A Virtual Laboratory for the 4 Bed Molecular Sieve (4BMS) of the Carbon Dioxide Removal Assembly (CDRA)

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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

• Life Support Systems Project (LSSP):
  • mature environmental subsystems
  • derived directly from the ISS subsystem architecture
  • reduce developmental and mission risk
  • demonstrate concepts for human missions beyond Earth orbit

• Have developed a Predictive Virtual Laboratory model of CDRA 4BMS
• Needed to know inputs such as sorbent behavior and thermal coupling
The CDRA 4BMS Beds

- Multiple sorbent layers: RK38 (5A), G544 (13X), Sorbead WS (SG), Sylobead B125 (SG)
- Multiple sorbates: CO$_2$, H$_2$O
- Variable flow rates, concentrations, and temperatures
- CO$_2$ bed desorbed with vacuum and in-situ heaters

- Insulated
- Square-ish cross sections
- Narrow RK-38 channels separated by heaters/spreaders
Model Approach

- Use Toth isotherms from other work
  - Describes how the sorbate and sorbent interact
- Use dimensionless correlations (Re, Nu, Pe, Pr)
  - Derives mass dispersion and thermal transfer coefficients
- Assume binary mass diffusion is valid
- Assume constant porosity in each bed layer
- Use Rumpf-Gupte permeability relationship
- Assume 1-D Darcy Flow
- Fit the single model parameter (LDF) using Cylindrical Breakthrough Test (CBT) data
Use COMSOL Multiphysics to solve in 1-D (for each layer in each bed):

- Transport of Concentrated Species (sorbate)
  - includes reactions, diffusion, and advection
  - time-dependent Mass Fraction inlet condition
- Heat Transfer
  - in solids for Can, Sorbent, and Insulation
    - Sorbent has sorption and heater Heat Sources
  - in fluids for Gas mixture
    - ideal gas with constant ratio of specific heats
    - inlet Temperature boundary condition
  - all are coupled via thermal coefficient Heat Sources
  - temperature-dependent material properties
- Darcy’s Law (pressure and superficial velocity)
  - inlet Mass Flux boundary condition
  - constant outlet Pressure (except for vacuum desorption phase – see next slide)
  - includes Mass Source due to sorption
- General Form PDE: pellet loading via LDF & Toth
- General Equations: heater switches
Vacuum desorption of the CO$_2$ bed:
• The adsorption effluent end is closed off
  • BC changed from ‘pressure’ to ‘no flow’
• Desorption effluent end of the bed is piped back to the cabin with a pump for ~ 10 minutes
  • ‘air save’ mode removes N$_2$ and O$_2$ still in bed
  • single strand of the bed heaters is turned on too
• At the end of air-save:
  • 2$^{nd}$ heater strand is turned on
  • effluent end of the bed is piped to space vacuum
• The low-pressure BC is applied to the effluent with a P(t) based on test data
• Bump due to pure CO$_2$ desorbing from bed
• Separate Physics Nodes and Steps for each bed
• Switch BC types for each half-cycle using Physics Tree
• Fine temporal and spatial resolution required to capture fronts and BC changes
• Boundaries between bed layers marked by ●
• Runtime on a desktop is slightly faster than real time
• No user interaction (‘nursing’) is required
This is what the model looks like in COMSOL.

Each half-cycle (HC) consists of a steady solve (to get the last HC results) and 4 time-dependent solves (one for each bed).
## CDRA-4EU CO₂ Removal Results

<table>
<thead>
<tr>
<th>HC (min)</th>
<th>flow rate (SCFM)</th>
<th>CO₂ removal rate (kg/day)</th>
<th>efficiency</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>data</td>
<td>model</td>
<td>delta %</td>
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<tr>
<td>155</td>
<td>20.4</td>
<td>3.65</td>
<td>3.35</td>
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<tr>
<td>96</td>
<td>34.0</td>
<td>5.69</td>
<td>5.82</td>
</tr>
</tbody>
</table>

- All cases match removal rate and efficiency to better than 10%
- Test inputs (dew point, inlet temperature, ambient temperature, heater power, flow rate) vary from test to test and within a test
- Expected model uncertainty ~10%, so the Virtual Laboratory works!
2 torr CO$_2$, 25 SCFM, and 154 min HC
Desiccant influent & effluent shown
‘burp’ at start of HC reproduced
Slight break-through at end of HC
Heavy CO$_2$ loading of the 13X desiccant layer predicted
Competing CO$_2$/H$_2$O isotherm and/or P(t) issues for spike?
4BMS-X Optimization

- Four person crew for exploration (fewer than ISS)
- 13X desiccant layer reduced in size (had excess capacity)
- CO\textsubscript{2} sorbent bed layer reduced (had excess capacity)
- Various new CO\textsubscript{2} sorbents modeled (have more capacity)
- Different heater methods modeled (reducing power requirements)
- Aiming to reduce equivalent mass and improve -ilities

Virtual Laboratory says:
- can remove 50% of the 13X and 30% of the 5A
- with new sorbents, can remove as much as 60% of the CO\textsubscript{2} sorbent
- average heater power can be reduced by ~50%
- verification of these predictions are now underway!
Summary

- Have constructed a *predictive* CDRA 4BMS 1-D Comsol model
  - Calibrated with CBT on various sorbates, sorbents, flow rates, concentrations
- Applied to CDRA-4EU Baseline data
  - Shows sorbent bed CO$_2$ breakthrough for nominal operation
  - Shows impact of the 13X CO$_2$ ‘reservoir‘ behavior
    - quantitatively can be improved with better competition model
  - Matched test results to better than 10% for all tests
- Now being used to inform next generation CDRA (4BMS-X) optimization

→Virtual Laboratory of any 4BMS System open for work!