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

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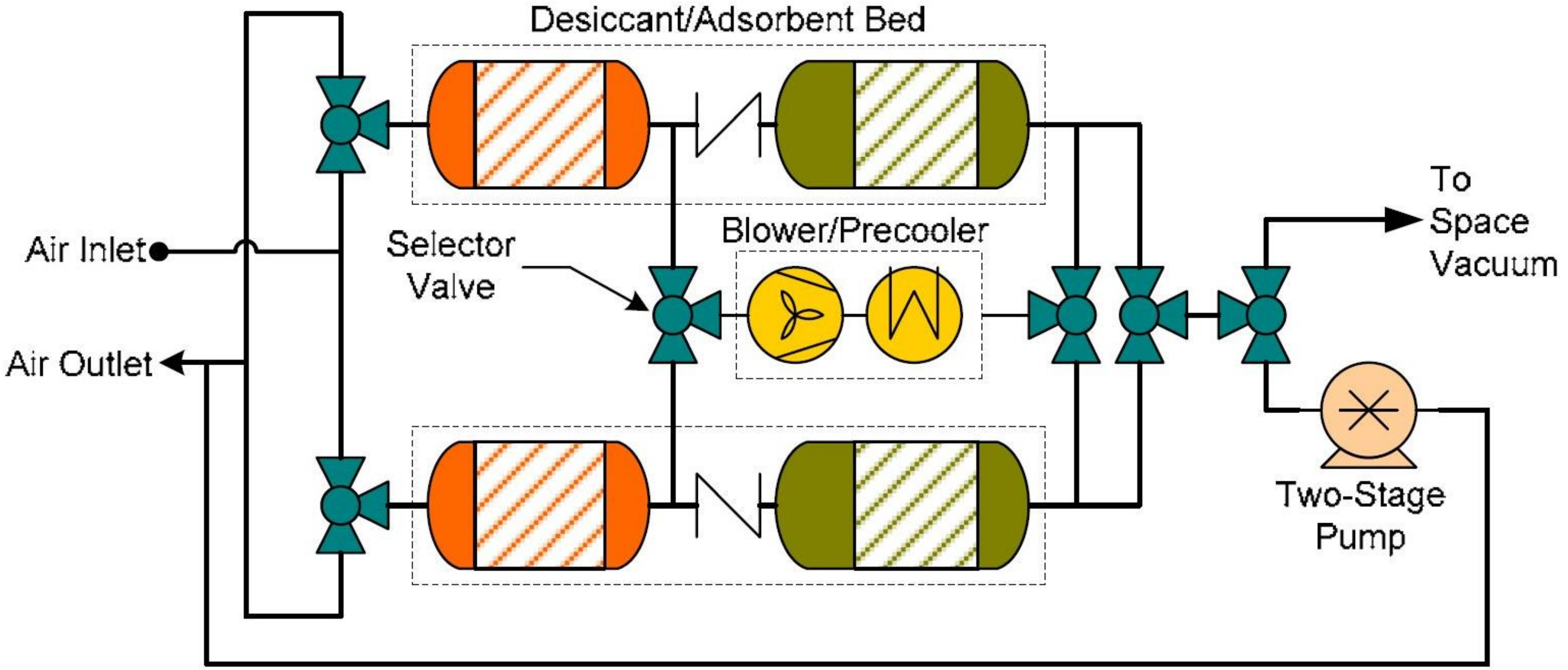
Introduction

- 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

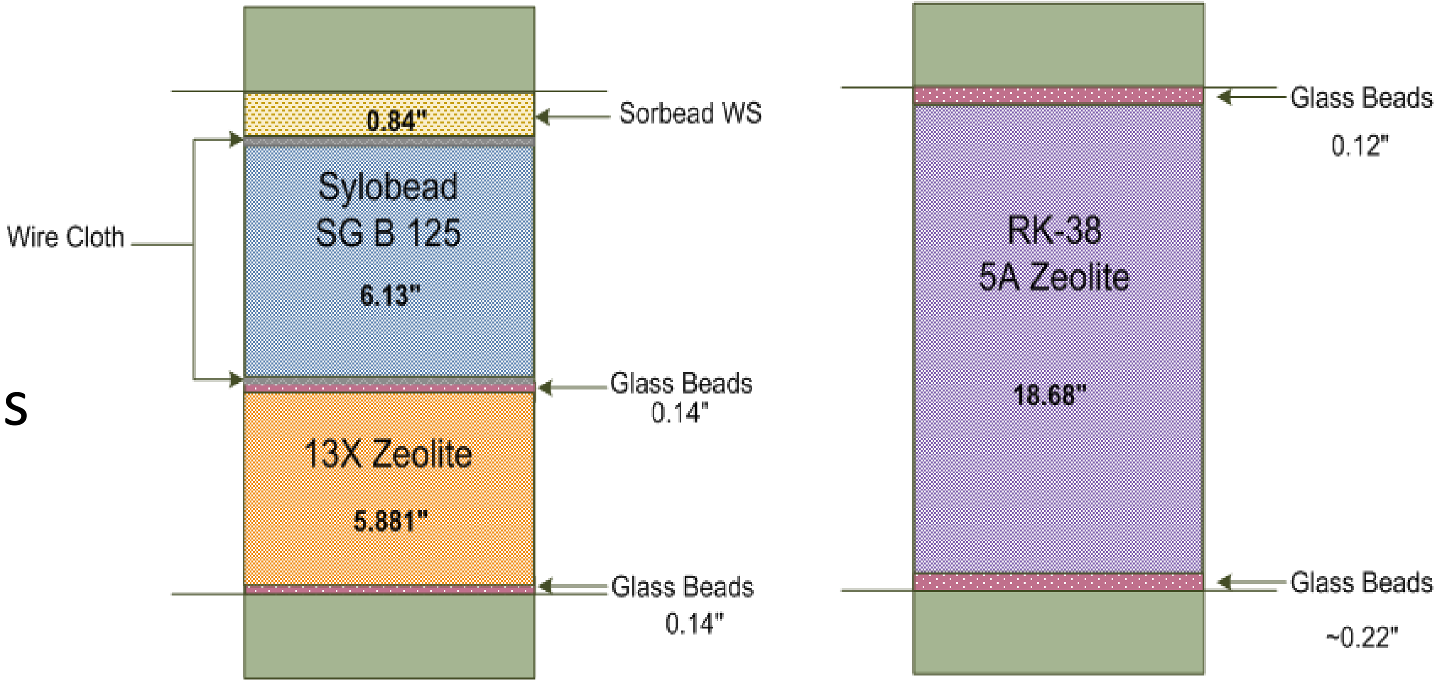
- Have developed a *Predictive* Virtual Laboratory model of CDRA 4BMS
- Needed to know inputs such as sorbent behavior and thermal coupling



The CDRA 4BMS Beds

- Multiple sorbent layers:
  RK38 (5A), G544 (13X), Sorbead WS (SG), Sylobead B125 (SG)
- Multiple sorbates: CO_2, H_2O
- 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



H_2O CDRA-4 Bed

CO_2 CDRA-4 Bed

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

COMSOL 4BMS Model

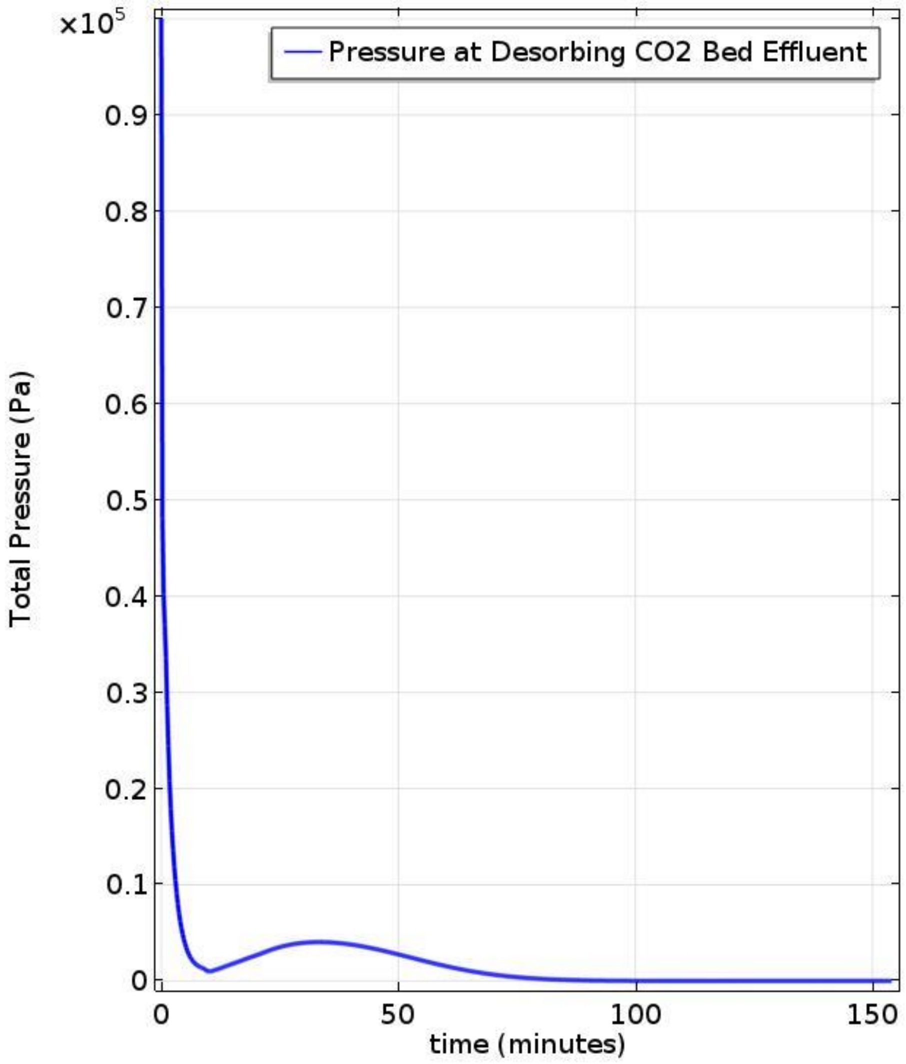
Use COMSOL Multiphysics to solve in 1-D (for each layer in each bed):

- 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

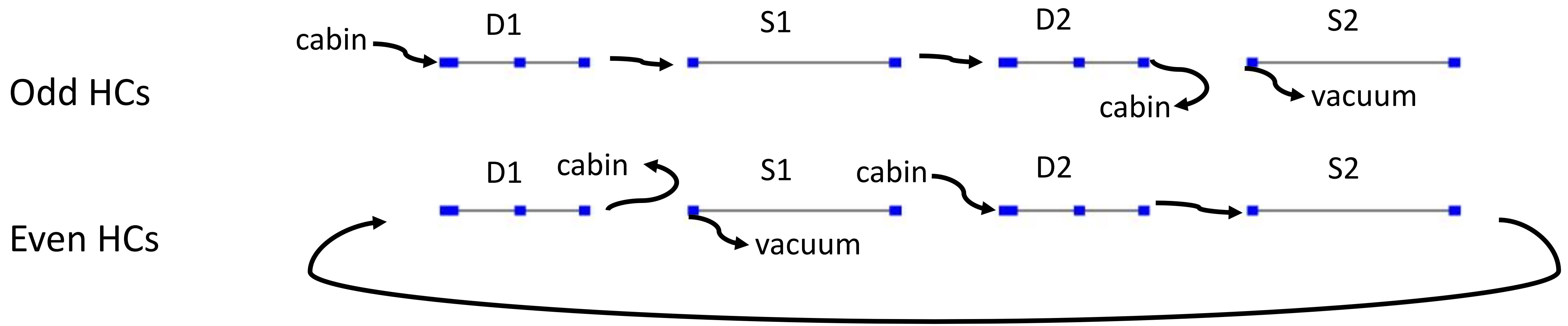
COMSOL 4BMS Model

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:
  - 2nd 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



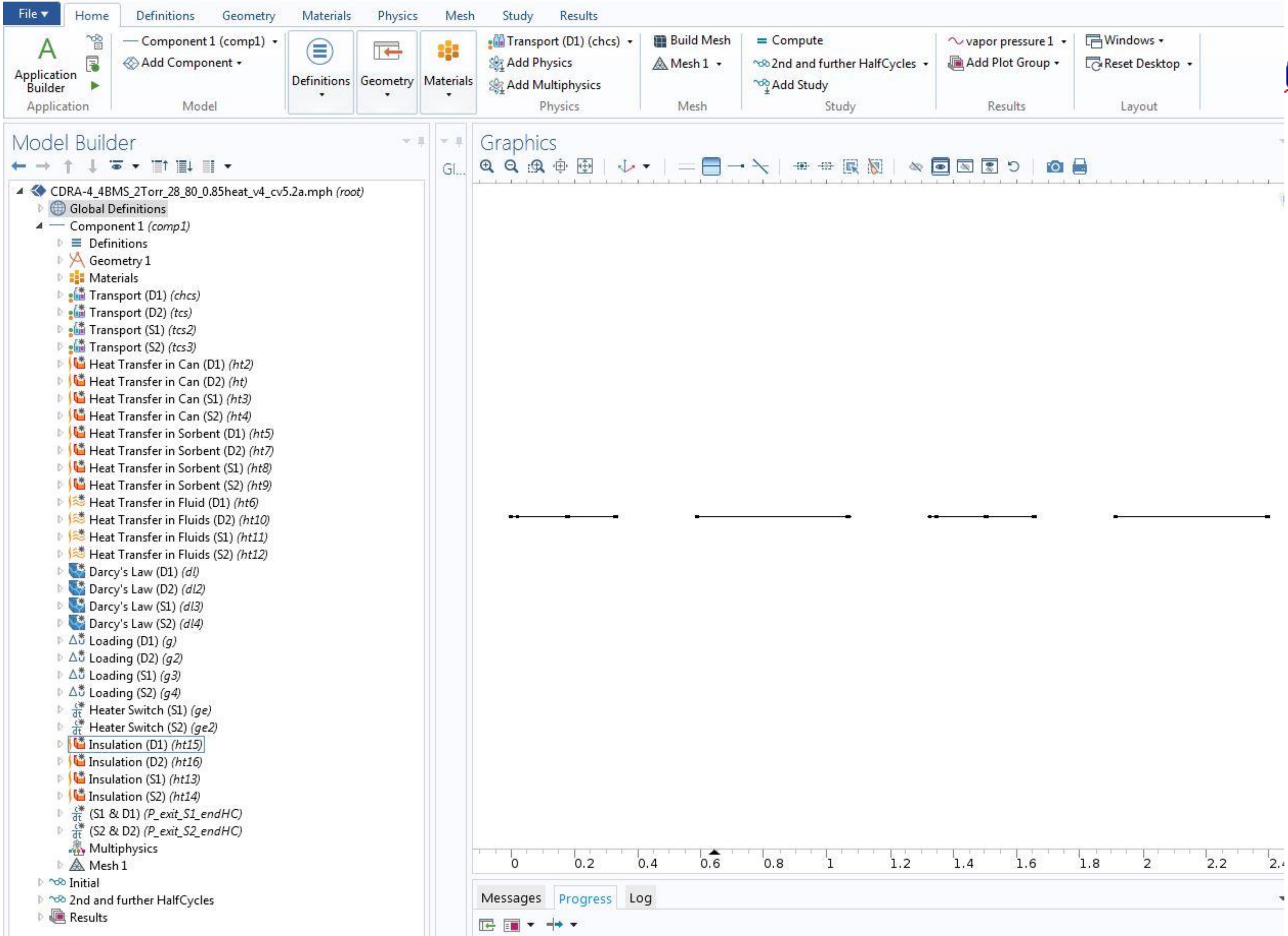
1-D Model



- 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).



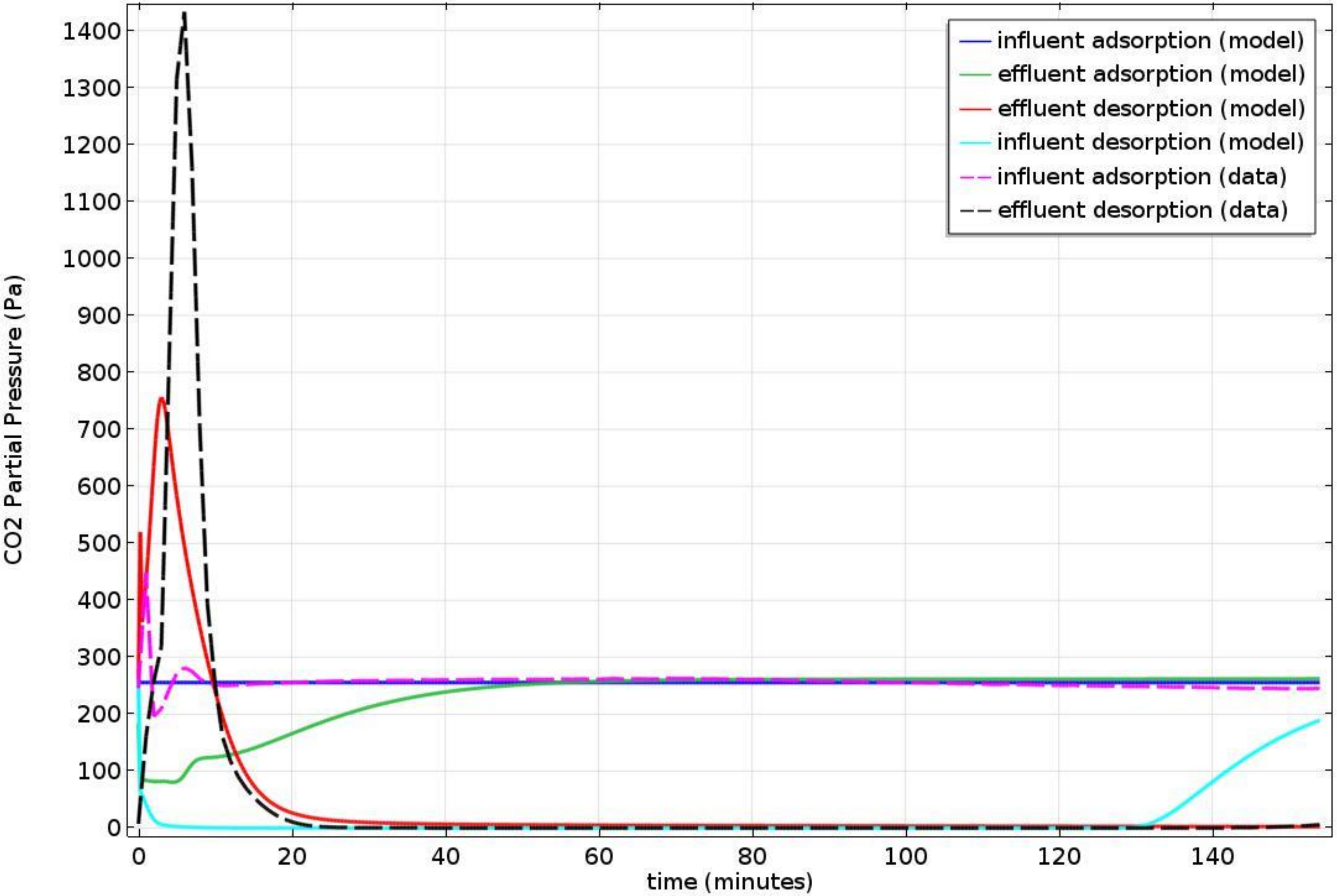
CDRA-4EU CO_2 Removal Results

HC	flow rate	CO2 removal rate (kg/day)			efficiency		
(min)	(SCFM)	data	model	delta %	data	model	delta %
155	20.4	3.65	3.35	8.2	0.843	0.789	6.4
90	25.0	4.11	3.73	9.2	0.772	0.716	7.3
90	24.0	3.76	3.70	1.6	0.745	0.696	6.6
215	20.0	3.18	3.12	1.9	0.779	0.749	3.9
172	25.0	4.05	3.90	3.7	0.783	0.749	4.3
144	30.0	4.83	4.62	4.3	0.740	0.740	0.0
123	34.0	5.18	5.44	-5.0	0.712	0.769	-8.0
195	20.0	3.49	3.41	2.3	0.813	0.818	-0.6
154	25.0	4.19	4.30	-2.6	0.812	0.826	-1.7
124	30.0	5.14	5.18	-0.8	0.781	0.830	-6.3
96	34.0	5.69	5.82	-2.3	0.810	0.822	-1.5

- *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!

CDRA-4EU CO_2 Predictive Results

- 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_2O 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_2 sorbent bed layer reduced (had excess capacity)
- Various new CO_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_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!