COMSOL CONFERENCE
2015 BOSTON

A 1-D Model of the 4 Bed Molecular Sieve of the Carbon Dioxide Removal Assembly

Robert Coker and Jim Knox

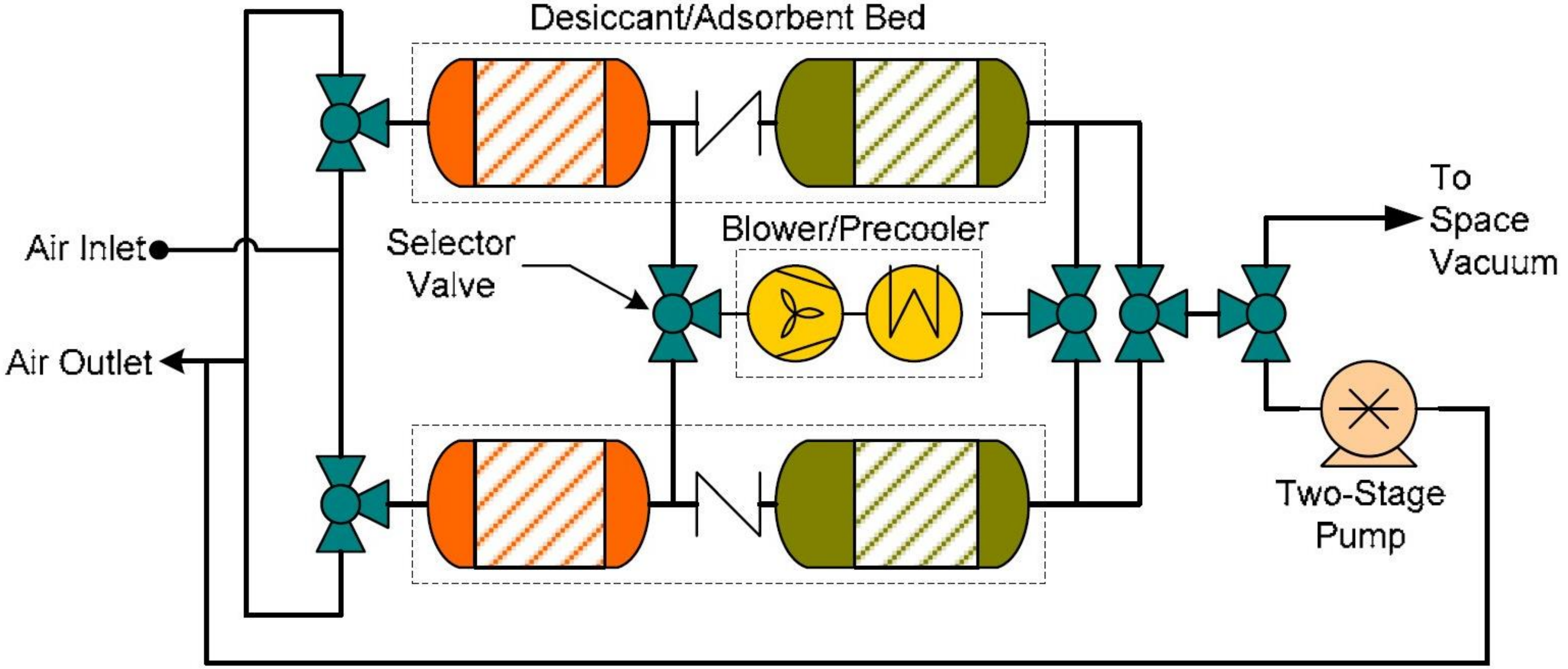
NASA Marshall Space Flight Center, Huntsville, Alabama, 35812, USA

October 7-9, 2015

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

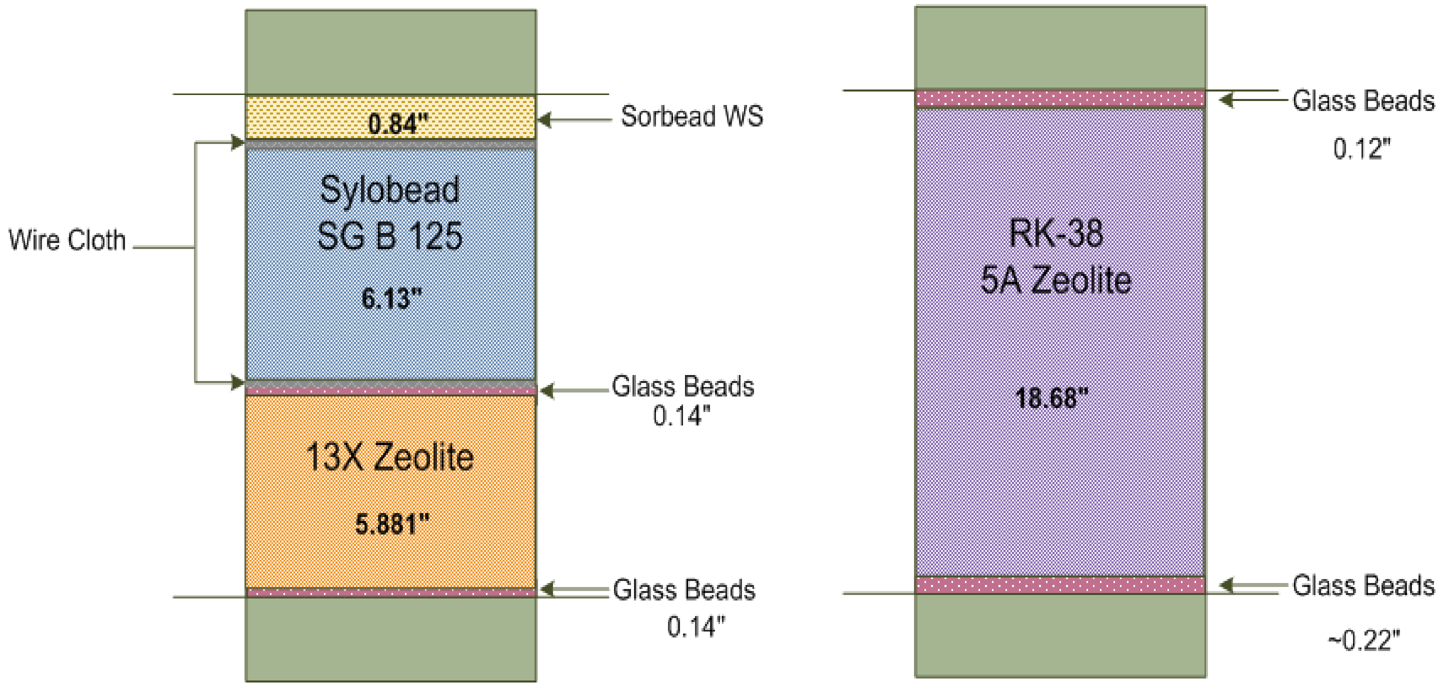
- Goal: *Predictive* model of the Carbon Dioxide Removal Assembly (CDRA)
- Here, focus on the 4 Bed Molecular Sieve (4BMS)
- Need to know sorbent behavior (isotherms, LDF, etc.)



The CDRA 4BMS Beds

- Multiple sorbents:
  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



H_2O CDRA-4 Bed

CO_2 CDRA-4 Bed

Model Approach

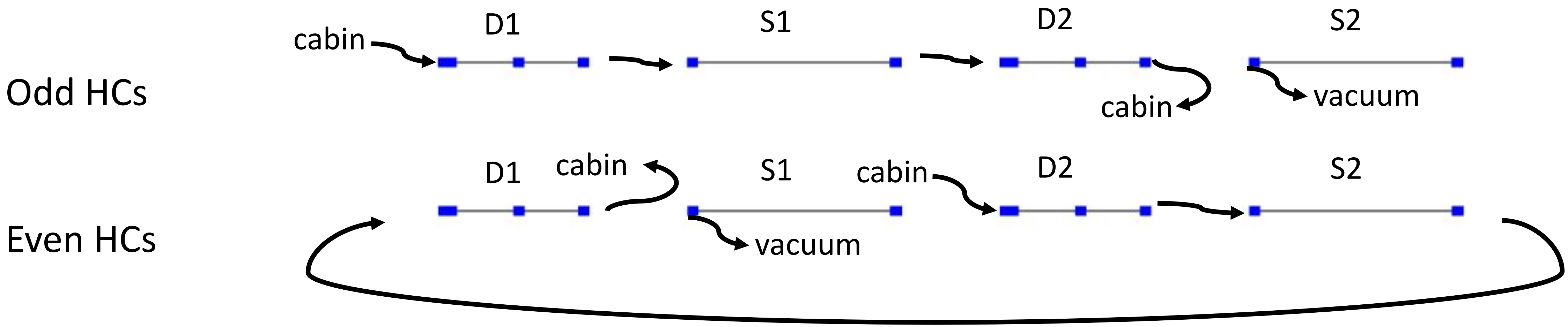
- Use Toth isotherms from other work
- Use dimensionless correlations (Re, Nu, Pe, Pr, Sc)
  - Derives mass dispersion and thermal transfer coefficients
- Assume binary mass diffusion is valid
- Assume constant porosity
- Use Rumpf-Gupte permeability relationship
- Assume 1-D Darcy Flow
- Fit the single model parameter (LDF) using CBT data

COMSOL 4BMS Model

Use COMSOL Multiphysics to solve in 1-D:

- 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
    - time-dependent inlet Temperature condition
  - all are coupled via thermal coefficient Heat Sources
  - temperature-dependent material properties
- Darcy's Law (pressure and superficial velocity)
  - time-dependent inlet Mass Flux
  - estimated constant outlet Pressure
  - includes Mass Source due to sorption
- General Form PDE: pellet loading via LDF & Toth
- General Equations: heater switches

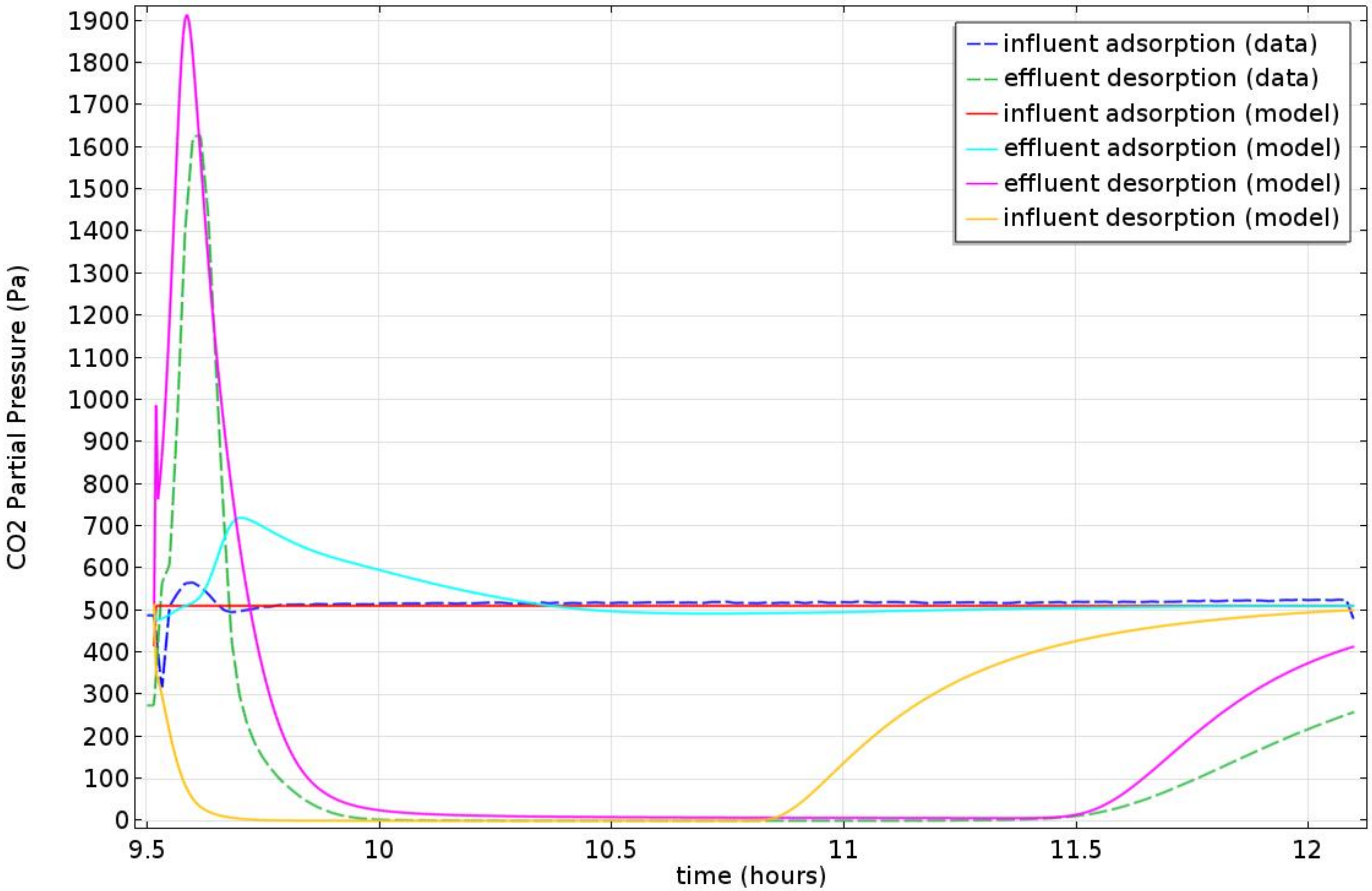
1-D Model



- Separate Physics Nodes and Steps for each bed
- Switch BC types for each half-cycle using Physics Tree
- Boundaries between sub-beds marked by ■

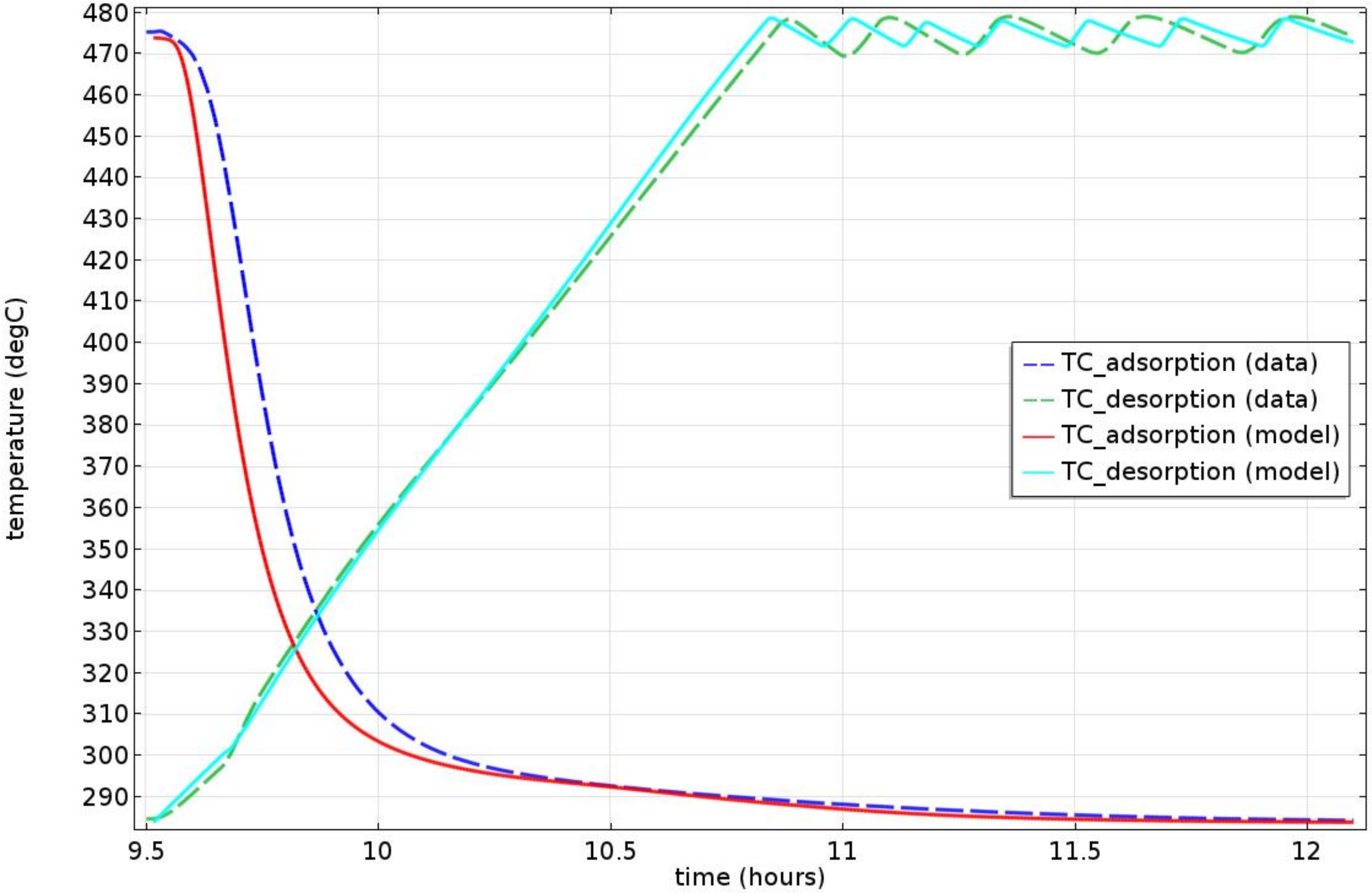
CDRA-4EU Test-bed CO_2 Results

- Competitive CO_2/H_2O on 13X (assumed 5 times 5A)
- '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
- 5A porosity of 55% (mass unknown)



CDRA-4EU Test-bed Temperature Results

- Model cools too slightly too quickly during adsorption
- Heater control set-points in test appear ‘soft’
- Slope, given thermal mass, dictates ~670W
- Model cools slightly too slowly during desorption when heaters off



Data only briefly heats at expected rate from 980W (but heater requirements say max 5 °F/min!)

Summary

- Have constructed a *predictive* CDRA 4BMS 1-D Comsol model
  - Calibrated with CBT on various sorbates, sorbents, flow rates, concentrations
- Generalize to 2D and 3D (?)
- 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 sorbent bed heater issue
- Approaching limits of 1-D
- Validate with more CDRA4-EU tests
  - Different flow-rates, half-cycle times, dew points, vapor pressures
- Inform CDRA optimization
- Genuine H_2O/CO_2 sorption competition model

→Virtual Laboratory of the CDRA System