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

• Goal: *Predictive* model of the Carbon Dioxide Removal Assembly (CDRA)
  • Here, focus on the Desiccant Beds (1D)
  • Need to know sorbent behavior (isotherms, LDF, etc.)
Cylindrical Breakthrough Test (CBT)

- Multiple sorbents: RK38, 13X G544, 5A G522, SG G40, SG B152
- Multiple sorbates: CO₂, H₂O
- Variable flow rates, concentrations, and temperatures

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

Use COMSOL Multiphysics to solve 7 PDEs:

- 1st order Ergun equation for interstitial velocity
- Gas pressure assuming ideal gas law
- Sorbate concentration via diffusion & advection
- Pellet loading via LDF & Toth
- Sorbent temperature with sorption physics
- Gas temperature (not in eqlbrm with sorbent)
- Wall housing temperature

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

\[
\rho_g \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left( \frac{\mu_g}{\epsilon} \frac{\partial (\epsilon u)}{\partial x} \right) = -\left( \frac{\partial P}{\partial x} + u \left( \frac{\epsilon \mu_g}{\kappa} + \epsilon^2 |u| \rho_g A + \frac{\partial q}{\partial t} \frac{(1 - \epsilon)}{\epsilon} M_a + \rho_g \frac{\partial u}{\partial x} \right) \right)
\]

\[
\frac{\epsilon}{R_s T_g} \frac{\partial P}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\epsilon u P}{R_s T_g} \right) + P \frac{\partial \left( \frac{\epsilon}{R_s T_g} \right)}{\partial t} = -\frac{\partial q}{\partial t} (1 - \epsilon) M_a
\]

\[
0 = \frac{\partial c}{\partial t} + (1 - \epsilon) \frac{\partial q}{\partial t} + \frac{\partial}{\partial x} \left( -D_x \frac{\partial c}{\partial x} - D_x \frac{c}{M_{mix}} \frac{\partial M_{mix}}{\partial x} + D_x \frac{c}{\rho_g} \frac{\partial \rho_g}{\partial x} + u \epsilon c \right)
\]

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

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

\[
\epsilon \rho_g c_{pg} \frac{\partial T_g}{\partial t} + \frac{\partial}{\partial x} \left( -k_g \epsilon \frac{\partial T_g}{\partial x} \right) = A h_{sg} (T_s - T_g) - \epsilon \rho_g c_{pg} u \frac{\partial T_g}{\partial x} + \frac{P_l h_{gc} (T_c - T_g)}{A_f}
\]

\[
\rho_c c_{pc} \frac{\partial T_c}{\partial t} + \frac{\partial}{\partial x} \left( -k_c \frac{\partial T_c}{\partial x} \right) = \frac{P_l h_{gc} (T_g - T_c)}{A_c} + \frac{P_o h_{Ac} (T_A - T_c)}{A_c}
\]
Example H₂O SG 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
- Model good enough to point out SLPM error
- Variability of testing conditions an issue
- Model has early temperature adsorption hump not seen in data
  - Not evident with higher flow rates or inlet dew points
Example CO$_2$ 5A CBT Results

- Carbon Dioxide on 5A zeolite RK38
- Flow is at 16 SLPM with an inlet partial vapor pressure of 5 Torr
- Consistently missing inlet sharp peak
- Temperature falloff and asymptotic behavior incorrect in models
- Excellent match to breakthrough curve
Summary

• Have constructed a *predictive* desiccant bed model
  • Applied to CBT
    • Various sorbates, sorbents, flow rates, concentrations
• Next: Generalize PDEs to 2D and 3D (!)
• Or: Use COMSOL modules
  • Velocity and pressure modules appropriate?
  • Have verified thermal modules give PDE results, but:
    • Assumption of $T_g \sim T_s$ not always valid
• Then: Apply same model methodology to CDRA Sorbent Beds
  • Complex 3D geometry
  • Including heaters
  • Uses vacuum desorption
  • Have to model $\text{H}_2\text{O}/\text{CO}_2$ sorption competition

→ Full System Predictive CDRA Model!