Virtual Design of a Four-Bed Molecular Sieve for Exploration

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Introduction: Aboard the International Space Station, CO_2 is removed from the cabin atmosphere by a four-bed molecular sieve (4BMS) process called the Carbon Dioxide Removal Assembly (CDRA).[1] This 4BMS process operates by passing the CO_2-laden air through a desiccant bed to remove any humidity and then passing the dried air through a sorbent bed to remove the CO_2. While one pair of beds is in use, the other pair is thermally regenerated to allow for continuous CO_2 removal.

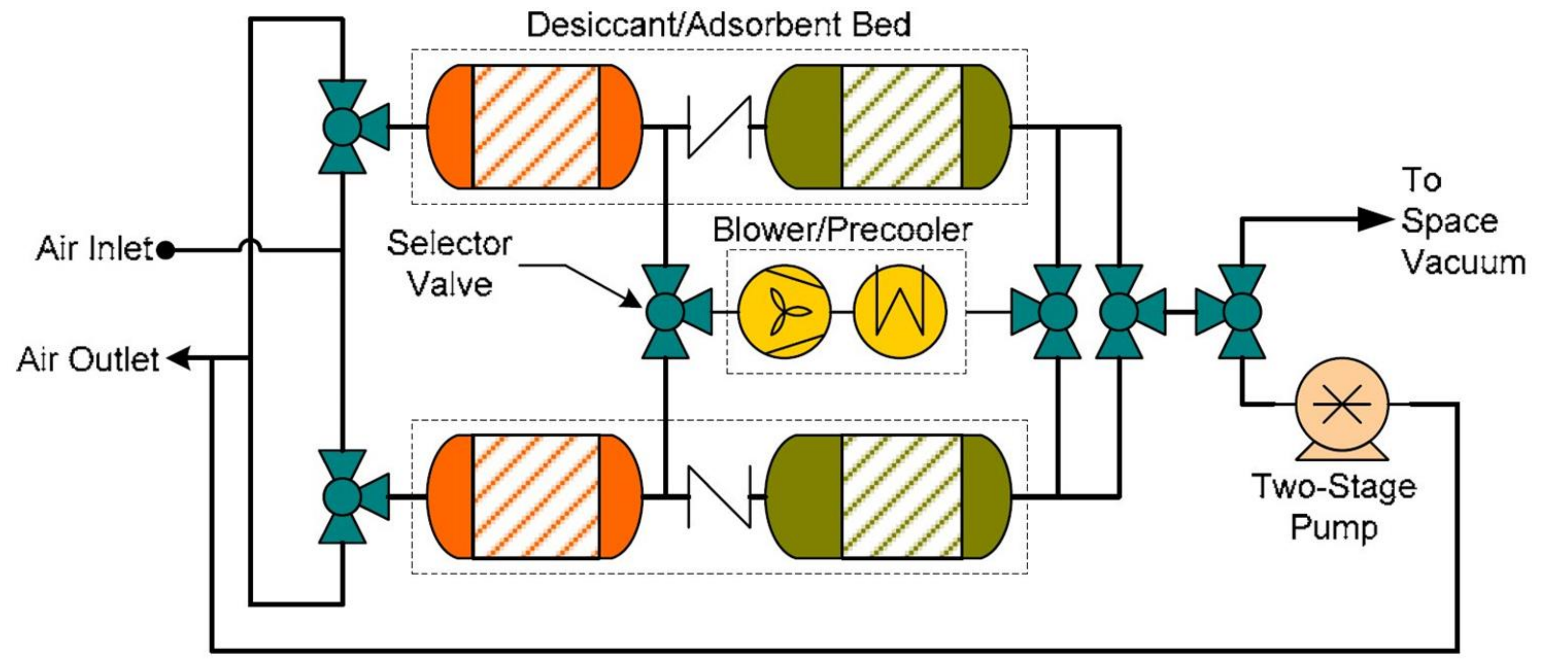
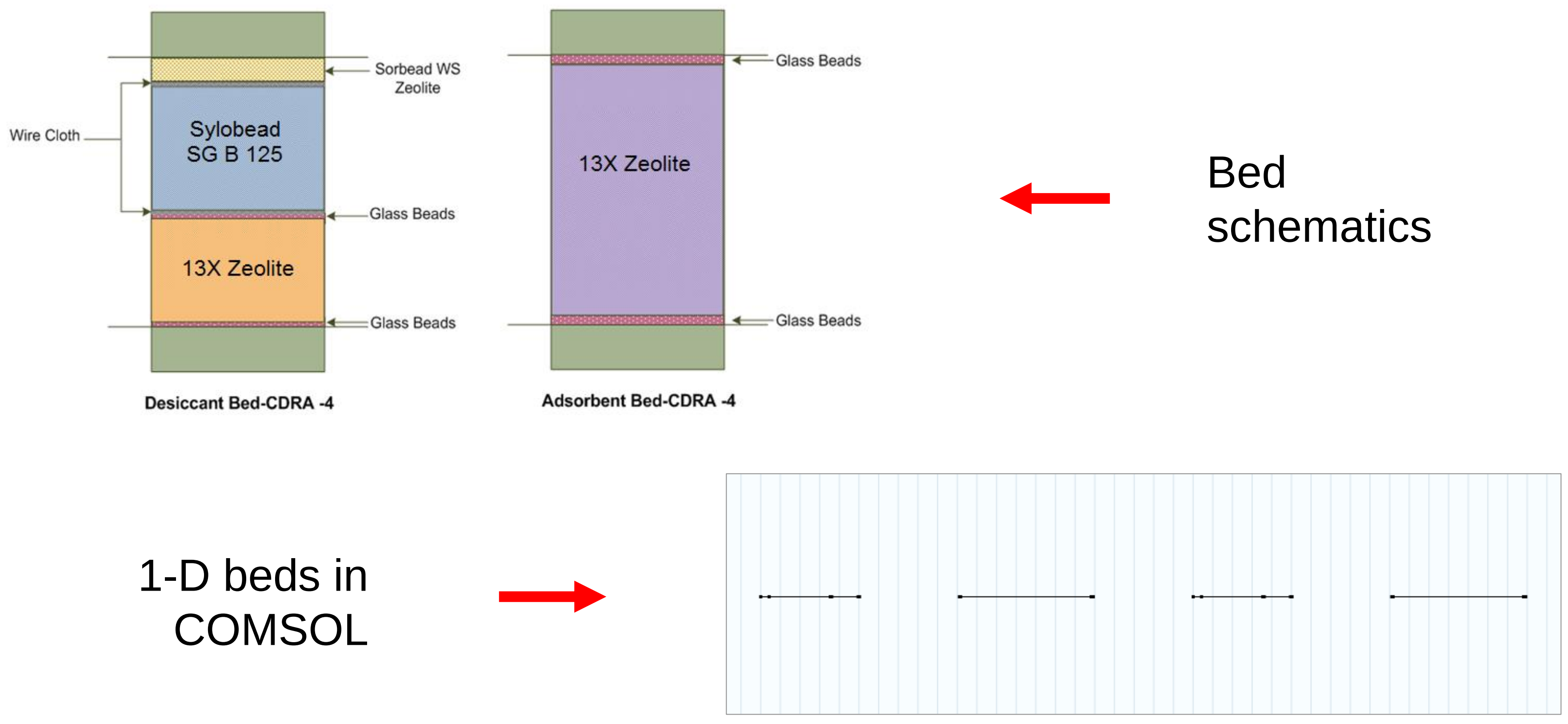


Figure 1. Carbon Dioxide Removal Assembly (CDRA) process schematic.

Though CDRA has effectively removed CO_2 throughout its lifetime, it has also experienced technical issues that have made maintaining the system difficult. One major issue is that the CO_2 sorbent has been observed to break down, producing dust which impedes gas flow in the system and can damage system components such as valves. It is also likely that the beds are oversized, increasing the system mass and power requirement unnecessarily. Accordingly, design changes to address these issues are being pursued for implementation in a next-generation 4BMS process. These changes include a new bed geometry, a new sorbent, revised heater design, and revised valve design. As changes in bed geometry (especially length) and in the type of sorbent used lend themselves well to investigation by simulation, COMSOL modeling is being used to help guide the design of the new 4BMS process.

Computational Methods: A 1-D plug flow model is used, with each bed being represented by a separate domain.[2]



Bed schematics

1-D beds in COMSOL

Figure 2. The simulated beds.

Though only 1-D, the model includes the majority of the relevant physics, including Darcy's law for flow in porous media; separate heat transfer solutions for sorbent, gas, can, and insulation; and diffusion in the gas phase. Moreover, experimental adsorption rate and equilibrium data[3] (Fig. 3 & 4) are used as inputs to the model, as these factors are the major drivers of model behavior. For further model details, see Knox, et al.[4]

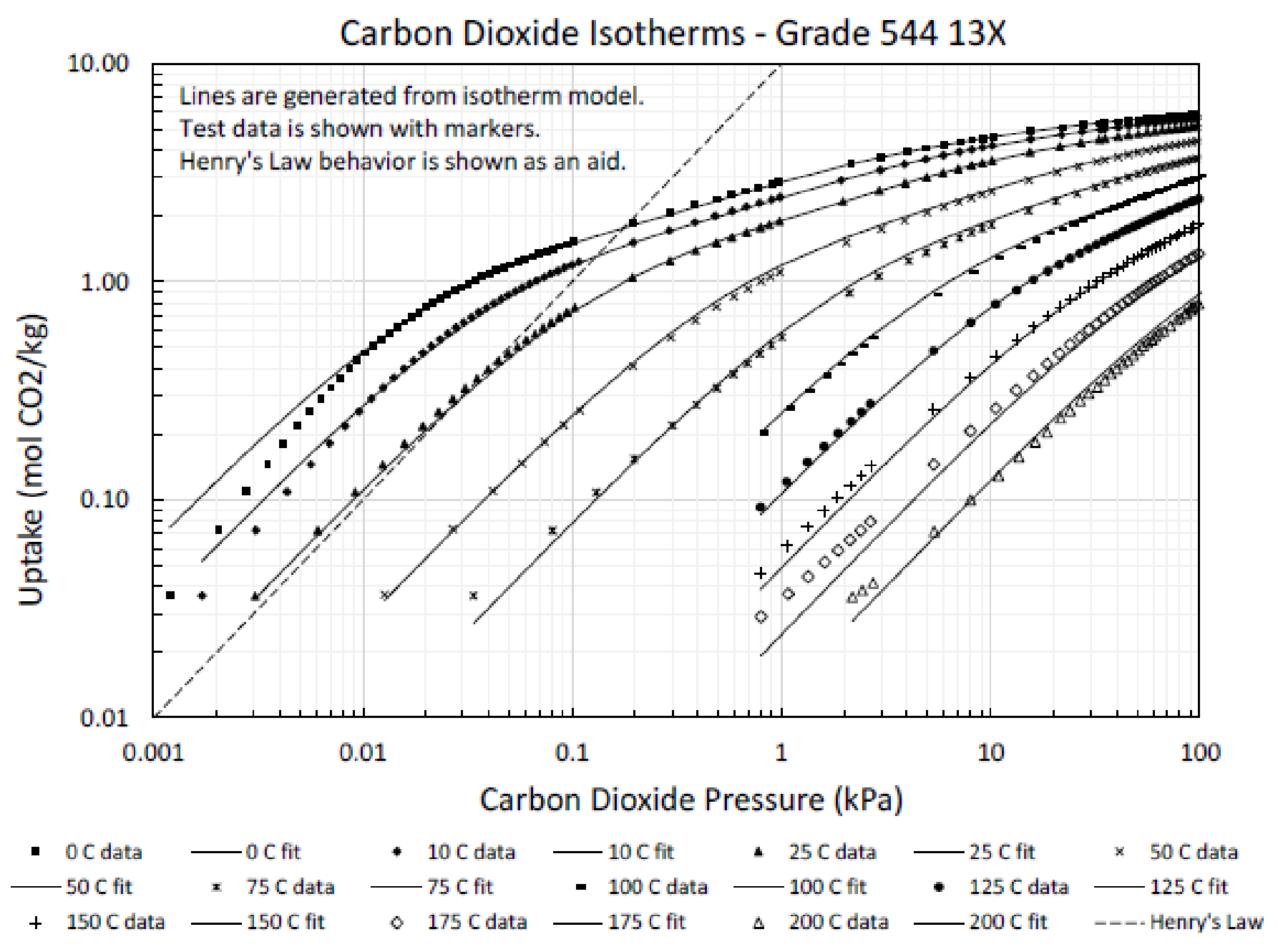


Figure 3. Adsorption equilibrium data.

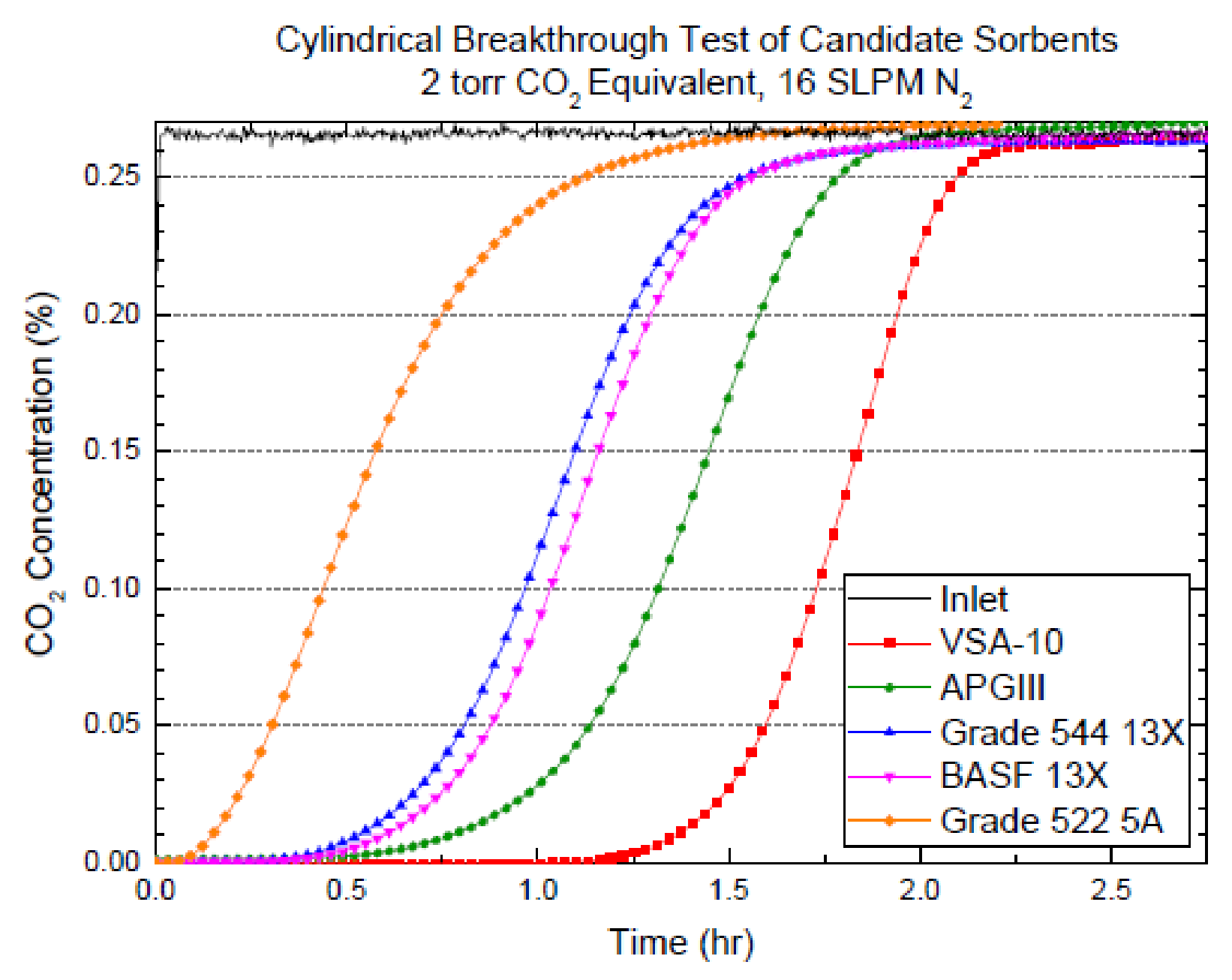


Figure 4. Adsorption breakthrough data.

Results: Six new process configurations were studied, including configurations with four new CO_2 sorbents. Candidate sorbents were identified based on their CO_2 adsorption capacity and on their resistance to dusting (Fig. 5 & 6).[3]

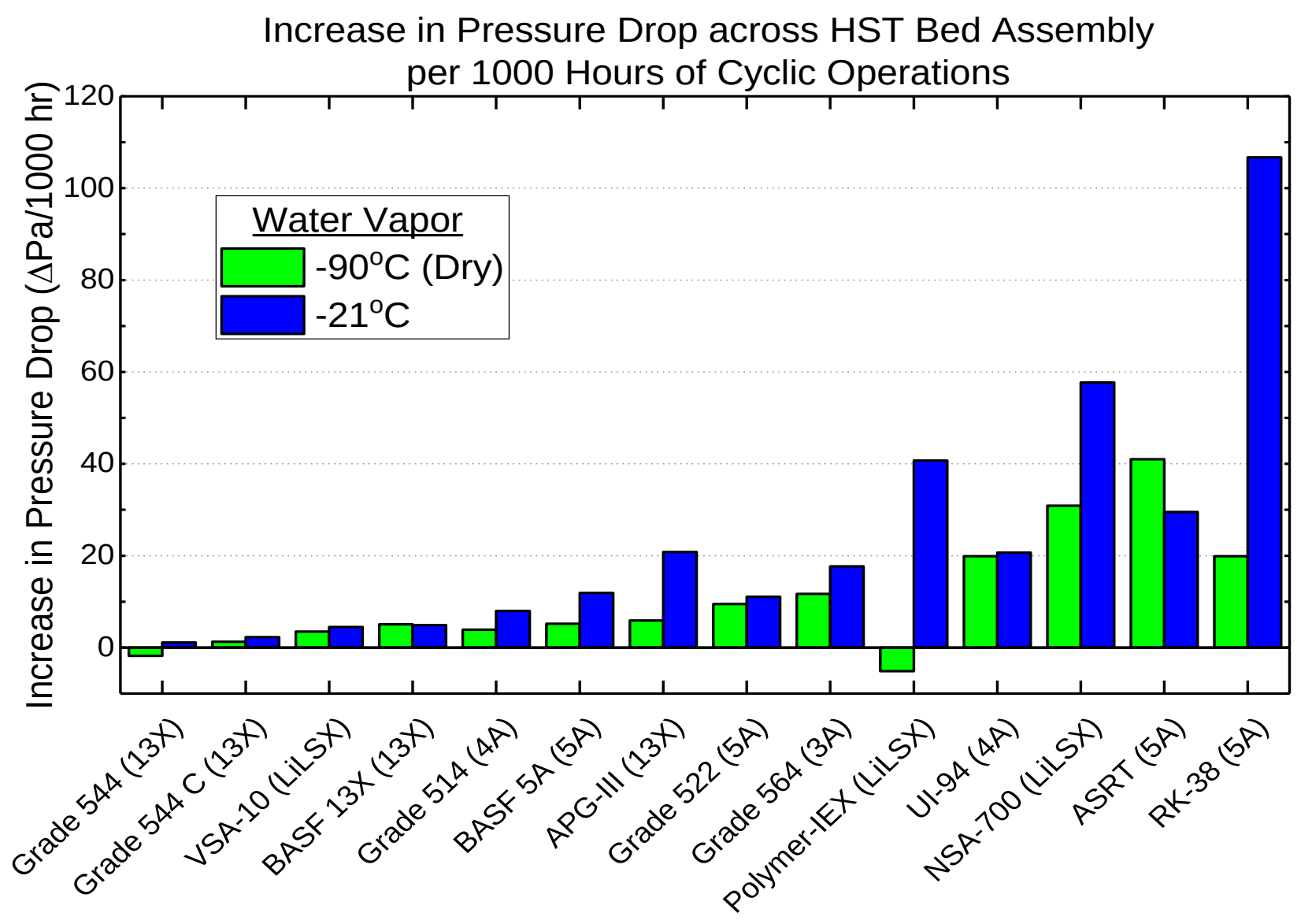


Figure 5. Sorbent dusting comparison.

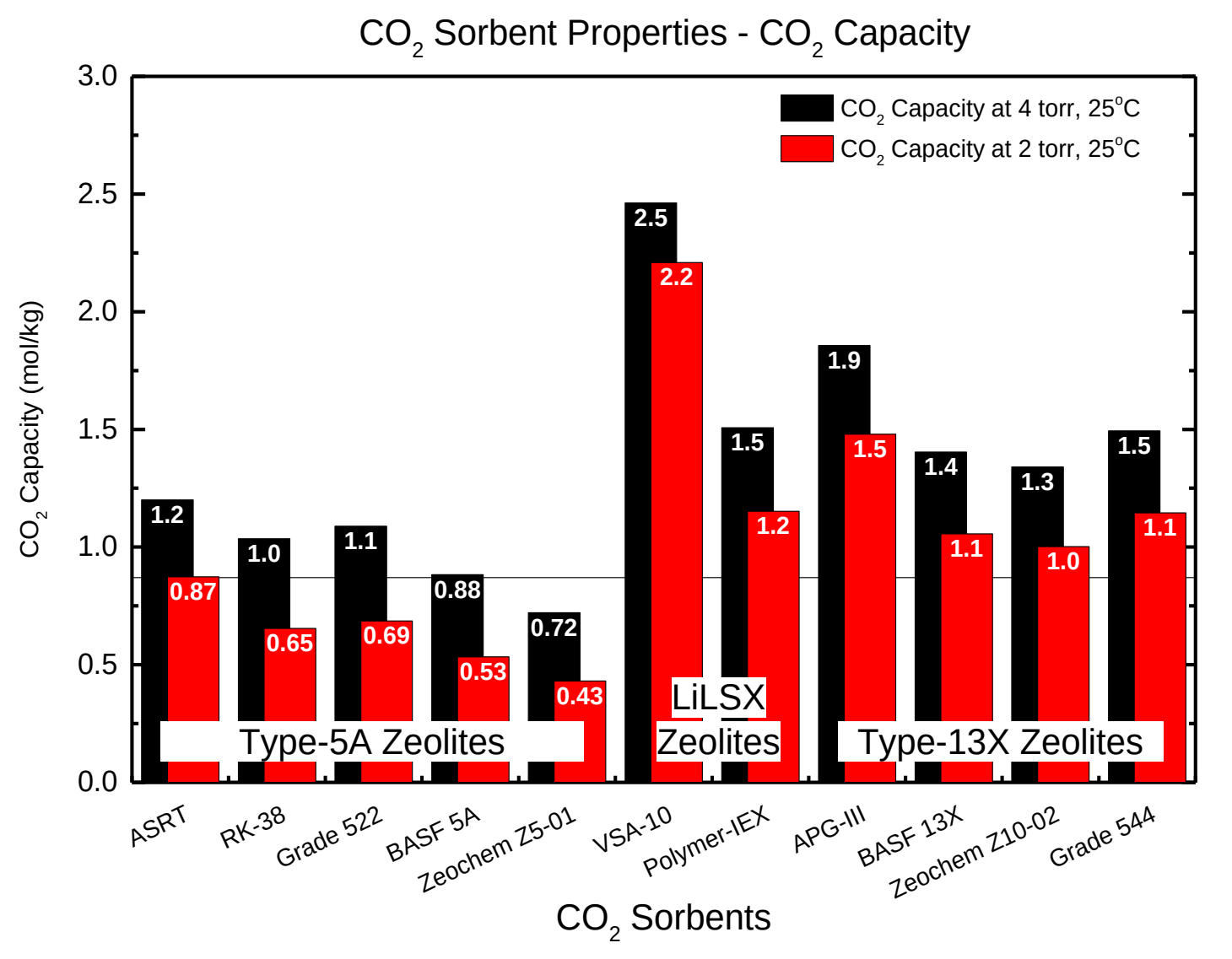


Figure 6. Sorbent CO_2 capacities.

For each configuration, the zeolite layer of the desiccant bed was reduced by 45%, and the sorbent bed size was reduced by 30-60%. For two of the sorbents (544 13X and APG III), two different flow rates were investigated. Each configuration uses a half-cycle time of 80 minutes. All six configurations exceed the daily CO_2 removal target for a four-person crew (4.16 kg).

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

Table 1. A summary of the simulation results.

Using COMSOL, the behavior of a configuration can be explored in more detail than is possible experimentally. Visualizing CO_2 concentration as a function of bed depth shows how close the bed is to breakthrough at the end of a half-cycle (Fig. 7). Plotting CO_2 concentration as a function of time shows when breakthrough occurs during a half-cycle, and how much CO_2 is exiting the sorbent bed (Fig. 8). This ability to visualize breakthrough is especially important since the six configurations studied all involve smaller bed sizes.

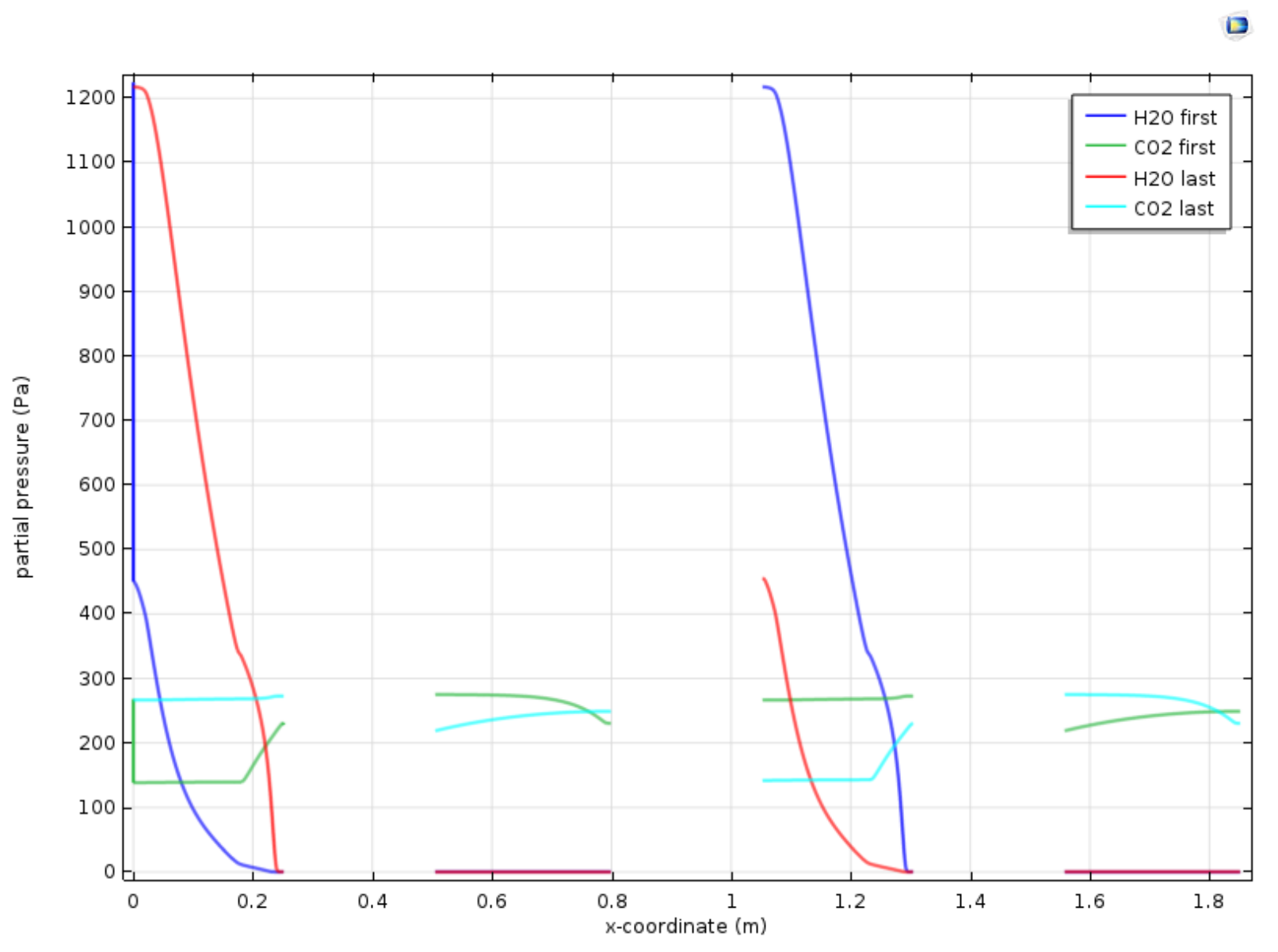


Figure 7. Bed concentration profiles.

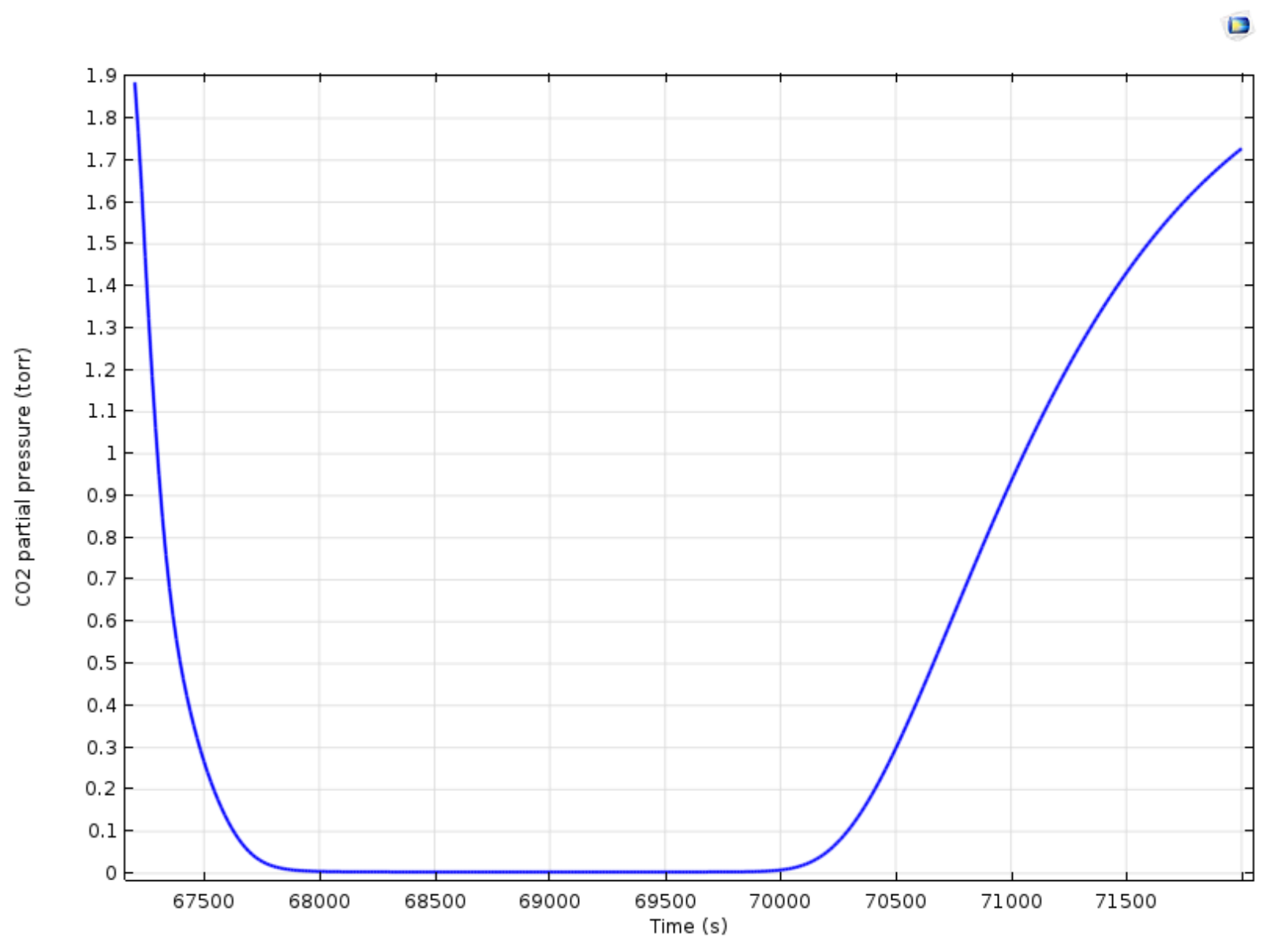


Figure 8. CO_2 outlet pp as f(t).

Conclusions: Six new configurations of a 4BMS process for CO_2 removal in space have been simulated. The configurations chosen focus on reducing the bed sizes and choosing a new sorbent for CO_2 adsorption. This work shows that reductions in bed size and changes in sorbent are feasible while still yielding a 4BMS process for space that meets the minimum requirement of 4.16 kg/day CO_2 removal. Future studies will focus on 544 13X as the sorbent due to its acceptable performance and its superior resistance to dusting. Bed size, half-cycle time, and flow rate will be optimized.

References:

1. Kay, R., International Space Station (ISS) Carbon Dioxide Removal Assembly (CDRA) Protoflight Performance Testing, *International Conference on Environmental Systems*, 1998.
2. Coker, R. F., and Knox, J. C., Predictive Modeling of the CDRA 4BMS, *46th International Conference on Environmental Systems*, 2016.
3. Knox, J. C., et al., Investigation of Desiccants and CO_2 Sorbents for Advanced Exploration Systems, 2015-2016, *46th International Conference on Environmental Systems*, 2016.
4. Knox et al., Limitations of Breakthrough Curve Analysis in Fixed-Bed Adsorption, *Ind. Eng. Chem. Res.*, 4734–4748, 2016.