45th International Conference on Environmental Systems

Computer Simulation and Modeling of CO_2 Removal Systems for Exploration

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Hilton Bellevue, Bellevue, WA

July 12-16, 2015

Introduction

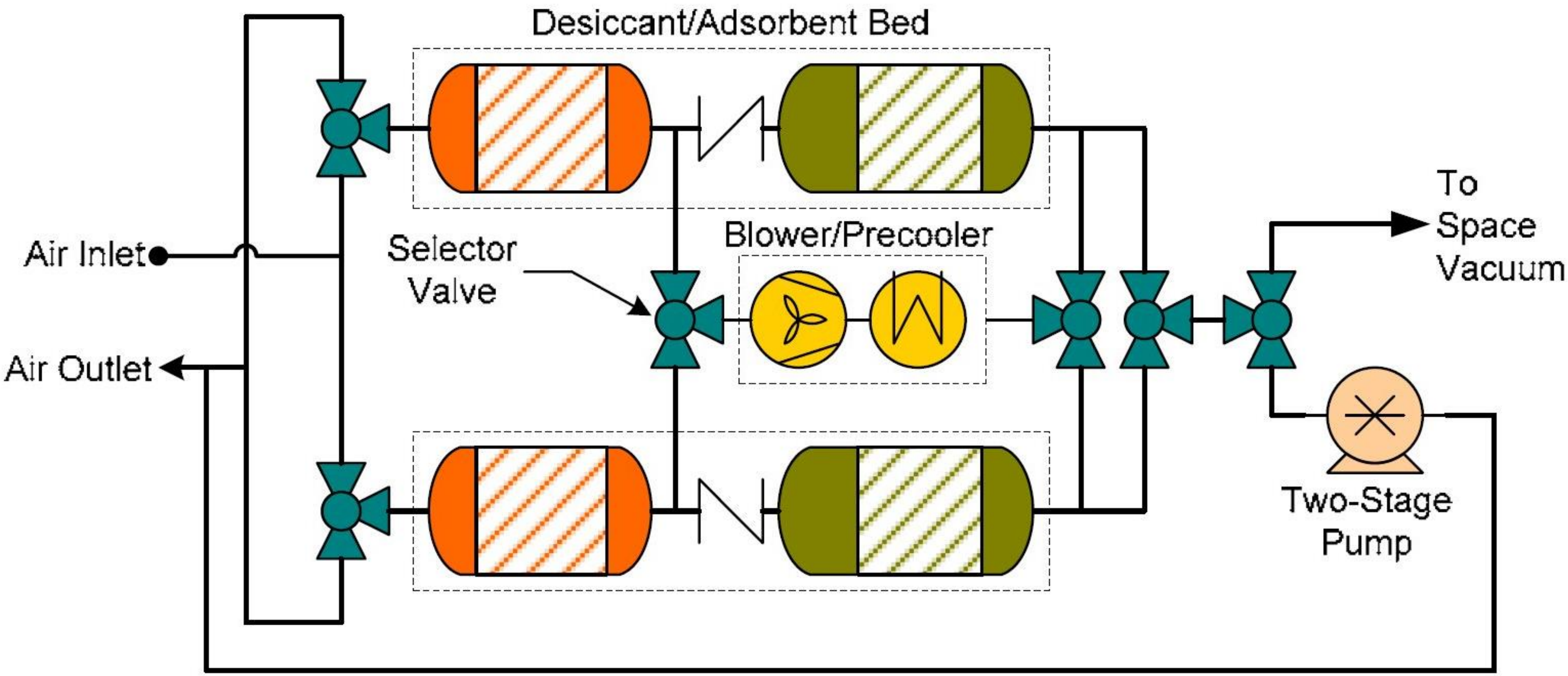
- Advanced Exploration Systems (AES) Program:
  - Atmosphere Resource Recovery and Environmental Monitoring Project (ARREM)
  - Now the Life Support Systems Project (LSSP)

- Rapid development of prototype systems
- Validation of concepts for human missions beyond LEO
- Reduce developmental and mission risk
- Derived directly from the ISS subsystem architecture

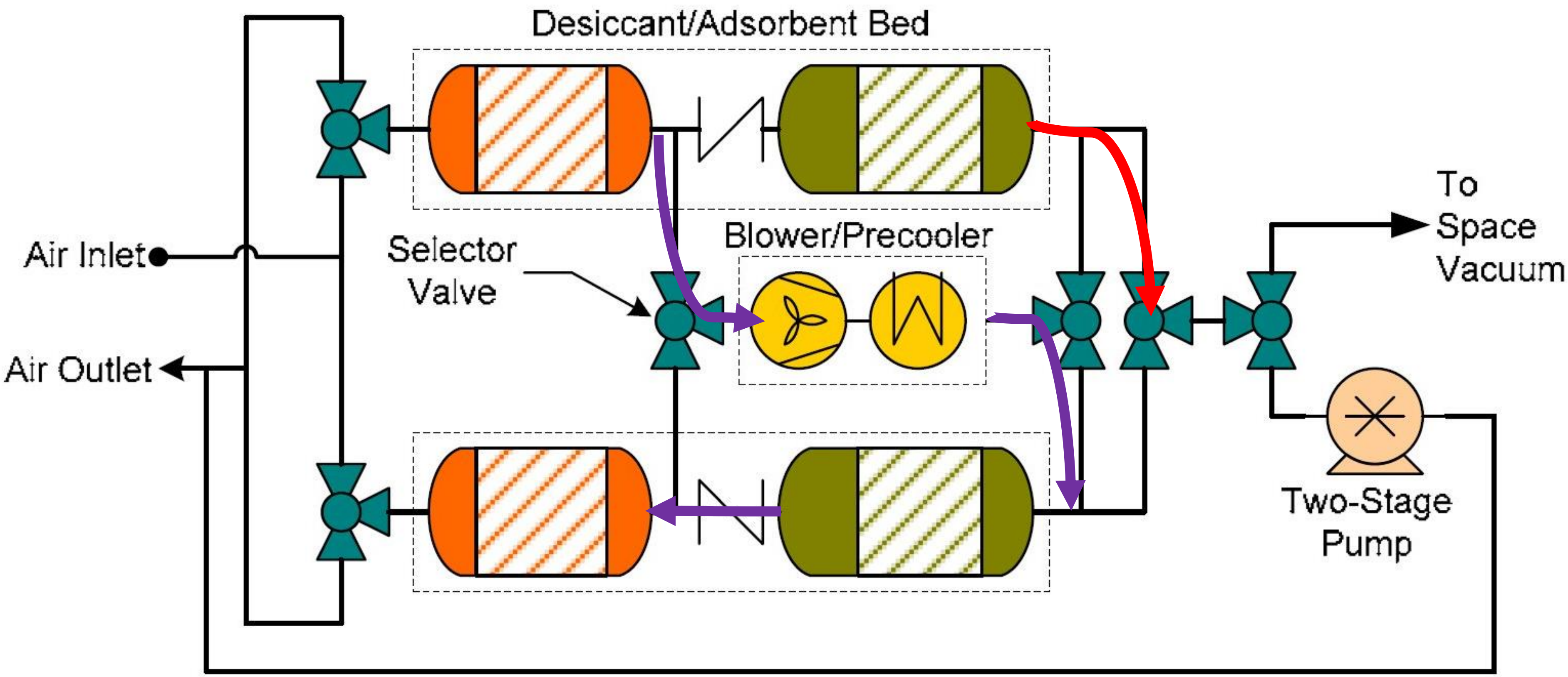
➢ Virtual Laboratory via Simulation

Carbon Dioxide Removal Assembly (CDRA)

- Goal: *Predictive* model of the CDRA-4EU test-bed
- Model the entire four Bed Molecular Sieve (4BMS) in 1-D
- Need sorbent/sorbate behavior (isotherms, LDF, etc.)
- Validated with Cylindrical Breakthrough Tests (CBT)



Carbon Dioxide Removal Assembly version 4 Engineering Unit (CDRA-4EU)



Every 'half-cycle' the system switches flow directions
Desorbing sorbent bed is heated & evacuated (red)
Desiccant beds (orange) remove and return H2O (orange),
Sorbent beds (green) remove CO2

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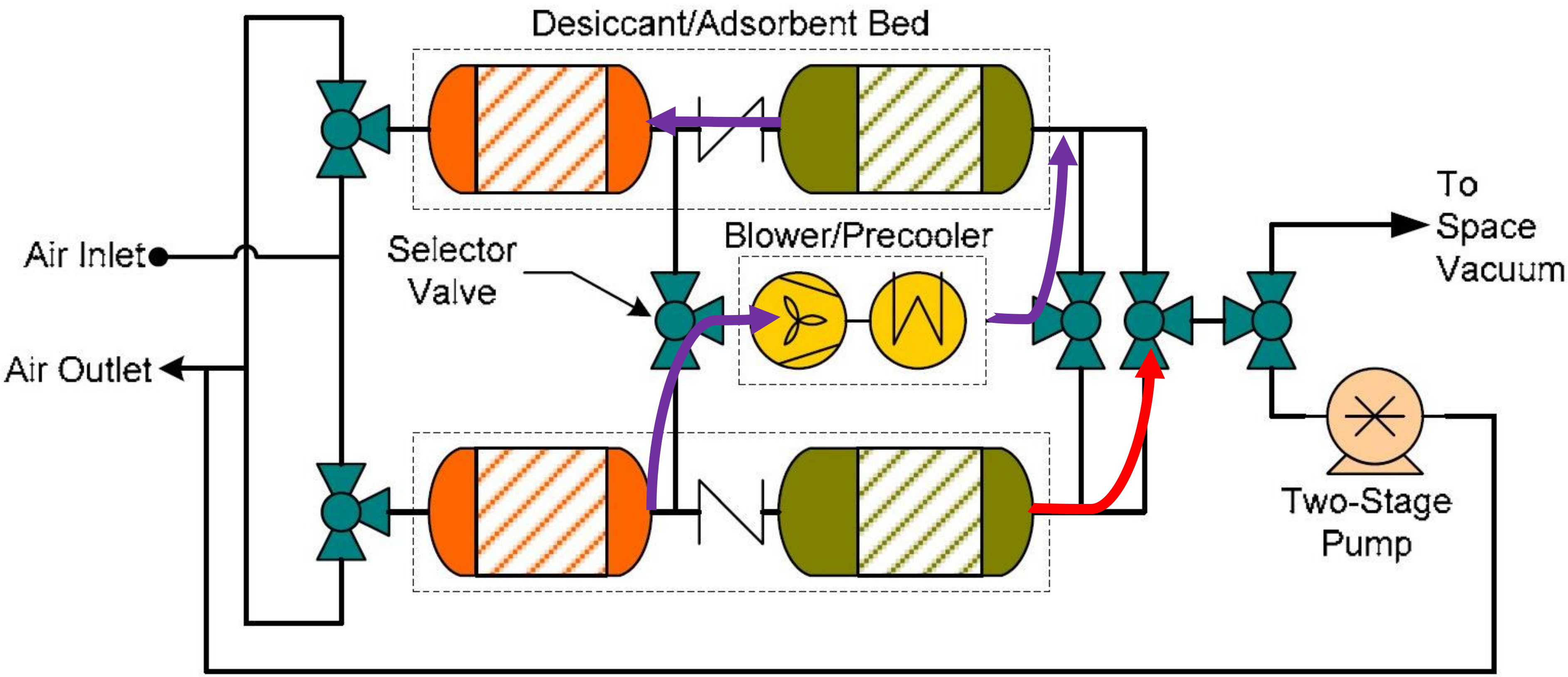

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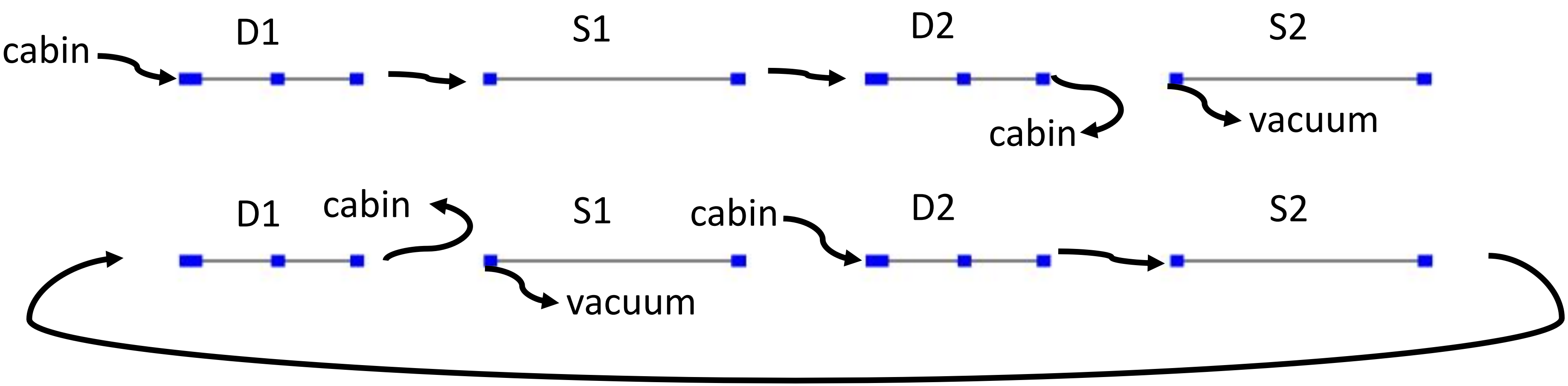
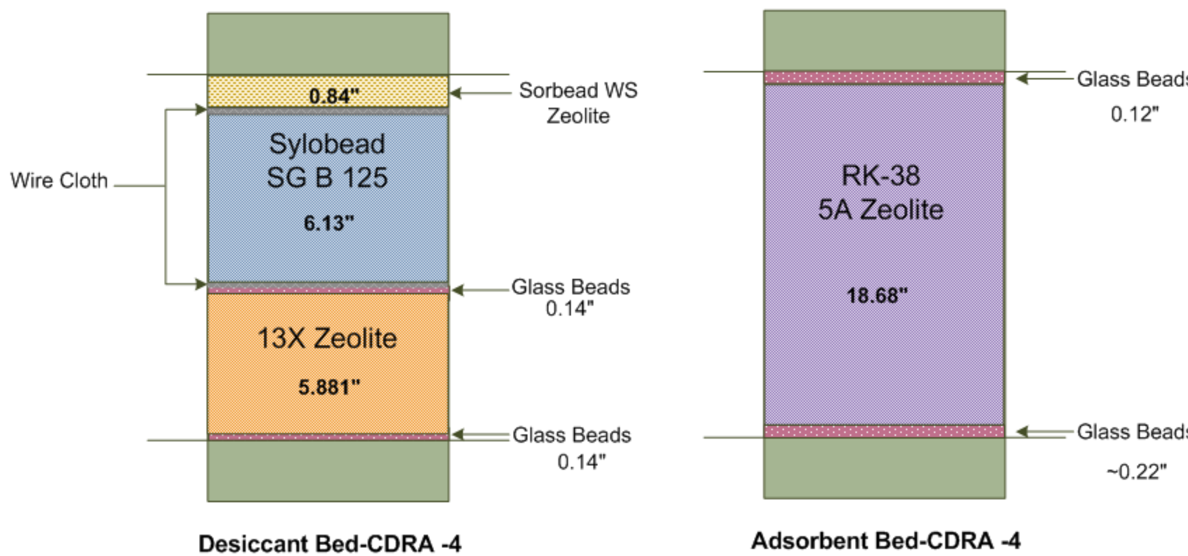
CDRA-4EU 4BMS 1-D COMSOL Model



- Changes boundary conditions
- Glass beads treated as inactive beds
- Separate thermal solutions for gas, sorbent, can, insulation
- Sorbate mass fraction outputs are inlet conditions for next bed
- Each container solved separately



Model Details: the Approach

- Use sorbent/sorbate inputs from other work
- Use dimensionless correlations (Re, Nu, Pe, Pr, Sc)
  - Derives mass dispersion and thermal transfer coefficients
- Some simplifying assumptions such as:
  - Darcy flow
  - binary mass diffusion
  - constant porosity
  - Rumpf-Gupte permeability
  - 1D ‘plug flow’ style model with wall corrections
  - single component isotherms
- Use CBT to calibrate k_m, ΔH, h, kappa, q, and porosity
  - Across-the-board validity of the 1-D LDF model?
- Use COMSOL Multiphysics modules to solve the PDEs
- Apply predictively to CDRA-4EU test-bed data

Model Details: the Physics

(constant gamma, ideal gas)

$$0 = -\left(\frac{\partial P}{\partial x} + \frac{u\mu}{\kappa_s}\right)$$

Darcy's Law

$$\frac{\partial(\rho\epsilon_s)}{\partial t} + \frac{\partial}{\partial x}(u\rho) + (1-\epsilon_s)M_s\frac{\partial q}{\partial t} = 0$$

P loss term

(now in mass fraction)

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

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

LDF parameter

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

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

(similar for insulation)

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

(heaters)

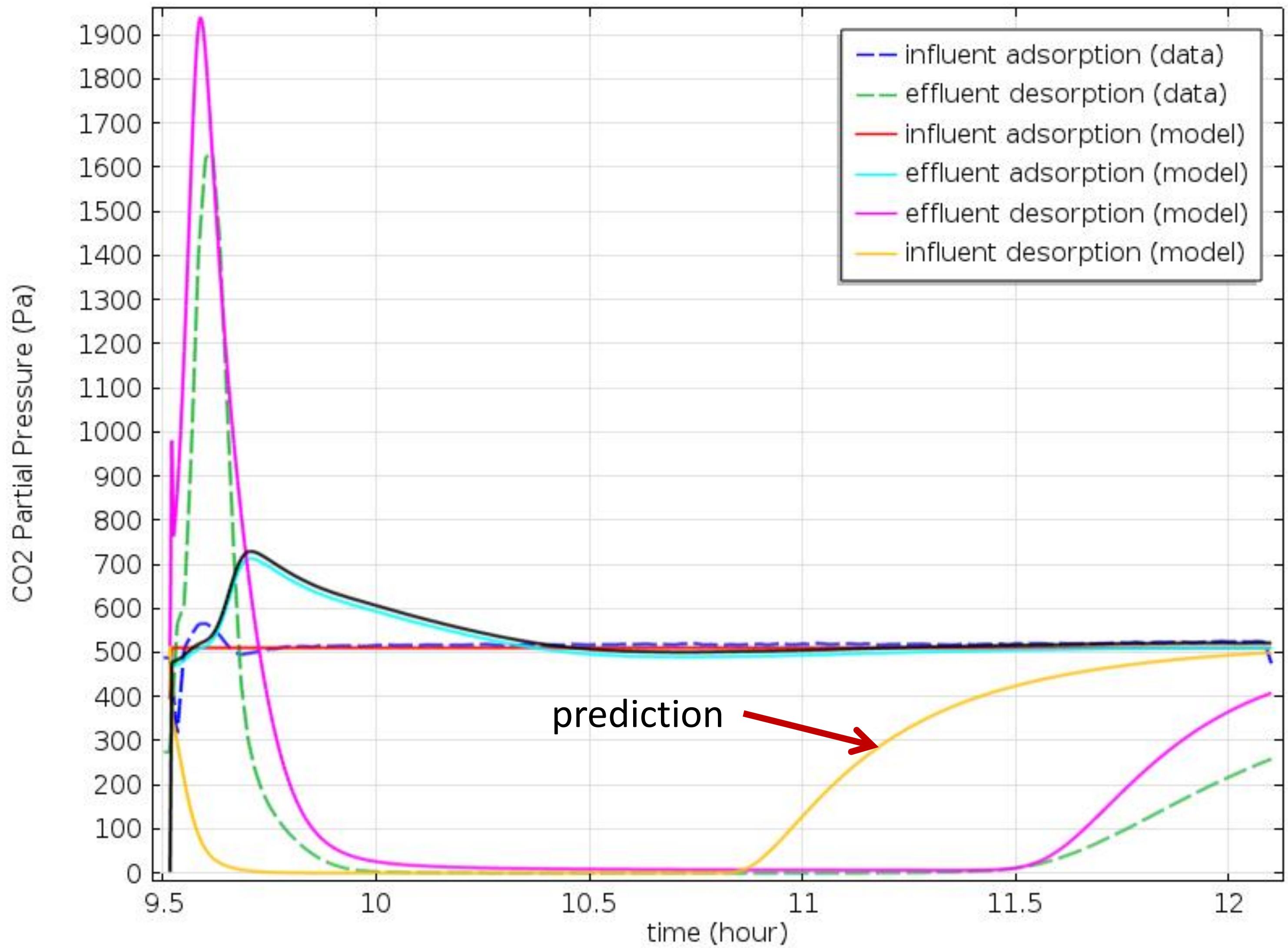
$$S_{new} = \mathrm{if}(T_h \geq T_{max}, 0, \mathrm{if}(T_h \leq T_{min}, 1, S_{old}))$$

Model Details: CDRA-4EU Application

- Cyclic with 155 min adsorption and desorption half-cycles
- 10 minute air-save mode on desorbing sorbent bed
- Sorbent bed heaters and vacuum desorption added
- Pseudo-binary CO2/H2O isotherm on 13X bed
- Heat capacity & thermal conduction of sorbent beds include fins
- 8x number of pellets across desiccant bed diameter, 2x P_{vap}, and 70x the flow rate (compared to CBT) but scaling assumed valid
- Heat-loss to desiccant bed from POIST
- Reduced sorbent bed heater power to 70%
- Results shown here run for 3 half-cycles (~converged)
- Run time is ~ real time
- Increasing scale factor on h as gas pressure drops (~$P^{-1/2}$)

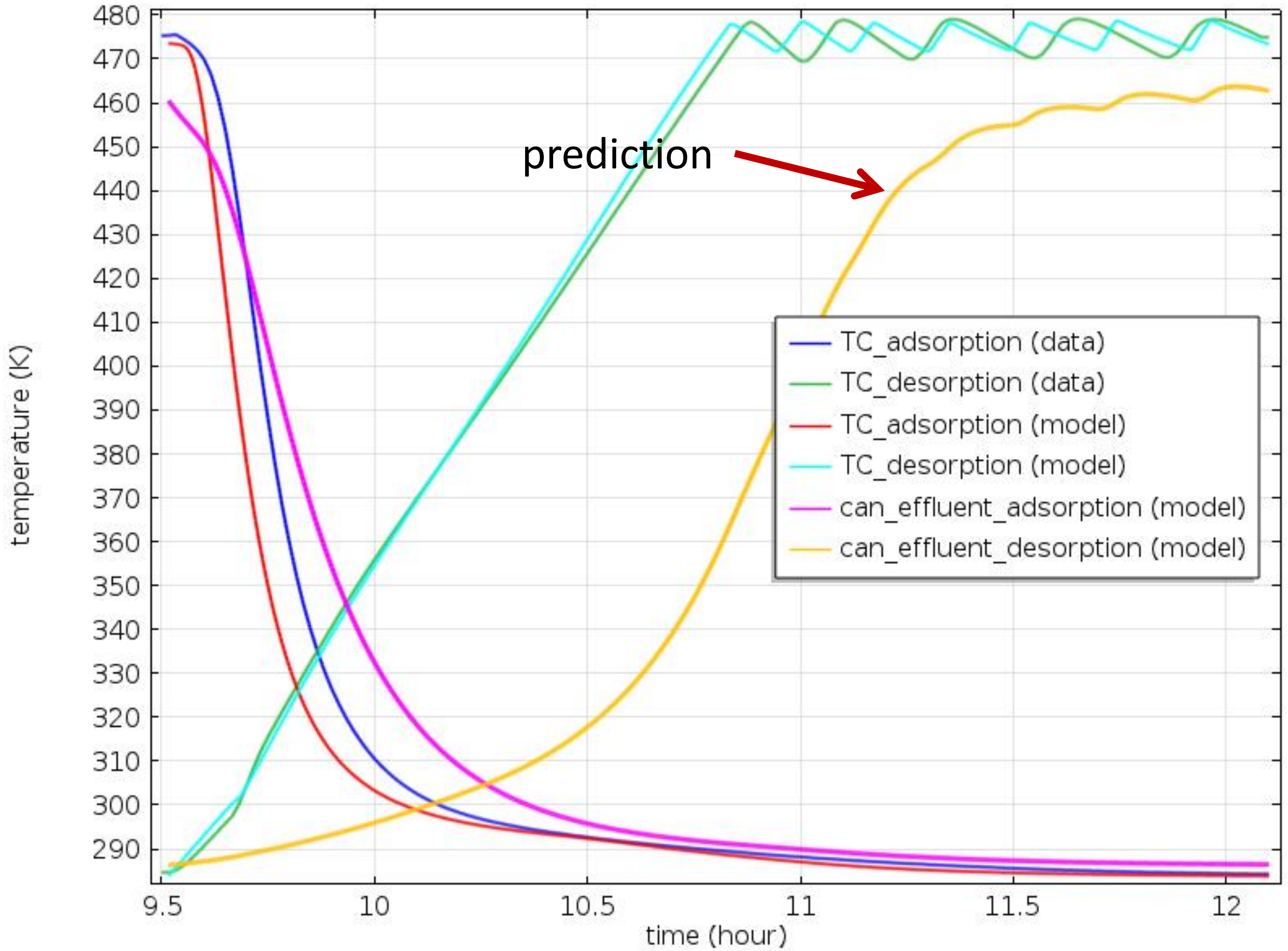
CDRA-4EU Test-bed Results: CO_2

- Competitive CO_2/H_2O on 13X (assumed 5x5A)
- 'burp' at start of HC reproduced
- Break-through at end of HC reproduced
- Requires heavy CO_2 loading of 13X and break-through of 5A
- Fudged 5A porosity 55% (channeling? large voids?)



CDRA-4EU Test-bed Results: Sorbent Bed T

- Model cools slightly too quickly during adsorption
- Heater control set-points in test appear 'soft'
- Slope, given thermal mass, dictates ~690W (vs 980W)

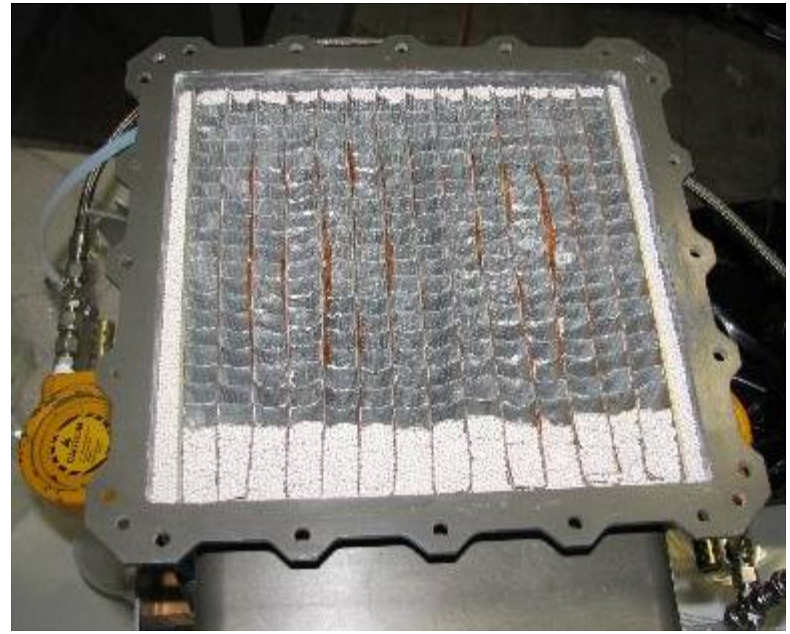


1-D Limitations

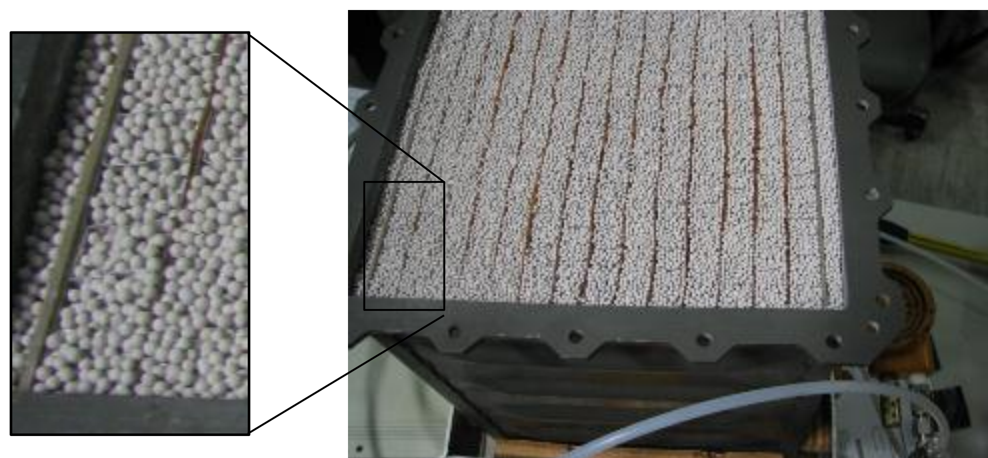
- 1-D is not expected to be able to capture behavior of full CDRA system
  - Desiccant bed: 2-D cylindrical channels
  - Sorbent bed: 3-D rectilinear channels
- Single value of porosity inherently limiting
  - Sorption processes driven by centerline mass (ϵ_s~min)
  - Flow processes driven by channeling effects (ϵ_s~1)
  - Cannot capture both c and T with single ϵ_s value!
    - Attempts to do so will get the right answer for wrong reason
      - Unusable for outside-the-box modeling

CDRA Sorbent Bed

- Develop a 3-D thermal/fluid model of a representative CDRA sorbent bed channel to provide insight into bed porosity, heat transfer and mass transfer via direct simulation.
- The sorbent beds are filled with a poly-disperse distribution of spherical UOP RK38 pellets that have a mean diameter of 2.1 mm.
- The individual CDRA sorbent channels are formed by the volume enclosed by aluminum heater plates and perpendicular fins.
- The individual CDRA sorbent passages are approximately 0.3” x 0.5” in cross section and 18” in length.
- Each channel span may only contain 5-6 pellets across. At this small size, wall effects may be laterally felt deep into the passage domain.



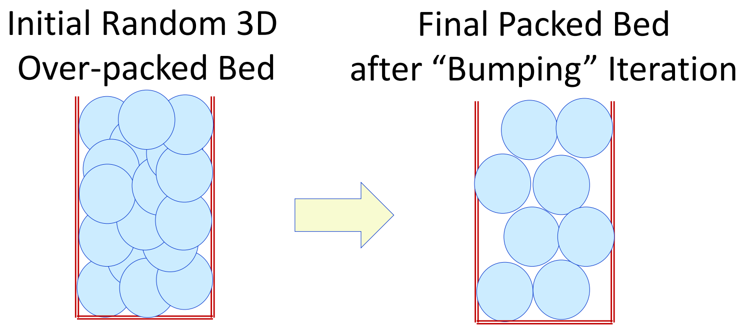
CDRA Sorbent Bed Cross Section

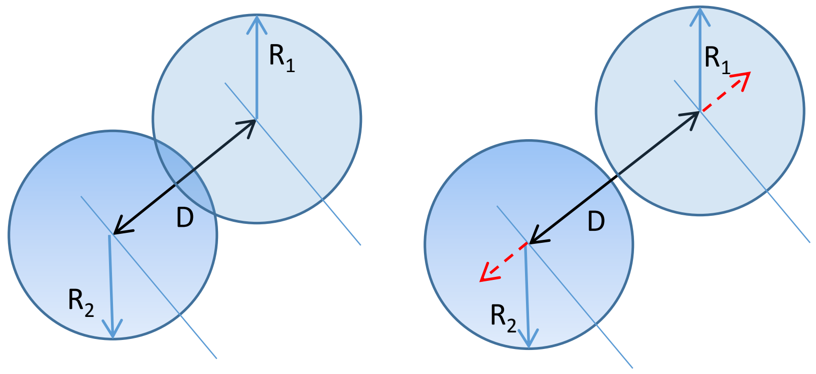


Detailed CDRA Sorbent Bed Channel

Spherical Packing Algorithms

- Two algorithms have been utilized to generate the spherical particle packings for this study--
- A simplified sphere packing algorithm to randomly place spheres inside of a truncated CDRA sorbent bed channel
  - Initialized with a random over filled channel of spherical pellets (i.e. overlapping spheres) and, through an iterative "bumping" process, excess spheres are removed
- LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is a classical molecular dynamics code that models an ensemble of particles in a liquid, solid, or gaseous state.
  - The granular discrete element method capabilities of LAMMPS are built upon in LIGGGHTS (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations).

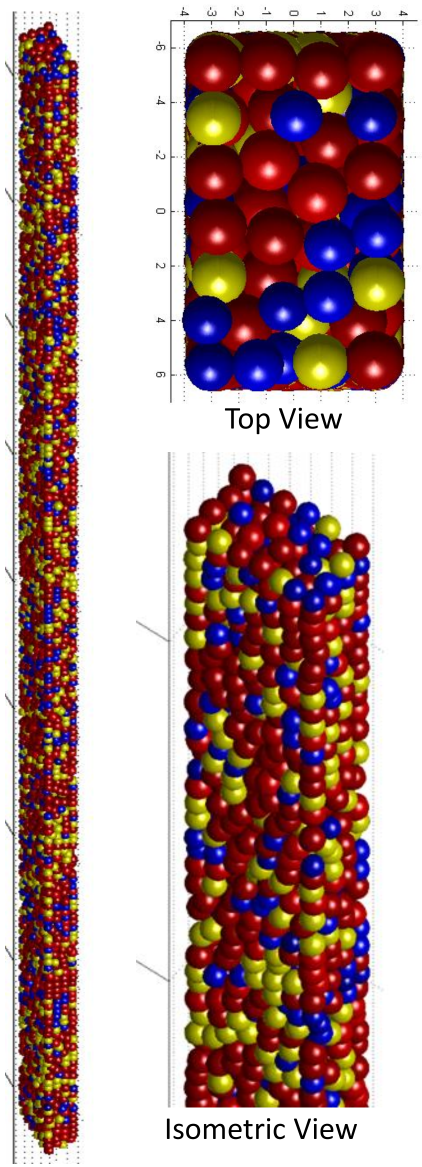




Sphere Bumping Iteration

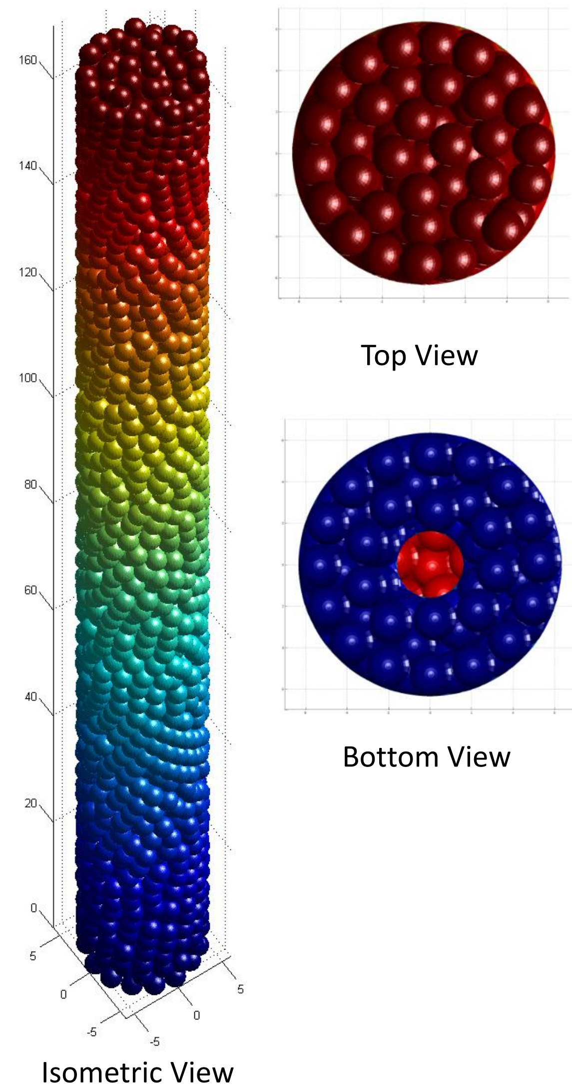
LAMMPS is developed and maintained by Sandia National Laboratories: http://lammps.sandia.gov/
LIGGGHTS is developed, distributed and maintained by DCS Computing: http://www.cfdem.com/

Spherical Packing Results



LAMMPS Packing of Individual CDRA Channel

- Developed poly-disperse packed bed model of CDRA channel over entire length using LAMMPS (see left). The pellets are colored according to size with blue the smallest and red the largest.
- Observed effective solid fraction of 56% in the CDRA channel with hard shell approximation to reduce particle overlap.
- Developed mono-disperse bed packing of Hydrothermal Stability Test Article with thermocouple void for correlation using BUMPS routine. Results indicate solid fraction of 53% versus measured of 57%.
- Importable and meshable in COMSOL



BUMPS Packing of HST Test Article

Summary

- Have constructed a *predictive* CDRA 4BMS model
- Applied to CBT to get correlations
  - Various sorbates, sorbents, flow rates, concentrations
- More data needed to narrow model constraints
  - Thermal coefficients, power, packing
- Applied to CDRA-4EU Baseline data
  - Shows sorbent bed CO_2 breakthrough
  - Shows 13X CO_2 'reservoir'
    - Do not remove 13X (without changing other things)!
  - Shows possible sorbent bed heater issue
- Approaching limits of 1-D
  - Developing 3-D models to inform needed adjustments

Future Work

- One more CBT iteration required (model has changed)
- Generalize to 2-D and 3-D (presently unviable)
- Genuine binary H_2O/CO_2 sorption competition
- Better sorbent/sorbate input parameters
- Validate with more CDRA4-EU tests
  - Different flow-rates, half-cycle times, dew points, vapor pressures
- Inform CDRA optimization

→Virtual Laboratory of the CDRA System