COMSOL CONFERENCE
2015 BOSTON

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

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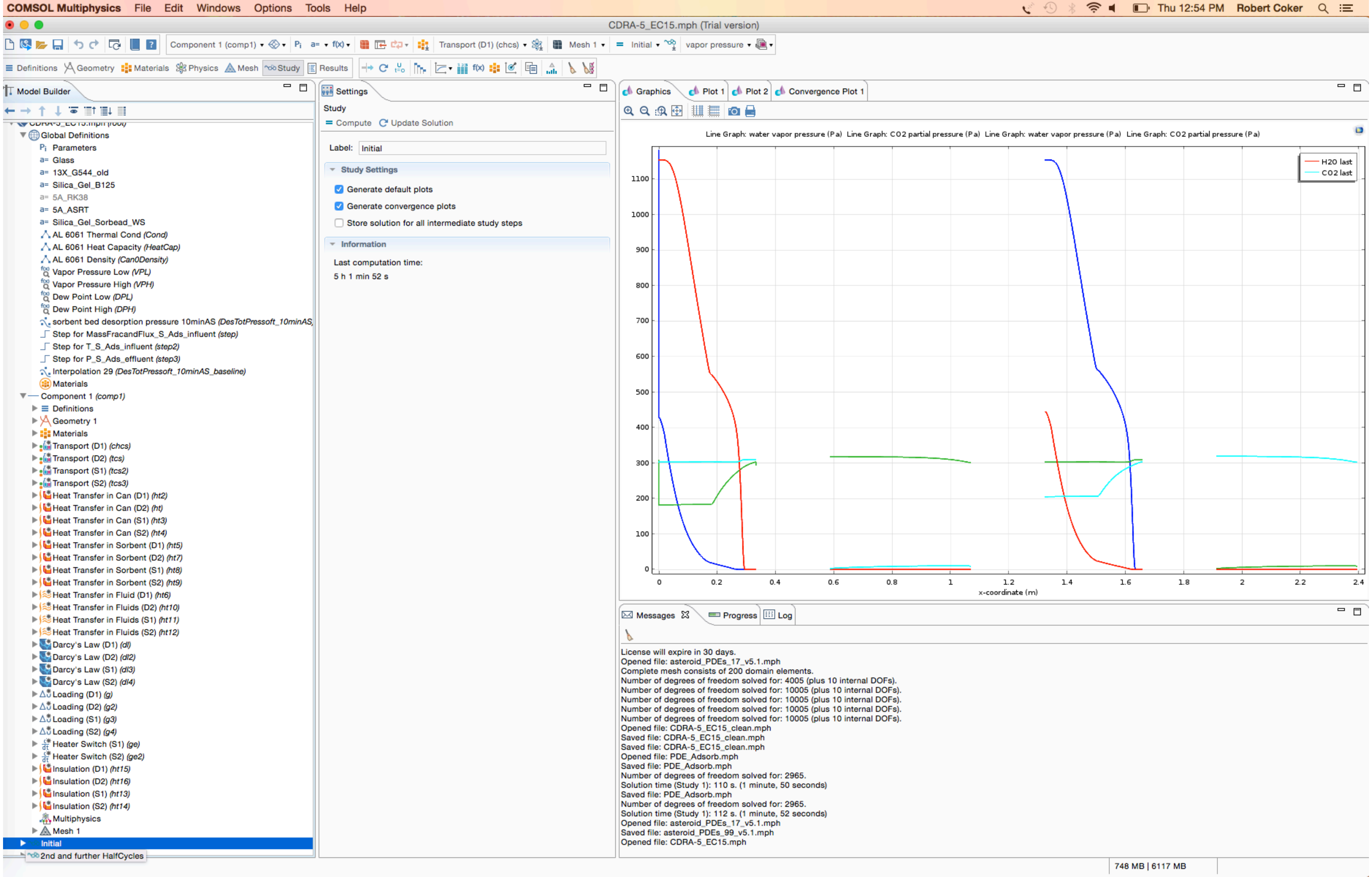
COMSOL Multiphysics File Edit Windows Options Tools Help
Thu 12:54 PM Robert Coker
CDRA-5_EC15.mph (Trial version)
Component 1 (comp1)
Transport (D1) (chcs)
Mesh 1
Initial
vapor pressure
Definitions Geometry Materials Physics Mesh Study Results
Model Builder
Global Definitions
Parameters
Glass
13X_G544_old
Silica_Gel_B125
5A_RK38
5A_ASRT
Silica_Gel_Sorbead_WS
AL 6061 Thermal Cond (Cond)
AL 6061 Heat Capacity (HeatCap)
AL 6061 Density (Can0Density)
Vapor Pressure Low (VPL)
Vapor Pressure High (VPH)
Dew Point Low (DPL)
Dew Point High (DPH)
sorbent bed desorption pressure 10minAS (DesTotPressoft_10minAS
Step for MassFracandFlux_S_Ads_influent (step)
Step for T_S_Ads_influent (step2)
Step for P_S_Ads_effluent (step3)
Interpolation 29 (DesTotPressoft_10minAS_baseline)
Materials
Component 1 (comp1)
Definitions
Geometry 1
Materials
Transport (D1) (chcs)
Transport (D2) (tcs)
Transport (S1) (tcs2)
Transport (S2) (tcs3)
Heat Transfer in Can (D1) (ht2)
Heat Transfer in Can (D2) (ht)
Heat Transfer in Can (S1) (ht3)
Heat Transfer in Can (S2) (ht4)
Heat Transfer in Sorbent (D1) (ht5)
Heat Transfer in Sorbent (D2) (ht7)
Heat Transfer in Sorbent (S1) (ht8)
Heat Transfer in Sorbent (S2) (ht9)
Heat Transfer in Fluid (D1) (ht6)
Heat Transfer in Fluids (D2) (ht10)
Heat Transfer in Fluids (S1) (ht11)
Heat Transfer in Fluids (S2) (ht12)
Darcy's Law (D1) (dl)
Darcy's Law (D2) (dl2)
Darcy's Law (S1) (dl3)
Darcy's Law (S2) (dl4)
Loading (D1) (g)
Loading (D2) (g2)
Loading (S1) (g3)
Loading (S2) (g4)
Heater Switch (S1) (ge)
Heater Switch (S2) (ge2)
Insulation (D1) (ht15)
Insulation (D2) (ht16)
Insulation (S1) (ht13)
Insulation (S2) (ht14)
Multiphysics
Mesh 1
Initial
2nd and further HalfCycles
Settings
Study
Compute Update Solution
Label: Initial
Study Settings
Generate default plots
Generate convergence plots
Store solution for all intermediate study steps
Information
Last computation time:
5 h 1 min 52 s
Graphics Plot 1 Plot 2 Convergence Plot 1
Line Graph: water vapor pressure (Pa) Line Graph: CO2 partial pressure (Pa) Line Graph: water vapor pressure (Pa) Line Graph: CO2 partial pressure (Pa)
H20 last
CO2 last
1100
1000
900
800
700
600
500
400
300
200
100
0
0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8 2 2.2 2.4
x-coordinate (m)
Messages Progress Log
License will expire in 30 days.
Opened file: asteroid_PDEs_17_v5.1.mph
Complete mesh consists of 200 domain elements.
Number of degrees of freedom solved for: 4005 (plus 10 internal DOFs).
Number of degrees of freedom solved for: 10005 (plus 10 internal DOFs).
Number of degrees of freedom solved for: 10005 (plus 10 internal DOFs).
Number of degrees of freedom solved for: 10005 (plus 10 internal DOFs).
Number of degrees of freedom solved for: 10005 (plus 10 internal DOFs).
Opened file: CDRA-5_EC15_clean.mph
Saved file: CDRA-5_EC15_clean.mph
Saved file: CDRA-5_EC15_clean.mph
Opened file: PDE_Adsorb.mph
Saved file: PDE_Adsorb.mph
Number of degrees of freedom solved for: 2965.
Solution time (Study 1): 110 s. (1 minute, 50 seconds)
Saved file: PDE_Adsorb.mph
Number of degrees of freedom solved for: 2965.
Solution time (Study 1): 112 s. (1 minute, 52 seconds)
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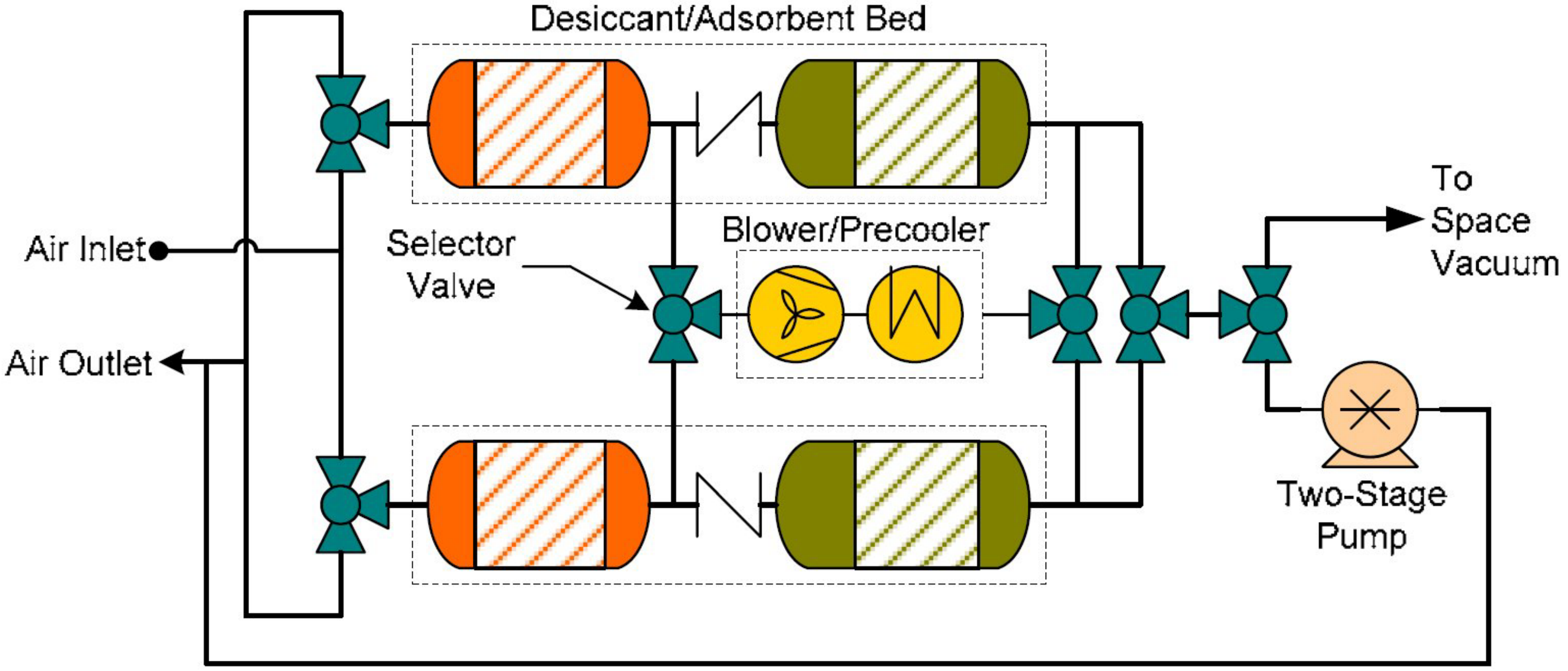
Saved file: asteroid_PDEs_99_v5.1.mph
Opened file: CDRA-5_EC15.mph
748 MB | 6117 MB

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

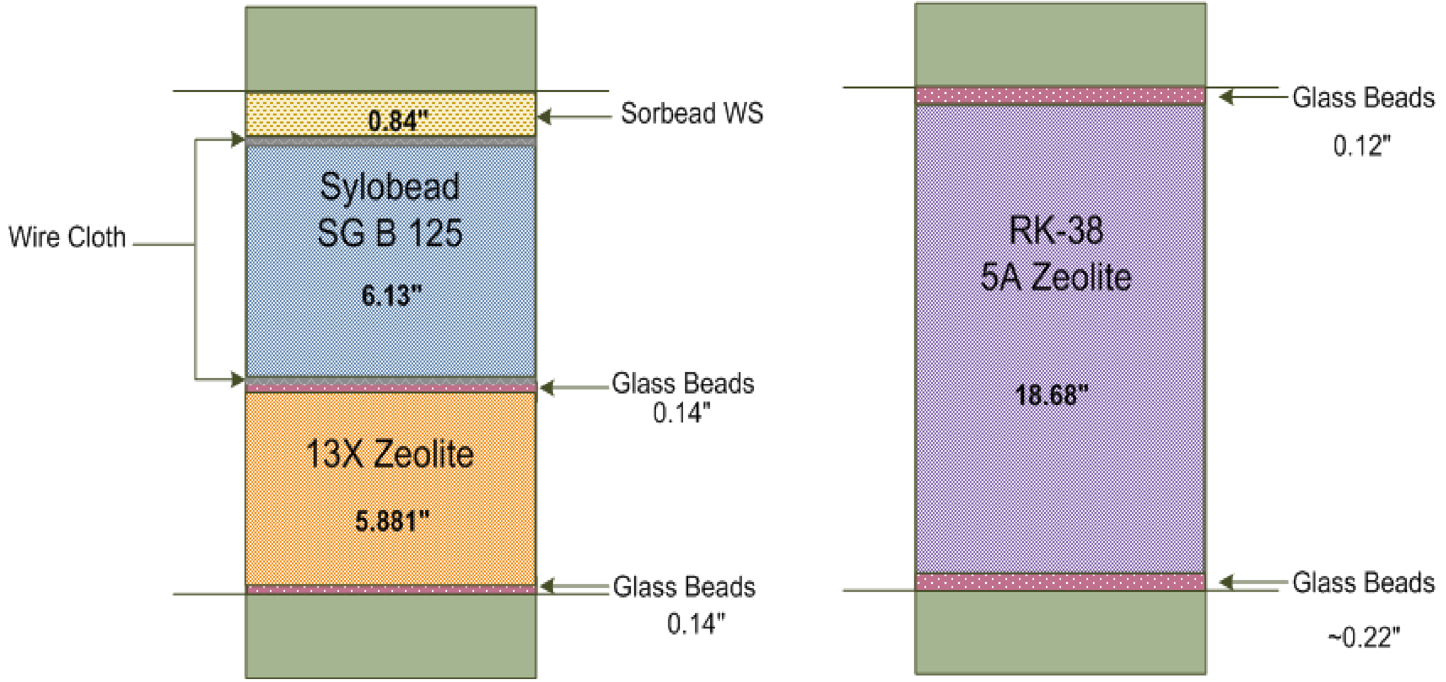
- Goal: *Predictive* model of the Carbon Dioxide Removal Assembly (CDRA)
- Here, focus on the 4 Bed Molecular Sieve (4BMS)
- Need to know sorbent behavior (isotherms, LDF, etc.)



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

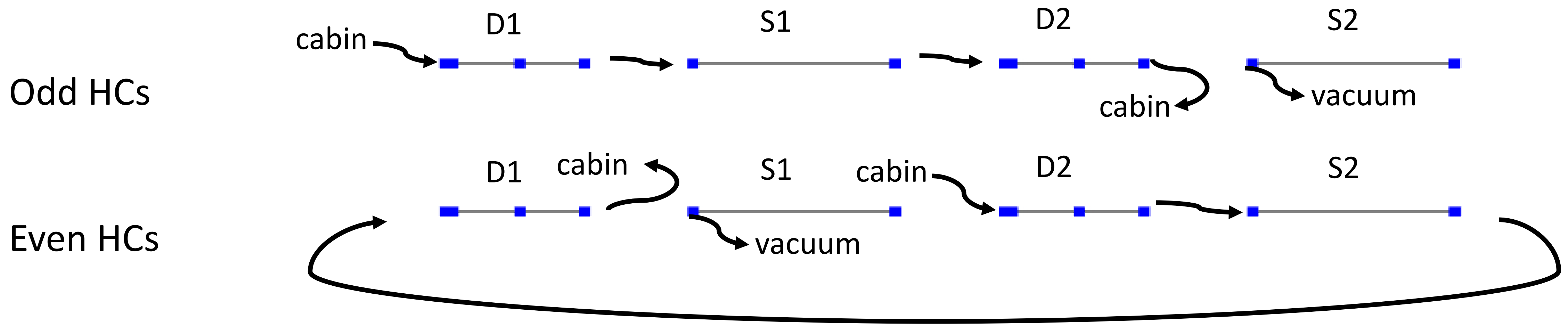
- Use Toth isotherms from other work
- Use dimensionless correlations (Re, Nu, Pe, Pr, Sc)
  - Derives mass dispersion and thermal transfer coefficients
- Assume binary mass diffusion is valid
- Assume constant porosity
- Use Rumpf-Gupte permeability relationship
- Assume 1-D Darcy Flow
- Fit the single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

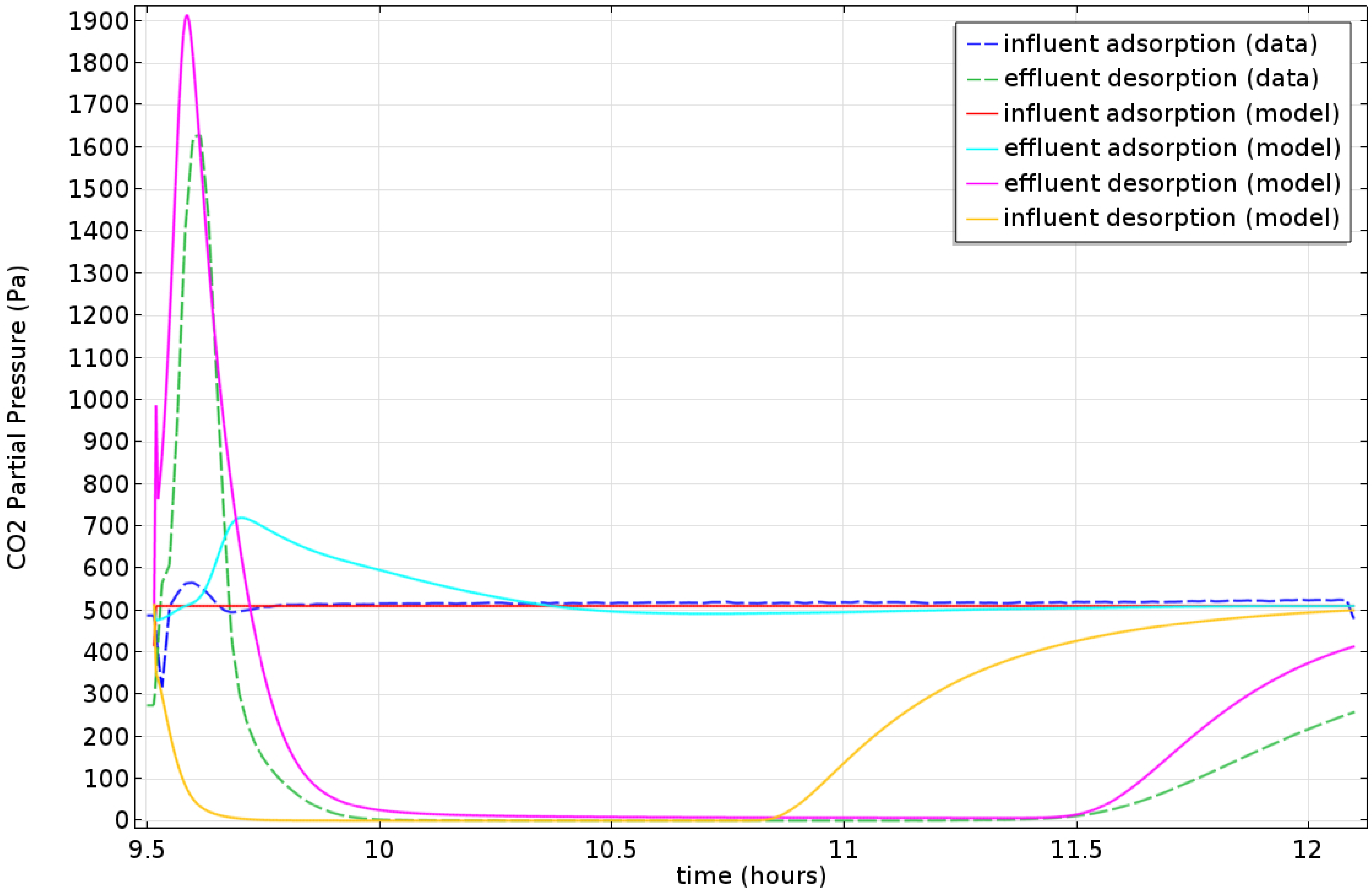
1-D Model



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

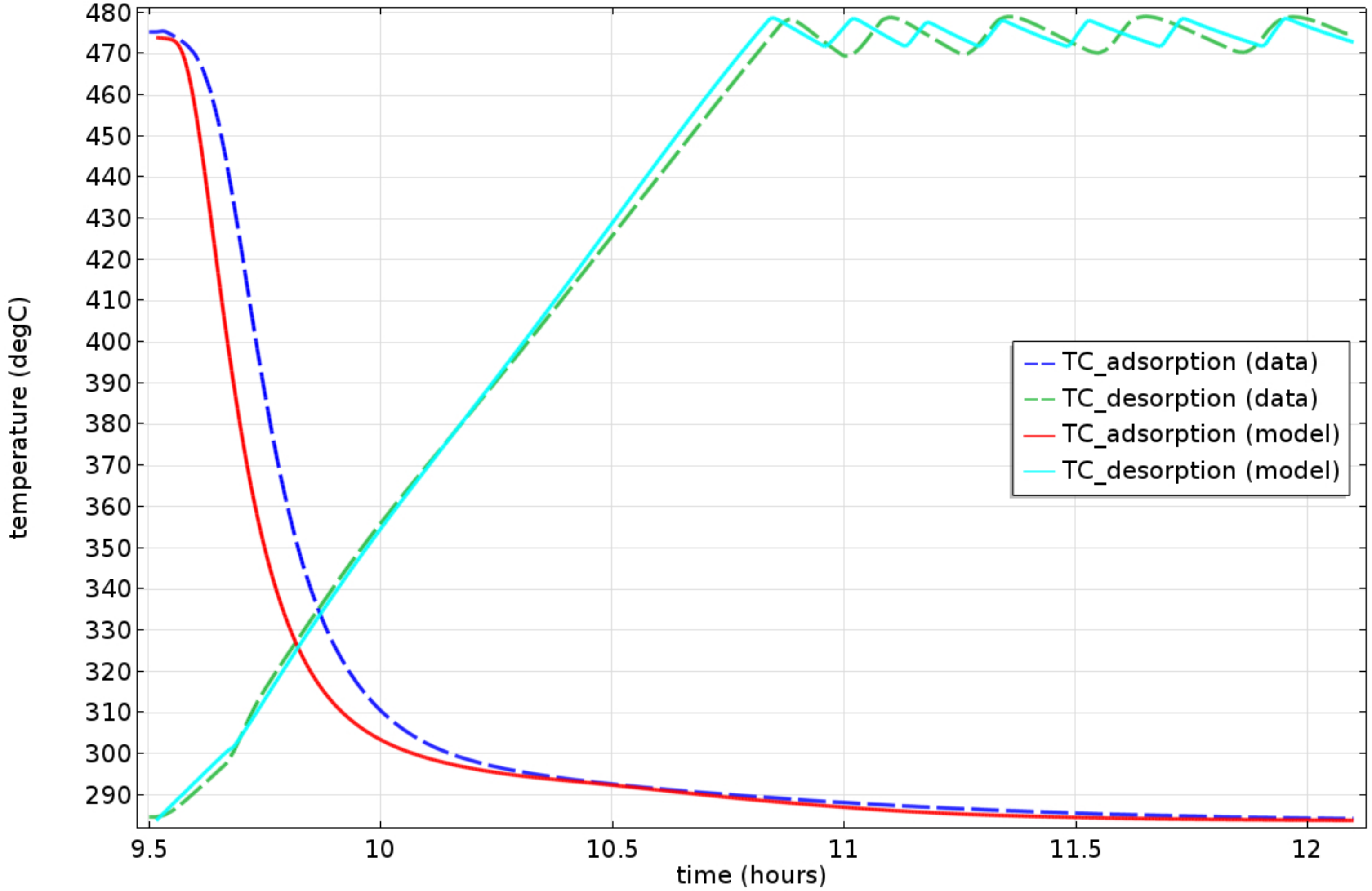
CDRA-4EU Test-bed CO_2 Results

- 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