Virtual Design of a 4-Bed Molecular Sieve for Exploration

Timothy J. Giesy[1], Robert F. Coker[2], Brian F. O'Connor[3], and James C. Knox[4]
NASA Marshall Space Flight Center, Huntsville, Alabama, 35812, USA

Simulations of six new 4-Bed Molecular Sieve configurations have been performed using a COMSOL model. The preliminary results show that reductions in desiccant bed size and sorbent bed size when compared to the International Space Station configuration are feasible while still yielding a process that handles at least 4.0 kg/day CO_2. The results also show that changes to the CO_2 sorbent are likewise feasible. Decreasing the bed sizes was found to have very little negative effect on the adsorption process; breakthrough of CO_2 in the sorbent bed was observed for two of the configurations, but a small degree of CO_2 breakthrough is acceptable, and water breakthrough in the desiccant beds was not observed. Both configurations for which CO_2 breakthrough was observed still yield relatively high CO_2 efficiency, and future investigations will focus on bed size in order to find the optimum configuration.

Nomenclature

4BMS = Four bed molecular sieve
4BMS-X = Four bed molecular sieve for exploration
CDRA = Carbon dioxide removal assembly
ISS = International Space Station
NASA = National Aeronautics and Space Administration
SCFM = Standard cubic feet per minute
SG = Silica gel

I. Introduction

In "NASA's Journey to Mars: Pioneering Next Steps in Space Exploration"[1] the stated goal for the agency is to "*extend human presence deeper into the solar system and to the surface of Mars*". As also stated therein, "*It is time for the next steps, and the agency is actively developing the capabilities that will enable humans to thrive beyond Earth for extended periods of time, leading to a sustainable presence in deep space*". The three phases required to reach these goals are defined as "Earth Reliant", Proving Ground", and "Earth Independent". In the first and current phase, "***Earth Reliant** exploration is focused on research aboard the ISS. On the space station, we are testing technologies and advancing human health and performance research that will enable deep-space, long-duration missions.* One of those technologies listed is "*Mars mission class environmental control and life support systems*". In this paper, efforts to develop CO_2 Removal technologies (part of a life support system) for Exploration missions are described. These efforts are focused on producing ISS flight demonstrations. Here the ISS will provide the platform for long-term system testing in a relevant environment, thus enabling the evaluation and certification of the technology candidates for future missions.

II. Background

Currently, CO_2 removal aboard the International Space Station (ISS) is accomplished by the Carbon Dioxide Removal Assembly (CDRA), which utilizes a Four-bed Molecular Sieve (4BMS) arrangement to effect separation of CO_2 from air. However, as discussed by Knox et al.,[2] numerous improvements to ISS CDRA are desirable to

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[1] Aerospace Engineer, Environmental Control and Life Support Development Branch/ES62
[2] Aerospace Engineer, Thermal and Mechanical Analysis Branch, Space Systems Dept./ES22
[3] Thermal Engineer, Thermal and Mechanical Analysis Branch, Space Systems Dept./ES22
[4] Aerospace Engineer, Environmental Control and Life Support Development Branch/ES62

address reliability and capability issues before deploying 4BMS for future exploration missions. This has led to the development of the next generation of 4BMS, designated 4BMS-X, to address these issues.

To aid in the design and development of 4BMS-X, a fully predictive computational model has been developed in COMSOL Multiphysics.[3] This model was shown to predict accurately the bulk behavior of the beds in the 4BMS, despite being a 1-D approximation of the system. Furthermore, the model allows the user to control a variety of model inputs, including bed size, sorbent and desiccant choices, half-cycle time, heater temperatures, flow rate, etc. Accordingly, the model can be used not just to predict the behavior of the current CDRA configuration, but also to guide design decisions for future configurations. Using predictive modeling, changes to the 4BMS configuration can be explored virtually, without the added time and expense of experimentation.

Figure 1 shows a schematic representation of the ISS CDRA 4BMS. This system consists of two sorbent beds for removing CO_2 from the air as well as two desiccant beds for protecting the sorbent beds from water vapor. During operation, cabin air flows through the first desiccant bed, where water vapor is removed, and into the first sorbent bed, where CO_2 is adsorbed. From there, the air flows through the second desiccant bed in order to remove the water adsorbed during the previous half-cycle and to send it back to the cabin. At the same time, the second sorbent bed undergoes an "air save" mode, which captures most of the air still in the sorbent bed, after which the sorbent bed is heated and exposed to vacuum to remove the adsorbed CO_2 in preparation for the next cycle. Further details about CDRA can be found elsewhere.[4-5]

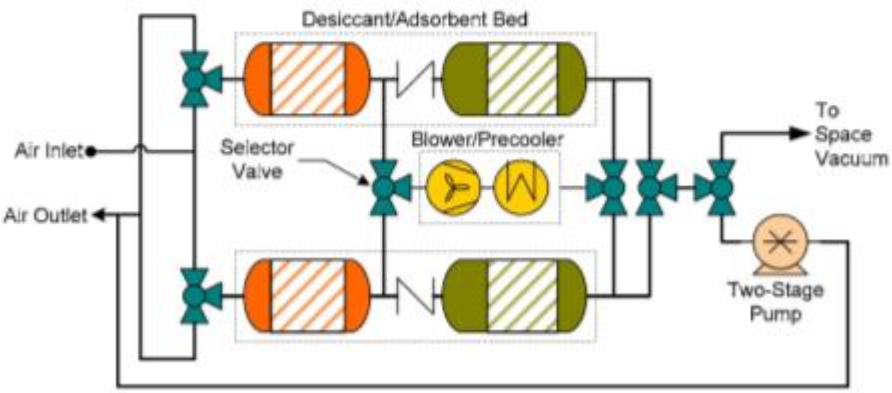

Figure 1. A schematic representation of the ISS CDRA four bed molecular sieve process. The sorbent beds are the larger pair of beds on the right side of the figure.

Figure 2 shows a schematic representation of the desiccant and sorbent beds from the ISS CDRA. The desiccant beds show three different desiccant material layers referred to respectively as the guard layer (Sorbead WS), the bulk desiccant (SG B 125), and the residual desiccant (13X zeolite), as well as multiple inert glass bead layers. Conversely, the sorbent beds each have only one sorbent layer (RK-38).

Of the design improvements that are necessary for a next-generation 4BMS, the ones that lend themselves most readily to examination by computer simulation are the reduction in residual desiccant, the reduction in CO2 sorbent, and changes in sorbent identity. These changes could result in a 4BMS system that is lighter, smaller, and uses less energy than the current configuration. For new configurations with different desiccants/sorbents and bed sizes, the model also allows optimization of the process by varying flow rate and half-cycle time.

This paper presents some preliminary simulations of alternate 4BMS configurations, making changes in sorbent identity, bed size, cycle time, and flow rate compared with the current CDRA 4BMS. These simulations form the groundwork for guiding 4BMS-X design decisions.

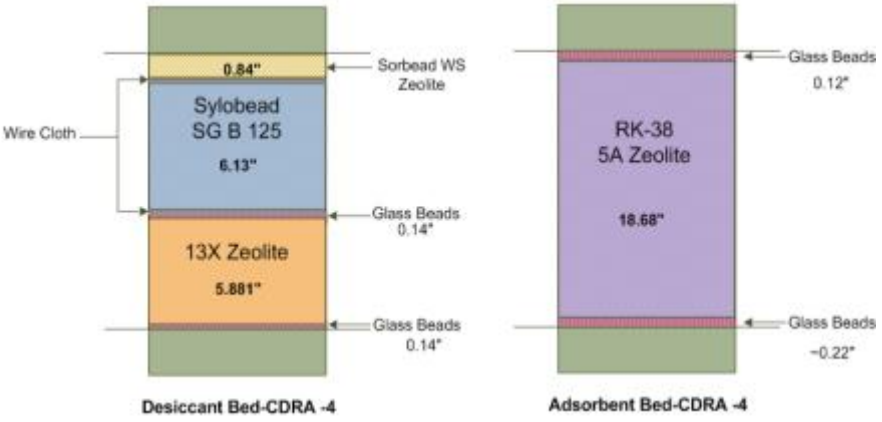

Figure 2. A schematic showing the sorbent layering in both the desiccant and sorbent beds of the CDRA 4BMS.

III. Results and Discussion

A summary of the preliminary results is shown in Table 1. Six studies were carried out, each with a different 4BMS configuration. Simulations were carried out using 80-minute half-cycles and a 2 torr partial pressure of CO_2 and a 10°C dew point at the system inlet. Other relevant model parameters can be found in Coker and Knox.[3] For each of the six studies, the residual desiccant amount was reduced to 45% of the ISS CDRA value. Furthermore, four different CO_2 sorbents, including a 13X zeolite (544), one LiLSX zeolite (VSA-10), a 5A zeolite (RK-38), and zeolite APG III were studied as candidates for the CO_2 sorbent. In each configuration, the sorbent bed size was decreased when compared with the CDRA sorbent beds, with the amount of the decrease depending on the sorbent. For both the 544 and APG III studies, two different inlet flow rates were compared. Table 1 reports the sorbent, flow rate, half cycle time, calculated CO_2 removal rate, sorbent bed size (as a fraction of the CDRA beds), and CO_2 efficiency. Each study resulted from the simulation of 11-15 half-cycles. For comparison, recent 4BMS experimental results using 544 13X (71.5% of nominal CDRA bed) as the CO_2 sorbent, a 50% reduction in residual desiccant, and a flow rate of 27.8 SCFM showed a CO_2 removal rate of 4.75 kg/day with an efficiency of 0.82.

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 from the six 4BMS configurations considered in this work. Listed are the CO_2 sorbent, the process flow rate, the sorbent bed size as a percentage of the ISS CDRA sorbent bed size, and the calculated CO_2 removal rate and CO_2 efficiency.

Of the data listed in Table 1, the primary value of interest for each configuration is the CO_2 removal rate. Each of the six configurations simulated in this work gives a CO_2 removal rate well above 4.0 kg/day, which is the average CO_2 production rate of a four-member crew.[6] Moreover, CO_2 efficiency values are similar to those achieved in simulations of the full-size CDRA 4BMS.[3] These results show that reductions in both residual desiccant and CO_2 sorbent are possible while still yielding a process that meets the CO_2 removal need of a four-person crew. The results also show that changing the CO_2 sorbent is feasible.

While the CO2 removal rate is the most useful piece of information in determining the viability of a configuration, there are additional details to consider about the operation of a cycle that determine whether or not a cycle is worth pursuing experimentally. First, it is of interest to show for configurations with reduced desiccant and sorbent bed sizes that such a bed size decrease does not cause problems with the cycle operation. Particularly, if the desiccant bed is undersized, water vapor could break through the desiccant, allowing water to reach the zeolite of the sorbent bed, which would negatively impact the CO_2 capacity of the zeolite and decrease the effectiveness of the overall process. Figure 3 shows the partial pressure of water vapor in the desiccant bed at the end of the adsorption half-cycle as a function of position for the 544 13X configuration with a flow rate of 26.75 SCFM. This configuration was chosen as a representative sample of the configurations tested in order to demonstrate the features of the model and to characterize the results. This figure shows that though the desiccant bed has been decreased in size, the water vapor partial pressure at the outlet of the desiccant beds is still very low, indicating that the desiccant beds are not experiencing water vapor breakthrough. The absence of water breakthrough was also observed for the other five configurations presented in this work.

Similarly, if CO_2 breaks through the sorbent bed a long time before the end of an adsorption half-cycle, the CO_2 efficiency of the process will suffer, as much of the CO_2 is simply sent back to the cabin atmosphere without being adsorbed. Thus, in investigating smaller bed sizes, it is necessary to show that the bed size isn't small enough to allow premature breakthrough of CO_2. Figure 4 plots CO_2 partial pressure at the outlet of the sorbent bed for the same configuration (544 13X and 26.75 SCFM) throughout an adsorption half-cycle. As is clear from the figure, CO_2 has indeed broken through by the end of the half-cycle, with the outlet partial pressure at the end of the half-cycle almost reaching the inlet composition. Similar behavior was observed for the 544 13X and 28 SCFM configuration, while CO2 breakthrough was not observed for any of the other four configurations. It should be noted that some degree of breakthrough is acceptable here, as it allows for longer half-cycle times and the minimization of unused adsorbent.[4] While the CO_2 efficiency numbers for the 544 13X configurations are reasonable, they are the lowest of the six configurations tested, and this breakthrough behavior is likely responsible for this difference in efficiency. These results show that the sorbent bed for these configurations may be undersized, and that if 544 13X is chosen as a replacement CO_2 sorbent, the sorbent beds may need to be larger than those simulated here. Nevertheless, these results show the value of using predictive modeling to explore new 4BMS configurations before any physical experimentation.

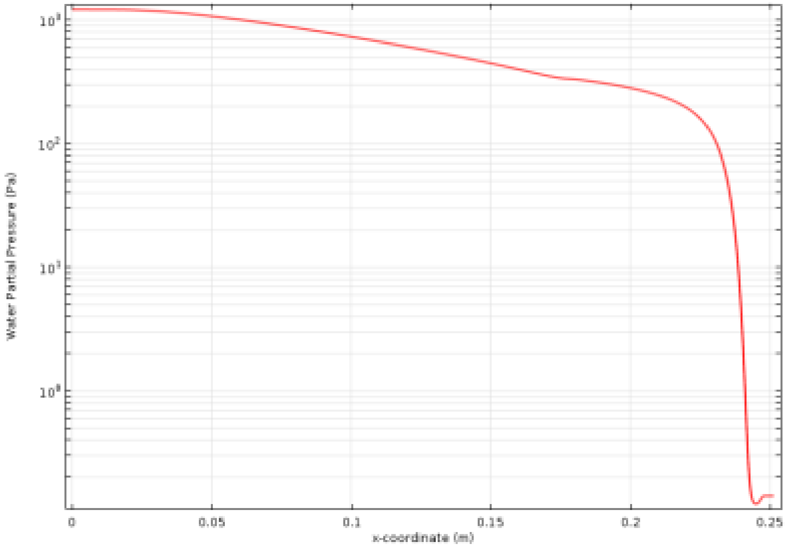

Figure 3. Partial pressure of water vapor in the desiccant bed as a function of position at the end of an adsorption HC. The data shown is from the 544 13X, 26.75 SCFM configuration. This figure shows that the desiccant bed does not experience water breakthrough.

In Figure 4, the initial-time part of the breakthrough curve shows a relatively high partial pressure of CO_2 leaving the sorbent bed. This behavior can be explained by the high temperature of the sorbent bed during this period of the adsorption phase. Figure 5 shows the sorbent temperature as a function of the length coordinate in the sorbent bed at the beginning of an adsorption half-cycle. As can be seen in the figure, the temperature throughout the bed is approximately 202°C. At the beginning of a half-cycle, the bed that is about to undergo adsorption has just been thermally regenerated. As there is no way for the sorbent bed to cool down before adsorption begins, the sorbent remains hot during the first part of the adsorption phase. This higher temperature reduces the capacity of the sorbent until the sorbent cools down.

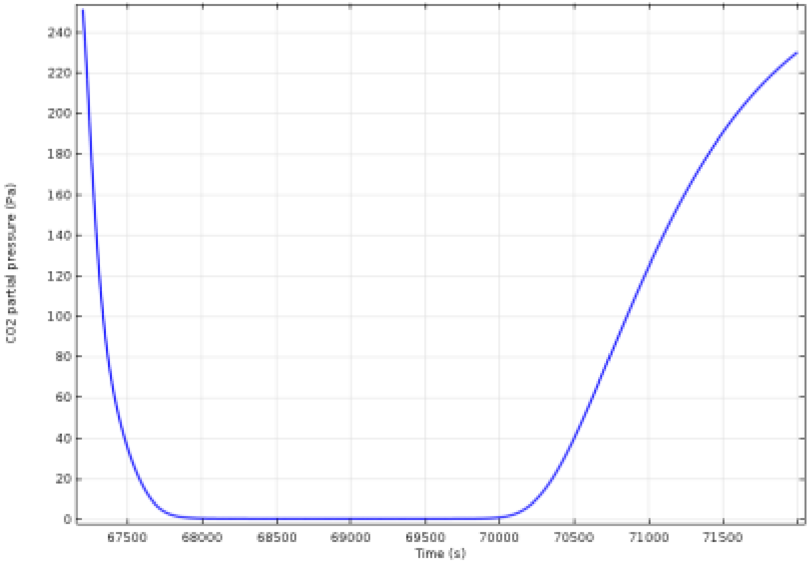

Figure 4. CO_2 partial pressure at the outlet of the sorbent bed as a function of time. The data from this plot are from the 544 13X, 26.75 SCFM configuration. This figure illustrates CO_2 breakthrough in the sorbent bed.

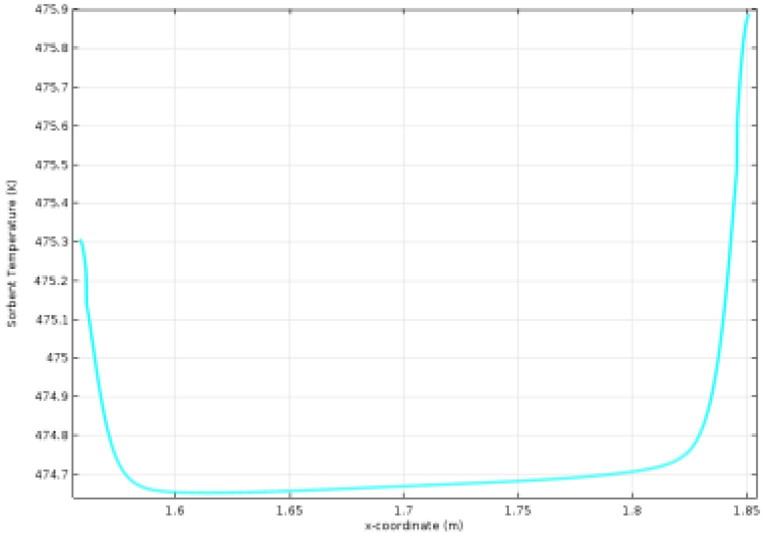

Figure 5. Temperature profile of the sorbent in the sorbent bed at the beginning of an adsorption half-cycle. The sorbent at this point in a half-cycle is still at high temperature from the thermal regeneration of the previous half-cycle.

Figure 6 shows CO_2 loading in the 13X zeolite layer of the desiccant bed. While 13X is used in the residual desiccant layer for its water capacity, it is also a good CO_2 sorbent. When cabin air passes through the desiccant bed, the air loses CO_2 in addition to water vapor, and this CO_2 is later returned to the cabin during desiccant bed regeneration. Thus, having a large residual desiccant 13X layer negatively impacts the CO_2 efficiency of the overall process. This figure shows that the CO_2 loading in the residual desiccant layer increases from the beginning of an adsorption half-cycle to the end. These data indicate that the decrease in the residual desiccant layer thickness may have a positive effect on the CO_2 efficiency.

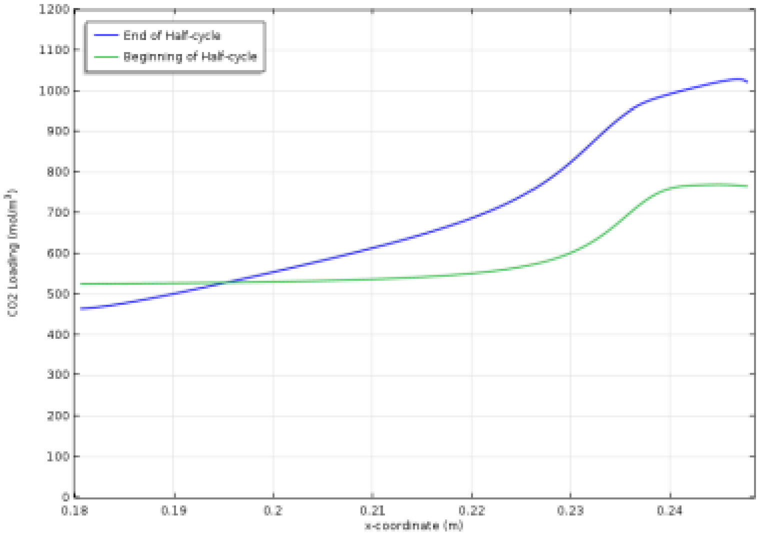

Figure 6. The CO_2 loading profile in the residual desiccant layer of the desiccant bed, comparing the profile at the beginning of an adsorption half-cycle with the profile at the end of the half-cycle. This figure illustrates the CO_2 efficiency losses that occur due to adsorption in the desiccant bed.

The results presented here show the benefits of using predictive simulation to explore future 4BMS configurations. These preliminary results have shown that it is possible to make significant reductions in desiccant and sorbent bed sizes while still yielding a process with high CO_2 removal capacity. The results also show that, besides the sorbent currently in use, there are other candidate sorbents that could be used to adsorb CO_2 effectively. The COMSOL model allows visualization of bed outlet compositions and loading profiles, which show that depending on the identity of the sorbent, the flow rate, and the magnitude of the bed size decrease, CO_2 breakthrough can occur in the sorbent bed. Furthermore, though water breakthrough was not observed in the six configurations simulated in this work, the COMSOL model allows investigation of this possibility, which becomes especially important when investigating decreases in desiccant bed sizes.

For giving adequate guidance to 4BMS-X design decisions, much simulation work remains. In this work, only one bed size decrease was investigated for each sorbent. The goal of investigating new bed sizes is to identify the optimum bed size for reducing system mass and energy consumption without any sacrifice of performance. Accordingly, future work will involve simulating multiple bed size configurations. Future work may also include simulating multiple half-cycle times and flow rates to find the best configuration for a new bed size. Given that the results show CO_2 adsorption in the 13X layer of the desiccant bed, future configurations considered may also replace the 13X residual desiccant layer with a sorbent with lower CO_2 capacity. Finally, to ensure that the configurations are sized properly to avoid breakthrough, future configurations will undergo simulation of more half-cycles (i.e., longer run times).

IV. Conclusions

Simulations of new 4BMS configurations have been performed with the view of guiding future 4BMS-X design decisions. Six configurations were considered, each with significant reductions made in the sizes of the desiccant beds and the sorbent beds. Among the six configurations, four CO_2 sorbent candidates were considered; for the 13X and APG III zeolite varieties, two different flow rates were considered. The results show that reducing desiccant bed and sorbent bed sizes is feasible while still maintaining a system that can handle at least 4.0 kg/day CO_2. Furthermore, changing the CO_2 sorbent is also possible. For guiding 4BMS-X design decisions, further simulation studies are to be performed to study the effect of bed size, CO_2 sorbent, residual desiccant, flow rate, and half-cycle time. These results will drastically reduce the time and cost of determining the best 4BMS configuration for future exploration missions.

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