Multi-Dimensional Adsorption Model of CO2/H20 Sorbent Bed

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Introduction

- The objective of this simulation effort is to develop and correlate a 2D axisymmetric adsorption model of the Vacuum Characterization test article in order to capture 3-D radial effect during adsorption.
- A 1-D baseline model has been created to understand the multi-physics being used during the adsorption process. However, this model only captures axial effects such as velocity, CO2 concentration and temperature

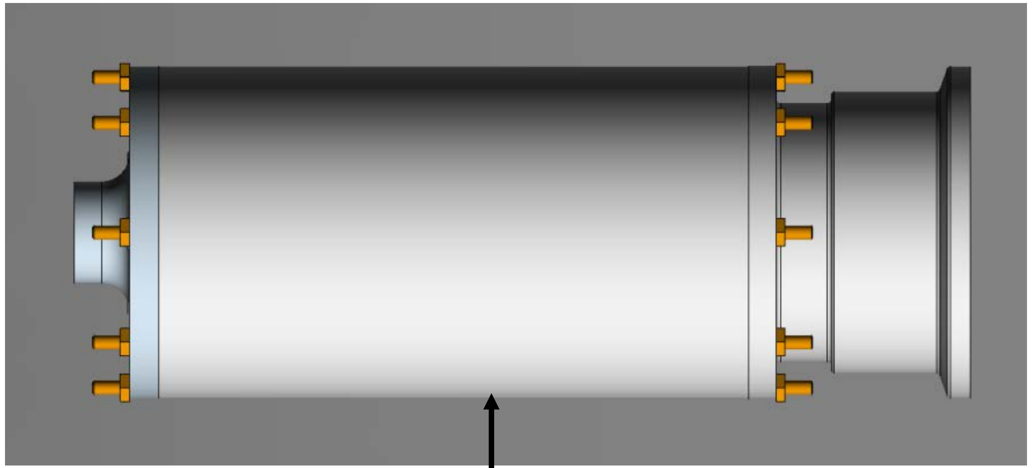
Approach

- The 2-D axisymmetric adsorption model has been developed to find and understand 3-D radial effects that a 1-D model cannot capture. Understanding these effects can help establish predictive capabilities that can be used to modify 1-D models for improved test correlations.

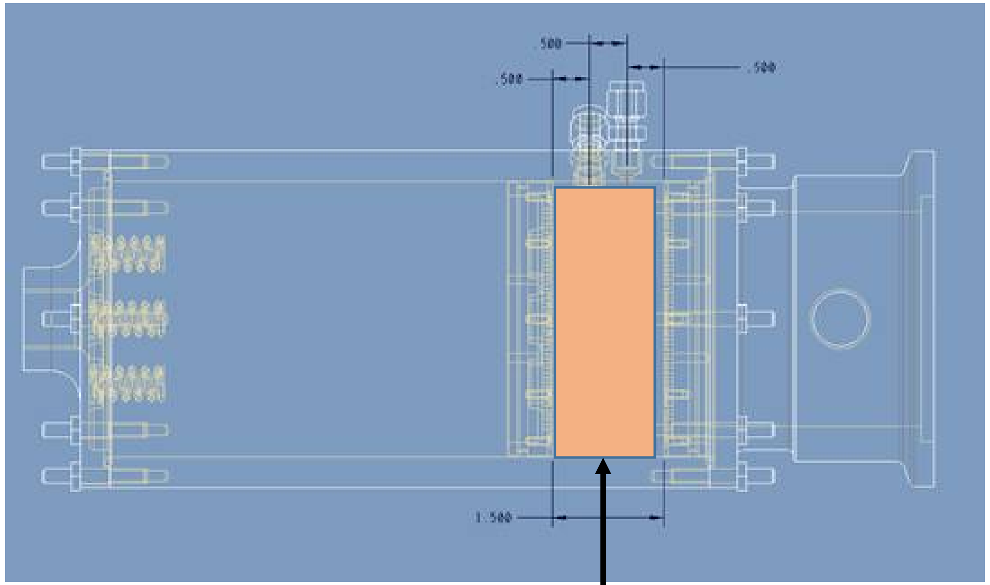
- This 2-D axisymmetric model includes COMSOL built-in Brinkman porous media flow interface which accounts for the fluid velocity and pressure fields in both the radial and axial direction.

Test Canister

- The canister contains a pelletized adsorption bed which is used to adsorb H_2O and/or CO_2.

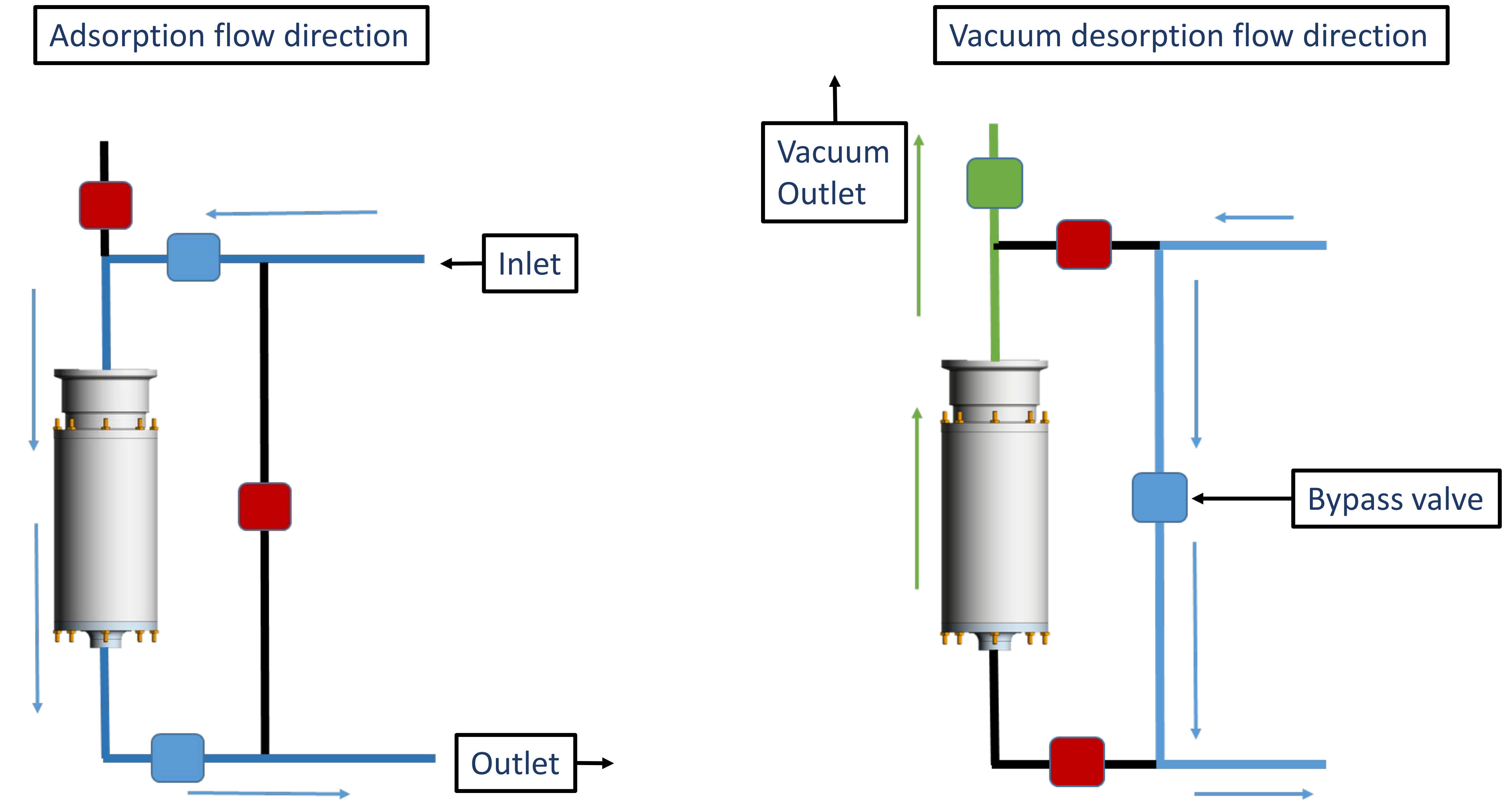


6061 Aluminum canister with a 3.4” inner diameter

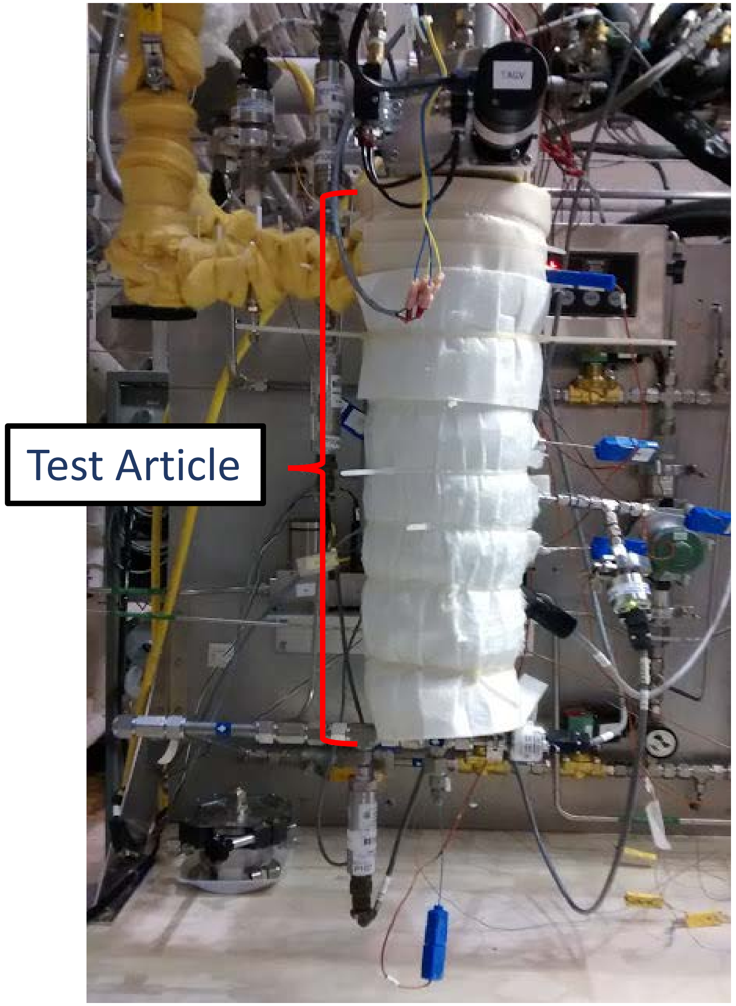


The bed length can be adjusted from 1” to 6”

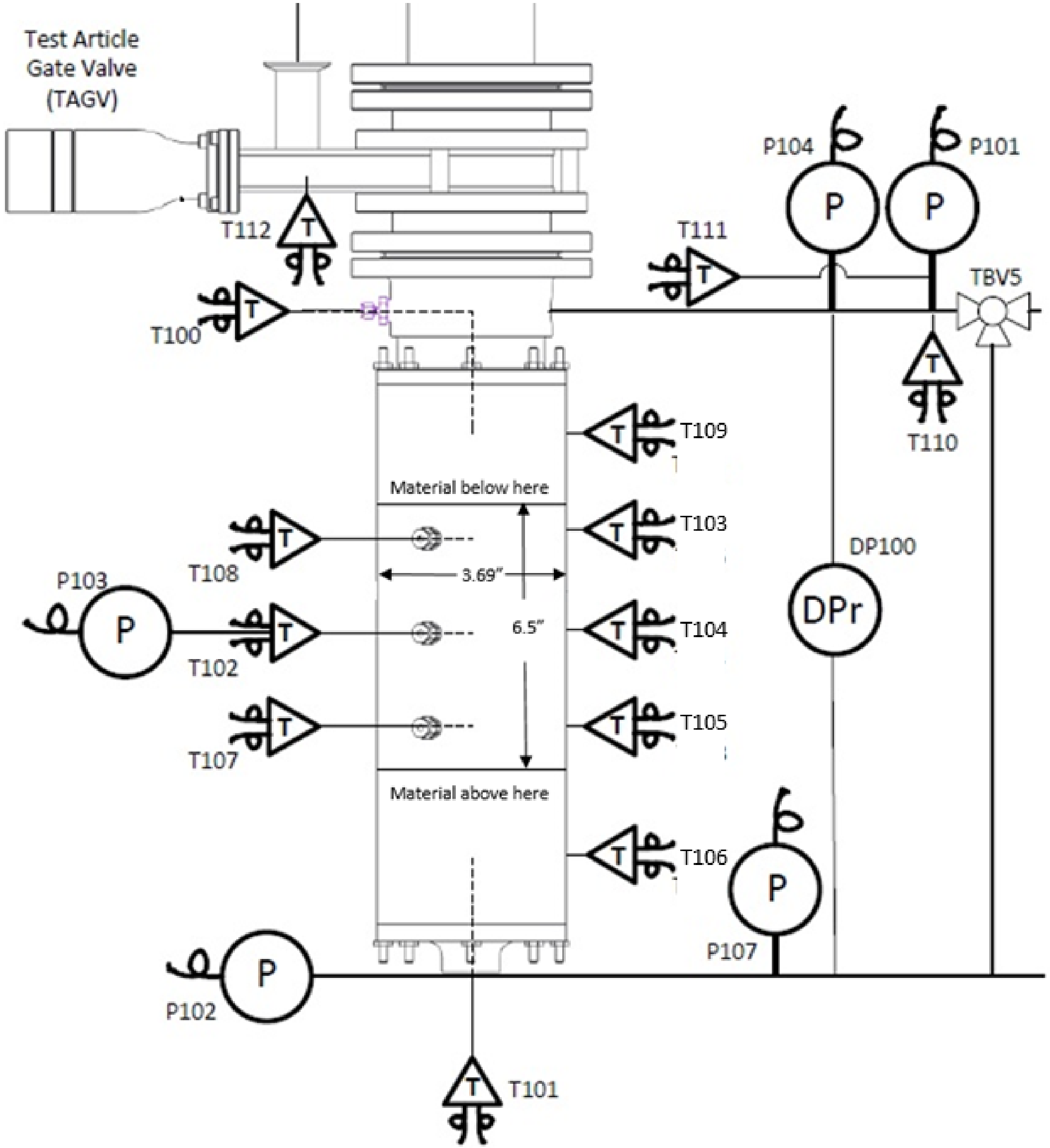
Adsorption/Desorption Apparatus



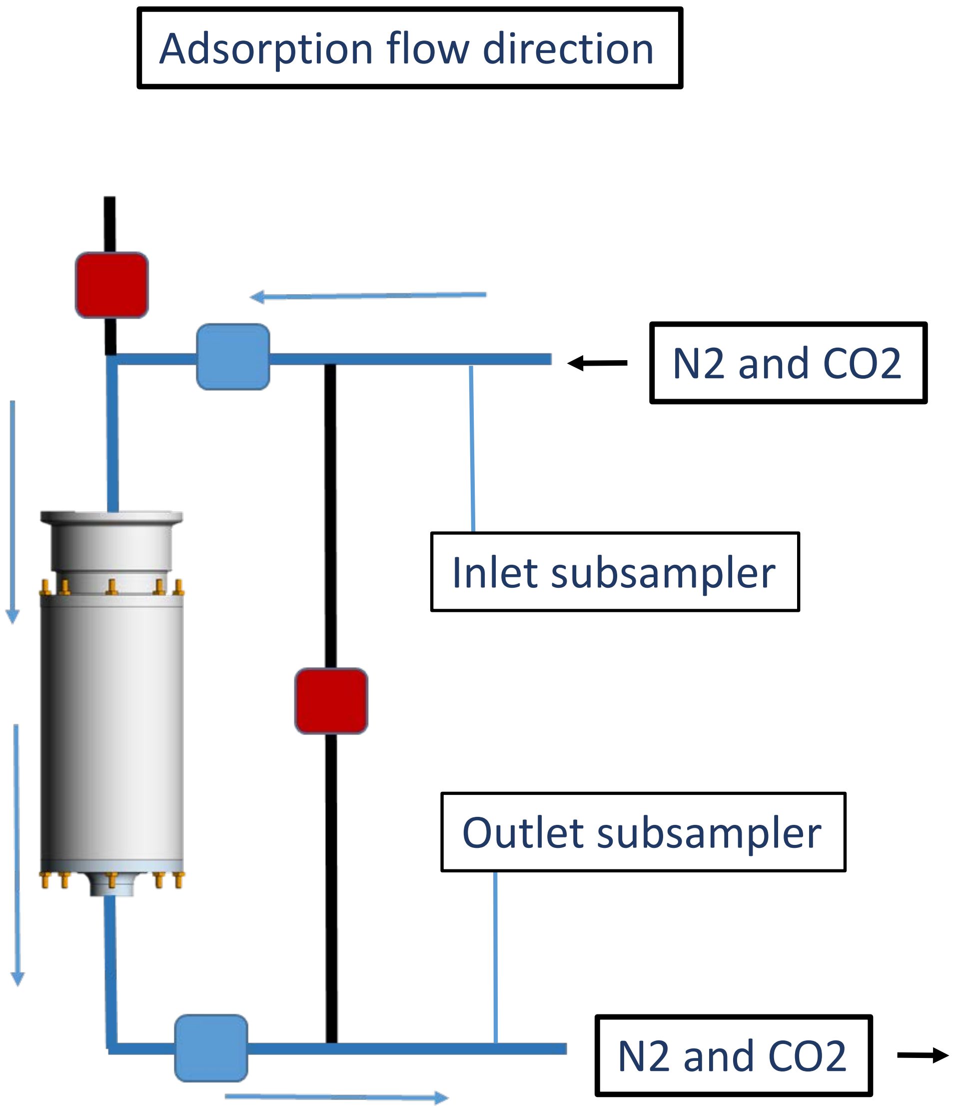
Test Article



Photograph of test article covered in pyropropel (yellow) & fiberglass (white) insulation (taken 6-26-2015)



Vacuum Characterization Breakthrough Test



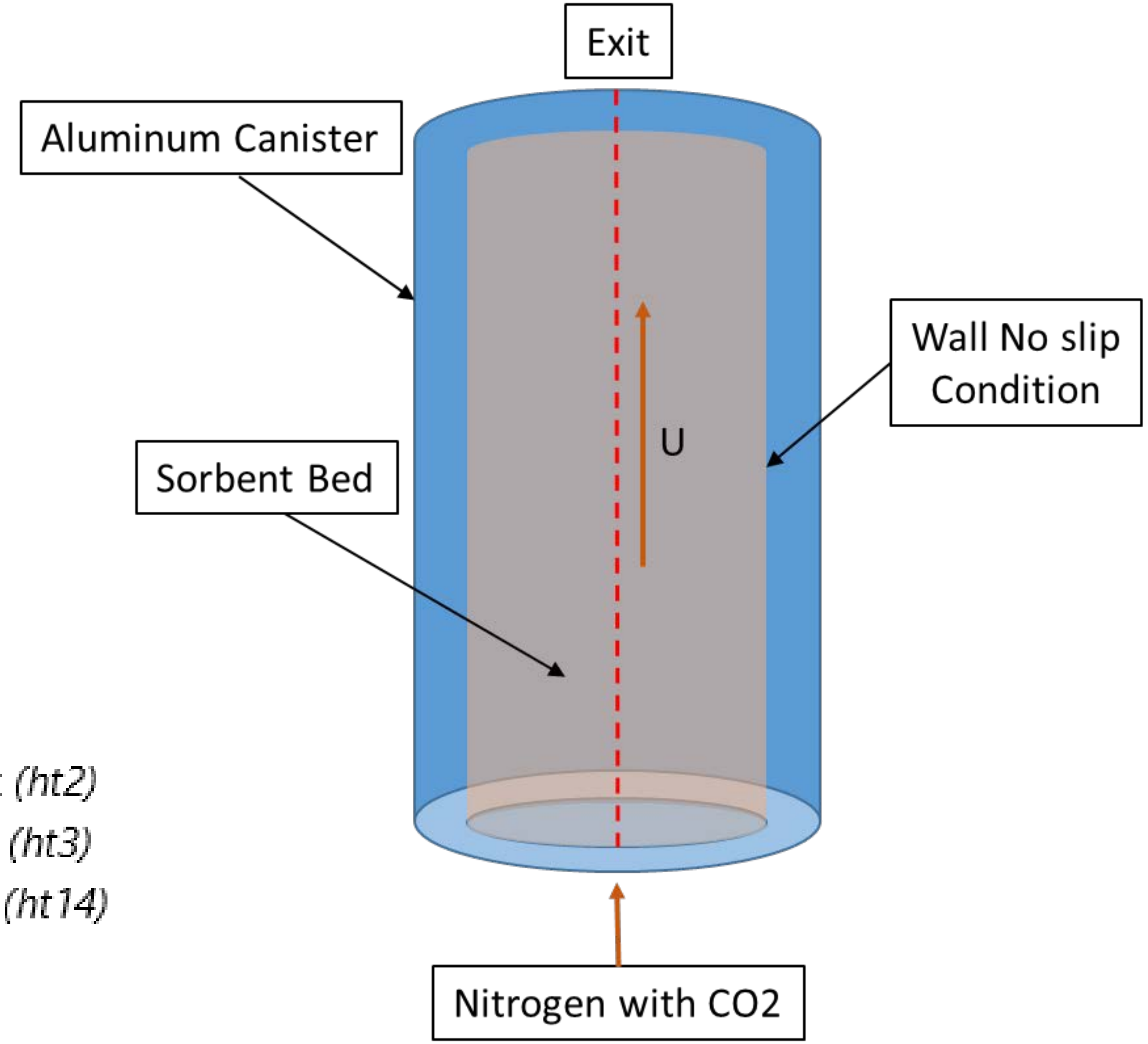
- Nitrogen is used as a carrier gas in this experiment. Nitrogen and CO2 are introduced at the inlet. The total flow is controlled by the Nitrogen flow controller
- Two CO2 subsamplers are used to measure the influent and effluent CO2 partial pressure
- The total mass flow, system pressures, CO2 partial pressure, and inlet temperatures measurements are used as COMSOL model inputs.
- Internal and external temperature data are used to help correlate to the COMSOL model

COMSOL Breakthrough Test Setup

Created a 2D axisymmetric model of the VC breakthough test and compared results to test data

Model parameters:

- 135 L/min
- Nitrogen and CO2
- 5A-RK38
- Constant Void Fraction/Variable Void Fraction



1D Modules

- Transport (S2) *(tcs3)*
- Heat Transfer in Can *(ht)*
- Heat Transfer in Sorbent *(ht2)*
- Heat Transfer in Fluid *(ht3)*
- Insulation (S2) *(ht14)*
- Darcy's Law (S2) *(dl4)*
- Loading (S2) *(g4)*

2D Modules

- Transport (S2) *(tcs3)*
- Heat Transfer in Can *(ht)*
- Heat Transfer in Sorbent *(ht2)*
- Heat Transfer in Fluids 3 *(ht3)*
- Heat Transfer Insulation *(ht14)*
- Loading (S2) *(g4)*
- Brinkman Equations *(br)*

CO2 Loading PDE

Mass transfer rate represented in COMSOL

Transport of Concentrated Species

Reaction: $-\frac{\partial q}{\partial t} M_{CO2}(1-\varepsilon)$

Heat Transfer in Sorbent

Heat Source: $-dh\frac{\partial q}{\partial t}(1-\varepsilon)$

Brinkman Porous flow

Mass Source: $-\frac{\partial q}{\partial t} M_{CO2}(1-\varepsilon)$

Linear Driving force

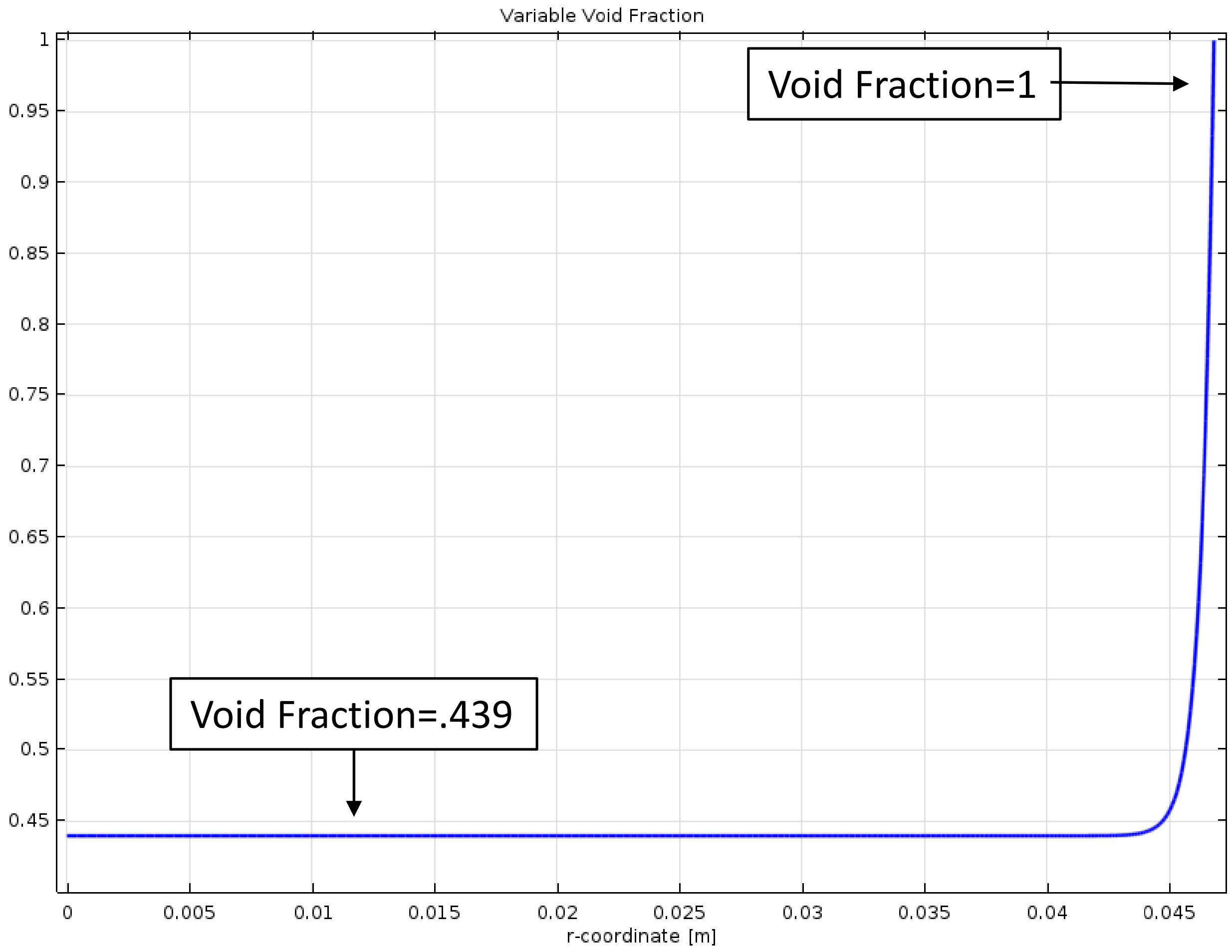
$$\frac{\partial q}{\partial t} = k_m(q^* - q)$$

Governing Equation PDE

Variable Void Fraction

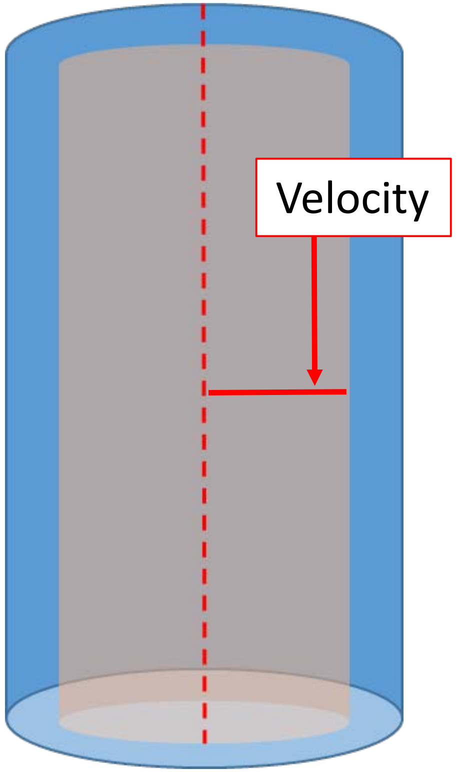
Eps_p=VoidFraction*(1+C*exp(-N*max(0.[m],(ColRad-r))/EqPelDia))

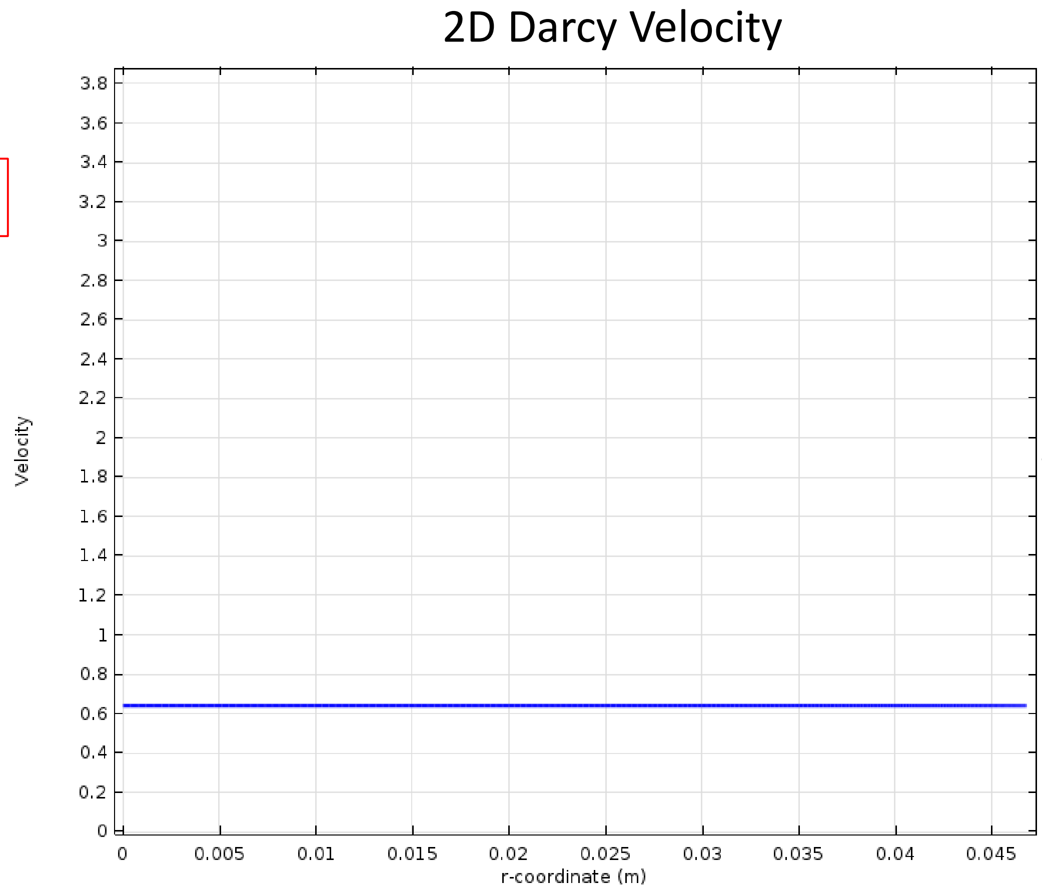
Tobias and Vortmeyer

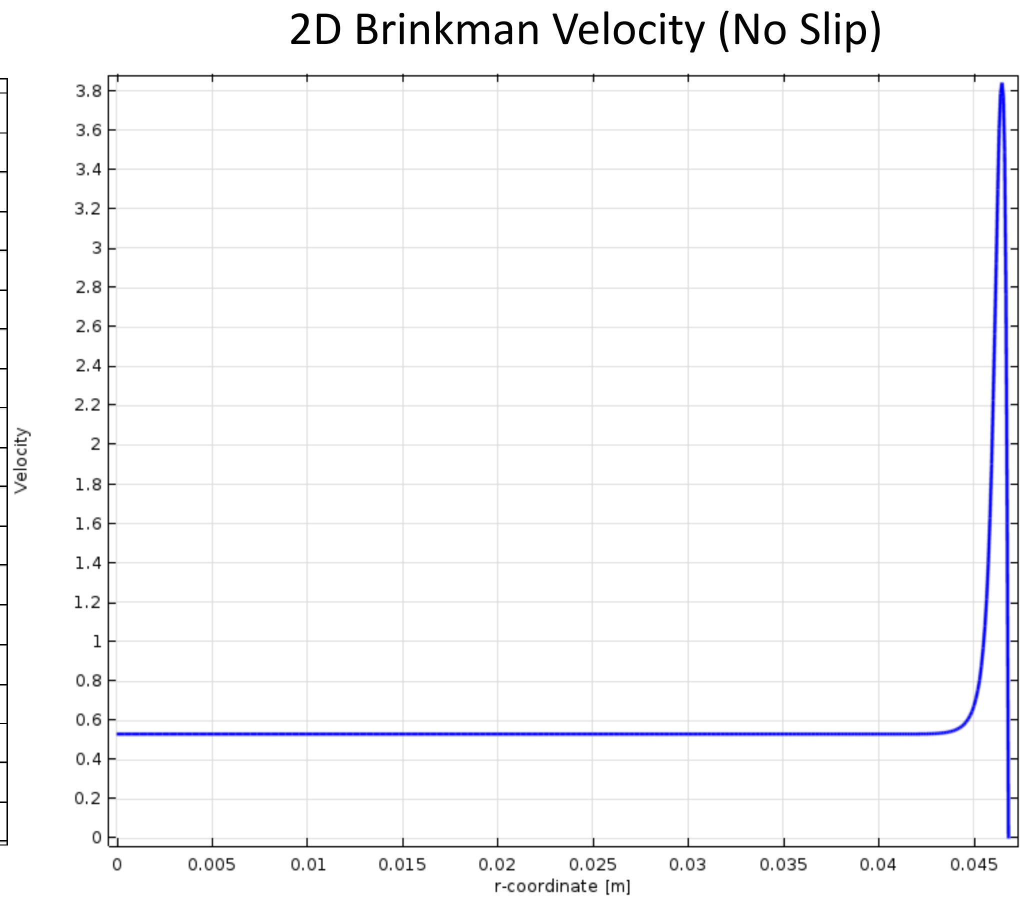


- The porosity varies sharply near the wall for a spherical packed bed since the geometry of packing is interrupted there. As a result, the velocity profile inside the packed bed is severely distorted near the wall.
- This phenomenon is known as flow channeling. A channeling effect was added to the model by using an expression that varies the porosity and increases it exponentially as it reaches the wall.

Kappa Variable Void Fraction

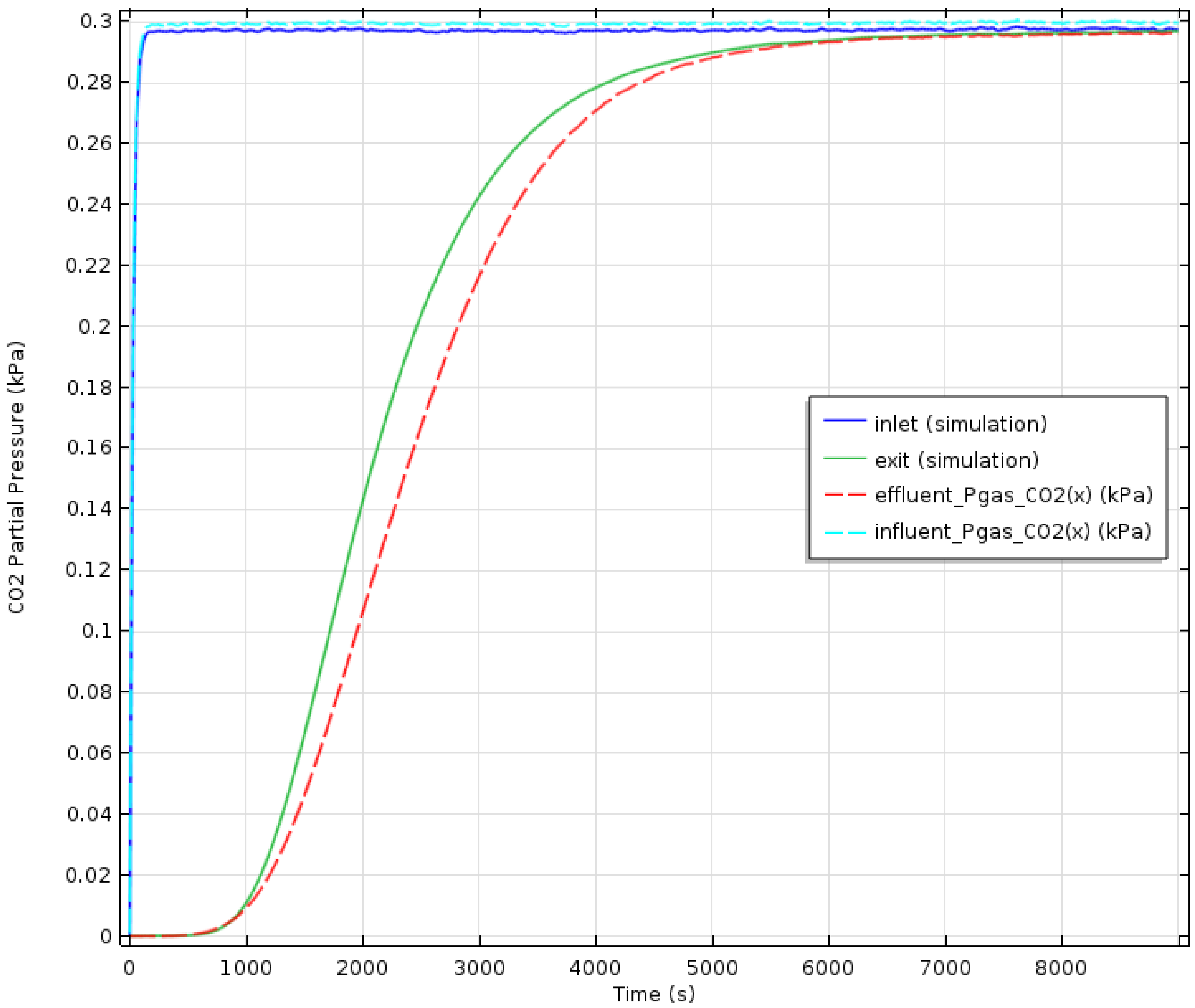




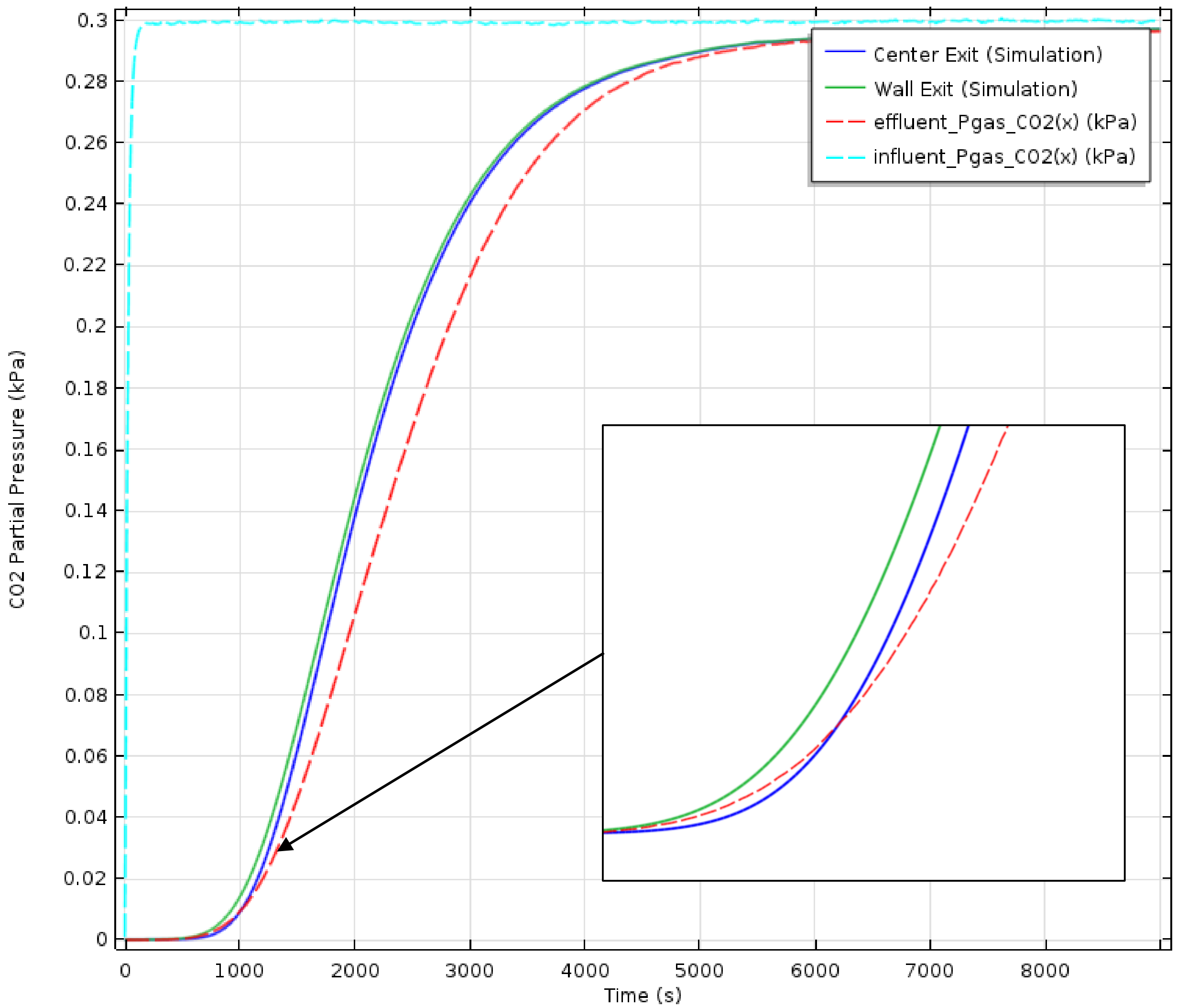


Breakthrough Curve

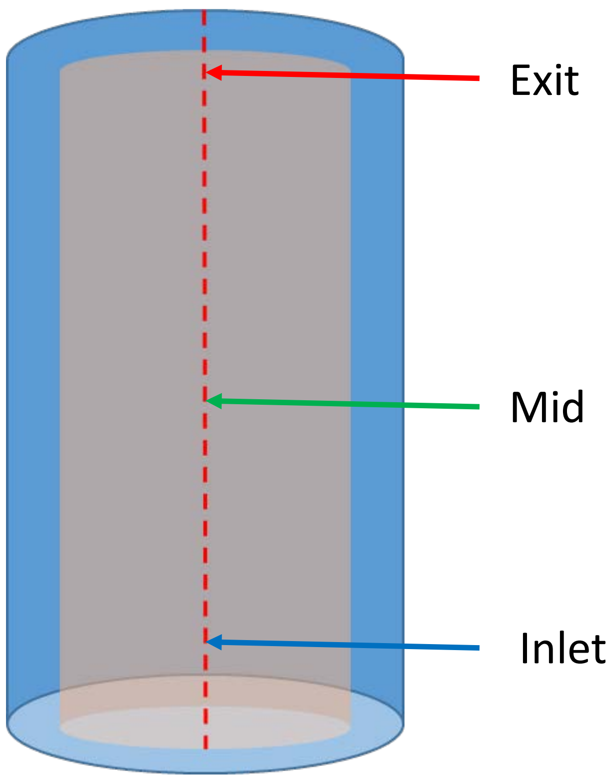
1D Darcy

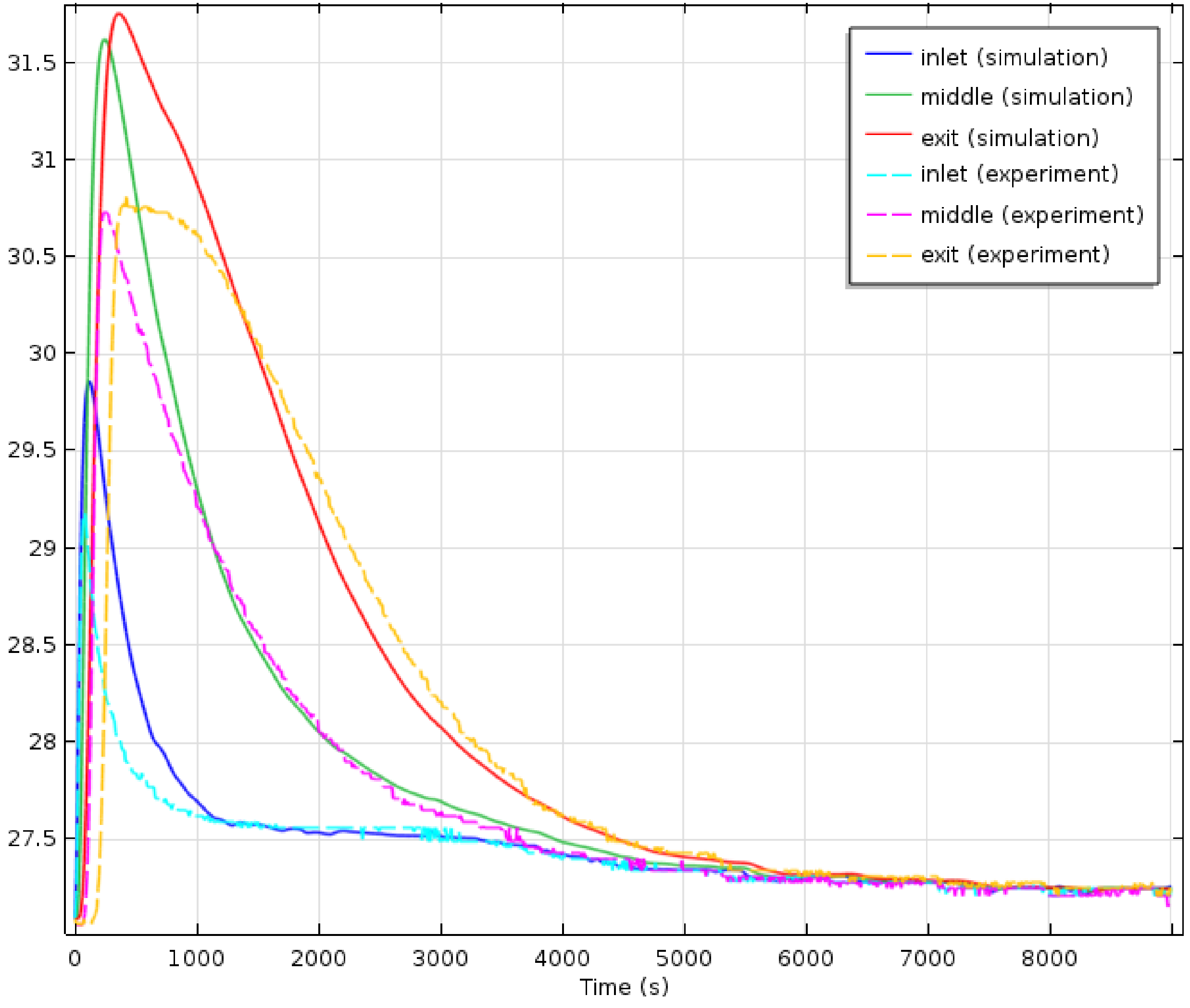


2D Brinkman Velocity (No Slip)

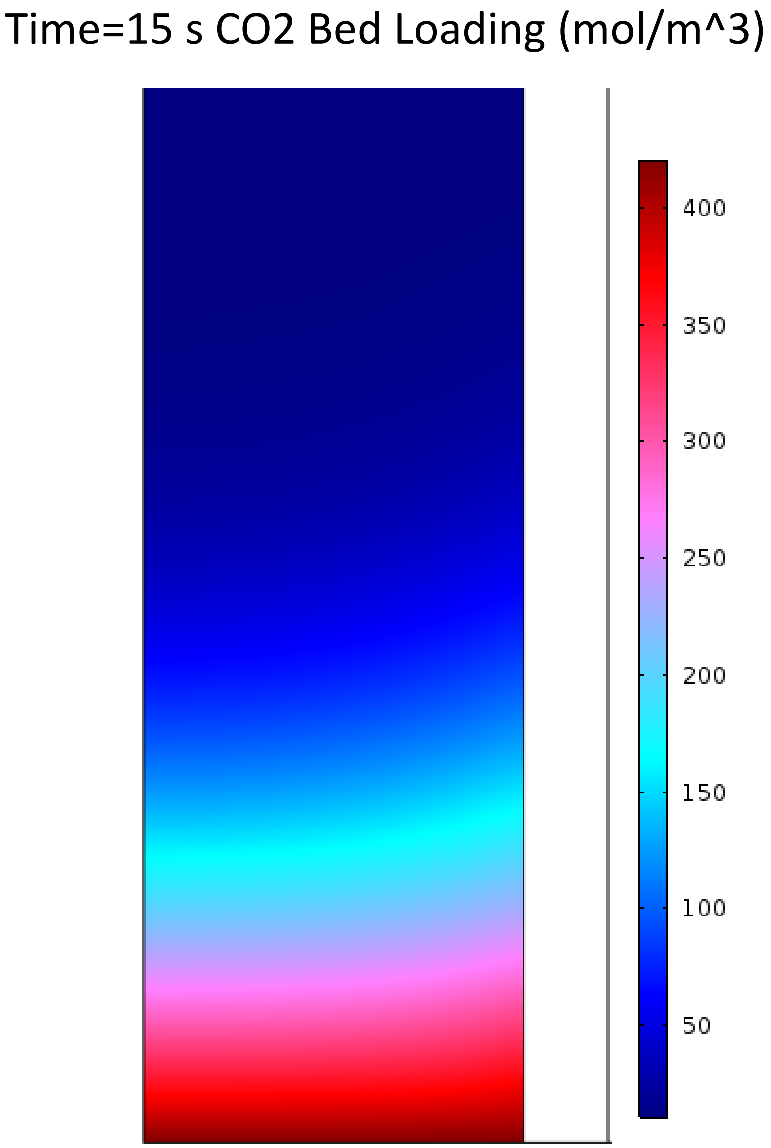


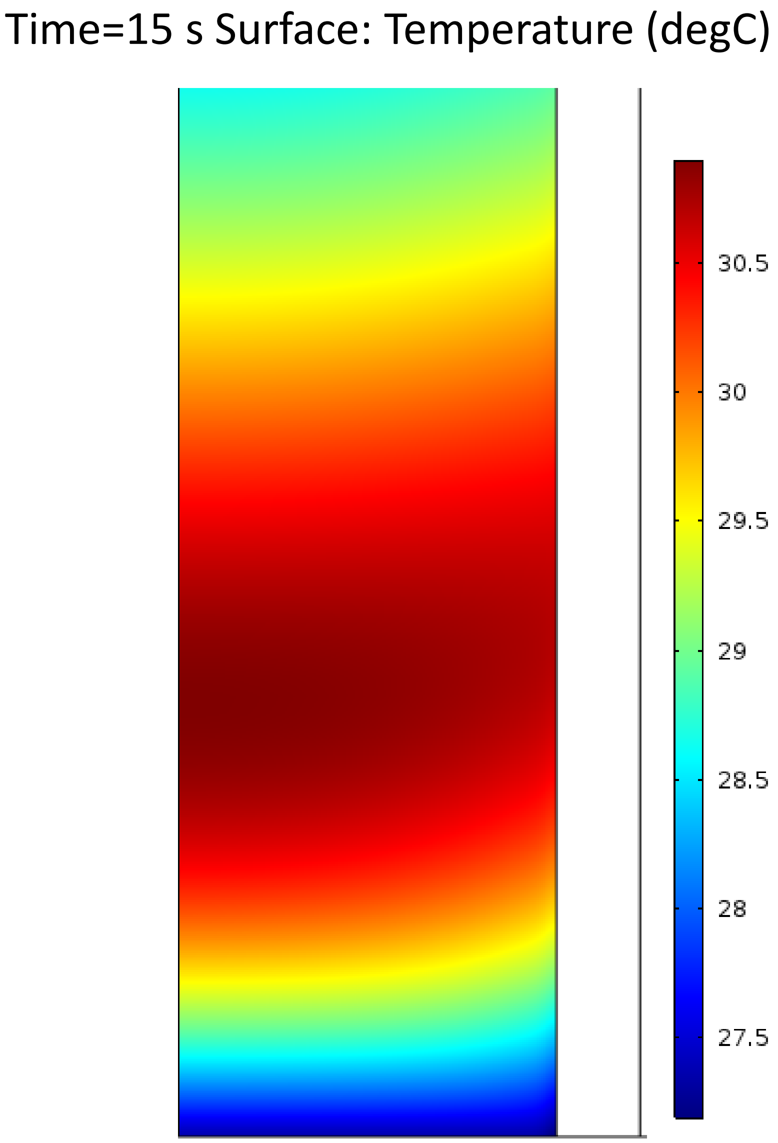
Axial Temperature



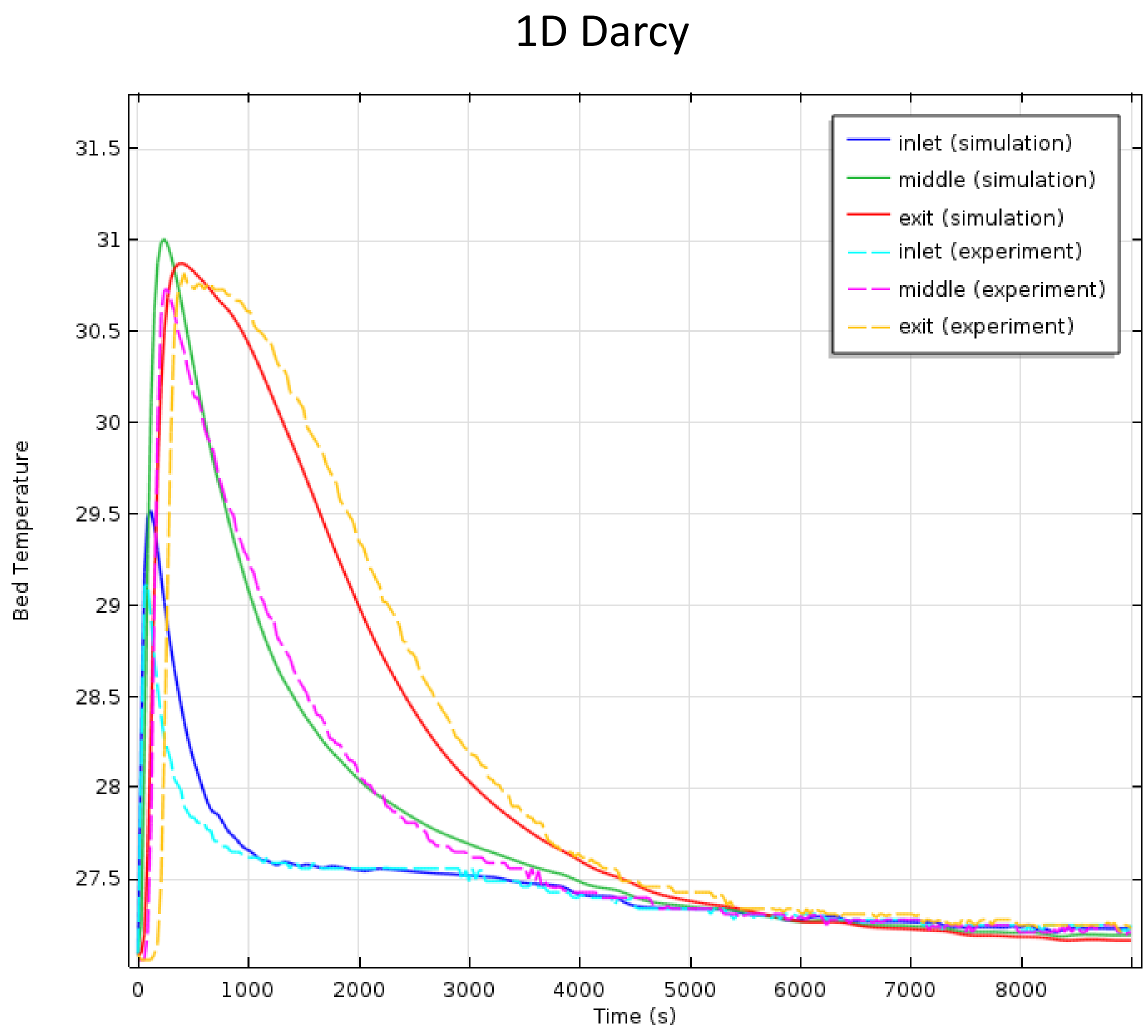


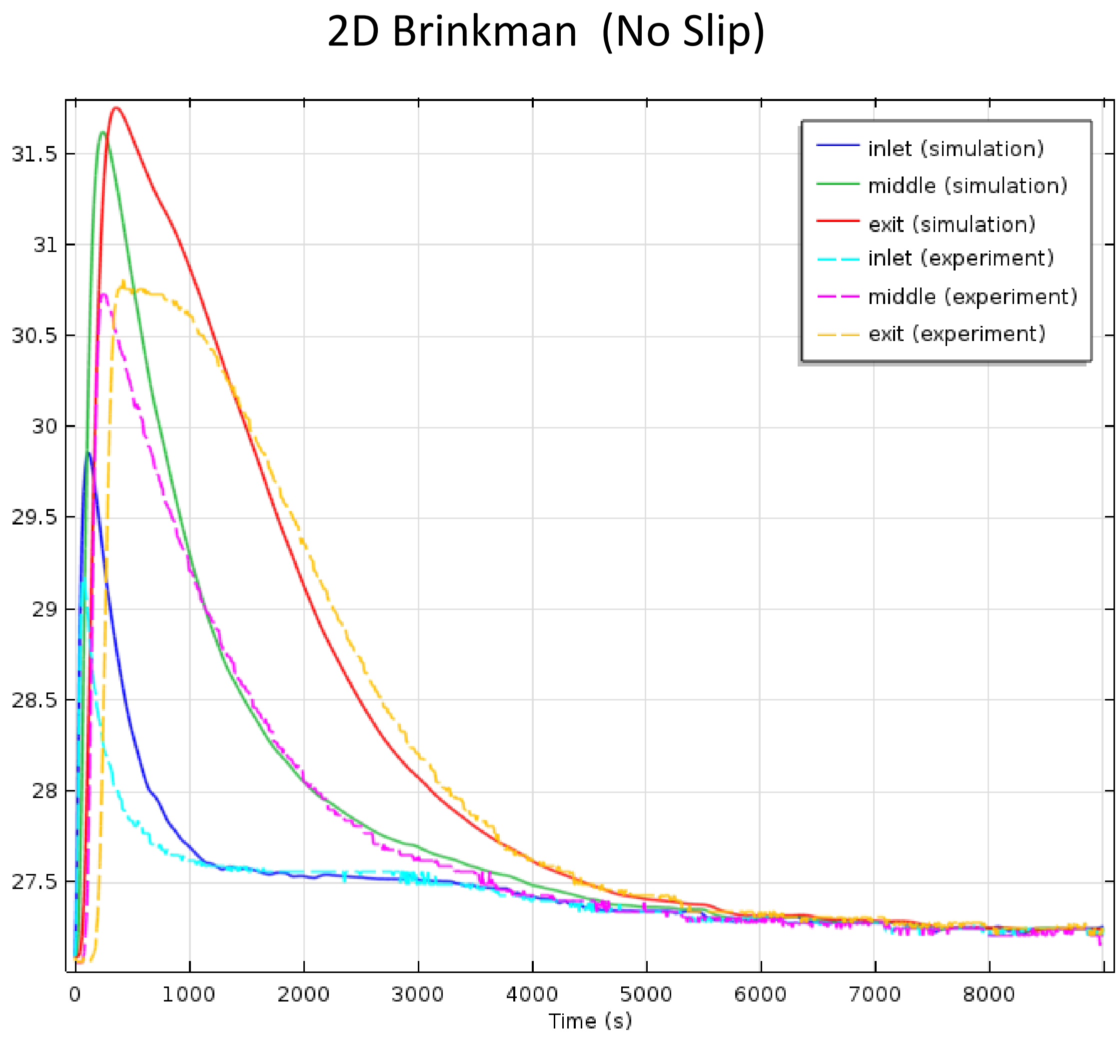
Bed Loading and Temperature





Temperature Comparison





Conclusion/Future Work

- It’s the first step in understanding how to model channeling at the wall with a no slip condition
- Learn and modify assumptions to improve correlations
- Upgrade to Free and Porous Media
- Vacuum Characterization test has been modified with vacuum instrumentation. Post processes desorption data
- Compare COMSOL desorption model to VC test data