Predictive Modeling of the CDRA 4BMS

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As part of NASA's Advanced Exploration Systems (AES) program and the Life Support Systems Project (LSSP), fully predictive models of the Four Bed Molecular Sieve (4BMS) of the Carbon Dioxide Removal Assembly (CDRA) on the International Space Station (ISS) are being developed. This virtual laboratory will be used to help reduce mass, power, and volume requirements for future missions. In this paper we describe current and planned modeling developments in the area of carbon dioxide removal to support future crewed Mars missions as well as the resolution of anomalies observed in the ISS CDRA.

Nomenclature

T_{in}	=	gas temperature at CDRA influent, K
T_{amb}	=	ambient temperature outside the CDRA, K
T_{pc}	=	pre-cooler gas temperature, K
$P_{in,CO2}$	=	partial pressure of CO_2 at CDRA influent, Pa
$P_{in,H2O}$	=	partial pressure of H_2O at CDRA influent, Pa
$Po_{,S}$	=	effluent adsorbing sorbent bed total gas pressure, Pa
$Po_{,S}$	=	effluent adsorbing desiccant bed total gas pressure, Pa
NASA	=	National Aeronautics Space Administration
AES	=	Advanced Exploration Systems
CDRA	=	Carbon Dioxide Removal Assembly
ISS	=	International Space Station
4BMS	=	Four Bed Molecular Sieve
SG	=	Silica Gel
LSSP	=	Life Support Systems Project
SCFM	=	standard (1 atm, 0 ºC) cubic feet per minute
CBT	=	Cylindrical Breakthrough Test
LDF	=	linear driving force
HC	=	half-cyle
PDE	=	partial differential equation
CDRA-4EU	=	CDRA Version 4 Engineering Unit

I. Introduction

Predictive simulation tools have been developed to reduce the hardware testing requirements of the Life Support Systems Project (LSSP) as part of the National Aeronautics Space Administration's (NASA) Advanced Exploration Systems (AES) program[1,2]. Although sub-scale testing is required to establish the predictive capability of the simulations, the much greater cost of extensive full-scale testing can be limited to that required for the confirmation of analytical design optimization studies. Once predicative capability is established, geometric reconfiguration of a model is usually straightforward. A predictive simulation capability provides improved understanding of complex processes since process conditions (temperature, pressure, concentrations, etc.) may be examined anywhere in the sorption column. Weaknesses in a prototype design can be readily identified and improvements tested via simulation. Finally, the predictive simulation provides a powerful tool for virtual troubleshooting of deployed flight hardware. Here, we discuss using the COMSOL Multiphysics code[3] to model

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the combined water desiccant and carbon dioxide sorbent subsystems, together known as a 4 Bed Molecular Sieve (4BMS), of the Carbon Dioxide Removal Assembly (CDRA) as it presently operates on the International Space Station (ISS).

Figure 1 illustrates the operation of the ISS CDRA 4BMS. Cabin air is sent through a desiccant bed, where water vapor is adsorbed. Then a precooler and blower pre-condition the dry air and send it through a sorbent bed where CO_2 is removed. The dry and (nominally) CO_2-free air then goes through the second (desorbing) desiccant bed, where water vapor is added back to the air stream. This is then returned to the cabin. Meanwhile, the second sorbent bed, after a short (~10 min) 'air save' mode that recovers the bulk of the air trapped in the sorbent bed, has one end closed off and is heated while being vented to vacuum. This releases the CO_2 from the bed. Such a 'half-cycle' (HC) is typically on the order of 150 minutes long. On the next HC, the valves are switched so that the two adsorbing beds become desorbing and vice versa.

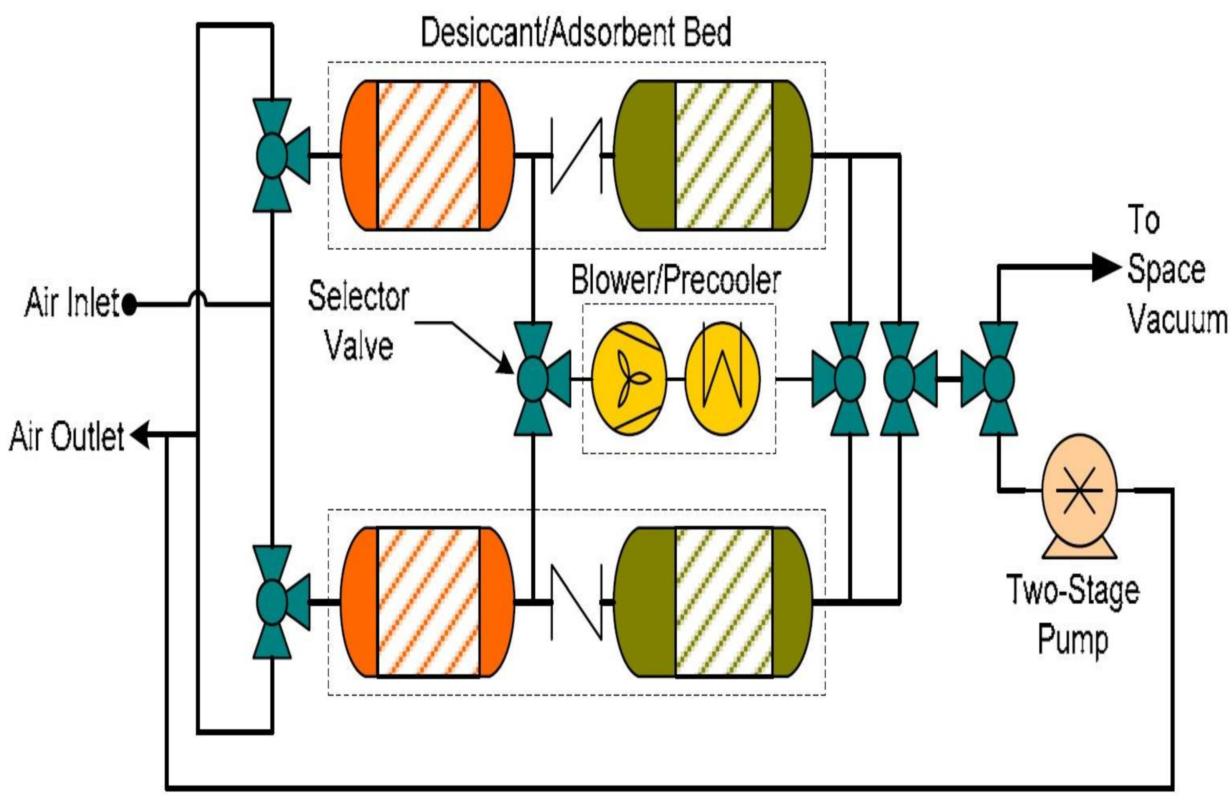

Figure 1. Schematic of the CDRA 4BMS. *Air comes in from the cabin, has water vapor removed in a desiccant bed (orange), is cooled by the precooler (yellow), has CO_2 removed in a sorbent bed (green), gets water vapor put back in in the 2^{nd} desiccant bed, then is returned to the cabin. Meanwhile, the 2^{nd} sorbent bed is heated and evacuated to space.*

II. 1-D Full System Model

For the bulk separation of CO_2 and H_2O, temperature changes due to the heat of adsorption are significant, requiring the simulation of the heat balance equations through the beds and the housing, as well as the equations for sorption processes, mass balance, and fluid flow. 1-D models have proven accurate enough for predictively driven system design[4,5,6]. The sorbent beds are not cylindrical and the heaters used to assist in CO_2 desorption make for a potentially complex multi-dimensional flow path, but, in practice, the dry air flows fairly uniformly through the channels, so that, nonetheless, a 1-D approximation is sufficient to capture the bulk behavior of the beds. At the present time, full 3-D models are computationally prohibitive, so to guide the design of the next generation CDRA, 1-D models will be used.

The 4BMS is modeled as a fully coupled system, with the calculated CO_2 and H_2O mass fractions output as a function of time from one bed used as the inlet boundary condition for the next bed in the flow path. As discussed elsewhere, the 1-D COMSOL model is calibrated to test data from simple cylindrical breakthrough tests (CBT)[4,5]. Thus, there are no knobs to turn and the model should be purely predictive. In fact, the initial models quickly showed that the sorbent bed heaters were not efficiently depositing their heat into the sorbent pellets[6]; this turned out to be due to, at least in part, an undocumented thermal path between the sorbent and desiccant beds.

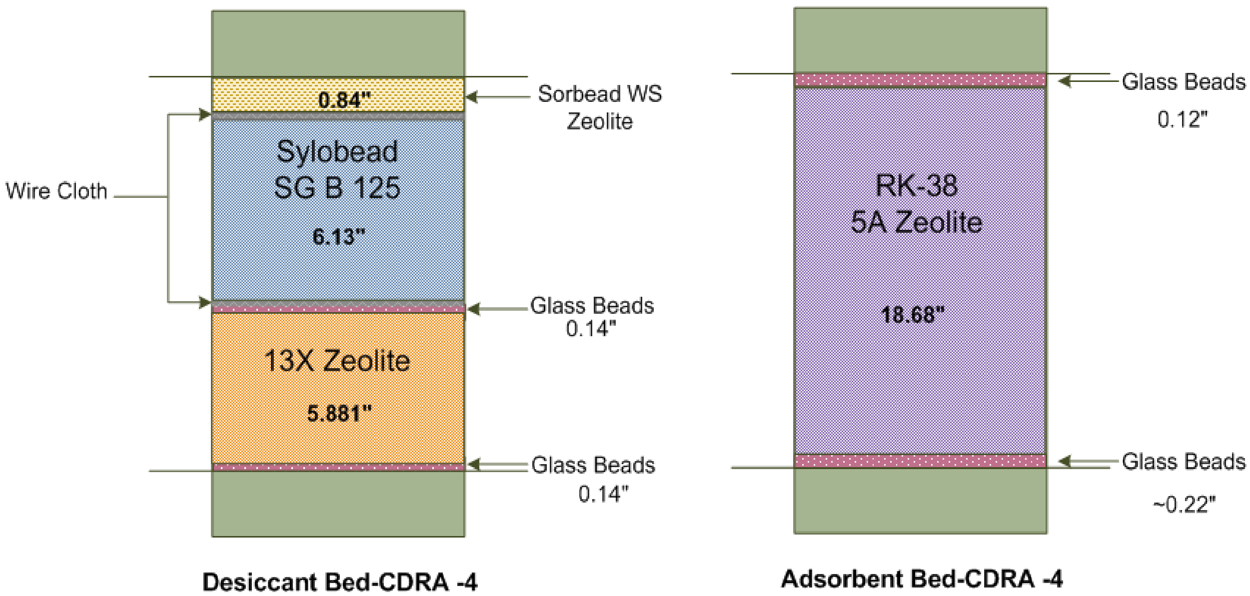

Figure 2 Idealized schematic of 4BMS model. *Only the glass beads (red) and sorbents (orange, yellow, blue, and purple) are modeled. The inlet and outlet regions (green) and thin wire cloths (grey) are not modeled.*

The 1-D models of the ISS CDRA 4BMS were constructed using the COMSOL Multiphysics code using their chemical transport, Darcy flow, and thermal transport modules to solve for concentrations, pressures, and temperatures, respectively. Each one of the four beds is modeled as a separate domain with its own physics nodes, boundary conditions, and solver settings. Within each of these domains, the temperature of the sorbent, gas (including the sorbate), surrounding can, and insulation are determined through separate heat transfer physics nodes. Domain partial differential equation (PDE) nodes are used to solve for the local pellet loading. Only the glass bead and sorbent-containing parts of the beds, as illustrated in Figure 2, are modeled. The glass bead layers are treated in the same way as the sorbent layers, but with zero adsorption and desorption capacity for H_2O and CO_2. Other than a linear competition between CO_2 and H_2O on the 13X in the desiccant beds[6], both the transport and sorption of the two sorbates are treated independently, so that, e.g. the 5A does not interact with H_2O and the SG does not interact with CO_2. For further details of the 1-D COMSOL model, see Ref. 6. All model input parameters are determined from the CBT or other tests or models, so that the work presented here is entirely predictive of the CDRA 4BMS behavior.

Some required inputs, such as total sorbent mass and pressure drops across the beds, are not known for the ISS CDRA 4BMS ground engineering test unit (CDRA-4EU) that is discussed here. The pressure drops are only needed for the model initial conditions, so reasonable guesses were made and iterated upon for quicker convergence. The mass transfer of CO_2 on 13X is not well known; although this will be addressed in future work, here it is assumed that it behaves as on 5A. The heat transfer coefficient relationships (no longer scaled at atmospheric pressure, as in Ref. 6) are not valid at low pressures, so for the desorbing sorbent bed, a scale factor that goes as $\sqrt{(1\ \text{atm}/P)}$ was applied to the calculated coefficient. Although some test inputs (e.g., the adsorbing desiccant bed inlet temperature, the inlet H_2O partial pressure, and the desorbing sorbent bed effluent pressure) may also vary significantly over time and/or from test to test, the values used in the simulations here were not varied from model to model. Ambient temperature, system inlet CO_2 partial pressure, sorbent bed influent temperature, and influent total pressures are constant nominal values. Only flow rate and half-cycle time were varied from model to model to compare with CDRA-4EU test results. The nominal inputs used in the models presented here are given in Table 1. Note they are not the same as used in Ref. 6; the most significant differences are increases in the inlet temperature and dew point and a reduction in the inlet CO_2 partial pressure. Given these inputs, the COMSOL model should completely predict the behavior of the CDRA 4BMS, within the limits of the 1-D simplification, uncertainity of model inputs (e.g., Toth parameters), the inherent accuracy of the linear drifing force (LDF) model, and test to test variability. For faster runtime as well as increased numerical stability, the initial conditions for the bed loadings are set to be close to the expected final results. It should be noted that the initial conditions of the CDRA-4EU test bed for each test are unknown; thus only the final quasi-steady state is compared to the model.

Table 1. Model inputs for the CDRA-4EU

Input	Value
T_{in}	285 K
T_{amb}	294 K
T_{pc}	283 K
Air save mode	10 min
$P_{o,S}$	99,940 Pa
$P_{o,D}$	97,840 Pa
$P_{in,CO2}$	259 Pa
$P_{in,H2O}$	1218 Pa

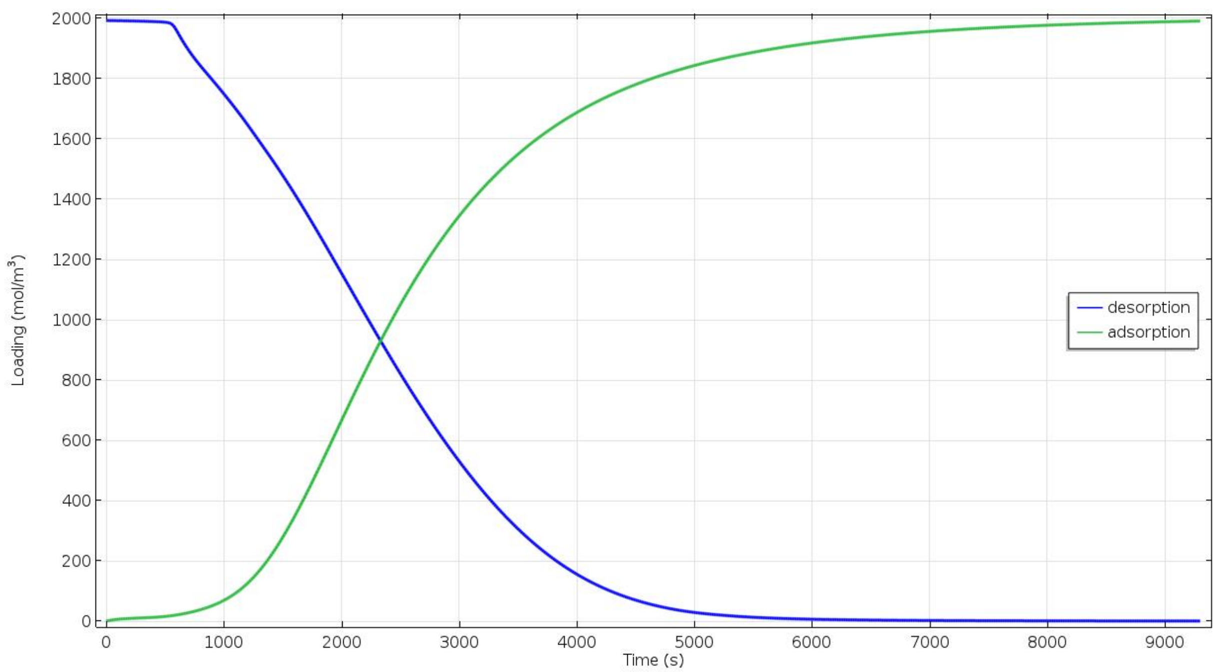

Figure 3 Sorbent bed loading. *Loading of the RK-38 5A pellets in the middle of the sorbent beds during desorption (blue) and adsorption (green) for old nominal operation of CDRA.*

III. Results

Loading results for the old nominal ISS CDRA operation at a 155 minute HC and a flow rate of 20.54 SCFM are shown in Figures 3 and 4; the old nominal conditions are the same as shown in Table 1 but with an inlet CO_2 partial pressure of 518 Pa. The pellet CO_2 loading in the middle of the sorbent beds at the end of a desorption (blue) and adsorption (green) HC are shown Figure 3. It can be seen that there is little desorption for the initial ~10 minutes due to the air save mode, followed by a roughly linear desorption profile. Also, by the middle of the HC, the middle of the sorbent bed has already reached over 85% of its CO_2 capacity. Figure 4 shows the modeled H_2O and CO_2

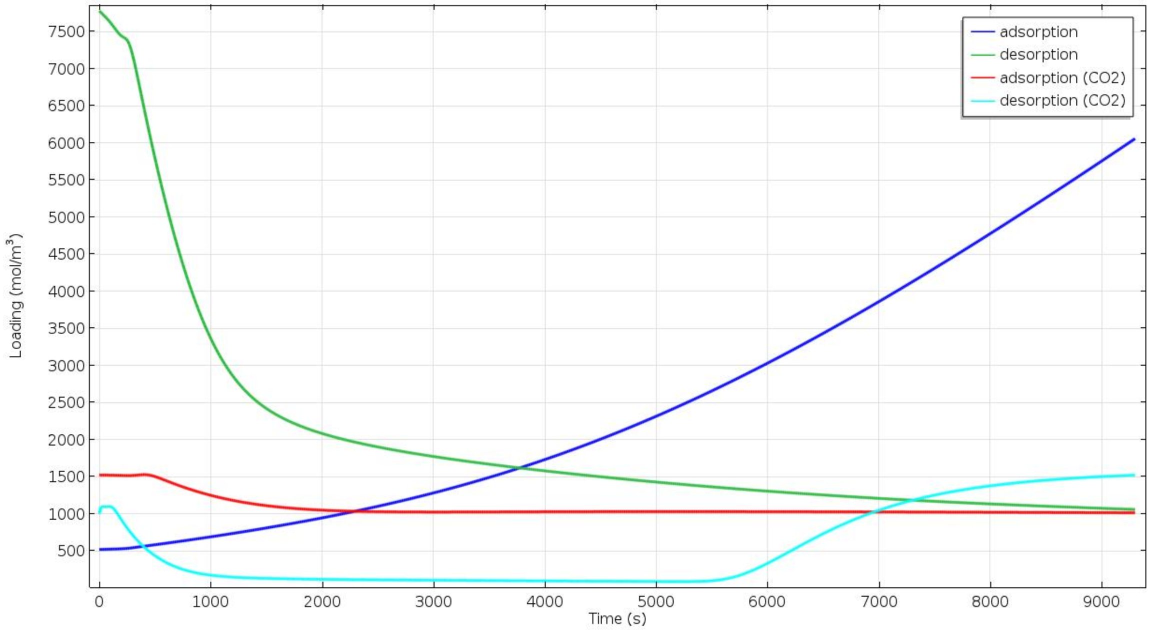

Figure 4 Desiccant bed loading for old nominal ISS CDRA. *Water loading of the SG pellets in the middle of the desicant beds during adsorption (blue) and desorption (green). Also shown is the CO_2 loading in the middle of the 13X beds during adsorption (red) and desorption (light blue).*

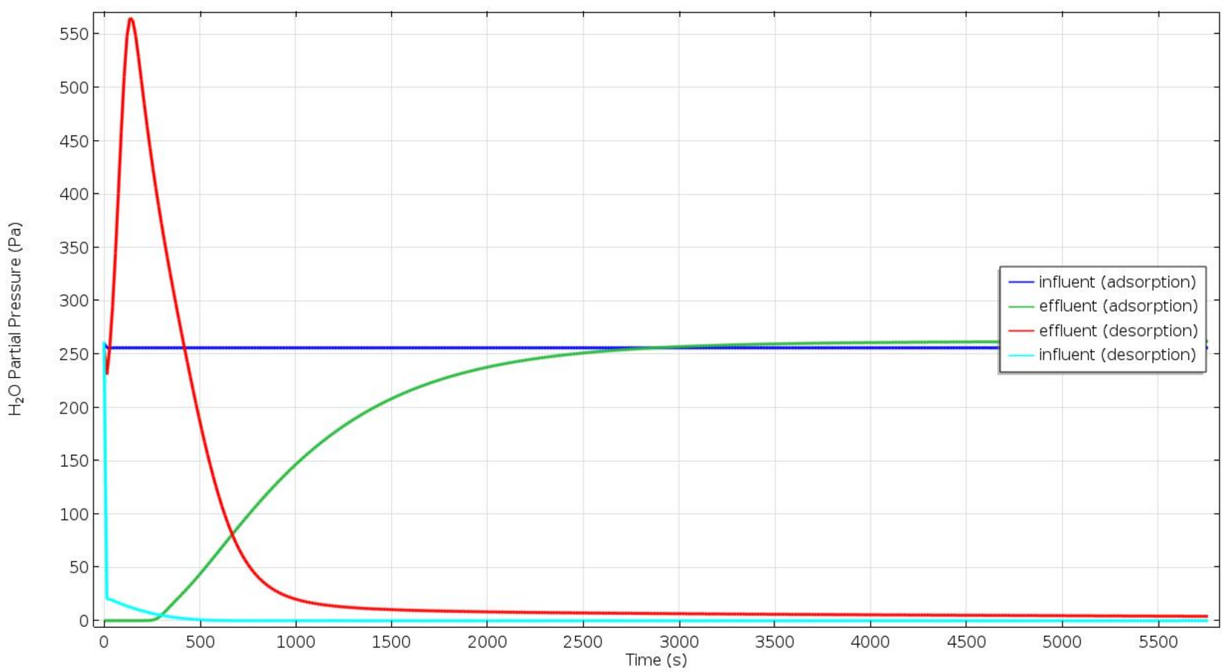

Figure 5 CO_2 Partial Pressure. *CO_2 partial pressure at inlet and exit of the desiccant beds during desorption and adsorption half-cycle for a flow rate of 34 SCFM and a HC of 96 minutes.*

loading after 5 HCs for the desiccant beds at the end of a desorption (blue) and adsorption (green) HC at a point halfway through the whole bed (thus close to the end of the SG layer). At this location, about half of the unloading occurs in the first 15 minutes of the desorption HC, whereas the loading during adsorption is gradual. Also shown in Figure 4 are the CO_2 loading of the 13X pellets in the middle of the 13X beds during adsorption (red) and desorption (light blue). In the intial 10 minutes of the adsorption HC, the pellets unload a little due to water competition. During the desorption HC, the high gas temperature unloads the CO_2 from the 13X within the first few

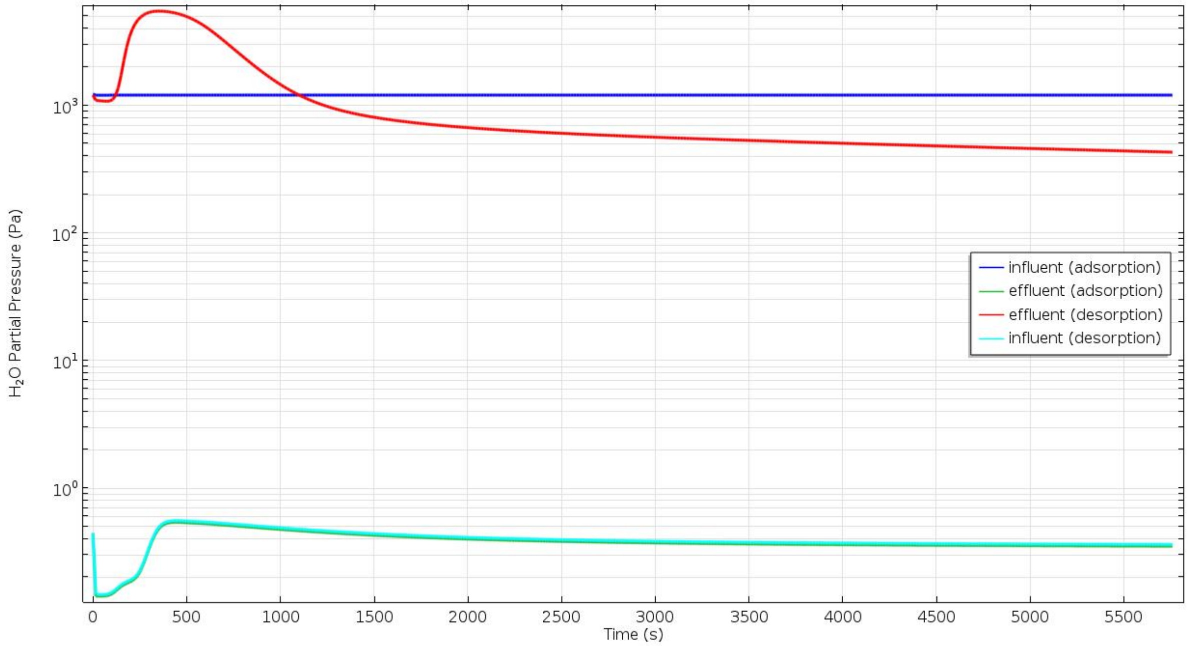

Figure 6 H_2O Partial Pressure. *Log plot of H_2O partial pressure at inlet and exit of the desiccant beds during desorption and adsorption half-cycles for a flow rate of 34 SCFM and a HC of 96 minutes.*

minutes. However, this CO_2 is replaced by the end of the HC as CO_2 that has broken through the sorbent bed returns to the desiccant bed.

Figure 5 shows model CO_2 partial pressure results for a HC of 96 minutes and a flow rate of 34 SCFM. This model has an inlet CO_2 partial pressure of 259 Pa. In this case, although the total air volume per HC through the CDRA is nearly the same as in the old nominal CDRA operation (~3200 SCF), due to the lower CO_2 partial pressure, the CO_2 does not significantly break through the sorbent bed (see Figure 7 below). The adsorption inlet (blue) is constant, whereas the exit (green) slowly rises as first the 13X CO_2 capacity is reached and then some CO_2 gets pushed off by H_2O. The brief rise at the influent during desorption (light blue) is due to the sorbent bed not being fully evacuated during the relatively short half-cycle (see Figure 7 below). The 'burp' at the effluent during desorption (red) is due to the 13X desorbing its load of CO_2. The magnitude of this burp has a substantial impact on the final CO_2 removal rate when the sorbent bed is operating below capacity.

Figure 6 shows the model desiccant H_2O partial pressure results for the same model as shown in Figure 5. Since the sorbent bed merely transports H_2O, the adsorption effluent (green) and desorption influent (light blue) are nearly indentical. The desorbing effluent (red) partial pressure exceeds the constant influent partial pressure (red) when the air is hot enough to drive off most of the H_2O from the SG; the initial dip is due to the dry air coming from the sorbent bed before significant unloading can occur. That is, the flow timescale is shorter than the sorption timescale. It should be noted that due to the higher inlet dew point of this model compared to the old ISS CDRA model, about ¾ of the 13X bed is loaded with water by the end of an adsorption HC.

Figure 7 shows the model CO_2 partial pressure in the sorbent beds for the same model as shown in Figures 5 and 6. Note that the left hand side of the bed is the effluent during desorption and the influent during adsorption. The CO_2 front during adsorption (blue) does not reach the effluent. During desorption, when the right hand side boundary is sealed and the left hand side is exposed to vacuum, the bed is not fully emptied of CO_2; note however that the remaing CO_2 has been desorbed from the sorbent during the HC. The dip on the right hand side is due to the

Table 2. CO_2 removal rates and efficiencies

HC (min) & flow rate (SCFM)	Measured Removal Rate (kg/day)	Calculated Removal Rate (kg/day)	Measured Efficiency	Calculated Efficiency
124 & 30	5.13	5.18	0.78	0.83
144 & 30	4.85	4.62	0.74	0.74
96 & 34	5.69	5.82	0.81	0.82

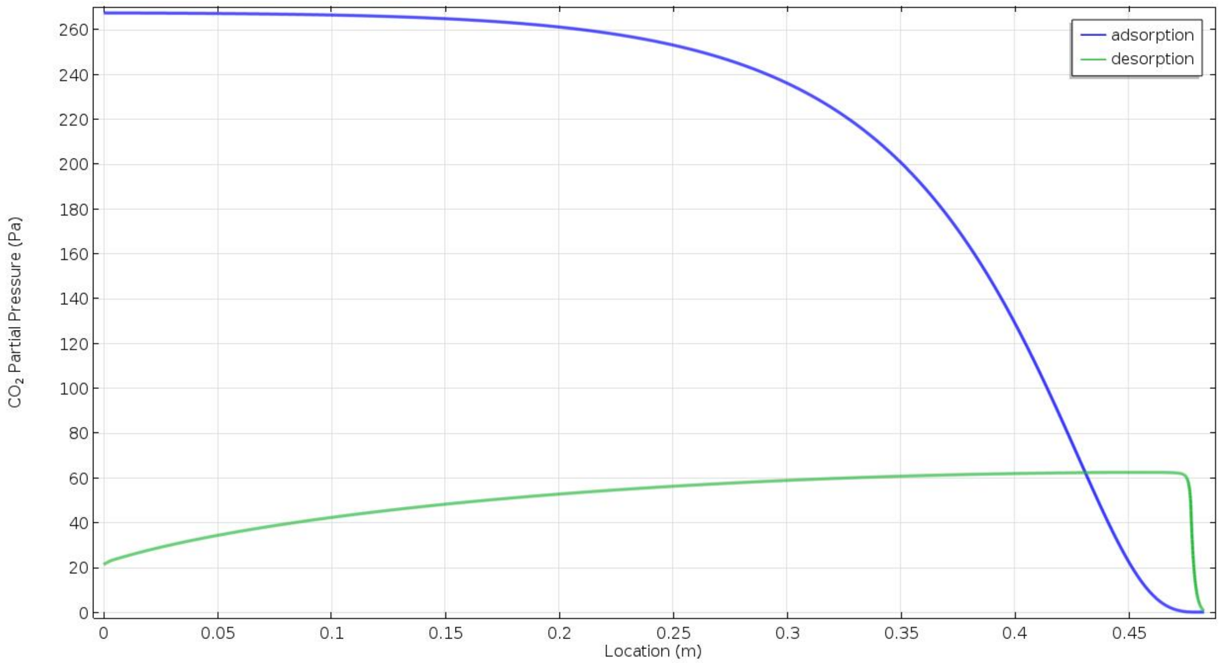

Figure 7 CO_2 Partial Pressure. *CO_2 partial pressure in the sorbent beds at the end of an adsorption (blue) and desorption (green) half-cycle for a flow rate of 34 SCFM and a HC of 96 minutes.*

fact the glass beads do not have any CO_2 to desorb.

Although other metrics must be met (e.g., the maximum water dew point out of the desiccant bed), the primary diagnostic of the CDRA-4EU performance is the CO_2 removal rate in kg/day. The results for the removal rate predicted by COMSOL and those experimentally measured are given in Table 2. Also listed are the estimated efficiencies. With all of the uncertainties in both the test data as well as the model, the agreement is remarkable.

The model is now being used to determine where in HC and flow rate parameter space ISS CDRA can achieve the maximum CO_2 removal rate. Tentatively this is estimtated to be 145 minutes and 26 SCFM. This fills the 13X layer of the desiccant bed with water while maximally using the CO_2 capacity of the sorbent bed; a lower inlet dew point would provide even more margin. Further, the model is being used to design the optimal exploration (4BMS-X) system where mass is at a premium. Here, since in nominal operation much of the 13X layer does not see water, the goal is to remove as much 13X as possible while not impacting the adsorbing effluent dew point. The tentative 4BMS-X model is removing 75% of the 13X layer and running at a HC of 80 minutes and a flow rate of 33 SCFM. An illustration of the relative behavior of the removal rate in this parameter space is given in Figure 8. The highest rates are achieved at the shortest HC times and highest flow rates. However, the minimum HC time is limited by the rate of heating of the sorbent bed during desorption; in the present design it takes ~80 minutes to reach the set point of 475 K.

IV. Summary & Conclusion

The objective of this work was to establish a virtual CDRA 4BMS testbed capability at MSFC. The constructed COMSOL model shows great promise in predictively modeling the ISS CDRA 4BMS, even with some appoximate approaches to the 1-D modeling of a 3-D system. It is now being used as a virtual laboratory at MSFC to explore optimization of the 4BMS sub-system on ISS, trouble shoot present ISS CDRA operation, and design future exploration life support systems. Clearly the actual system is not 1-D and further empirical work will be needed, particularly to model the non-cylindrical channels of the sorbent beds. 2-D and 3-D analysis is underway to further refine the model. Together, these tools will help decrease cost and turnaround time for developing the next generation life support systems.

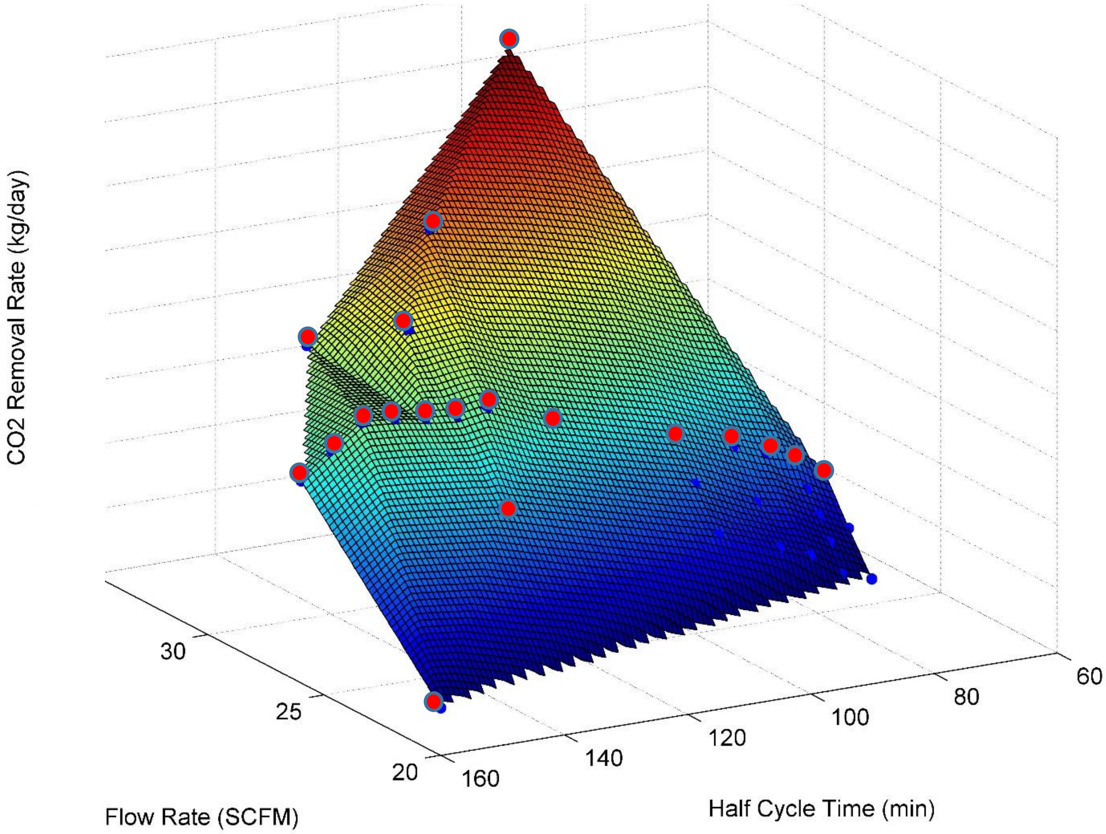

Figure 8 Predicted CO_2 Removal Rate. *An illustration of the relative removal rate behavior of the CDRA system in HC/flow rate space. Red dots show calculated points; the surface is interpolated from these.*

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