Modeling of Atmosphere Revitalization

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Introduction

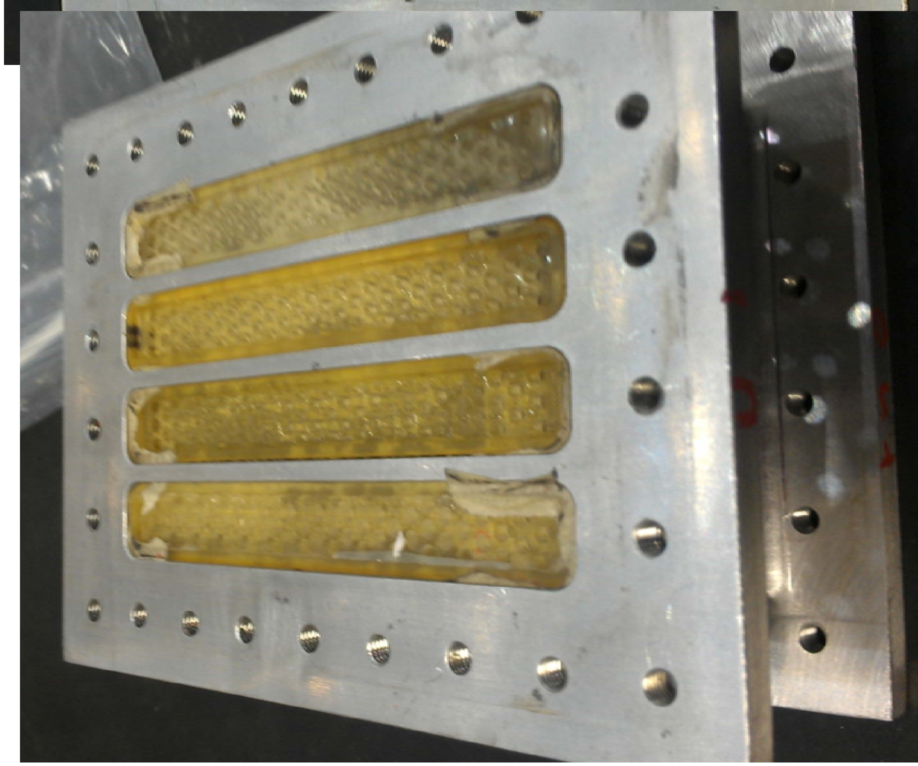
- NASA's AES is pioneering new approaches for future human missions beyond Earth orbit.
- All spacecraft systems must be minimized with respect to mass, power, and volume.
- Here, we show work related to improving system efficiency and reliability for water separation systems on crewed vehicles
  - the initial development of COMSOL simulations in support of the Atmosphere Revitalization Recovery and Environmental Monitoring (ARREM) project

Isothermal Bulk Desiccant

- Simultaneous desorbing and adsorbing flows
- Two paths are thermally linked
  - Adsorption more efficient due to heat loss
  - Desorption more efficient due to heat gain
- Linking can be done in variety of ways
  - e.g., Meshes or grids filled with sorbent
  - Here, simply a thermally conductive housing (Al)
- Flow paths alternate every ‘half-cycle’
- Can be driven by different means
  - e.g., vacuum
  - Here, driven by slight pressure differences from atmospheric

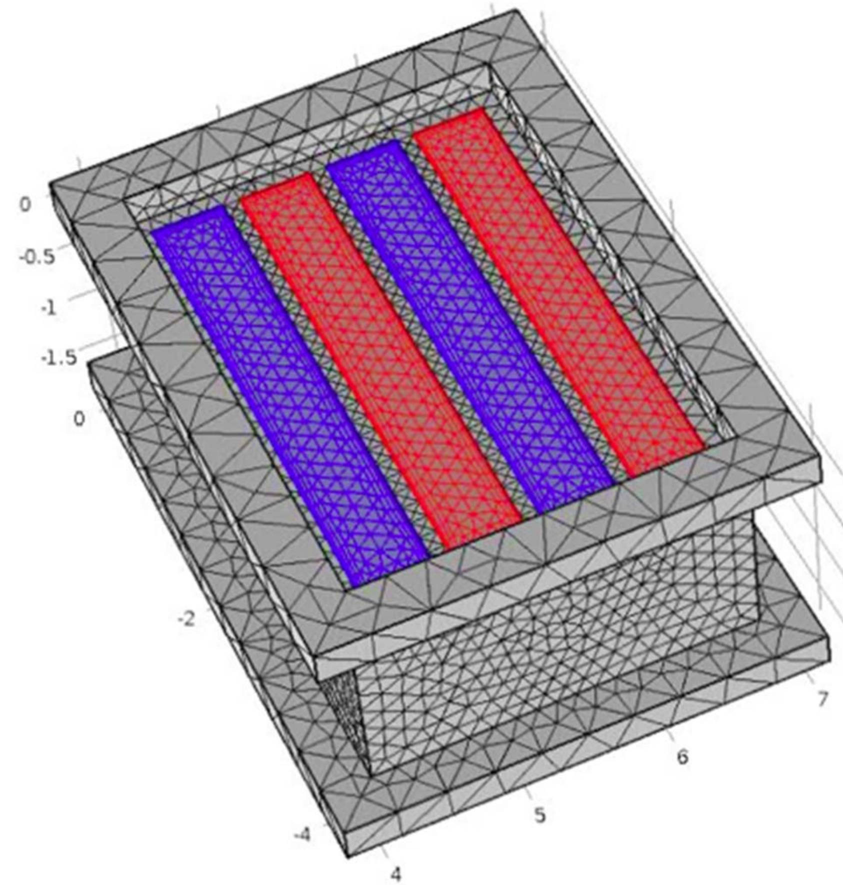
Isothermal Bulk Desiccant

- Geometry choice impacts mass
- Tested a sub-scale 4-cell IBD version
- Used 13X sorbent (large and fragile pellets)
- Both a plastic (unlinked) and Al 6061 (linked) housing
- Covered inlet and exit with mesh-covered baffles



Isothermal Bulk Desiccant

- Imported IGS CAD file directly into COMSOL
- Meshed immediately
  - Working with an un-converged mesh
- Red/blue domains are paired regions of wet/dry flow
- Baffles and manifold not modeled here



The size of the IBD bed in the three dimensions are shown in inches

IBD Comsol Model Description

- Physics Nodes:
  - Free and Porous Media Flow with Forchheimer Drag
  - Dilute Species Transport with Convection, Diffusion, and Reactions
  - Heat Transfer in Porous Media with a Heat Source
  - Heat Transfer in Solids
  - Domain ODE
  - Wall Distance (modified Eikonal equation)
- Transport of a dilute species, H_2O, in a carrier gas, N_2, modeled as free and porous media flow with pressure boundaries.
- The sorption rates and pellet loading were determined from solving a distributed ODE.
- Heat transfer in the porous media and the solid housing were modeled with the respective physics nodes.
- A wall-distance calculation was required to determine the local packing density of the pellets.
- Boundary conditions (inflow/outflow and wet/dry air) were switched after every half-cycle of the desiccant bed.

IBD Comsol Model Inputs

- Porosity model: $$\varepsilon(D) = \varepsilon_0 (1 + (\frac{1}{\varepsilon_0} - 1) e^{-4D/d_p}$$

  where D=distance to nearest wall, d_p =pellet diameter, ε_0=center-line porosity
- Permeability model (BKZ): $$\kappa(\varepsilon) = \frac{d_p^2 \varepsilon^3}{150(1-\varepsilon^2)}$$
- Sorbent mass balance (LDF approximation): $$\frac{dq}{dt} = k_m (q^* - q)$$

  where k_m = mass transfer coefficient, q*=equilibrium loading
- Reactions: $$R_i = -\frac{dq}{dt} \frac{(1-\varepsilon)}{\varepsilon}$$
- Heat source: $Q = -(1-\varepsilon) \frac{dq}{dt} \delta H$ where δH=heat of adsorption
- Forchheimer Drag Coefficient: $$\beta_F = 1.75 \rho_g \sqrt{\frac{\varepsilon}{150\kappa}}$$

Equilibrium Loading

- Loading from Toth equations:

$$q^* = \frac{\rho_S a p}{(1 + (bp)^t)^{1/t}}$$

$$b = b_0 e^{E/T} \quad a = a_0 e^{E/T} \quad t = t_0 + c_0 / T$$

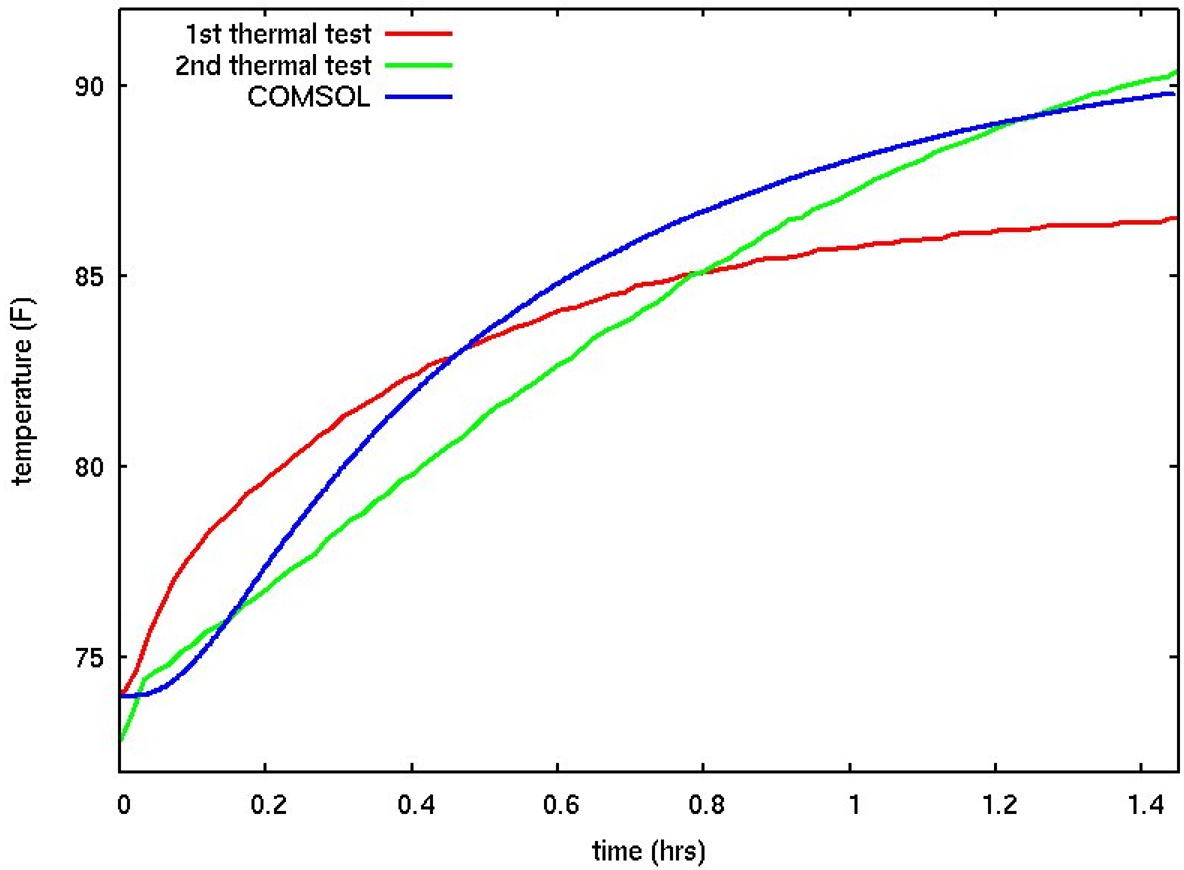
where a_0, b_0, c_0, and E are the Toth constants for H_2O on 13X

Physical Inputs

- Empirically determined:
  - mass transfer coefficient: 0.033 s^{-1}
  - dispersion coefficient: 0.0012 m^2/s
  - center-line porosity: 0.3
- Physical details of Sorbent and Housing:
  - density
  - heat capacity
  - heat transfer coefficient
  - thermal conduction
- Flow details: flow rates, inlet temperatures, inlet and exit pressures, inlet H_2O concentration

Results: Thermal Characterization

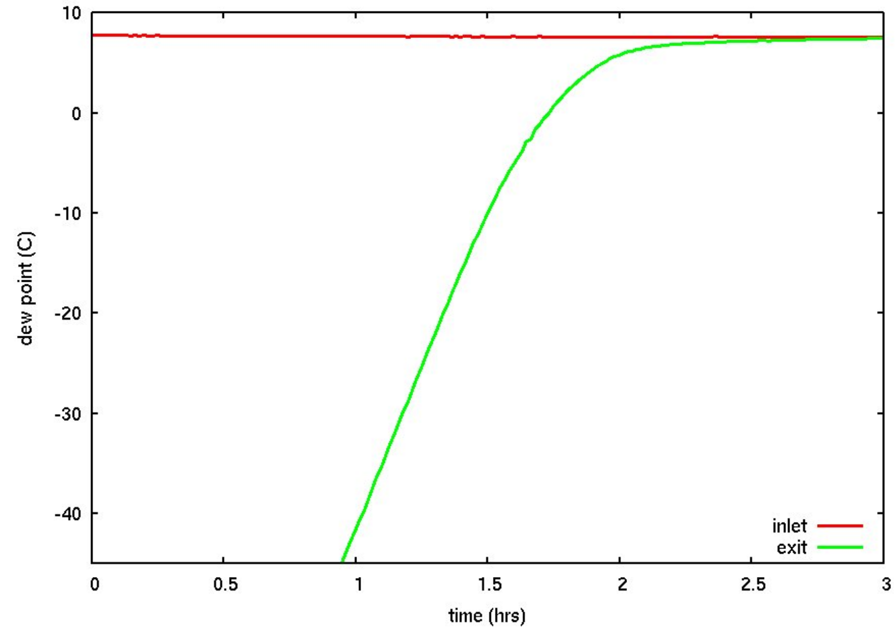
- Experiment not initially intended for this purpose
- Match to data requires ‘unreal’ physical parameters
- Test article boundary conditions very complex (thermal leaks and sinks)
- Nominally insulated

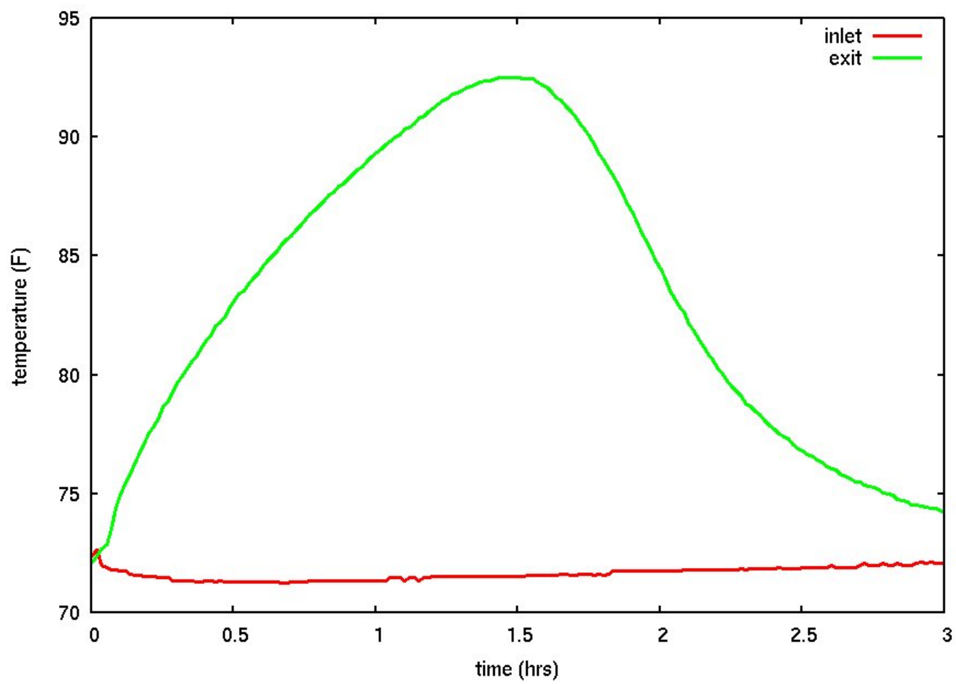


Nominal physical values (k, κ, cp, h) result in a much too rapid rise (<.2 hrs) to the inlet 115 °F value. Plastic housing.

Results: Breakthrough

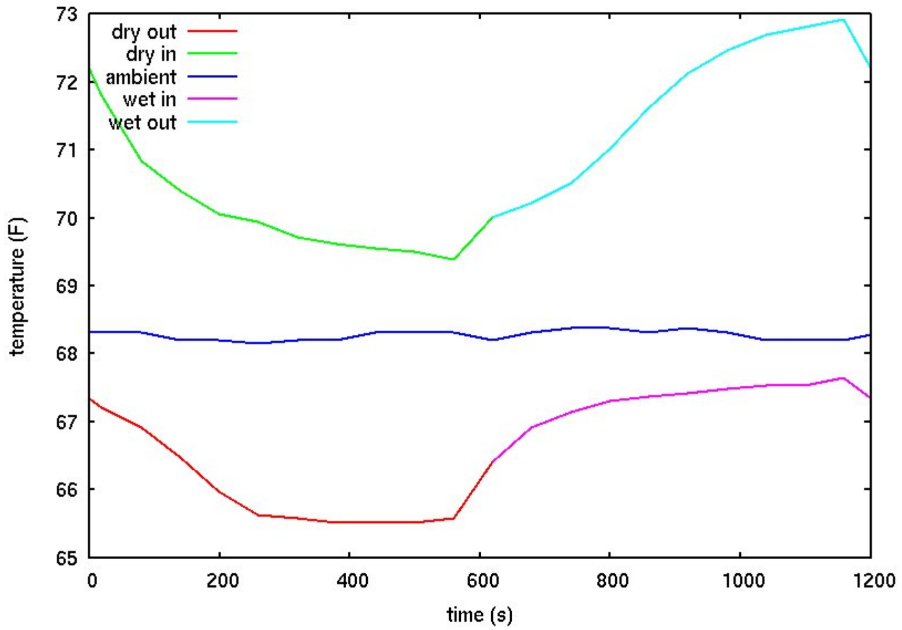
- Not yet modeled with Comsol due to time-step crashes
- Test not well diagnosed
- Packing not well constrained
- Likely suffering from dusting and clogging

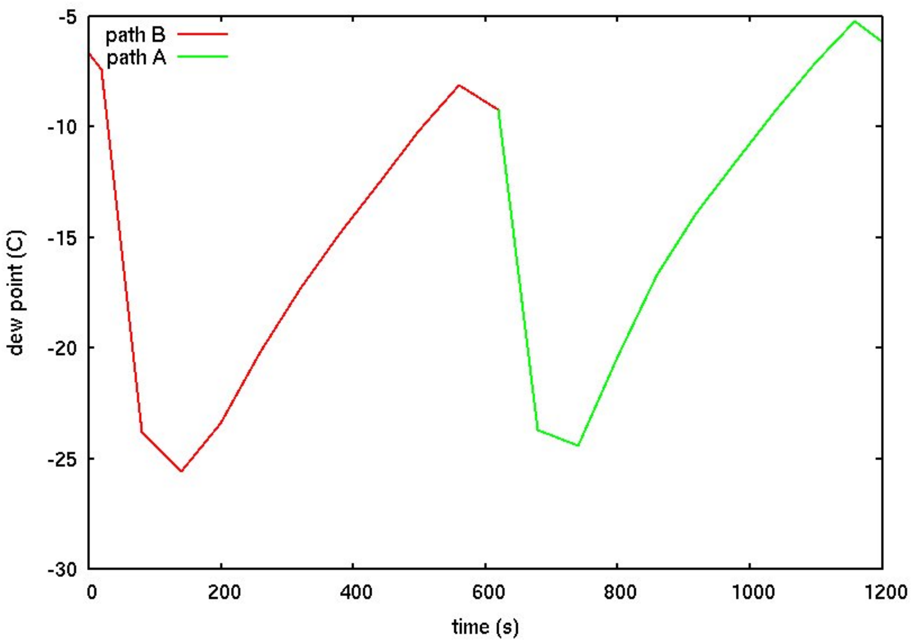




Results: Time-Dependent

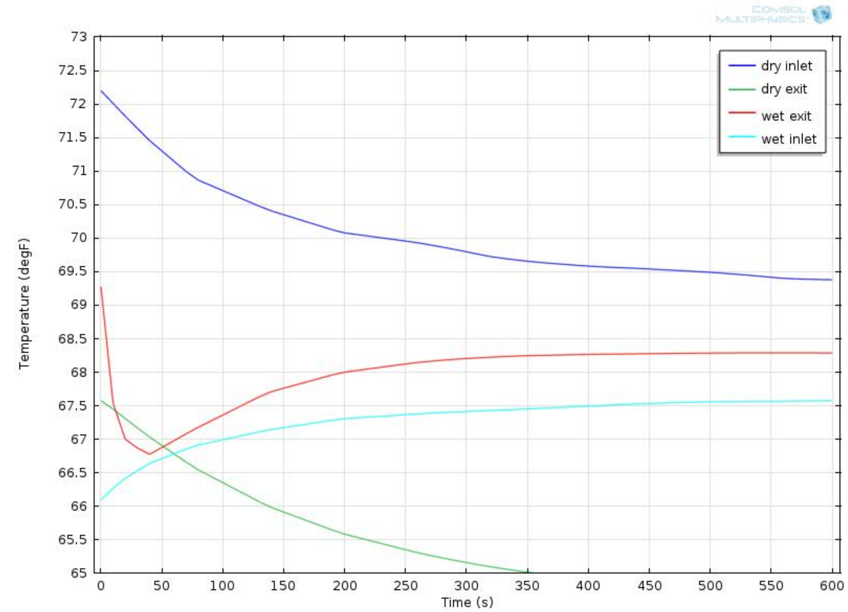
- Required checks to ensure positive quantities (concentration, gas density, flow rate, pressures, loading)
- 13X isotherm is flat at low vapor pressures, so large initial loading required
- Takes extremely long time to run-time converge (i.e. months of calendar time!)
- Aluminum housing.
- End of 8 hour experiment.
- Reached symmetry around the ambient temperature.
- Inlet dew point 8 °C, so peak efficiency here is ~93%.

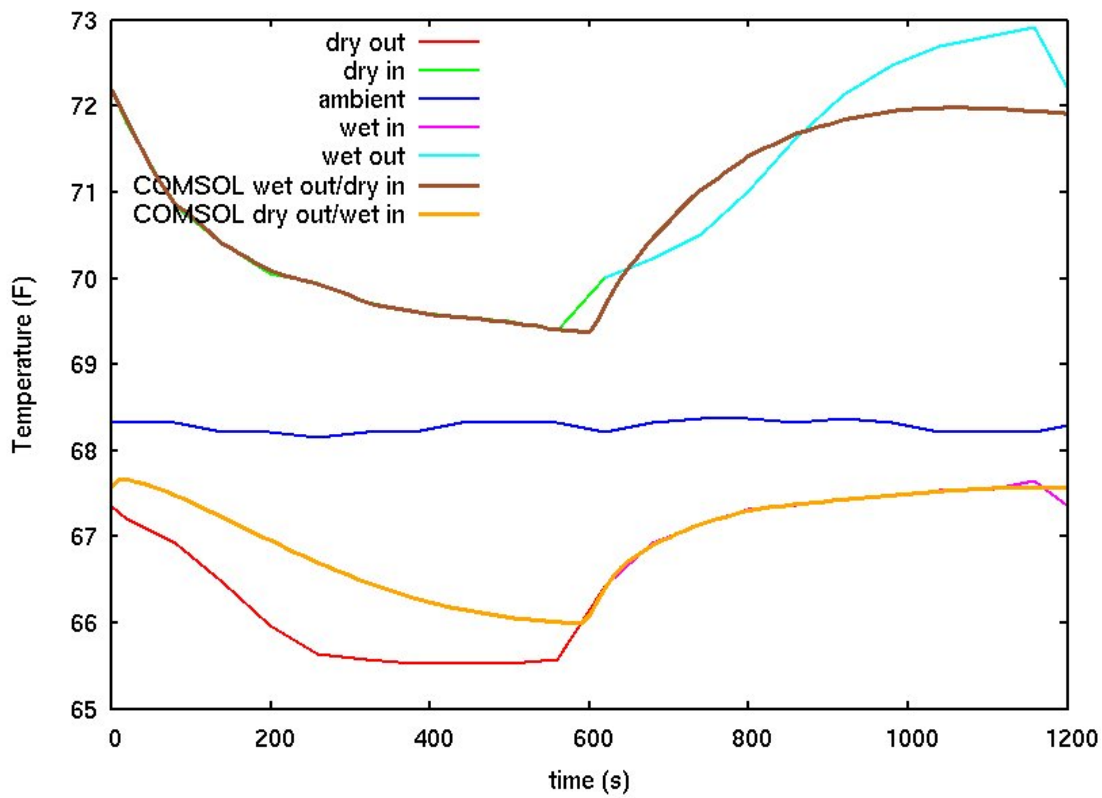




Results: Time-Dependent

- System is 'unloading' very slowly from saturated initial conditions
- Concentration still too high as well (only ~60% efficiency)
- Using MATLAB script to automate





Summary

- Just starting to use Comsol for NASA AES ARREM problems
- Initial tests with silica gel seem more numerically robust
- Very sensitive to initial conditions (e.g., loading) and boundary conditions (e.g., volumetric flow inlet does not converge well)
- Not yet spatially converged (takes weeks to run on a server)