Virtual Design of a 4-Bed Molecular Sieve for Exploration

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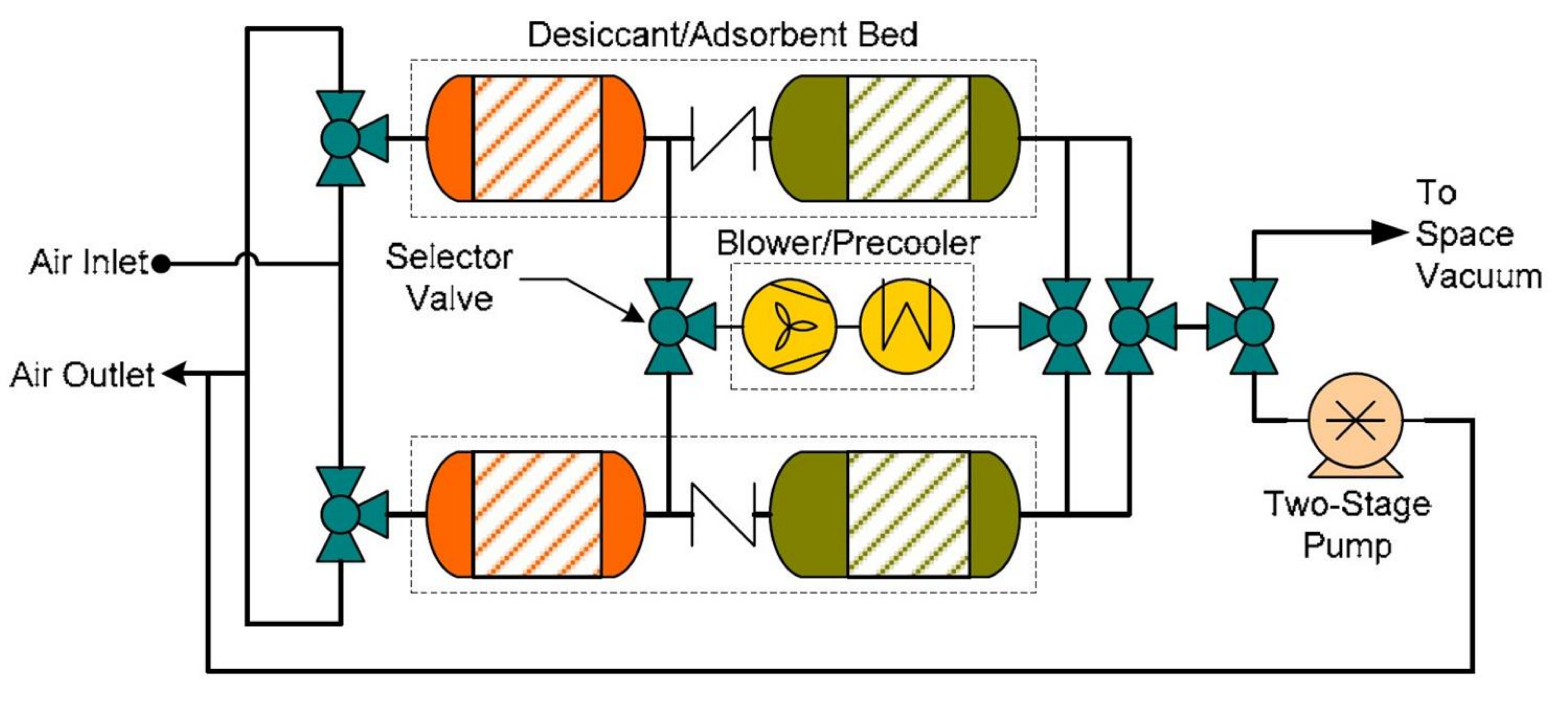
Overview

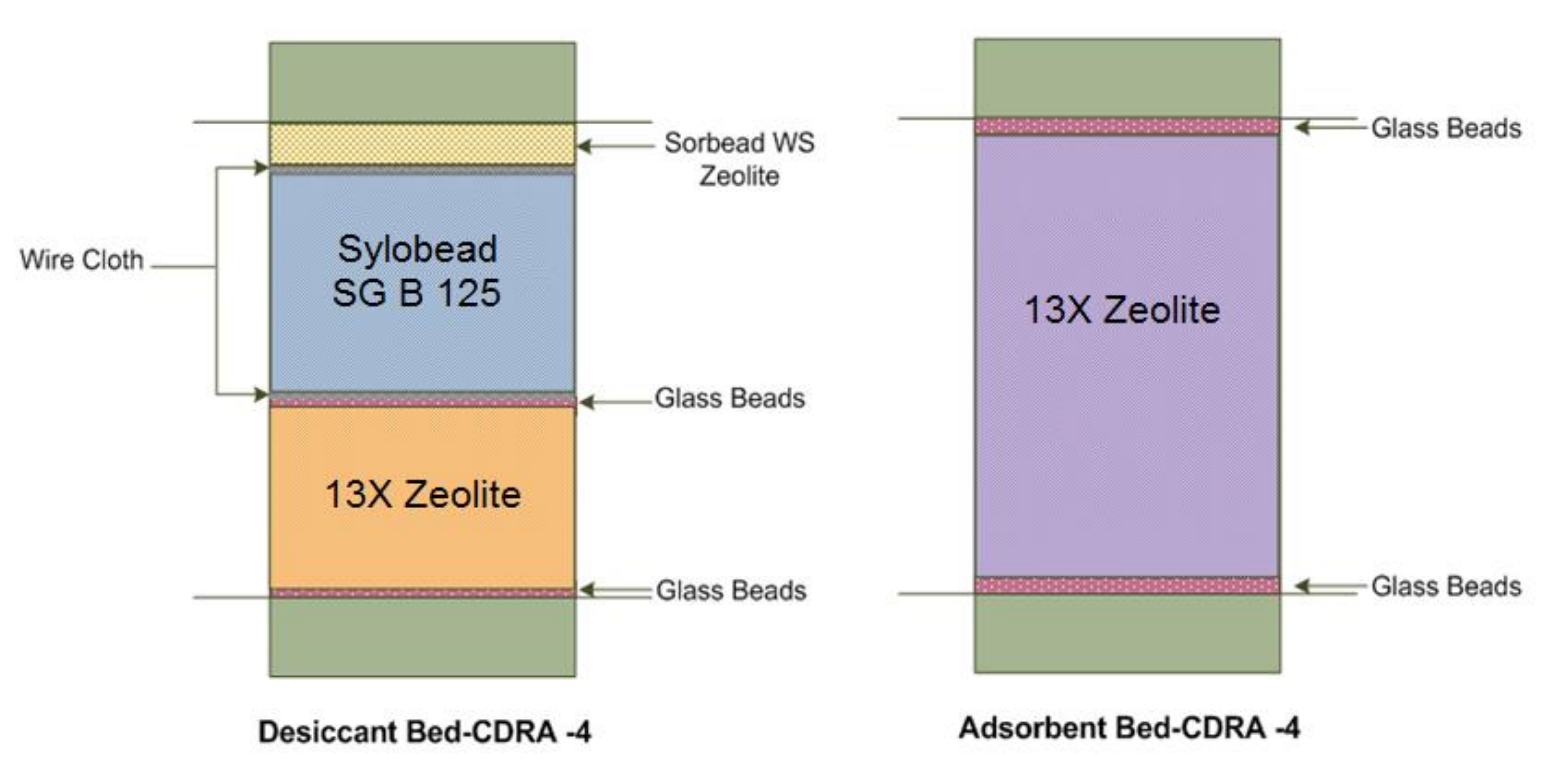
- Background: from CDRA to 4BMS-X
- 4BMS-X modeling using COMSOL
- Current modeling results

Background



Carbon Dioxide Removal Assembly (CDRA)

Background


Wire Cloth
Sorbead WS Zeolite
Sylobead SG B 125
Glass Beads
13X Zeolite
Glass Beads
Desiccant Bed-CDRA -4
Glass Beads
13X Zeolite
Glass Beads
Adsorbent Bed-CDRA -4

Background

- CDRA has known issues
  - Dusting
  - Possibly oversized
- Modeling can assist in guiding next-generation design:
  - Sorbent selection
  - Bed size
  - Half-cycle time
- A 4-bed model has been developed in COMSOL at MSFC
  - Presented at last year's ICES
  - Shown to agree with data from 4-bed system (4EU)

Model Basics

- Four one-dimensional domains, plug flow
- Each domain represents one of the four beds, with the different properties of each material layer accounted for in the model

Other Model Characteristics

- Darcy's law for flow in a porous medium
- Separate heat transfer in sorbent, gas, can, and insulation
- Diffusion in gas phase
- Sorbent loading using experimental isotherm data
- Adsorption rate by experimental LDF parameters
- For further details see reference:

Coker, R.F. and Knox, J.C., "Predictive Modeling of the CDRA 4BMS," *46th International Conference on Environmental Systems*, Vienna, Austria, ICES-2016-92, 2016

Validation of Model

HC	flow rate	CO2 removal rate (kg/day)			efficiency		
(min)	(SCFM)	data	model	delta %	data	model	delta %
155	20.4	3.65	3.35	8.2	0.843	0.789	6.4
90	25.0	4.11	3.73	9.2	0.772	0.716	7.3
90	24.0	3.76	3.70	1.6	0.745	0.696	6.6
215	20.0	3.18	3.12	1.9	0.779	0.749	3.9
172	25.0	4.05	3.90	3.7	0.783	0.749	4.3
144	30.0	4.83	4.62	4.3	0.740	0.740	0.0
123	34.0	5.18	5.44	-5.0	0.712	0.769	-8.0
195	20.0	3.49	3.41	2.3	0.813	0.818	-0.6
154	25.0	4.19	4.30	-2.6	0.812	0.826	-1.7
124	30.0	5.14	5.18	-0.8	0.781	0.830	-6.3
96	34.0	5.69	5.82	-2.3	0.810	0.822	-1.5

- Model was compared with data from CDRA-4EU
- Shown to predict CO_2 removal rate and efficiency to within 10%

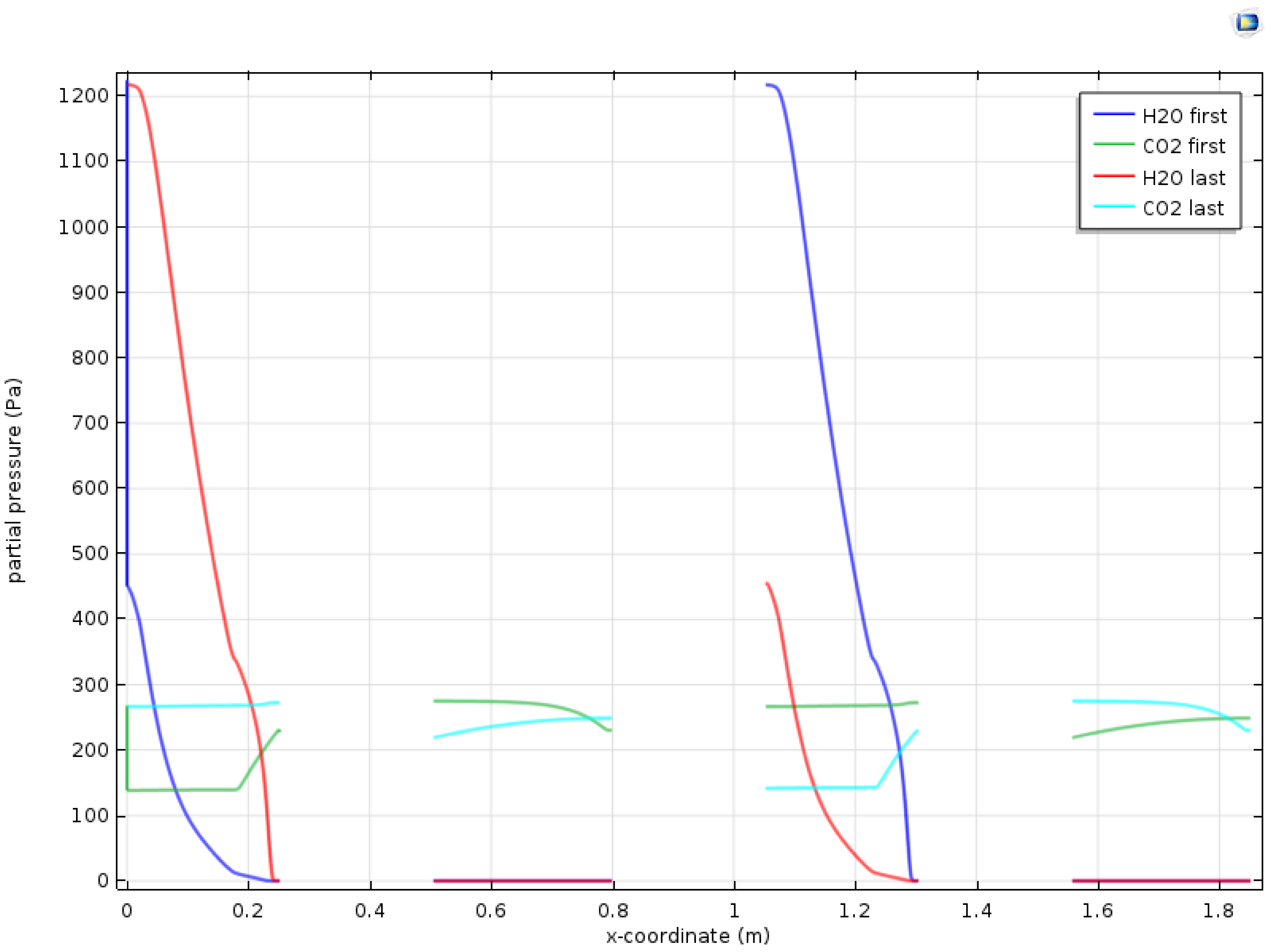
Current Efforts

- Reduced the size of the 13X layer in the desiccant bed by 55%.
- Reduced the sizes of the sorbent beds by 30-60%, depending on sorbent.
- Use four different CO_2 sorbents: Grade 544 13X, RK38 (5A zeolite), APGIII, and VSA-10 (LiLSX zeolite)
- 80 min half cycles
- Flow rates from 24.25 to 28 SCFM
- 2 torr inlet CO_2 partial pressure
- Targeting a CO_2 removal rate > 4.16 kg/day

Current Efforts: Results Summary

CO_2 Sorbent	Flow Rate (SCFM)	% of Nominal CDRA bed	CO_2 Removal Rate (kg/day)	CO_2 Efficiency
RK-38	24.25	70	4.21	0.81
VSA-10	24.25	40	4.32	0.84
544 13X	28	60	4.50	0.76
544 13X	26.75	60	4.47	0.79
APG III	28	55	5.14	0.86
APG III	24.25	55	4.26	0.82

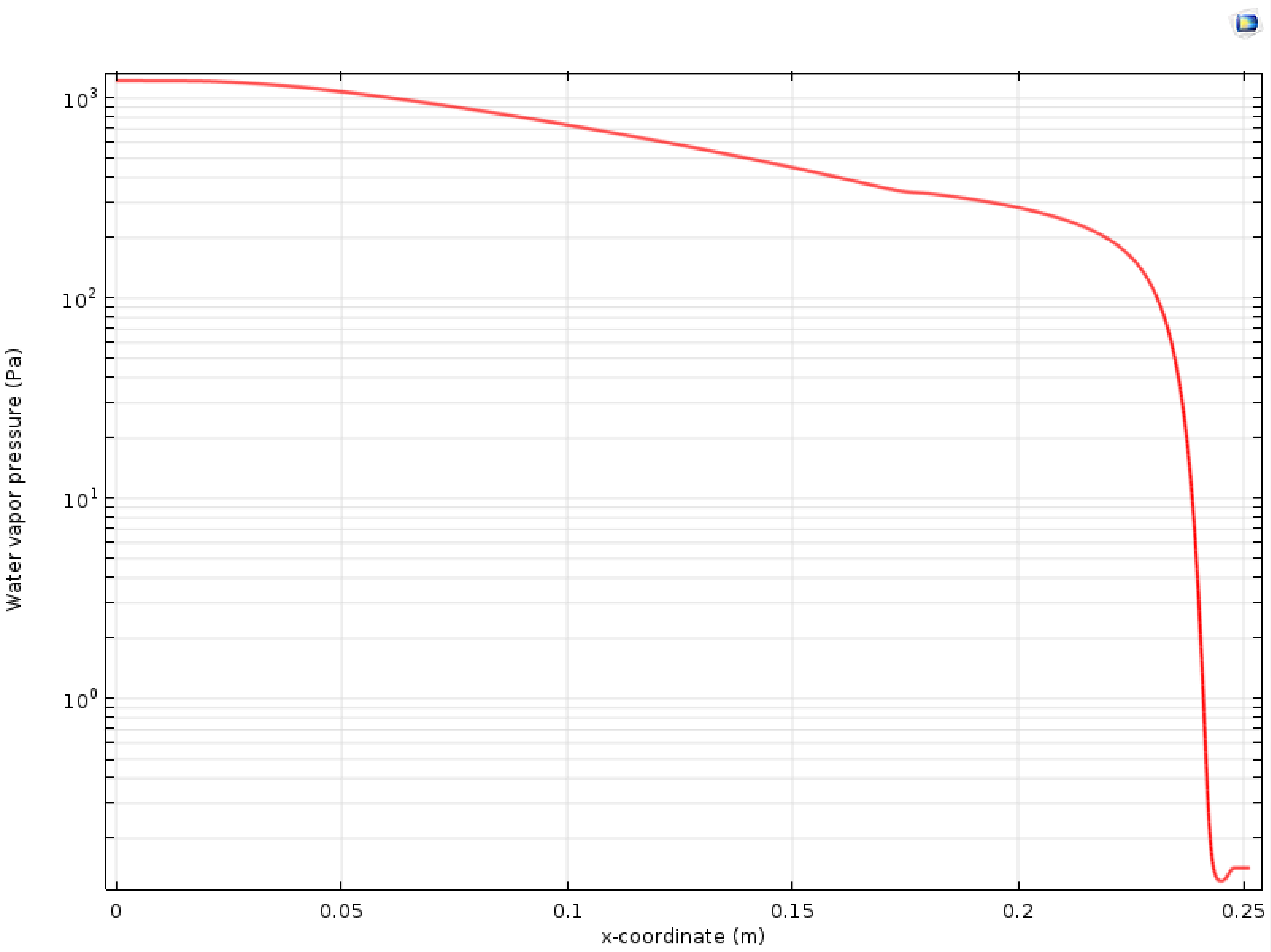
System Snapshot



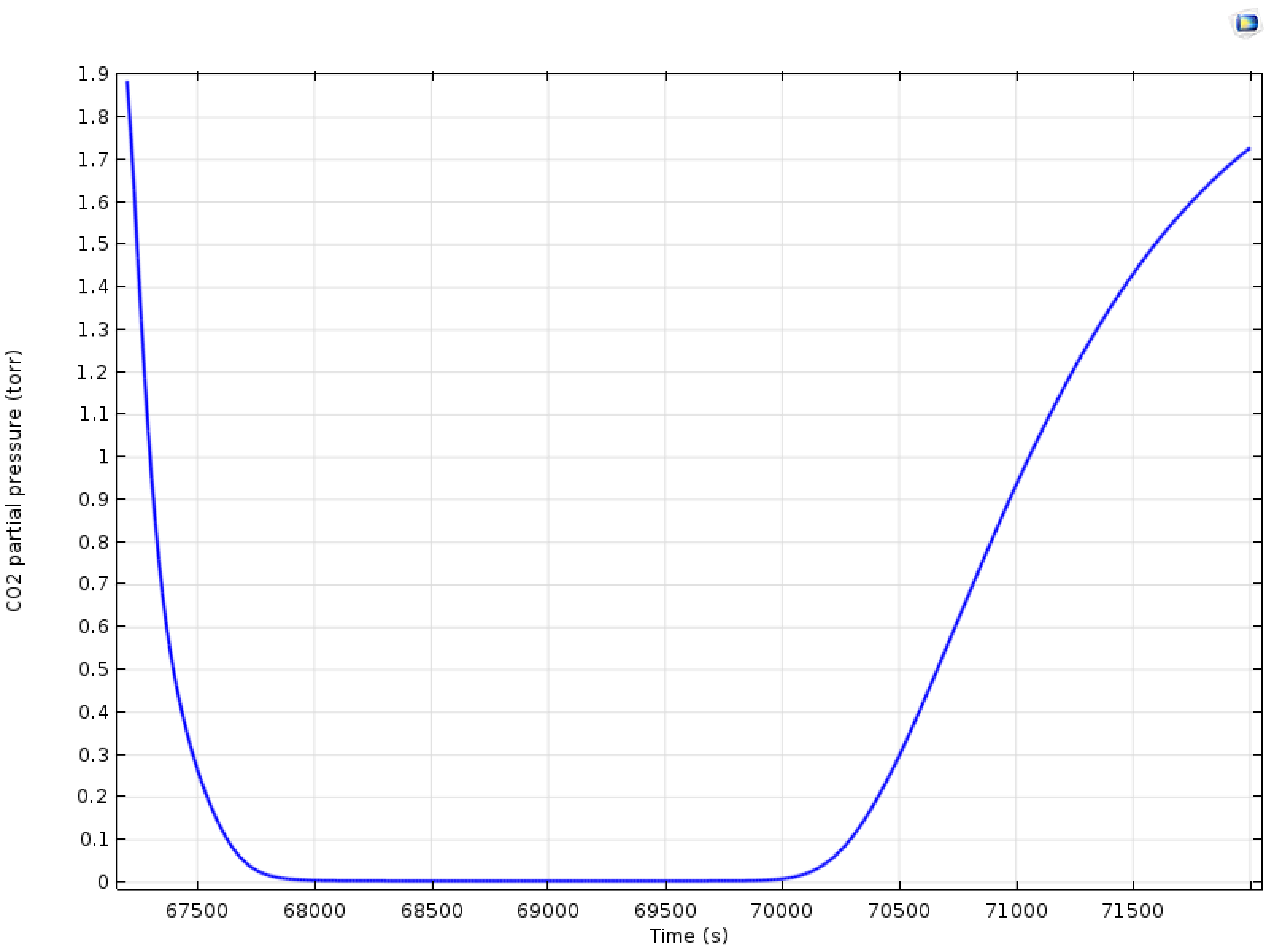
- Example: Grade 544 13X at 26.75 SCFM
- Gas-phase concentration of CO_2 and H_2O included in the model.
- Cycles are run until "converged" (i.e., desiccant/sorbent bed pairs are symmetrical).
- Breakthrough of either gas in any of the beds can be easily visualized.

Water Breakthrough

- Since desiccant bed sizes are smaller than current CDRA configuration, it must be shown that water does not break through desiccant beds.
- Water breakthrough was not observed for the desiccant bed in any of the configurations tested.



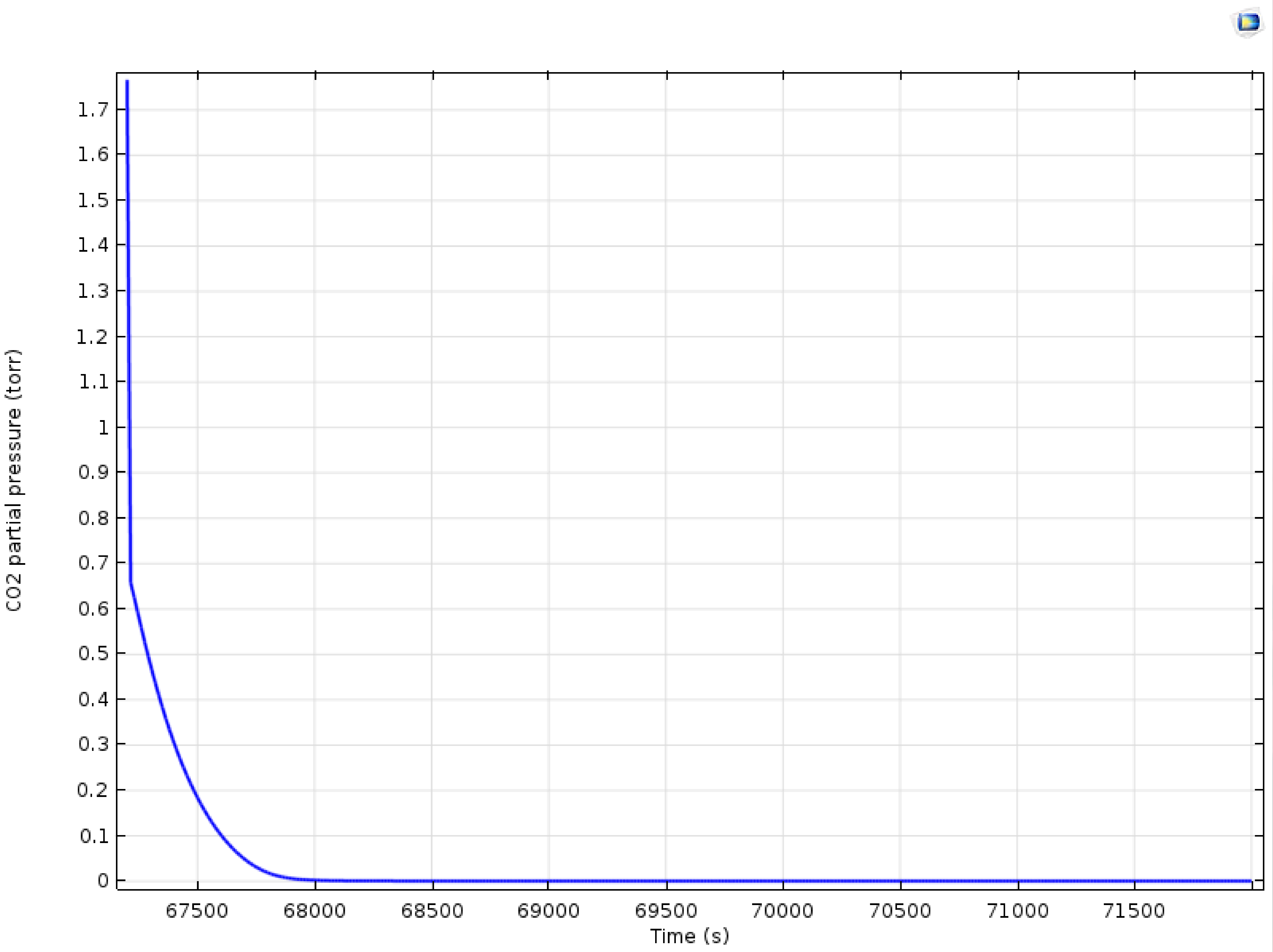
CO_2 Breakthrough



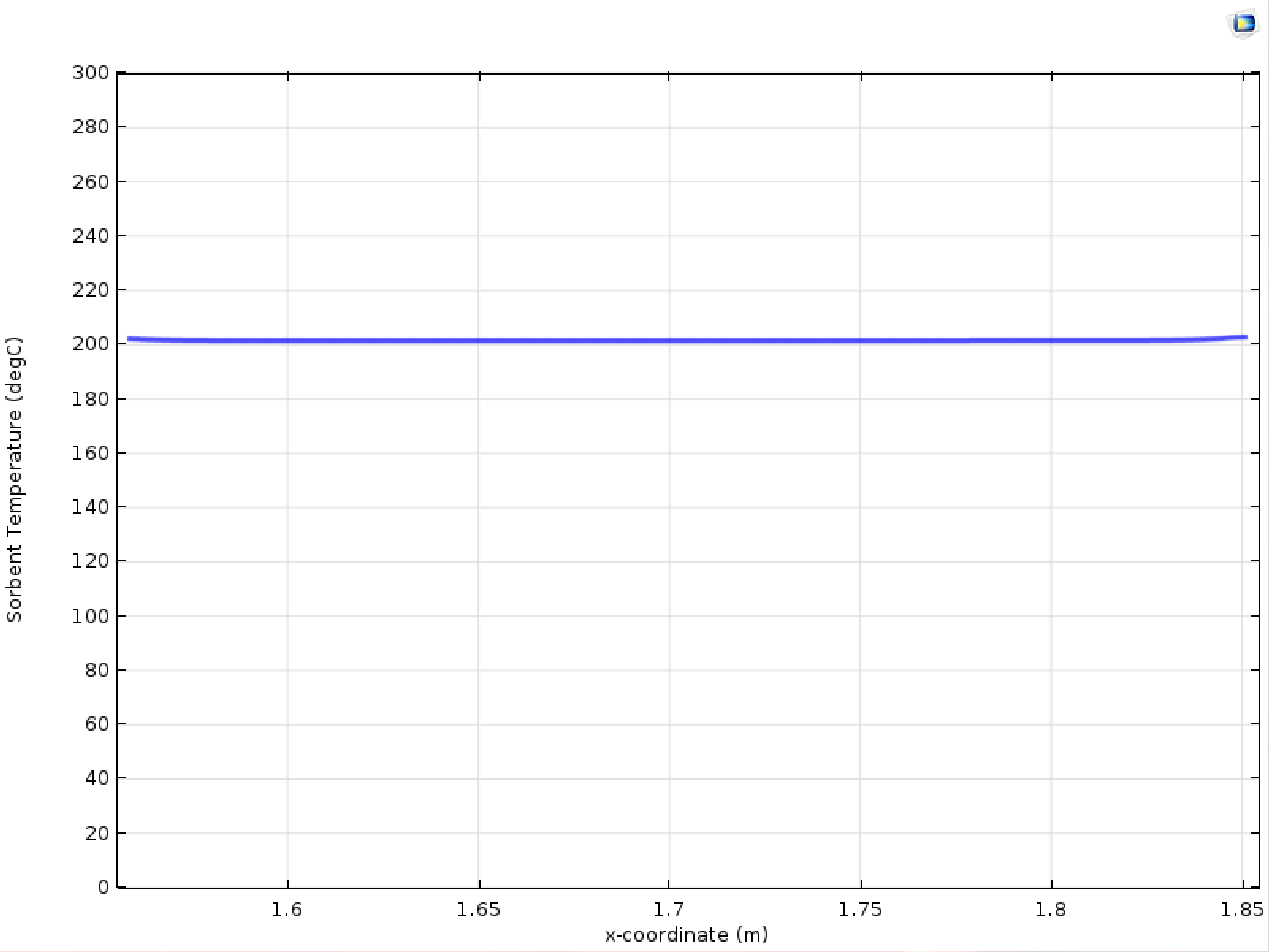
- Can also plot system variables as f(t) at a specific point in the geometry.
- Example: Grade 544 13X at 26.75 SCFM: outlet of sorbent bed
- For this case, the outlet concentration of CO_2 almost reaches the inlet concentration.

CO_2 Breakthrough (RK38)

- Example: RK38 at 24.25 SCFM
- CO_2 breakthrough not observed, with the concentration at the outlet of the desiccant bed remaining approximately zero.

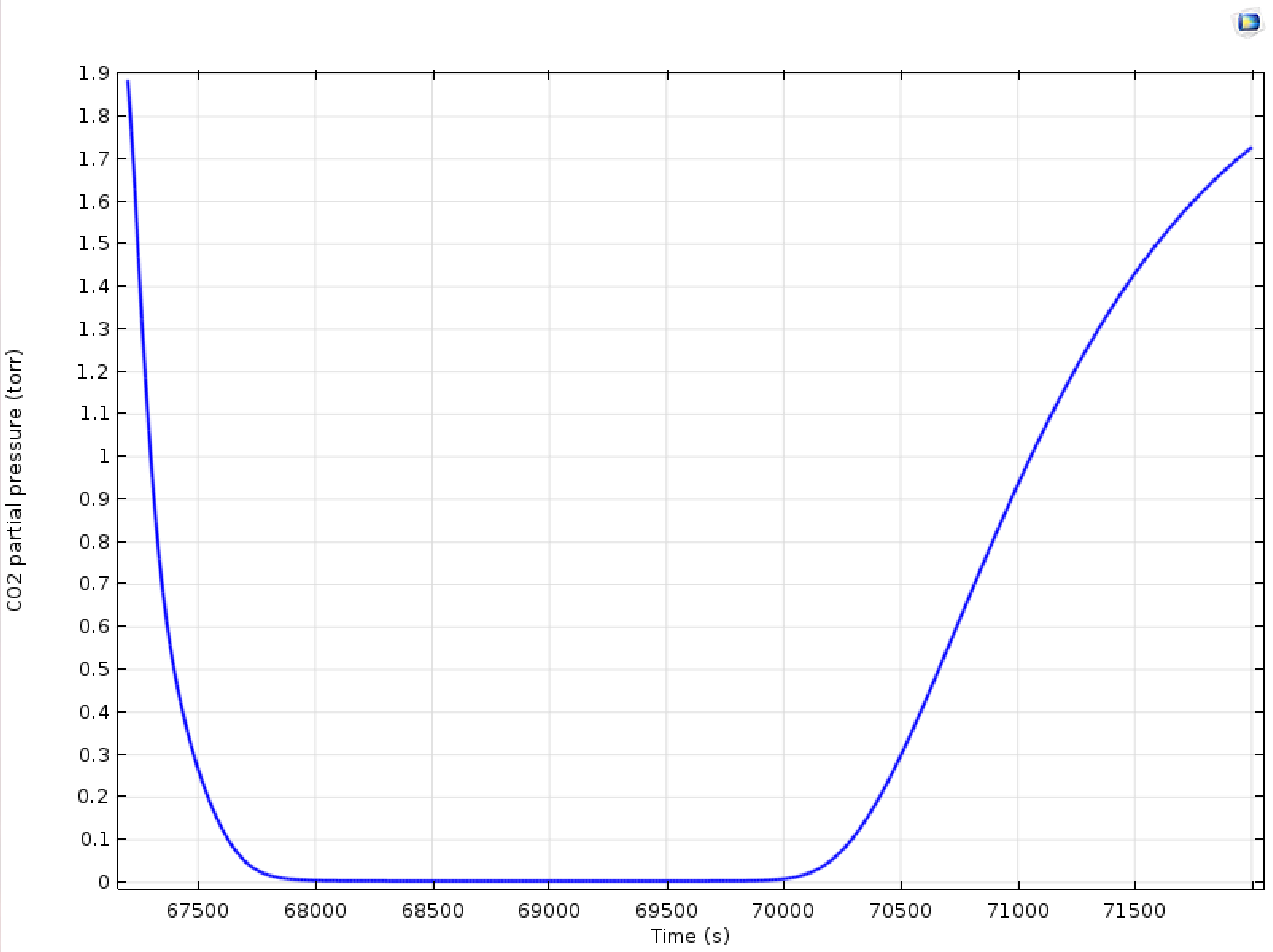


Bed Temperatures

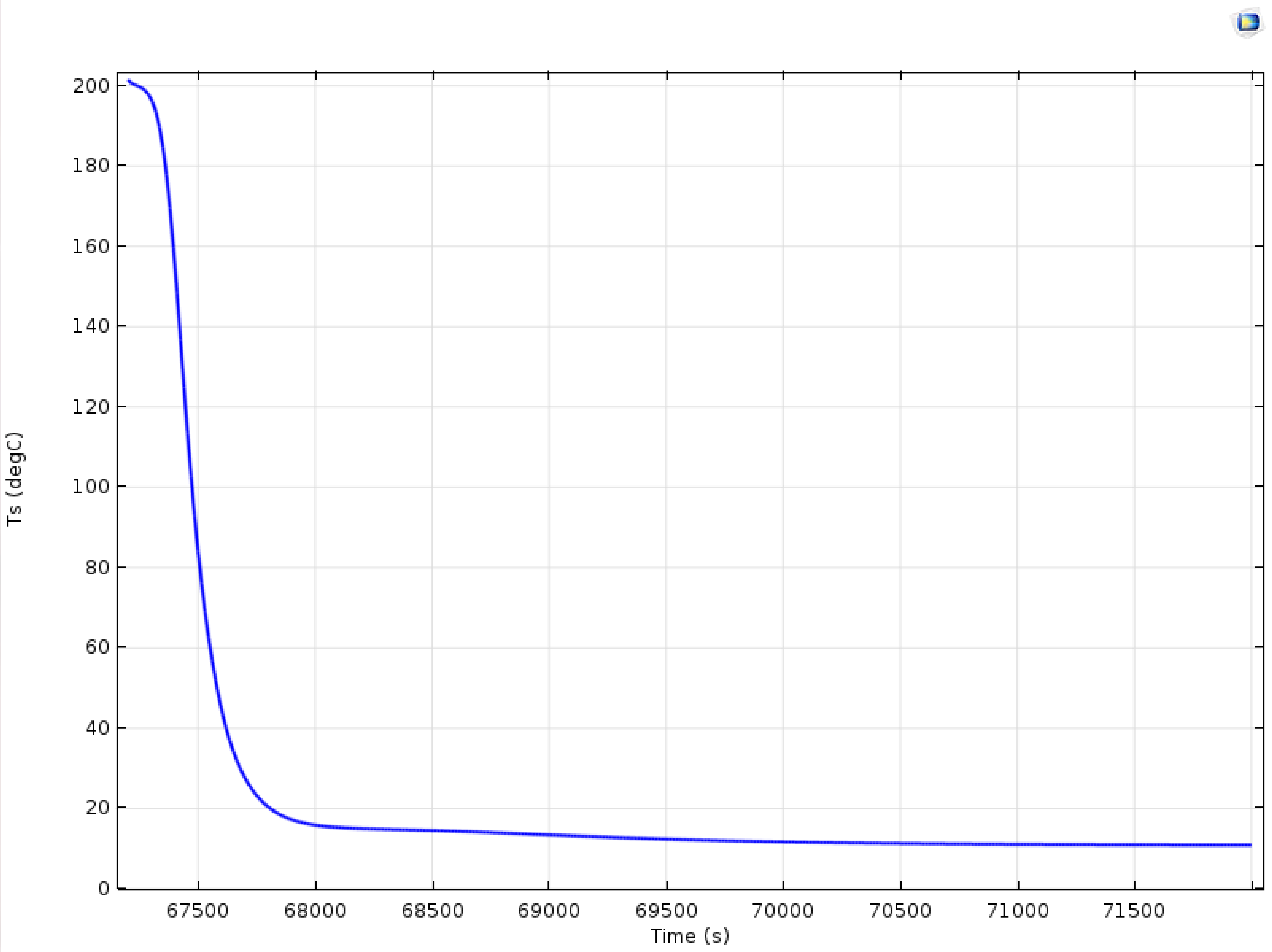


- Example: Grade 544 13X sorbent bed at the beginning of an adsorption half-cycle.
- High bed temperatures explain the non-zero CO2 outlet concentration at the beginning of an adsorption half-cycle. High temp → low adsorption.

Bed Temperatures



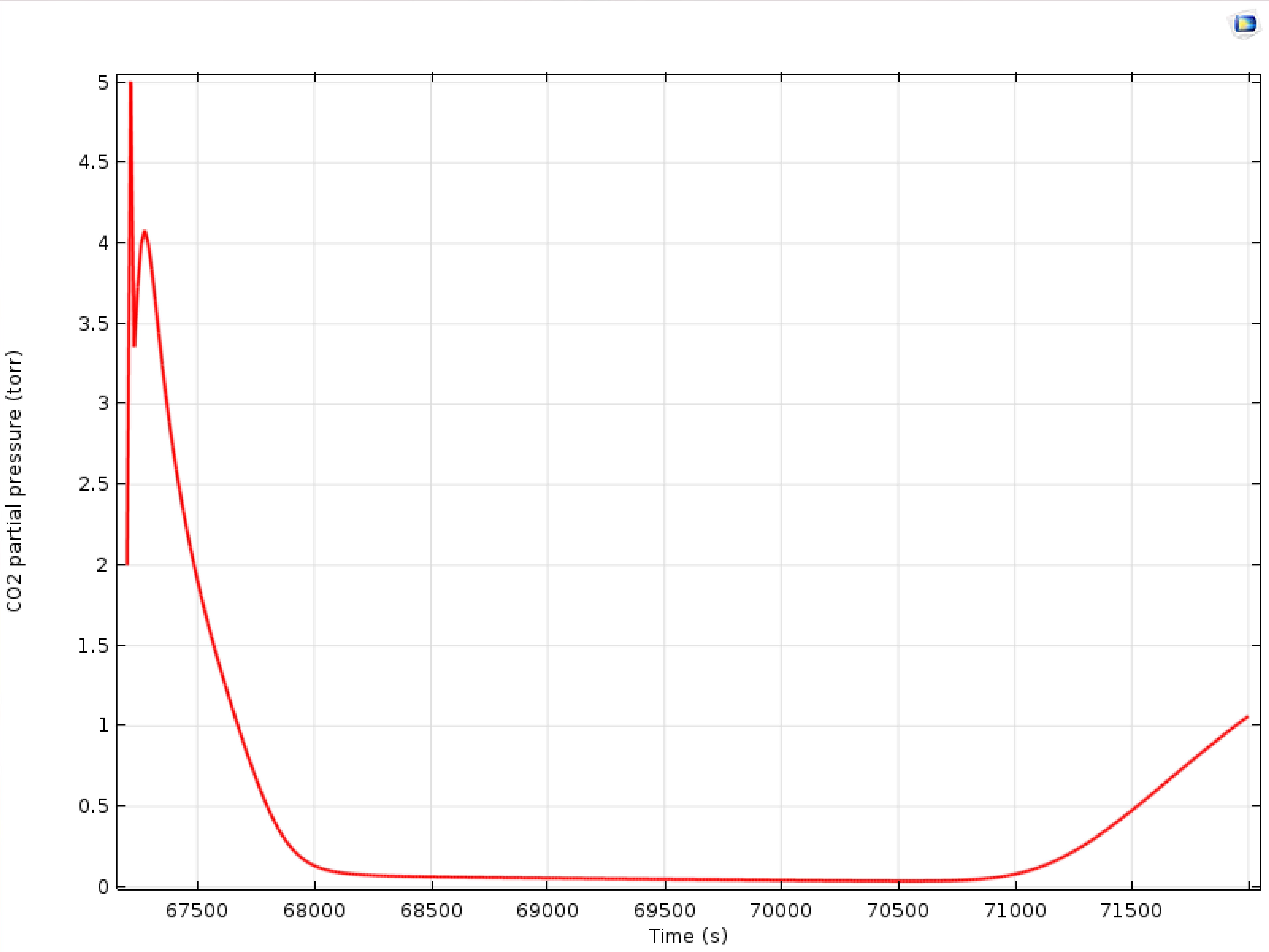
CO2 Breakthrough



Sorbent temperature (center of bed)

Overall System Outlet

- Example: Grade 544 13X at 26.75 SCFM
- 13X layer of the desiccant bed adsorbs CO_2, playing a significant role in the overall efficiency of the process



Summary

- Six possible new 4BMS configurations have been studied using a 1-D COMSOL model
  - Four different sorbents
  - Different flow rates
  - Smaller bed sizes
- The studies show that changes in sorbent and decreases in bed size are possible while still yielding a process with adequate CO_2 removal capability.

Future Work

- Model will continue to be used to help finalize 4BMS-X design
- Future studies will likely focus on Grade 544 13X as the CO_2 sorbent
- Bed size will be optimized
- Finalize flow rate and half-cycle time
- Possibility of replacing the 13X layer in the desiccant bed with another material will be investigated