

Advancements in Carbon Dioxide and Water Vapor Separations Using COMSOL Multiphysics® Software

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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 multiphysics 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 provides an update on the development of atmosphere revitalization models and simulations in support of the ARREM project during 2012 and 2013. COMSOL Multiphysics® software 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 require the use of 2-D simulations as shown in Figure 1.

(2) One-Third Scale Isothermal Bulk Desiccant Development. Initial models of a new 2-column IBD shown in Figure 2 with heat exchanger plates were conducted using the COMSOL code. Modeling results are showing in Figure 3.

(3) Microlith Residual Desiccant Development. Figure 4 provides a cross-section of the Microlith concept and 3-D COMSOL results showing concentration and bed loading of the jelly roll. With the addition of adsorption physics in 2013, this model provides a means for

optimization of cyclic parameters for this hardware, and allows 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, Vail, 2013.
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

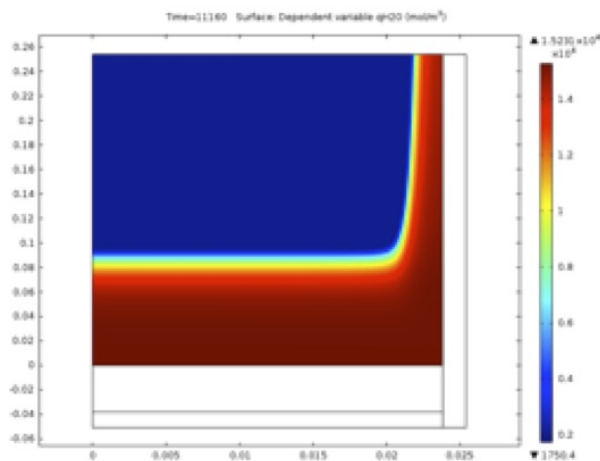
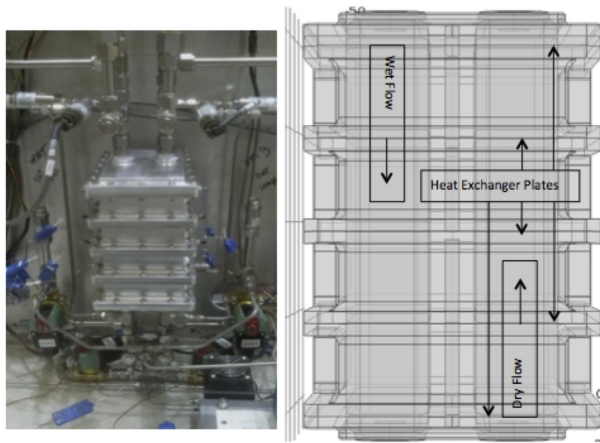


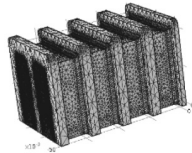
Figure 1: Concentration gradient in 2-D axisymmetric simulation of adsorption in a fixed bed.



1/3 scale of system required for 4 person crew.
 Cooled (60°F) air flow at 190/160 slpm with 10 °C dew point.

Figure 2: Photograph and diagram of isothermal bulk desiccant test apparatus.

IBD (model)



- Simplified 3D COMSOL model with HX plates as porous media
- Tracks concentration, temperature, flow path, loading
- Spatially varying porosity and permeability
- Qualitative match but not yet sufficiently quantitatively predictive

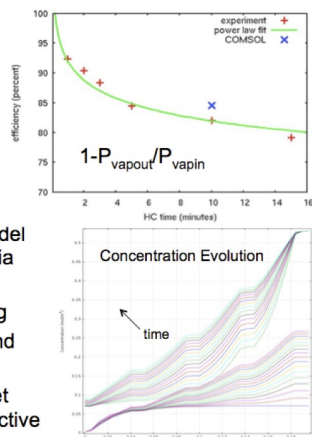


Figure 3: IBD model and results.

Microlith (model)

- Flow is from the top (meshes are upside down)
- Finely resolve mesh required
- Similar approach to IBD
- Constant porosity and permeability (fit to pressure drop)
- Thermal coefficients used
- Complex flow at bottom plate
- Breakthrough occurs non-uniformly
- Numerical issues (negative c and q)

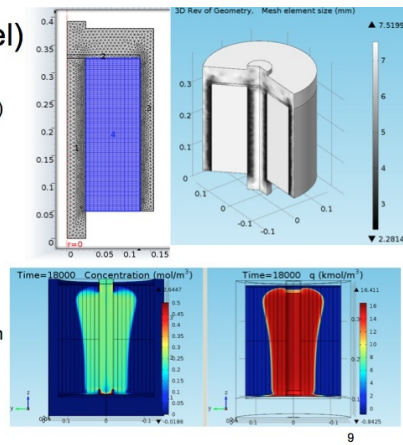


Figure 4: Microlith model and simulation results.