allows for the specification of superficial velocity at inlet

CFD - Velocity Contours at MOF and Amine Interface

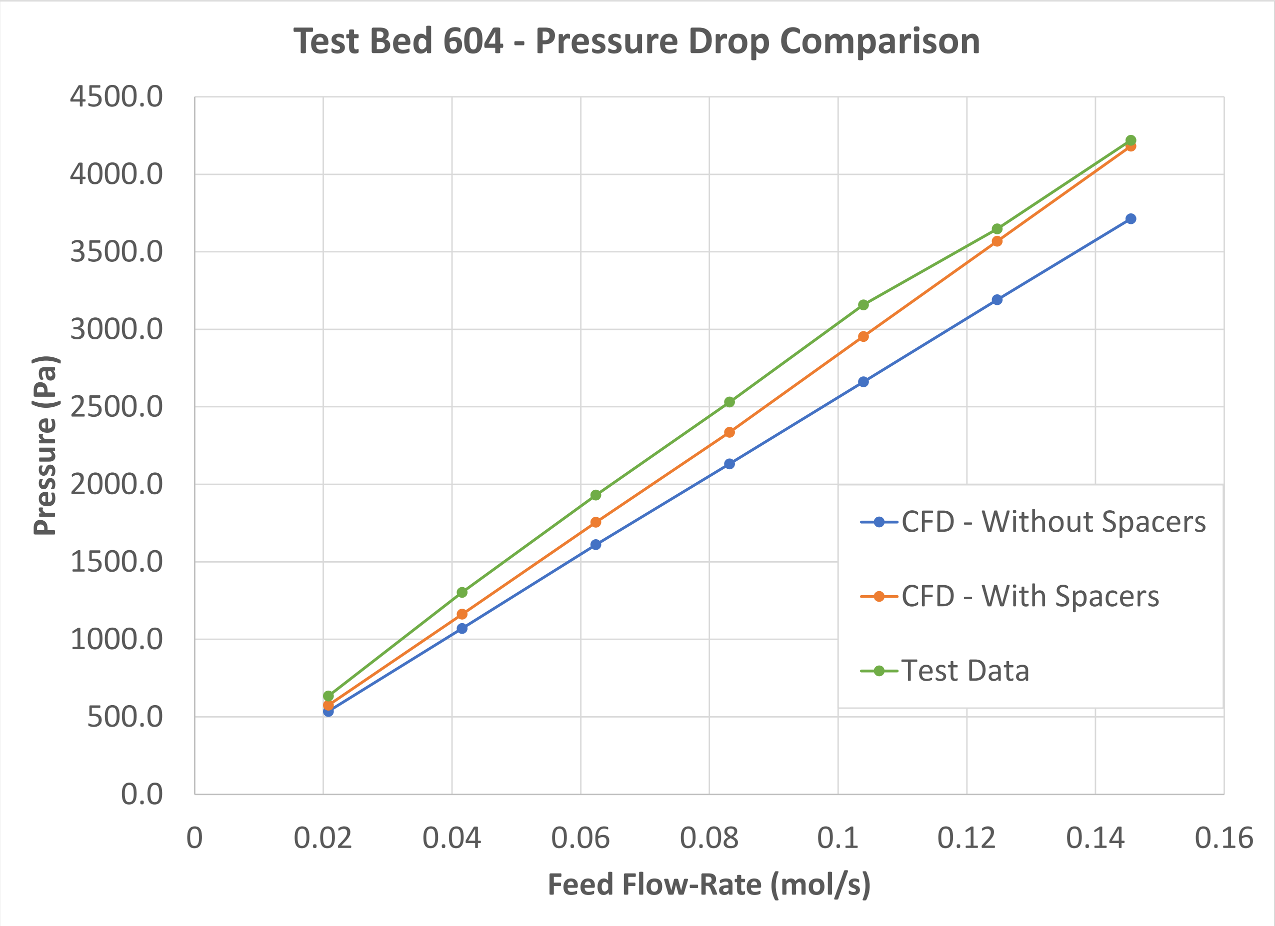
- Velocity spikes at the interface can be observed as well as flow around the spacers



Velocity Contours at MOF and Amine Interface for 0.15 mol/s Flow-Rate

Pressure Drop Comparison With and Without Spacers

- Graph shows the pressure drop values for CFD and testing at different feed flow rates
- By adding spacers in CFD model, pressure drop has increased, and the results match better with the test data
- Currently, the spacers are modelled as cylinders instead of dots. That might have some additional effect on the pressure drop



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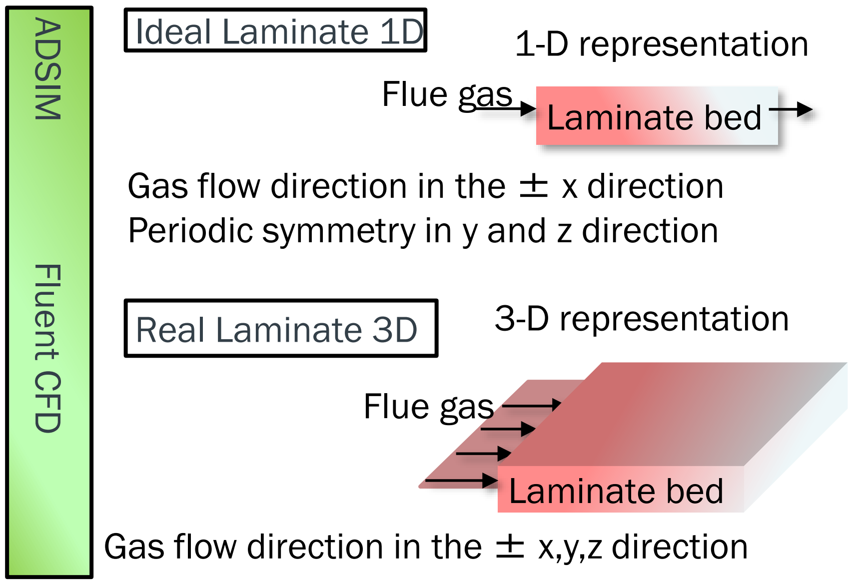
Fluent User defined function (UDF) Modelling

The Svante team is currently modelling the adsorption and desorption of gases in the structured adsorbent beds (SABs) in ANSYS Fluent. This work will allow to:



What can 1D1 adsorption not do well?

- Estimate flow mal-distribution / Flow channeling
- Estimate the gas dispersion in laminates
- Pressure drop under high throughput flows
- Pressure drop for complex geometries

Fluent CFD + Adsorption UDF - 3D adsorption simulation:

- Solve Mass & Momentum balance + Adsorption
- Solve Heat balance + Heat of Adsorption
- Validate the 3D Adsorption model as porous media
- Model Laminate bed

Validated models can help us optimized:

- **Geometry of the structure / Laminate**
- **Channel sizes / Laminate thickness / Spacer Pattern**

Final goal

- **Optimize laminate structures / segments**

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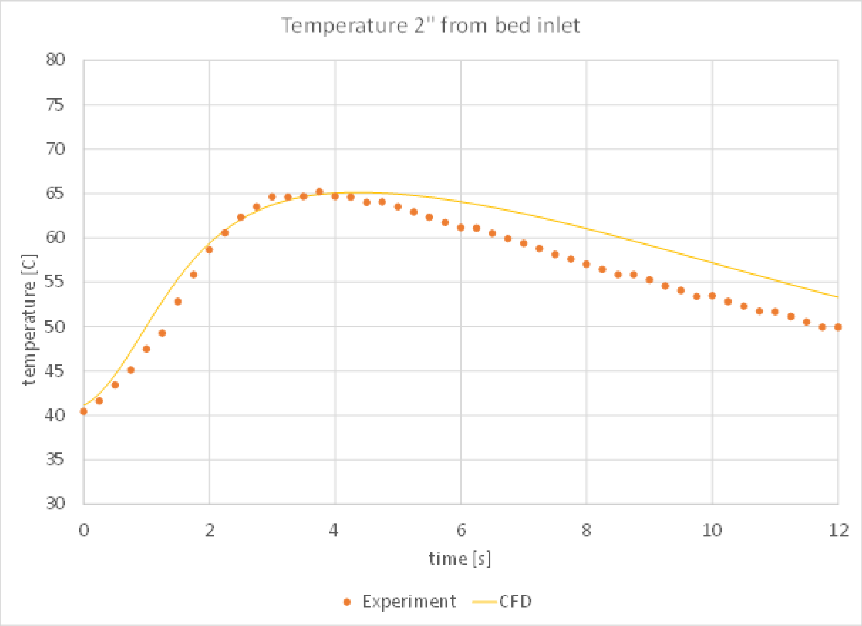
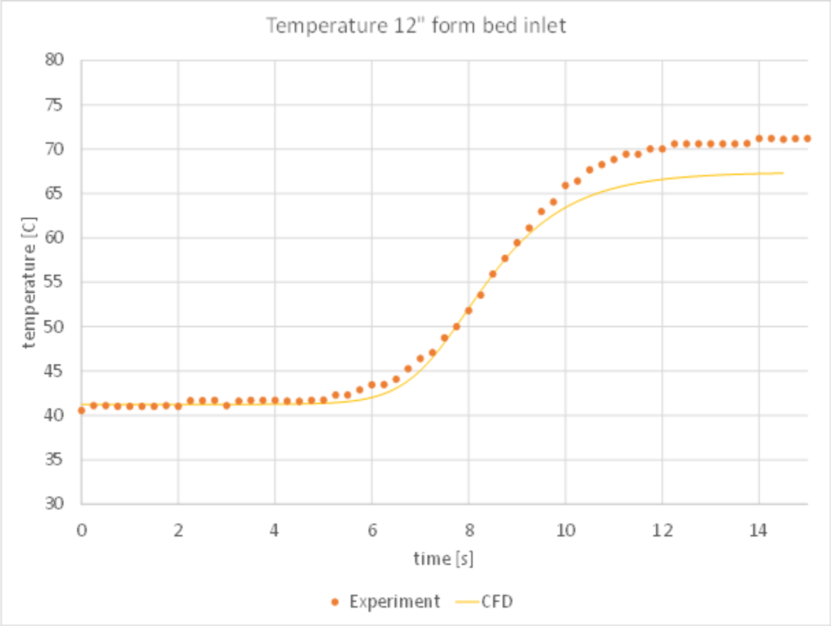
Model Verification

Results – Dry feed / Dry bed





- Bed contains and feed initially 100% N2
- 0.105 mole fraction CO2 added at inlet at time = 0 s
- Temperature measured 2” downstream of the bed inlet

- Bed contains and feed initially 100% N2
- 0.105 mole fraction CO_2 added at inlet at time = 0 s
- Temperature measured 12” downstream of the bed inlet
- Simulation of outlet CO_2 concentration in progress

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Future Tasks

- Long-term testing for both low concentrations (OTSG application) and high concentration (Cement applications) of the segmented bed geometry to confirm the initial KPIs and long-term stability (minimum of 2000 hours).

- Continue UDF (User Defined Functions)/Fluent model development for simulation adsorption and desorption of CO_2 - Adding effects of H_2O on adsorption and desorption

- TEA (Susteon) and maturation plan

Acknowledgment

This project was made possible by the support and hard work of an amazing team, including:

- DOE/NETL
  - Andrew Jones
  - Carl P. Laid
  - Jacqulyn M. Wilson
- Susteon
  - Ragubir Gupta
- BASF
  - Stefen Marx
- Electricore
  - Deborah Jelen
  - Sara Odom
  - Kathy Fagundo
- Svante R&D team

Appendix A: Organization Chart

ELECTRICORE, Inc. – Prime Contractor and Program Manager

Svante Inc. - Technical subrecipient, responsible for Adsorbent & Structured sorbent bed development and testing

R&D (material + process)
+
CFD
+
Manufacturing

Susteon, Inc. – Technical subrecipient, leading the techno-economic analysis (TEA)

DNV GL Technical subrecipient on Phase1 , responsible for process modelling and simulations

Appendix B: Program Schedule

Svante

Task Name
Task 15.0 – Segmented Bed CALF20/S4+(Gen 1) - Structured Adsorbent Bed Development
15.1 Optimize each Segment coating (density, thickness)
15.2 CALF20 & S4+ Segments length study Optimizing (each Segment length) for each category
15.3 Develop bed packaging for segmented bed concept
Task 16.0 – Segmented Bed CALF20/S4+(Gen1) - Process cycle Development and optimization for higher KPIs/longer bed lifetim
16.1 Bench-scale VTS testing
16.2 VTS beds data analysis
Task 17.0 – Segmented Bed CALF20/S4+ - Modeling of segmented bed to guide the bed design/process optimization
17.1: Modeling & simulations of individual segment
17.2: Segmented bed simulation and optimization
17.3: Test data analysis and model verification for final segmented bed optimization
17.4 2D modeling & simulation
Task 18.0 – VTS beds Autopsy, characterization in detail and report
Task 19.0 – High recovery mapping on final segmented beds
19.1 : Category 1/ 10% CO2 - High recovery mapping
19.2 : Category 2/ 16-17% CO2 - High recovery mapping
Task 20.0- Design and fabrication of multiple structured adsorbent beds for multi-bed cyclic steady-state performance assessmen
20.1: Sets of up to 8 or more full-length adsorbent beds will be produced, fabricated, and constructed
20.2: Process cycle design and mechanical implementation
Task 21.0- In-House PDU testing, data analysis, model verification and report
21.1: Unit commissioning and base case KPI demonstration testing of segmented bed
21.2: Durability test of segmented beds
Task 22.0- 2 PDU beds Autopsy, characterization in detail and report
Task 23.0- Design and Fabrication of optimized segmented bed for 1 TPD unit
23.1: Design of 1 TPD segmented bed
23.2: Fabrication of 1 TPD segmented beds/55 beds
Task 24.0- Process testing the optimized segmented bed unit

CFD: Ongoing

Completed

PDU Test: Ongoing

1 TPD Bed Building: Ongoing