ADVANCED STRUCTURED ADSORBENT ARCHITECTURES FOR TRANSFORMATIVE CARBON DIOXIDE CAPTURE PERFORMANCE

Project Number DE-FE0031732

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U.S. Department of Energy

National Energy Technology Laboratory

Carbon Capture

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Program Overview

- Total Funding: $3,774,983
  - Federal Funds: $2,999,904
  - Cost Share: $775,079
- Project PoP: May 2019 – July 2021
- Overall Project Objectives:
  1. Demonstrate energy reduction potential from Advanced Structure Adsorbent with greater than 30% reduction in Steam injection per MT of CO_2.
  2. Preserve other KPIs of RC-TSA* process and update TEA for new structure.

*Rotary Contactor (RC) – Temperature Swing Adsorption (TSA)

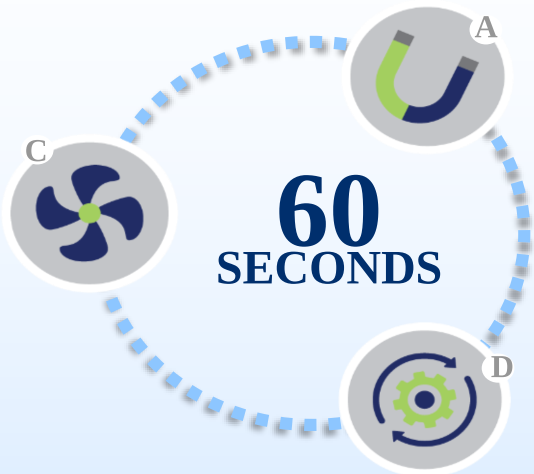
Program Overview

Project Participants:

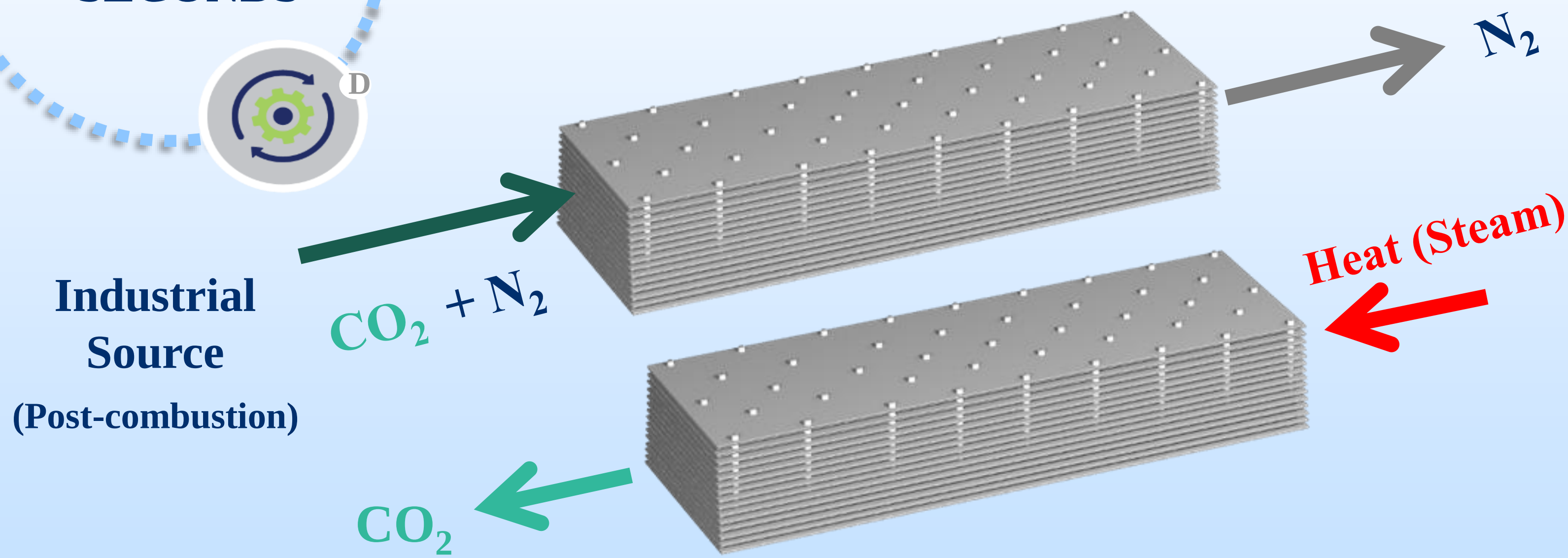
- Electricore, Inc. – Prime Contractor and Program Manager
- Svante, Inc. - Technical subrecipient, leader in large-scale CO_2 capture responsible for structured sorbent bed development and testing.
- DNV GL USA Inc. - Technical subrecipient, responsible for identification, development and updating critical documents including TMP and EH&S. DNV will also perform process modeling and simulations.
- Susteon, Inc. - Technical subrecipient, leading the techno-economic analysis (TEA).

*Rotary Contactor (RC) – Temperature Swing Adsorption (TSA)

Technology Background



RC- TSA with Structured selective CO_2 Adsorbent



- High bed productivity 10 Tonnes of CO_2 per m^3 of sorbent per day range
- Strong Capex advantage for contactor (RAM) at intermediate capture scale.
- Some energy penalty with difficult to recover heat stored in solids.

Technology Background

- Prior to program: demonstrated RC-TSA RAM technology with amines doped silica sorbent materials at 0.5 Tonnes / day scale.
- Identified potential MOF for RC-TSA with very good stability to moisture swing.

Fundamental performance enablers:

- **Very fast kinetics with contact time < 1s, 50-80s total cycle time.**
- **Contactor with very high surface area**
- **Low flow resistance of parallel channel structure.**
- **Low heat capacity relative to adsorption capacity.**

Significant challenges:

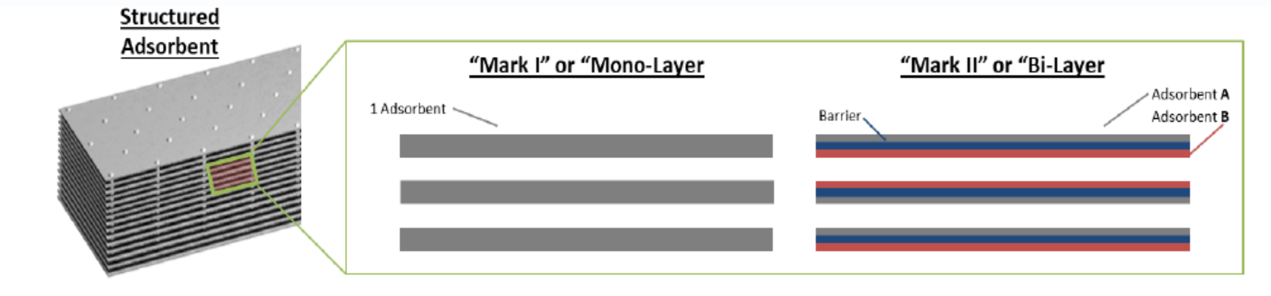
- **Sorbent lifetime needs to be years (3-5 yrs.)**
- **Cost of sorbent structure have to be modest (20-30 $/kg)**
- **Energy intensity of process needs to be minimized**

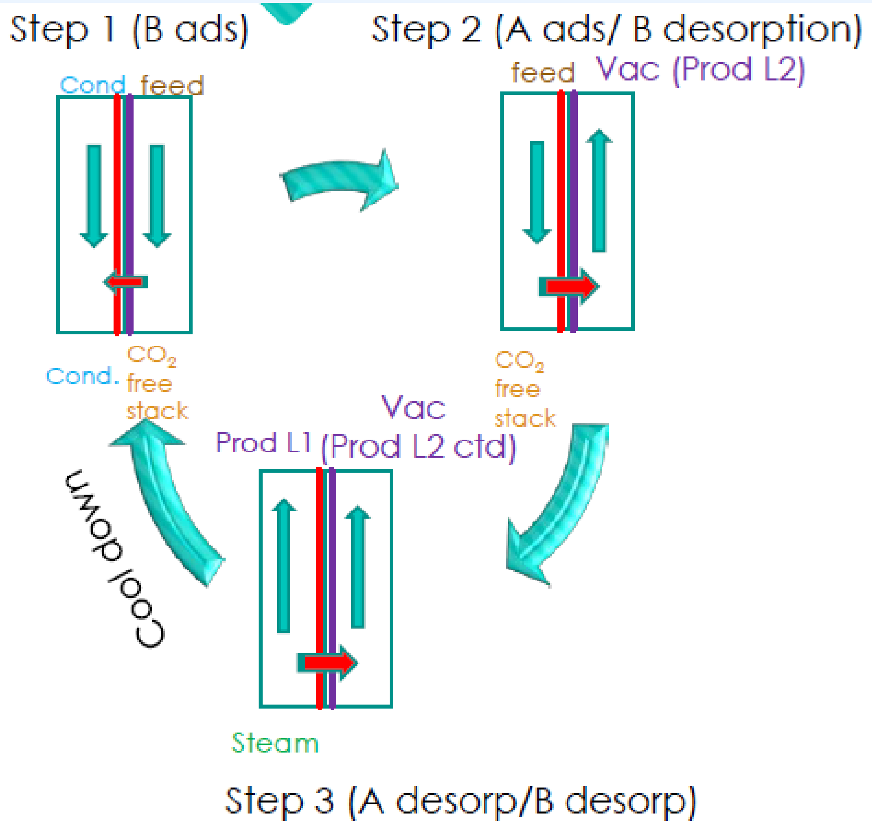
Technical Approach

Use new engineering design to create an advanced structure adsorbent for RC-TSA to:

- Optimize thermal management in Moisture Swing Adsorption –
  - Enable synergistic design and reduced amount of steam injection
- Create two different regeneration environments
  - Potential for increased capacity with high capacity sorbent material with fast regeneration.
- Expand the material choice to non-steam stable adsorption material (ex. MOF)
  - Part of the sorbent can have lower heat of desorption and use the heat generated in the other sorbent w/o using hot steam as a carrier gas

Structured Bed with Heat Exchange





Layer A:
-Steam compatible
-High heat of adsorption (>70kj/mole)
-Water promotes CO_2 ads
-Fast kinetic

Layer B:
-Low CO_2 heat of desorption (<40kj/mole)
-Air stable up to 120°C
-Stable to feed moisture content
-Fast kinetic

Project Scope – BP1 Complete

Task/Subtask Number	SOPO Task/ Subtask Title	Completion Date
1.0	Project Management and Planning	04/30/21
2.0	Technology Maturation Plan	04/30/21
3.0	Adsorbent Selection, Characterization and Synthesis (Phase I)	04/30/20
3.1	Finalize candidate adsorbent materials for Bi-Layer program	07/30/19
3.2	Thermodynamic equilibrium measurements of candidate adsorbents	04/30/20
3.3	Dynamic characterization of kinetic behavior of adsorbents	04/30/20
3.4	Flue gas compatibility study – contaminants, composition, and condition	04/30/20
3.5	Adsorbent Down-Selection and Production	04/30/20
4.0	Bi-Layer Laminated Structures Development (Phase I)	04/15/20
4.1	Barrier material selection and optimization	04/15/20
4.2	Bi-Layer coating development	04/15/20
4.3	Bi-Layer spacer and flow-path control printing	04/15/20
4.4	Bi-Layer laminate structure development	04/15/20
5.0	Bi-Layer Structured Adsorbent Bed Development and Design	05/31/20
5.1	Bi-Layer structures packaging development	04/30/20
5.2	Bi-Layer Bed fluid distribution analysis for independent process streams	12/31/19
5.3	Bi-Layer Bed Design	05/31/20
6.0	VTS Modifications for Bi-Layer Bed Testing	05/31/20
7.0	Bi-layer Bed Bench-Scale Testing (Phase I)	07/31/20
8.0	Computational Modeling and Process Simulation (Phase I)	07/31/20

Solid Sorbent Selection

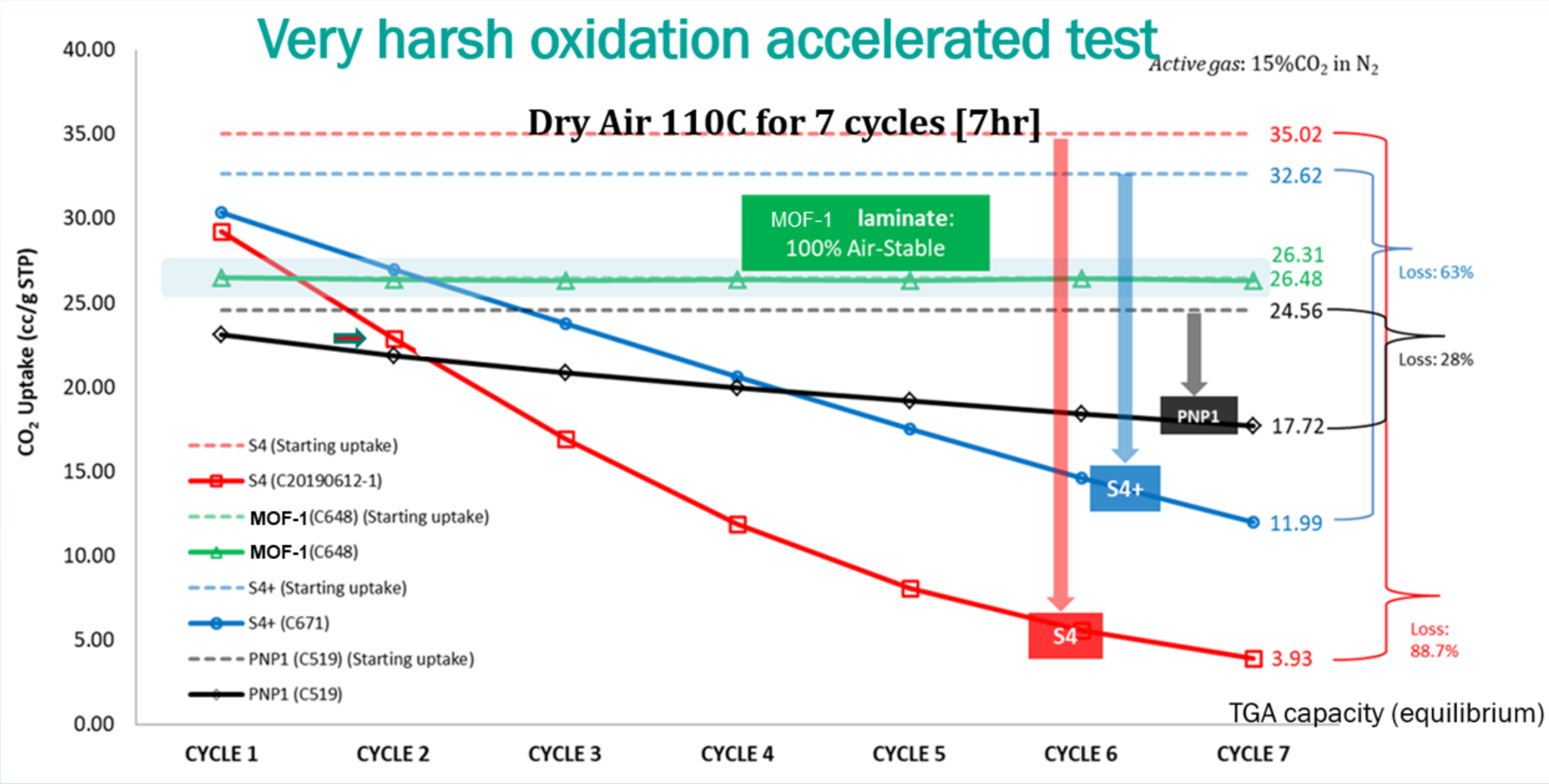
- **Subtask 3.1 - Finalize candidate adsorbent materials for Bi-Layer**
  - Down selection of the first set of sorbent material for Gen-0 Bi-layer bed design was based on the following criteria:
    - Critical Technology Element (CTE) criteria 1A and 1B,
    - Material availability, and
    - Prior demonstration of ability to form a laminate structure with the sorbent with minimal loss of adsorption capacity.
  - The list of down selected sorbent is provided below.

Side A sorbent	Water tolerance	Heat of CO_2 adsorption	Available at Kg scale	Laminate process
S4+ Doped silica	Very Good	about 90 kJ/mol	Yes	Yes
PNP-1 Porous polymer	Excellent	about 90 kJ/mol	Yes	To be optimized
S4 Doped silica	Vapor only	about 95 kJ/mol	Yes	Yes

Side B sorbent	Water tolerance	Heat of CO_2 adsorption	Available at Kg scale	Laminate process
MOF-1	Excellent	about 35 kJ/mol	Yes	Yes
MOF-2 (aminated)	Poor	about 56 kJ/mol	Yes	Yes

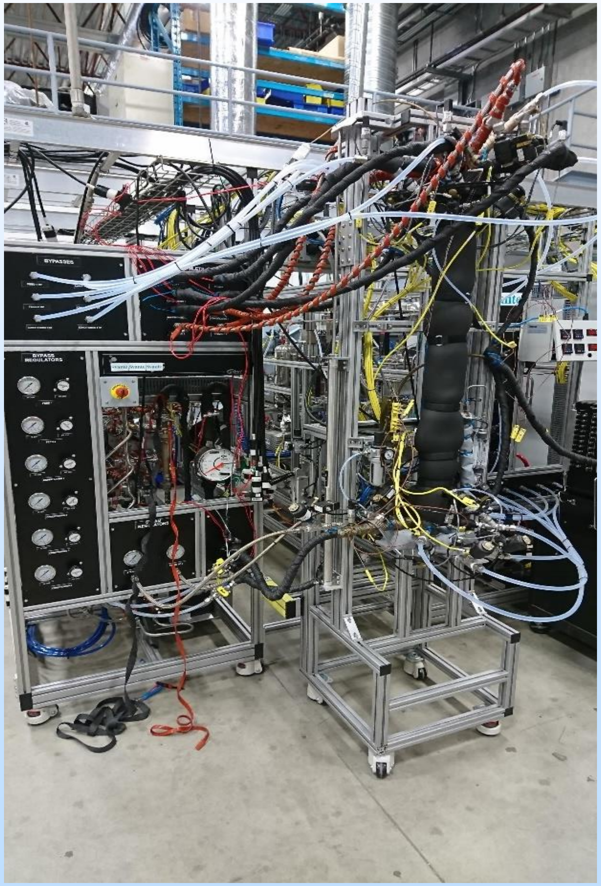
Solid Sorbent Stability

S4+ and MOF-1 showed good O_2 resistance in accelerated tests



RC-TSA – Single Layer KPIs

Subtask 3.3 - Dynamic characterization of kinetic behavior of adsorbents



Veloxotherm Testing Station II – picture – 0.5 to 1L adsorbent beds

- Multiple VTS testing beds were manufactured and optimized (structure sorbent and cycle) to match cycle times between the both sides of the bi-layered.
- Cycle time need to be short <60sec to minimize water pickup form the feed on MOF-1

10% CO_2, 5% H_2O in Feed	S4+ (PEIDS) bed	
Total Cycle time [Sec]	**50**	Fast Cycle
Productivity [CO2 T/m3 day]	**14.1**	Very high productivity
Recovery [%]	**81**	
Prod. Purity [%]	**85.5**	

17% CO2, 5% H2O in Feed	MOF-1 bed	
Total Cycle time [Sec]	**50**	Fast Cycle
Productivity [CO2 T/m3 day]	**9.6**	High productivity
Recovery [%]	**85**	
Prod. Purity [%]	**94.3**	

Material Scale Up

Subtask 3.5 - Adsorbent Down-Selection and Production

- Out of the five adsorbent candidates selected two were chosen
  - ❑ Side A: S4+
    - o Relatively high heat of adsorption, water and steam resistant, fast cycle, high productivity, better oxidation resistance
    - o Slurry and coating optimization still needs to be done for large scale
  - ❑ Side B: MOF-1
    - o Low HOA, **water and steam resistant**, low temperature (RT) and low pressure (1 ATM) synthesis using commercially available raw materials (**easily scalable**), high oxidation resistance
- The adsorbent and coating processes necessary for proof of concept for the Bi-layer bed design are complete.
- *> 200kg of the MOF-1 have been produced at Svante with evaluation of multiple suppliers leading to successful reduction in raw material and processing costs.*

Sorbent Process Model

Dynamic Computational Modeling and Process Simulation – single layer

- Single layer models for the preferred adsorbent layers have been developed and validated using VTS data. Objectives included:
  - ❑ Model the individual adsorbent layers to closely understand the dynamics of each layer during the process steps
  - ❑ Evaluate and validate modeling results in detail using test data under the same process condition
  - ❑ Deliver modeling inputs for the software capable of handling the Bi-layer modeling dynamics

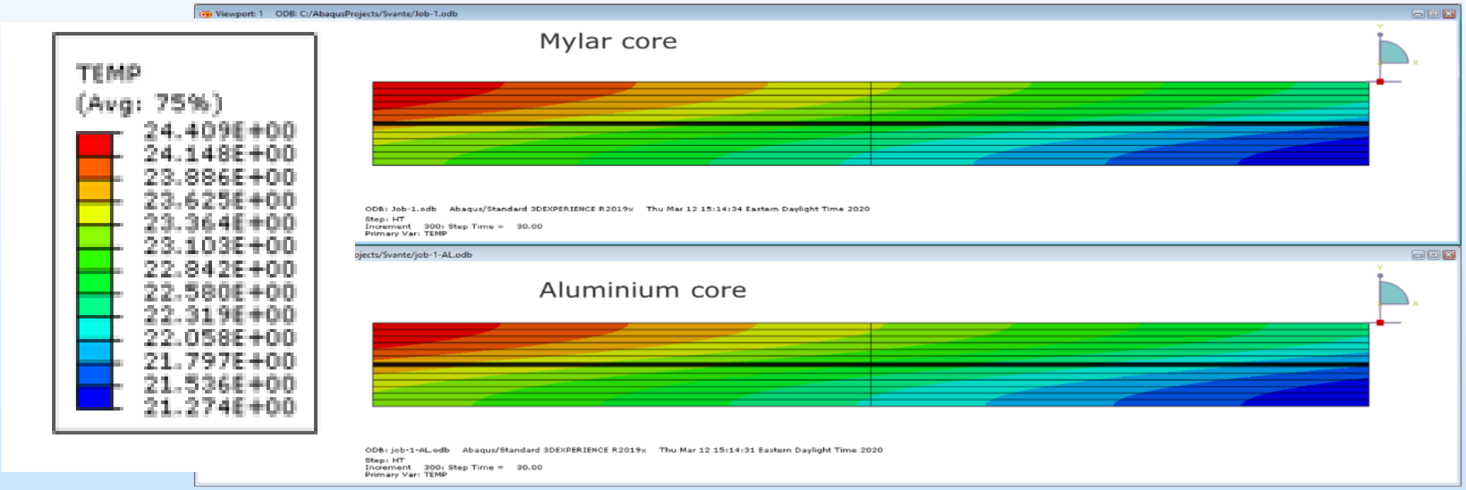
High level model verification results of two adsorbent candidates for bi-layer project

KPI	S4/S4⁺ - cycle without Reflux		Calf20 - cycle with Reflux	
	Test results	Dynamic model results	Test results	Dynamic model results
Recovery [%Out/In]	84%	85%	88%	91%
Purity [vol% CO_2]	88.5%	89%	89%	90%
Steam Ratio [wt H_2O/wt CO_2]	1.98	1.9	2.1	2.09

- ➢ Successfully modelled dynamic behavior and cycle KPIs using measured sorbent isotherms
- ➢ Provide greater insight in coupling of heat generation and desorption of CO_2 induced by H_2O adsorption and competitive CO_2, H_2O adsorption.

Modelling of Heat Released and Transferred Through the Barrier

Use transient adsorption model from single layer to compute heat duties to simulate bi-layer dynamic temperature profiles.



Modeling of 2D temperature profile through laminate (DNV-GL)

Down selected Aluminized Polymer-1 for process scale up to VTS bed size (m^2 scale)

Barrier thin enough for this application (~10um).

Bed Design and Assembly

Bi-Layer Bed fluid distribution analysis for independent process streams

- Built multiple 0.75L test beds with about 0.8m^2 of heat exchange surface and about 200g of active sorbent.

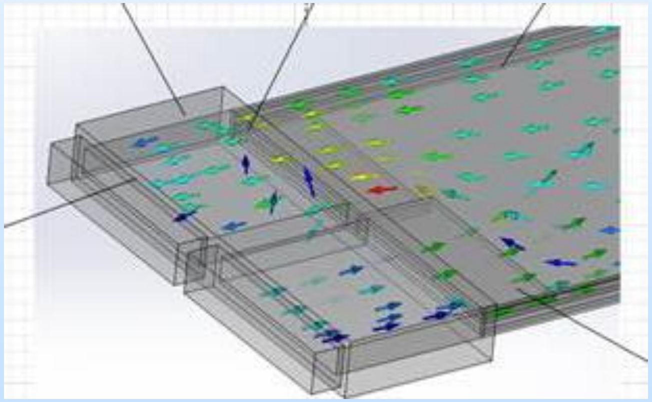


Illustration of flow arrangement (DNV-GL)

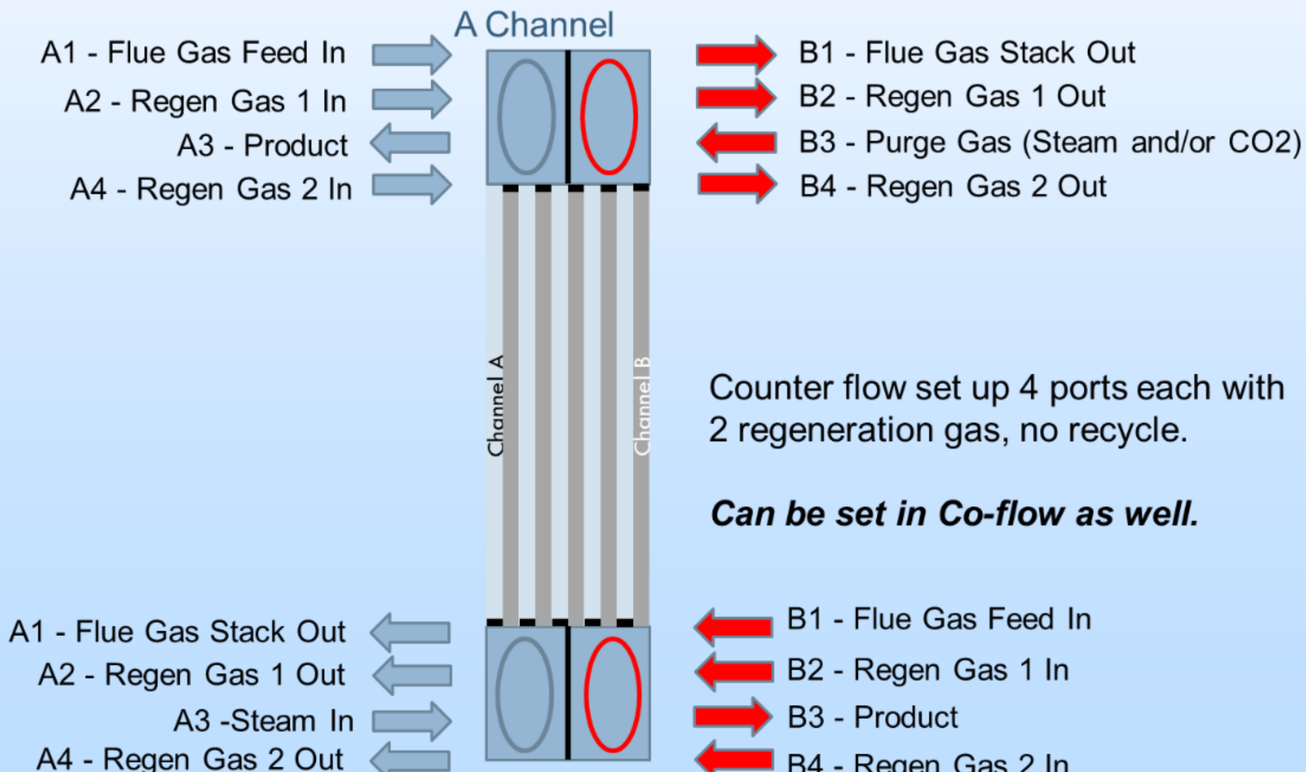
Inlet of 1.16m long bed

Bi-layer bed assembly

Process Testing

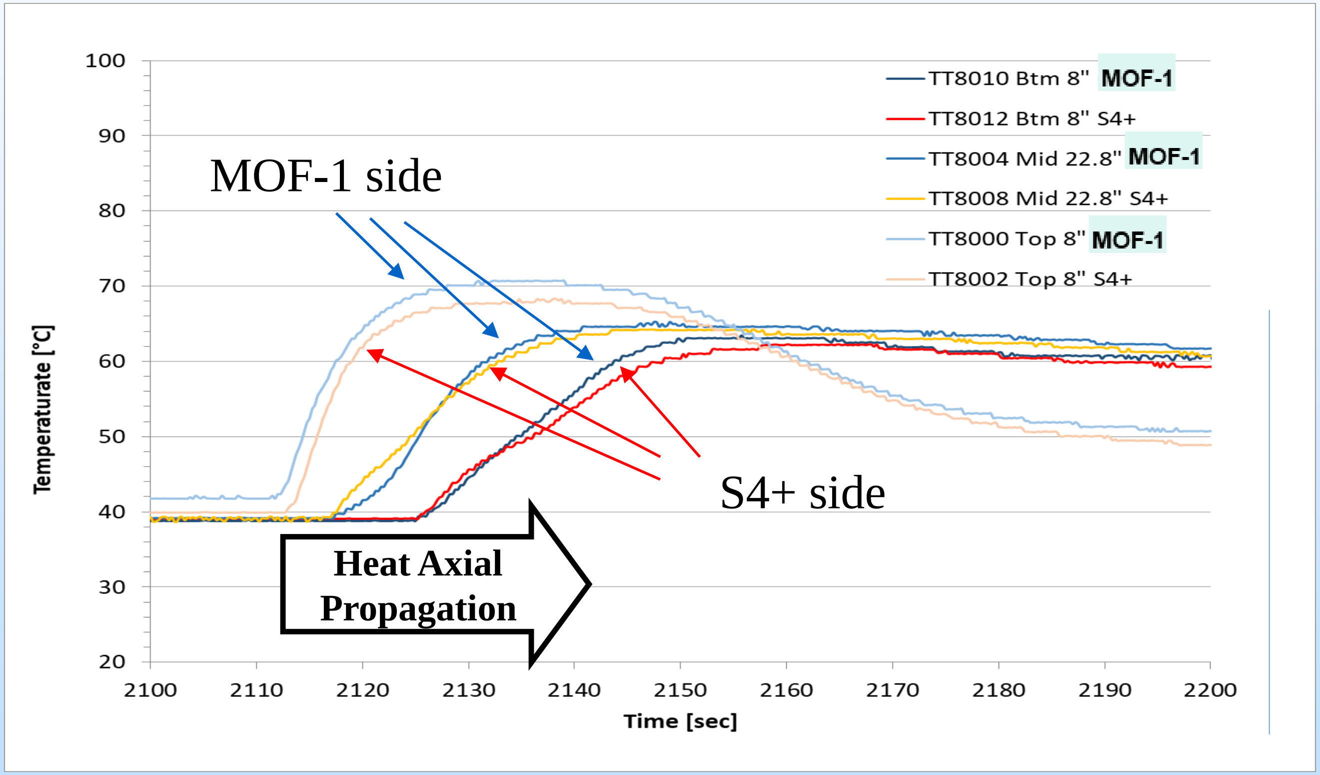
Task 7 - Bi-layer Bed Bench-Scale Testing

- The VTS 2 test station was used to test the single layer beds and commission the unit with its increased feed gas configuration flexibility. New connectors were built to distribute gas connections to channel A and B individually.



Testing – Heat Exchange Through the Barrier

Thermal transfer performance verified experimentally. Almost no lag in temperature rise between layers across the barrier material.

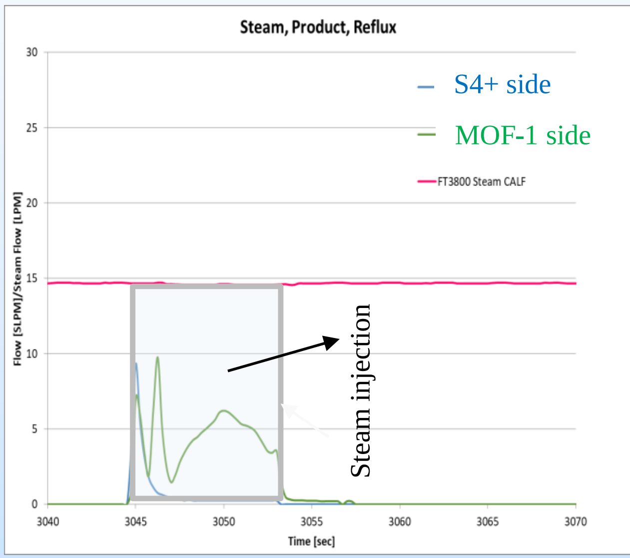


Temperature in A and B channels VS time during BT test

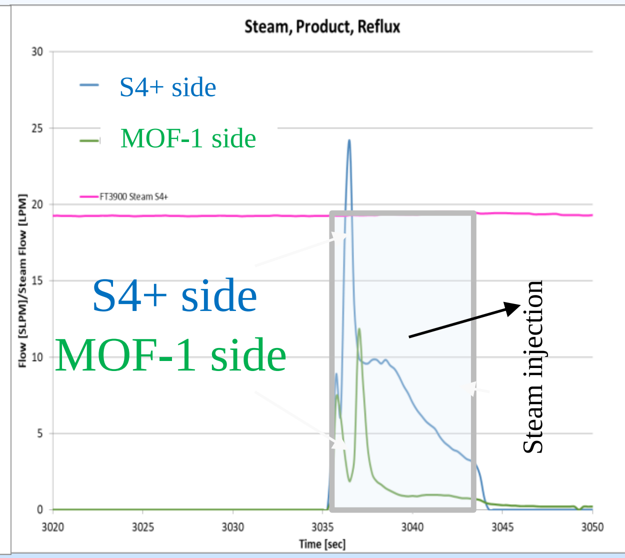
CO_2 injected on one side only (S4+ side)

Cyclic Process Testing – Product Flows

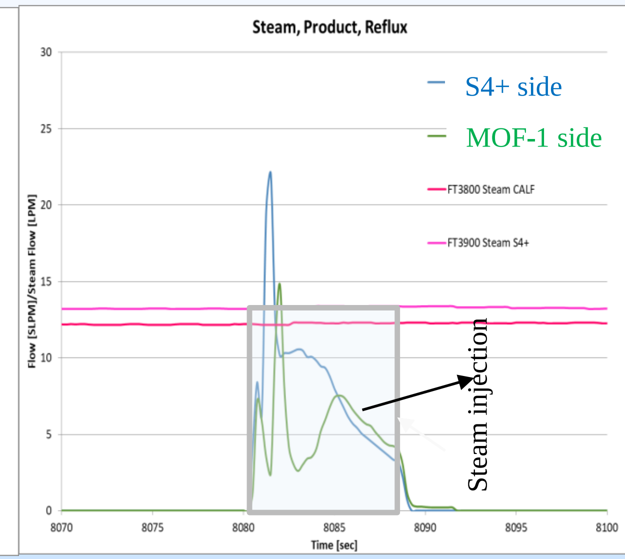
Steam MOF-1 side



Steam S4+ side



Steam On both sides



Comparison on Product flows for different steam injection strategies

- Desorption of CO_2 has large spike after 2s, followed by complex decay.
- Indirect heat fast desorption demonstrated.

Process KPIs for Bilayer Beds

Bed - #3

Steam	SR ratio (relative)	TPD / m3	Purity	S4 CO2/ Total CO2
Both side	1	3.4	77%	64%
S4+ side	0.85	2.7	80.4%	80%

Bed - #4

Steam	SR ratio (relative)	TPD / m3	Purity	S4 CO2/ Total CO2
Both side	1	5	73.3%	55%
S4+ side	**0.64**	2.8	87.2%	85%

Steam Ratio reduction successfully demonstrated twice.

- Steam Ratio dropped 15% and 35% respectively related to dual side steam injection.
  - Meets the end of year 1 success criteria for SR reduction.
- MOF-1 indirect regeneration demonstrated
  - Need flush gas or better vacuum to increase productivity
- Productivity, recovery need to improve.
  - Optimization of coating thickness and process

Summary

Development and initial testing of two very interesting CO_2 capture materials that could be important for CO_2 capture for carbon reduction/removal (Direct air capture, cement and SMR).

Built first successful dual channel parallel film heat exchanger with adsorbent with extremely low mass flow separator.

Demonstrated the manufacturability of device, as well as, effectiveness of heat transport between A and B sides.

Demonstrated fast indirect regeneration of sorbent across barrier layer and found a significant reduction (~35%) in the Steam Ratio by avoiding excess steam addition [In phase operation].

Budget Period 2 Goals

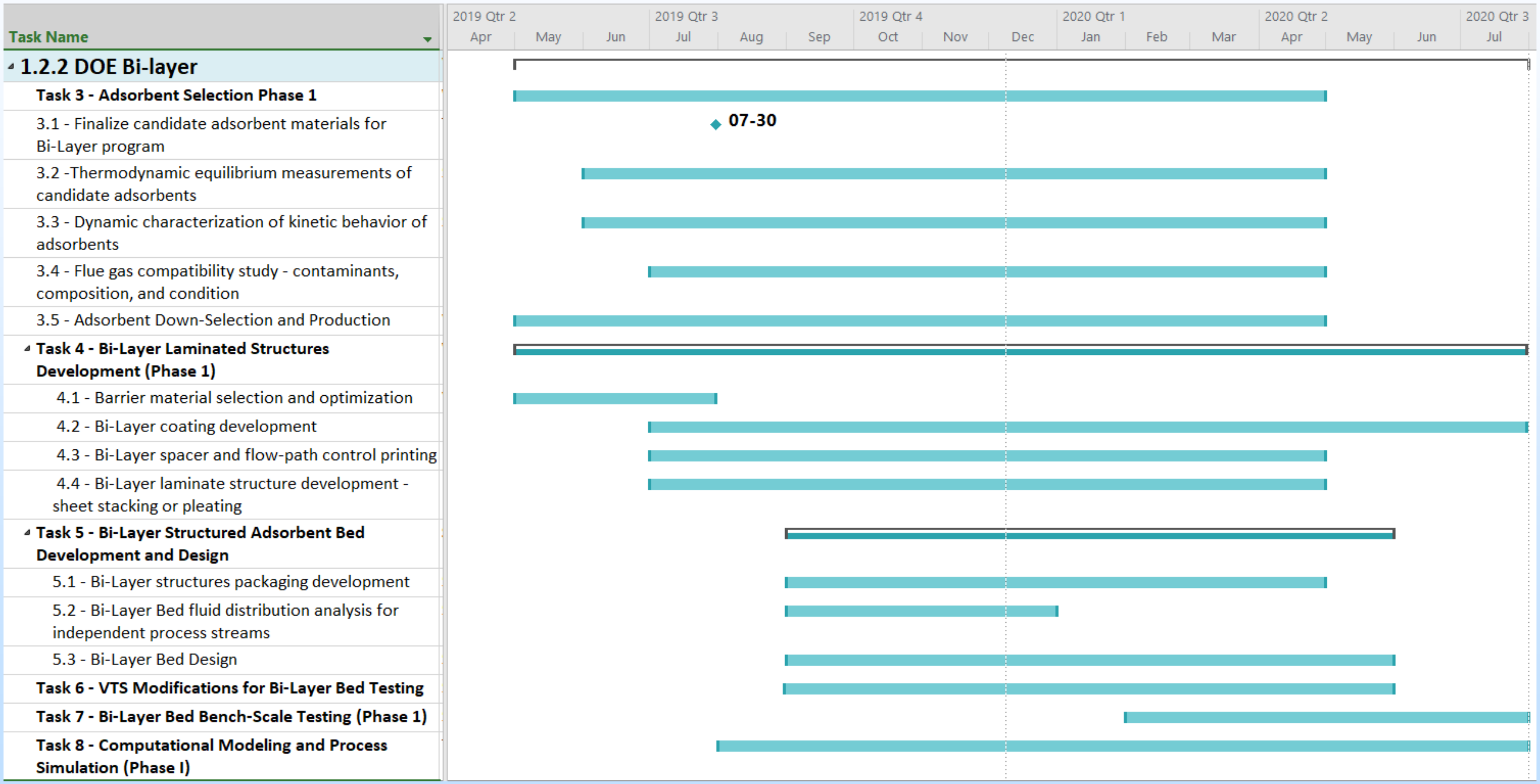
- Bi-layered optimization and testing of the optimized layers
  - Cycle development and optimization
  - Optimization of bed design (parallel vs alternative design)
  - Modelling energy balance
- Optimization of each layers in terms of material and process
  - MOF-1 and S4+
    - Scale-up efforts for MOF-1 (up to 1,000 Kg)
    - Optimized MOF-1 for lower SR
    - Long term field testing (Lafarge Cement site in Richmond BC, Canada, ~ 1TPD)
    - Long term testing of S4+ (synthetic flue gas composition (NG boiler) at external site, 0.1 TPD)
    - Slurry and Laminate optimization
    - Cycle optimization

Appendix

Organization Chart

- Electricore will serve as PRIME contractor and Project Director.
- Svante serves as the main technical point of contact for this project and technology provider.
- Susteon is leading the TEA.
- DNV is responsible for identification, development and updating critical documents for natural gas transmission stations and will perform process modeling and simulations.

Gantt Chart – BP1



Gantt Chart – BP2