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Full System Modeling and Validation of the Carbon Dioxide Removal Assembly

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Introduction

- Advanced Exploration Systems (AES) Program:
  - pioneering approaches for rapidly developing prototype systems
  - validating concepts for human missions beyond Earth orbit
- Atmosphere Resource Recovery and Environmental Monitoring Project (ARREM):
  - mature environmental subsystems
  - derived directly from the ISS subsystem architecture
  - reduce developmental and mission risk
  - demonstrate concepts for human missions beyond Earth orbit

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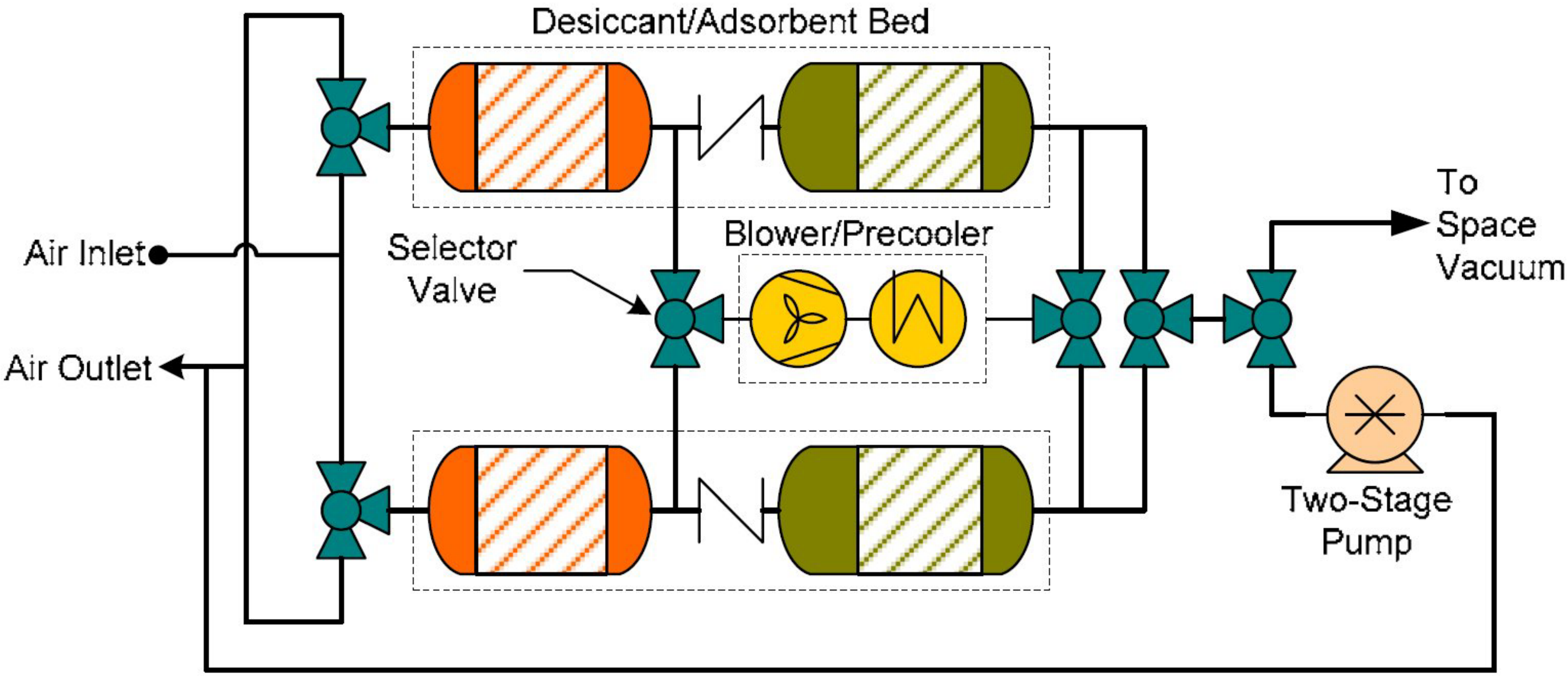
Carbon Dioxide Removal Assembly (CDRA)

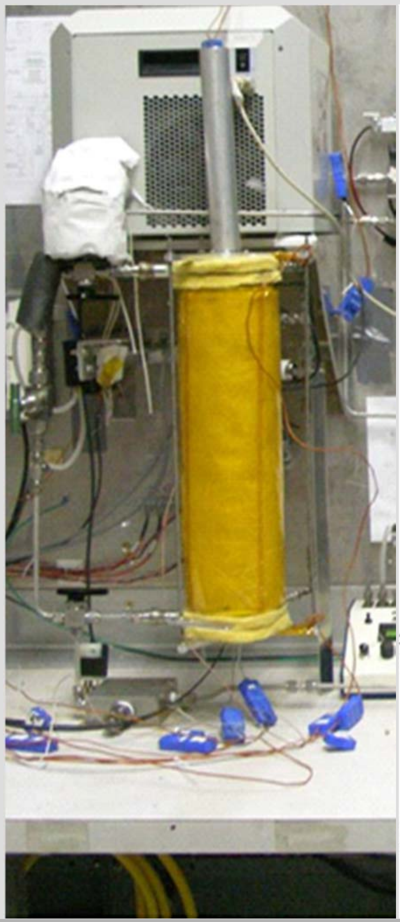
- Goal: *Predictive* model of the CDRA
- Here, focus on the Desiccant Beds (1D)
- Need sorbent behavior (isotherms, LDF, etc.)

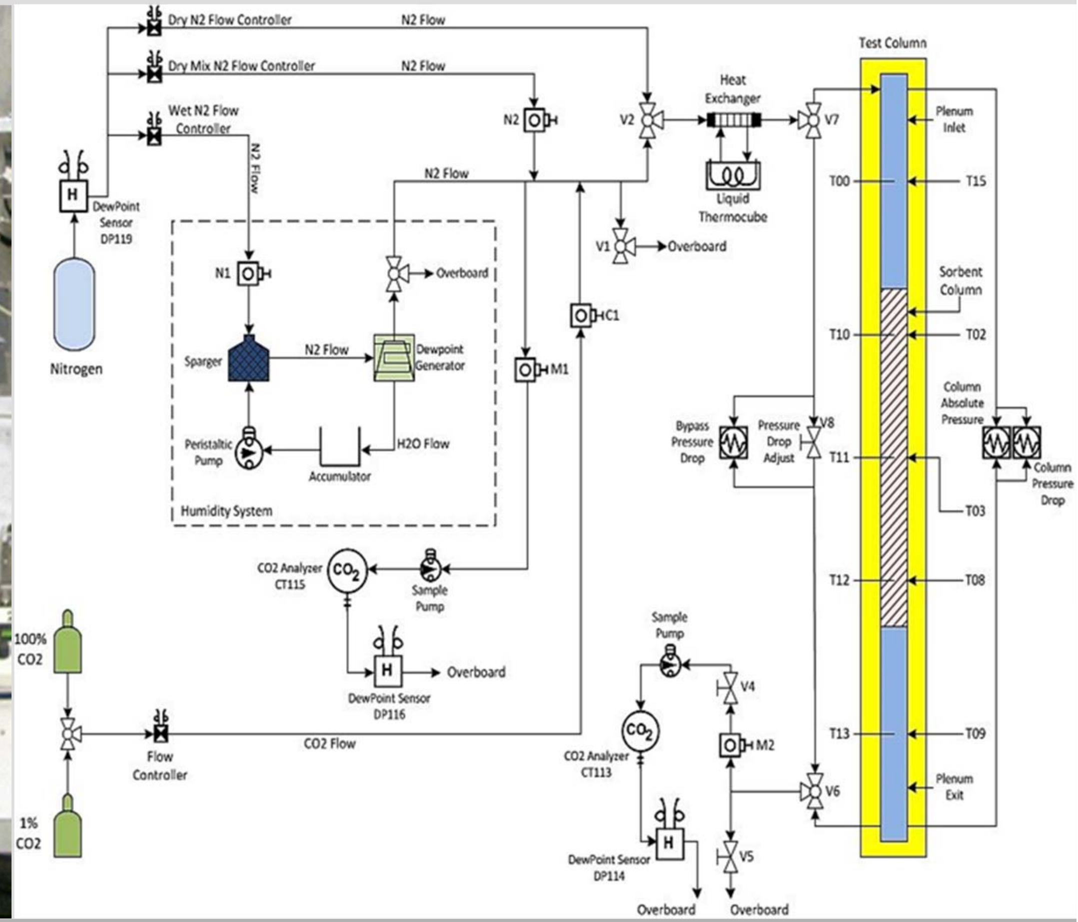


Cylindrical Breakthrough Test (CBT)

- Multiple sorbents: RK38, 13X G544, 5A G522, SG G40, SG B152
- Multiple sorbates: CO_2, H_2O
- Variable flow rates, concentrations, and temperatures

- Well diagnosed (TCs, FCs, DPs, PTs, masses)
- Insulated
- Surrogate for CDRA DBs





Modeling Approach

- Use Toth isotherms from other work
- Use dimensionless correlations (Re, Nu, Pe, Pr, Sc)
  - Derives mass dispersion and thermal transfer coefficients
- Assume binary mass diffusion is valid
- Assume constant porosity
- Use Rumpf-Gupte permeability relationship
- 1D 'plug flow' style model with wall corrections
- Fit the single remaining model parameter using CBT data
  - Across-the-board validity of the 1D LDF model?
- Apply predictively to POIST data
- Use for CDRA parameter study (size, flow, temperature)
- Use COMSOL Multiphysics Code to solve the PDEs

Model

Solve 7 PDEs:

- 1^{st} order Ergun equation for interstitial velocity
- Gas pressure assuming ideal gas law
- Sorbate concentration
- Pellet loading
- Sorbent temperature
- Gas temperature
- Wall housing temperature

- BCs tricky in COMSOL (applied only to flux terms)
- Time-dependent inlet conditions (flow rate, T_{gas}, concentration)
- Temperature-dependent material properties
- Adsorption and Desorption half-cycles with changing BCs

The PDEs

$$\frac{P}{R_s T_g}\frac{\partial u}{\partial t} = -\left(\frac{\partial P}{\partial x} + \frac{u\mu}{\kappa_s}\right) - \frac{u}{R_s}\frac{\partial\left(\frac{P}{T_g}\right)}{\partial t}$$

$$\frac{\epsilon_s}{R_s T_g}\frac{\partial P}{\partial t} + \frac{\partial}{\partial x}\left(\frac{uP}{R_s T_g}\right) - \frac{\epsilon_s}{R_s {T_g}^2} P \frac{\partial T_g}{\partial t} = 0$$

$$\frac{\partial c}{\partial t} + \frac{(1-\epsilon_s)}{\epsilon_s}\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(-D_x \frac{\partial c}{\partial x}\right) = -\frac{\partial}{\partial x}(uc)$$

$$\frac{\partial q}{\partial t} = (q_* - q)k_m$$

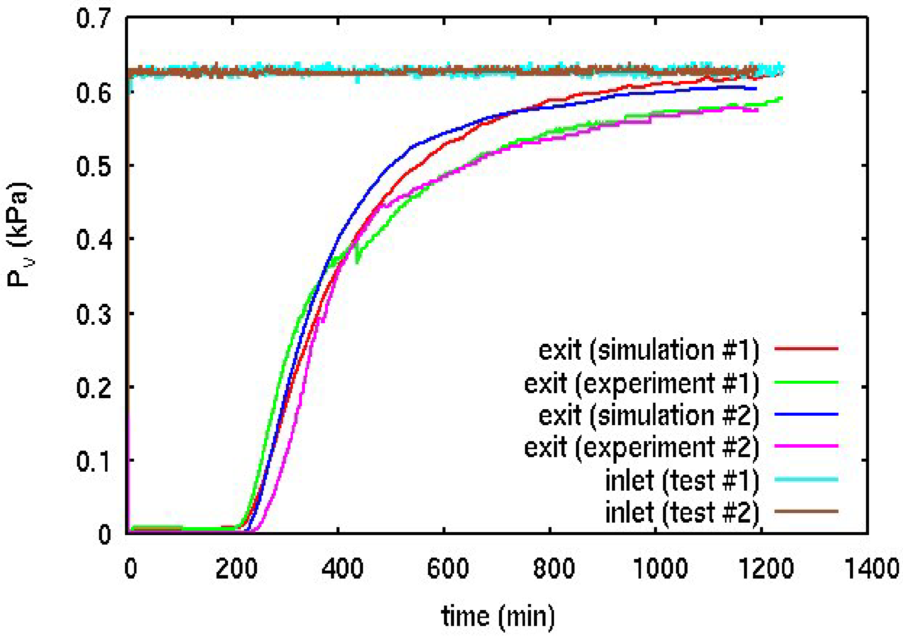
LDF parameter

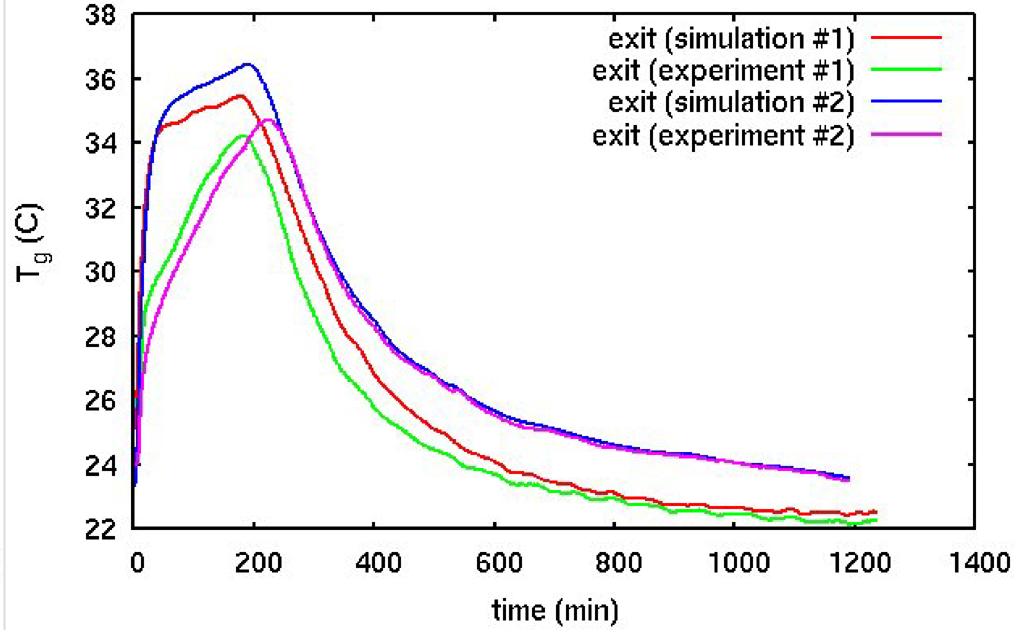
$$(1-\epsilon_s)\rho_s c_{ps}\frac{\partial T_s}{\partial t} + \frac{\partial}{\partial x}\left(-k_s(1-\epsilon_s)\frac{\partial T_s}{\partial x}\right) = \mathrm{A}h_{sg}(T_g - T_s) - \partial\mathrm{H}(1-\epsilon_s)\frac{\partial q}{\partial t}$$

$$\epsilon_s\rho_g c_{pg}\frac{\partial T_g}{\partial t} + \frac{\partial}{\partial x}\left(-k_{gx}\epsilon_s\frac{\partial T_g}{\partial x}\right) = \mathrm{A}h_{sg}(T_s - T_g) - \epsilon_s\rho_g c_{pg} u \frac{\partial T_g}{\partial x} + \frac{P_I h_{gc}(T_c - T_g)}{A_f}$$

$$\rho_c c_{pc}\frac{\partial T_c}{\partial t} + \frac{\partial}{\partial x}\left(-k_c\frac{\partial T_c}{\partial x}\right) = \frac{P_I h_{gc}(T_g - T_c)}{A_c} + \frac{P_O h_{Ac}(T_A - T_c)}{A_c}$$

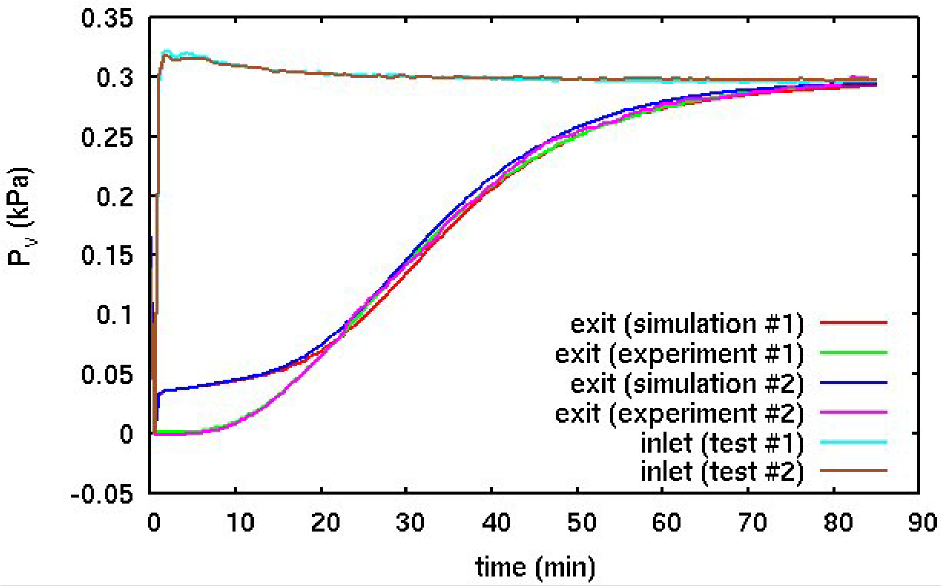
Example H_2O CBT Results

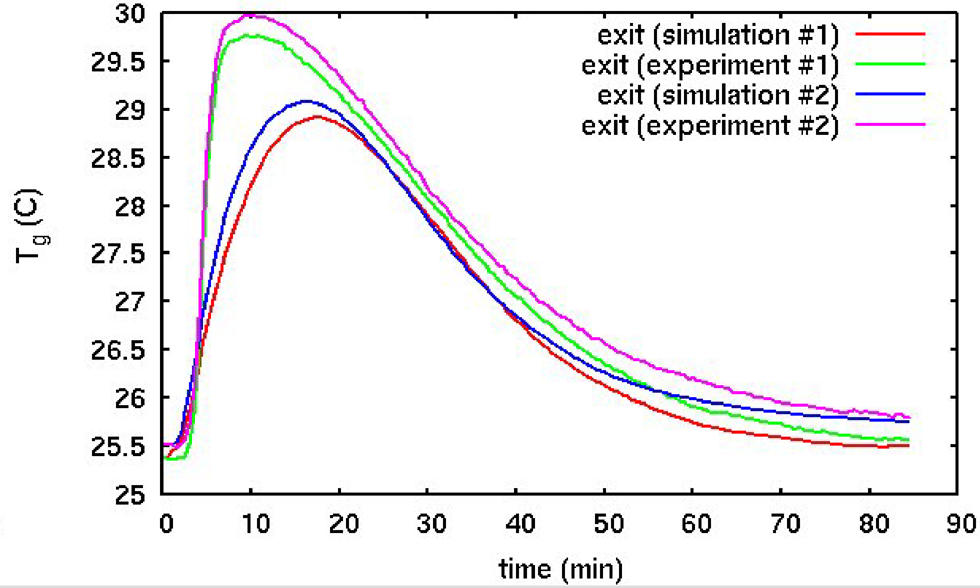




- Water vapor on Silica Gel Grade 40
- Flow is at 8 SLPM with an inlet dew point of 0.5°C
- Residuals dominated by *experimental* error in dew point sensors
- Variability of testing conditions evident in temperature
- Model has early temperature adsorption hump not seen in data
  - Not evident with higher flow rates or inlet dew points

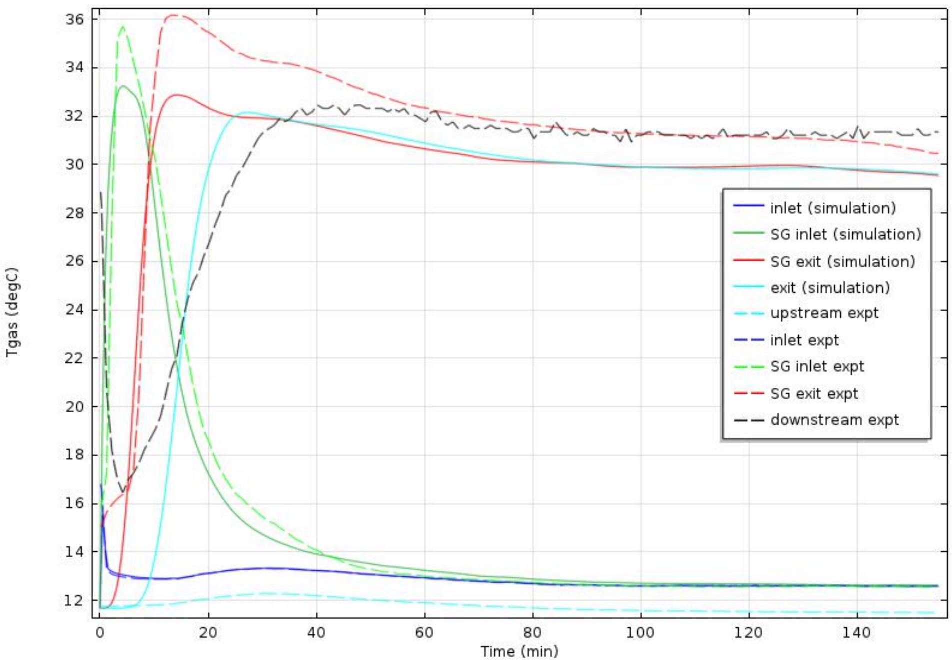
Example CO_2 CBT Results

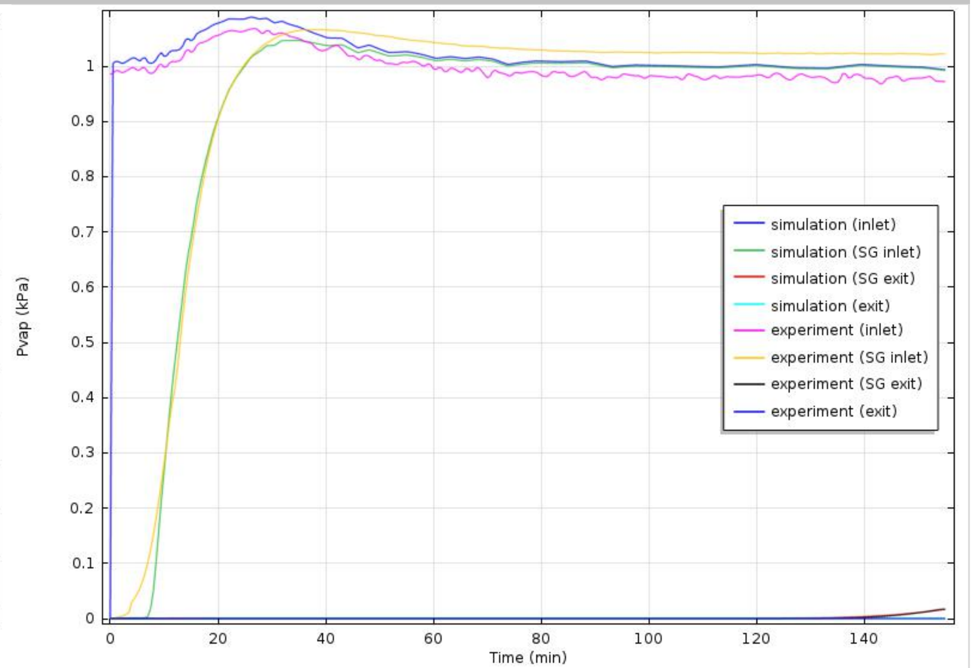




- Carbon Dioxide on 5A Grade 522
- Flow is at 16 SLPM with an inlet CO_2 partial pressure of 2.5 Torr
- Model has breakthrough ‘foot’ occurring very quickly
- Model has higher, steeper temperature rise at exit
- CO_2 models consistently worse than H2O
  - Inaccurate isotherms
  - CO_2/H_2O competitive adsorption

Integrated CDRA-3 Testbed Results





- Cyclic model with 155 minute adsorption and desorption half-cycles
- Not as well diagnosed as CBT (e.g., sorbent masses unknown)
- Flux inlet BC in COMSOL causes small shift in vapor pressure
- Note small rise in vapor pressure at SG exit (simulation and data overlay)
- Dominated by test uncertainties
- Used CBT-derived LDF parameters

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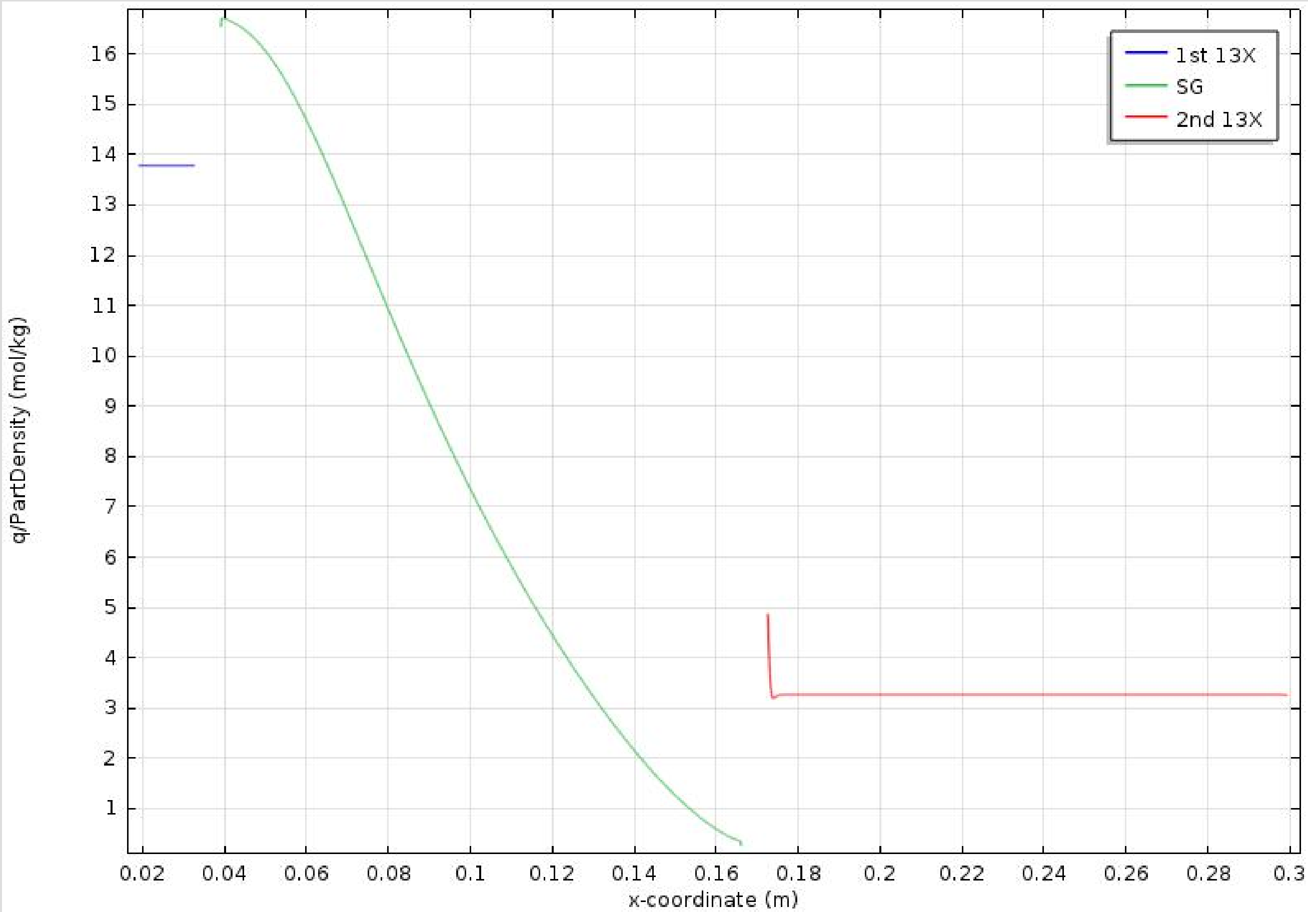
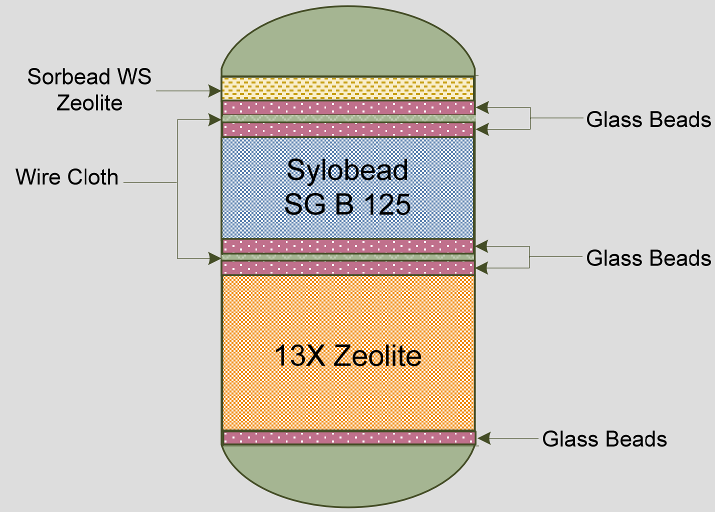


- Guard bed is fully loaded (never desorbs)
- Minimal loading at very front of 2nd 13X bed
- SG bed at ~half capacity with nominal CDRA operation

CDRA Application

- ISS CDRA-3 silica gel coming back with impaired capacity
- If SG is ‘poisoned’, can 13X still capture the water vapor?
- CBT showed B125 ~ G40 in capacity, performance
  - But not dusting or poisoning sensitivity
- Had to assume Sorbead ~ G544 13X

CDRA-4 model (with testbed BCs) says ‘yes’, but with a reduced half-cycle time



ISS CDRA-4 Desiccant Bed

Summary

- Have constructed a *predictive* desiccant bed model
  - Applied to CBT
    - Various sorbates, sorbents, flow rates, concentrations
  - Applied to CDRA-3 testbed
    - Matches data to within the experiment unknowns
  - Applied to CDRA-4 ISS desiccant bed issue
    - Used to help inform ISS half-cycle decision
    - Being used for sorbent decisions (13X vs SG)

Future Work

- Generalize PDEs to 2D and 3D
- Determine if COMSOL modules more efficient
- Inform CDRA Cycle II testing parameters
- Apply same model methodology to CDRA Sorbent Beds
  - Complex 3D geometry
  - Including heaters
  - Uses vacuum desorption
  - Have to model H_2O/CO_2 sorption competition

→Full System Predictive CDRA Model!