Advancements in Carbon Dioxide and Water Vapor Separations Using COMSOL

James Knox[1], Kenneth Kittredge[1], Robert F. Coker[1], Ramona Cummings[1], Carlos F. Gomez[1]

[1]NASA - Marshall Space Flight Center, Huntsville, AL, USA

Abstract

"NASA's Advanced Exploration Systems (AES) program is pioneering new approaches for rapidly developing prototype systems, demonstrating key capabilities, and validating operational concepts for future human missions beyond Earth orbit" [1]. Under the new Atmosphere Revitalization Recovery and Environmental Monitoring (ARREM) project [2], efforts are focused on improving current state-of-the-art systems utilizing fixed beds of sorbent pellets by evaluating structured sorbents, seeking more robust pelletized sorbents, and examining alternate bed configurations to improve system efficiency and reliability. These development efforts combine testing of sub-scale systems and multi-physics computer simulations to evaluate candidate approaches, select the best performing options, and optimize the configuration of the selected approach, which is then implemented in a full-scale integrated atmosphere revitalization test. Reference 3 discusses the hardware design and sorbent screening and characterization effort in support of the ARREM project within the AES program. This paper describes the development of atmosphere revitalization models and simulations in support of the ARREM project. COMSOL Multiphysics has been used in the following technology development efforts: (1) Development of 1-D and 2-D Axisymmetric Packed Bed Models and Comparison with Breakthrough Curves. Adsorption in fixed beds of pelletized sorbents is the primary means of gas separation for atmosphere revitalization systems. For the bulk separation of CO2 and H2O, temperature changes due to the heat of adsorption are significant, requiring the modeling and simulation of the heat balance equations. For columns with small tube diameter to pellet diameter ratios, as encountered in internally heated columns, flow channeling along the column wall can have a strong influence on overall performance [4]. In some cases, the influence is great enough to necessitate the use of 2-D simulations as shown in Figure 1. (2) Isothermal Bulk Desiccant Development. Initial models of the 4-column IBD with an aluminum (Al) foam lattice were conducted using the COMSOL Multiphysics code. For the porous flow part of the model, the code solves the low Mach number, compressible Brinkman equations modified by a Forchheimer drag term. Forchheimer drag adds a drag term that is proportional to the square of the fluid velocity, rather than just linear, as is the case in Darcy flow, with a coefficient given by βF = 1.75ρg*√(ε/150/κ). Heat transfer is modeled by solving the heat transfer equations separately for the porous medium (the beds) and the solid Al canister, with appropriate boundary conditions. Modeling results are showing in Figure 2. A second prototype test fixture, also shown in Figure 2, will be modeled following model validation. (3) Microlith Residual Desiccant Development. Figure 3 provides a cross-section of the Microlith concept and 3-D COMSOL velocity mapping of the jelly roll. This analysis provided important insight leading to successful corrective action for a flow channeling problem. Further uses of this model will be to map flow maldistribution following

corrective action. With the addition of adsorption physics, this model will provide a means for optimization of cyclic parameters for this hardware, and allow for design optimization studies for new Microlith designs.

Reference

1. NASA. "Human Exploration & Operations (HEO)." 2012.
2. Perry, J. L., Abney, M. B., Knox, J. C., Parrish, K. J., Roman, M. C., and Jan, D. L. "Integrated Atmosphere Resource Recovery and Environmental Monitoring Technology Demonstration for Deep Space Exploration," International Conference on Environmental Systems. AIAA, San Diego, 2012.
3. Knox, J. C., Gostowski, R., King, E., Thomas, J., Trinh, D., and Watson, D. "Development of Carbon Dioxide Removal Systems for Advanced Exploration Systems," International Conference on Environmental Systems. AIAA, San Diego, 2012.
4. Tobis, J., and Vortmeyer, D. "The near-wall channeling effect on isothermal constant-pattern adsorption," Chemical Engineering Science Vol. 43, No. 6, 1988, pp. 1363-1369.

Figures used in the abstract

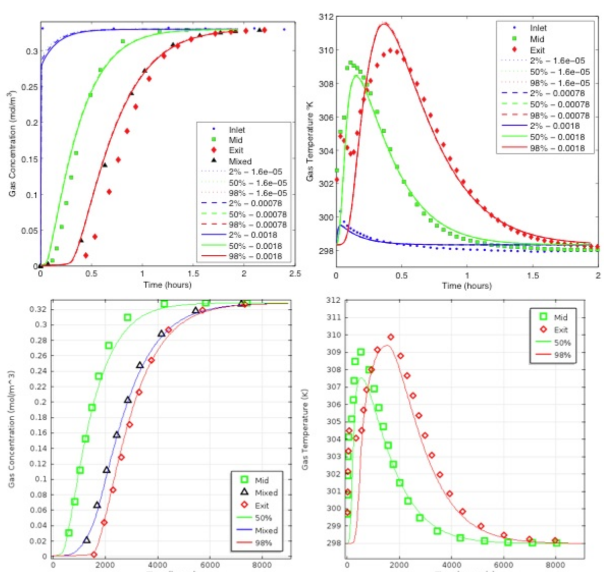

Figure 1. Breakthrough test data and 1-D (top) and 2-D axisymmetric (bottom) simulation results for CO_2 on zeolite CaA. *Concentration history (left) and temperature history (right). Experimental data are shown as symbols. Simulation data at the inlet (2%), midpoint (50%), and exit (98%) are shown as lines.*

Figure 1

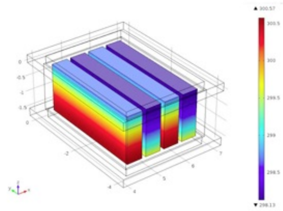

Figure 2. Temperatures (in K) on the bed surfaces at the end of the simulation (left); Cutaway of proposed Test Fixture (right) *Counting from left to right, columns 1 and 3 have wet air flowing downward and columns 2 and 4 have dry air flowing upward.*

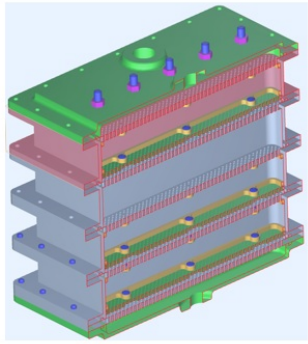

Figure 2

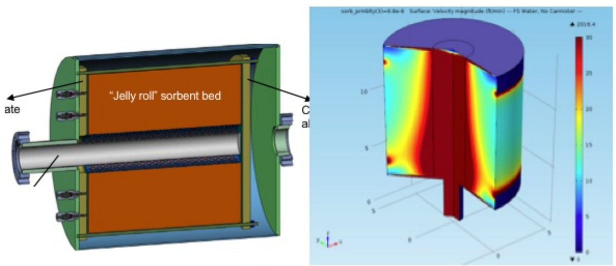

Figure 3. Internal cross-section view of the Microlith-based radial flow adsorber design concept (left) and 3-D Velocity Mapping of the Jelly Roll (right)

Figure 3