Adsorption Modeling: Governing Equation Construction of Micro-fluidic Dynamics

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THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

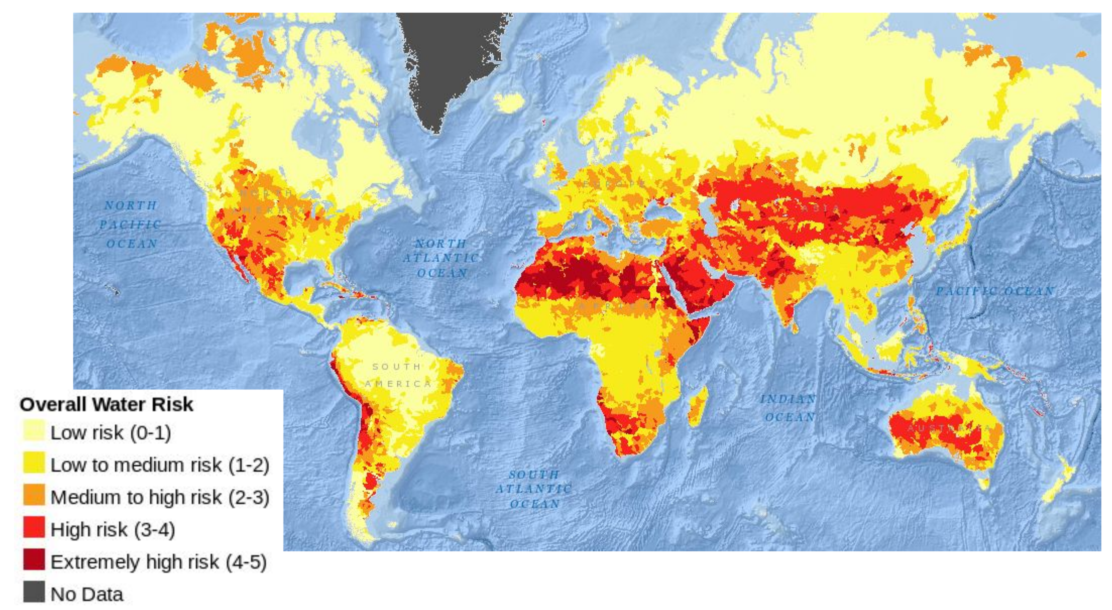
This project describes the computational work completed to answer the question, to what degree are the model factor approximations for a finite element adsorption model driving simulated results, and which constructions require the least amount of experimental work to adequately predict water harvesting capabilities of micro-porous adsorbents?

Introduction

Water scarcity is a serious concern and is expected to increase in severity in the coming years. One potential source of potable water is atmospheric humidity. Despite drought conditions humidity remains sufficiently high in suffering regions to prompt interest in its harvesting. Approximately 37.5 billion gallons of water remain largely untapped. We need tools to access atmospheric water at an energy cost that is economically feasible.

This poster describes work on a Zeolite 13X-water adsorption model made for use in collaboration with Dr. Sungwoo Yang's laboratory. The objective is to characterize novel materials for use in water vapor uptake/release by way of thermal conductivity shape optimization, porosity/permeabilities design, and next generation modeling kinetic assumptions.

The experimental research and model have direct application in atmospheric water harvesting, desalination, heat pump design, and battery development.



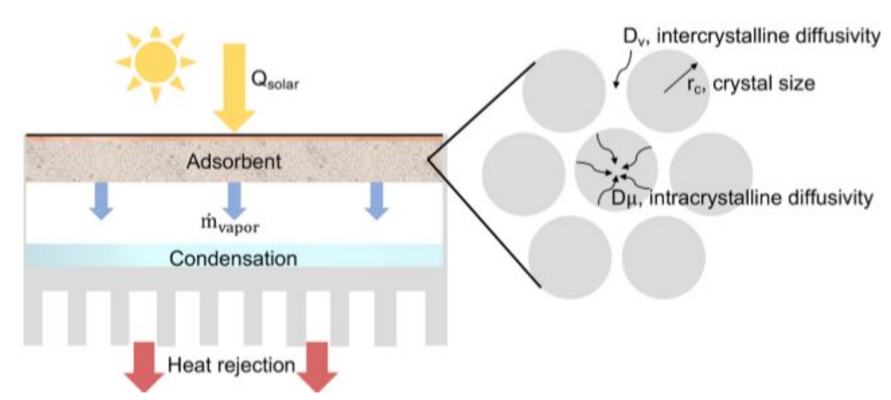
World Resource Institute: Water Risk, 2014

Major Decisions in Model Construction

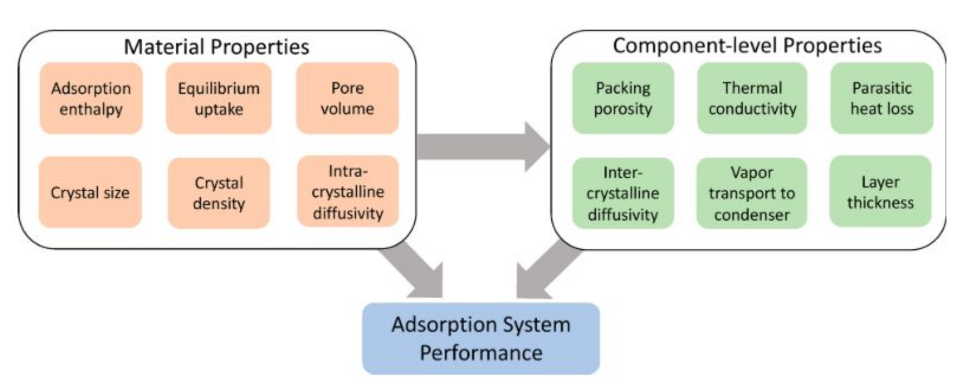
1) PDE in variational terms
Current build: Coupled Navier Stokes-Brinkman neglecting inertial forces and viscous forces, assuming local thermal equilibrium and ideal gas.

2) Numerical Implementation
Current build: Weak Forms are approximated by a mixed space finite element with nodal vectors Pressure, and Temperature. Q [kg Adsorbed / m^3 Adsorbent] is interpolated by shape function. A nonlinear solver approximates a solution field in a forward Euler calculation.

3) Properties Modeling
Current investigation: Adsorption modeling requires approximations for micro-porosities, macro porosities, adsorbed vapor density, vapor density(t), velocity gradient permeability, mass transfer resistance for adsorption, intra-particle gas diffusivity, vapor adsorption capacity, effective thermal conductivities, isosteric heat of adsorption, activation energies for adsorption and desorption, adsorbed vapor specific heat, vapor heat capacity, adsorption equilibrium density, adsorption isotherm, and adsorption saturation pressure.



Atmospheric Water Harvesting by way of Adsorption (figure source: LaPotin)



Properties for Laboratory and Computational Investigation (figure source: LaPotin)

Coupled Weak Formulation of Adsorption System

$$\frac{\varepsilon_t M_v}{R}\frac{1}{T}\frac{\partial P}{\partial t} - \frac{\varepsilon_t M_v}{R}\frac{P}{T^2}\frac{\partial T}{\partial t} + \frac{\partial Q}{\partial t} + \frac{M_v K_s}{R u_g}\frac{P}{T}\nabla P - \left(\frac{M_v K_s}{R u_g}\frac{P}{T}\nabla P\right)_\Gamma = 0$$

$$\frac{\partial Q}{\partial t} + GQ - GQ_{eq} = 0$$

$$\frac{\varepsilon_t C_{pv} M_v}{R}\frac{P}{T}\frac{\partial P}{\partial t} + C_{pv} Q\frac{\partial T}{\partial t} + (1-\varepsilon)p_s C_{ps}\frac{\partial T}{\partial t} - \varepsilon\frac{\partial P}{\partial t} + \frac{C_{pv} M_v K_s}{R u_g}\frac{P}{T}\nabla P \cdot$$
$$\nabla T + k_f \nabla T - |\Delta H|\frac{\partial Q}{\partial t} - \left(\frac{C_{pv} M_v K_s}{R u_v}\frac{P}{T}\nabla P \cdot \nabla T\right)_\Gamma - (k_f \nabla T)_\Gamma = 0$$

Micro-fluidic Property Models Under Study

Temperature dependent Adsorbed Density, ρ_{adv}

A critical parameter needed in Dubinin-Astakhov Isotherm (Q_{eq}).

1) Mugele equation
2) Hauer equation
3) Fitted from Ambrozek
4) Approximated from critical values

Isosteric Heat of Adsorption, ΔH

Describes the amount of heat released or required during adsorption/desorption.

1) Vant Hoff equation

Adsorption Equilibrium Isotherm, Q_{eq}

1) Dubinin-Astakhov Model (Fitted Values)
2) Dubinin-Astakhov Model (critical parameters)
3) Toth Isotherm
4) BET Isotherm

Permeability, K_s

1) Kozeny-Carman using Tortuosity
2) Kozeny-Carman using Kozeny constant
3) Kozeny-Carman using effective porosity

Mass Transfer Resistance to Adsorption, G

1) Fitted value from Ambrozek
2) Vasilev Adsorption Kinetics

Thermal Conductivities, k_f

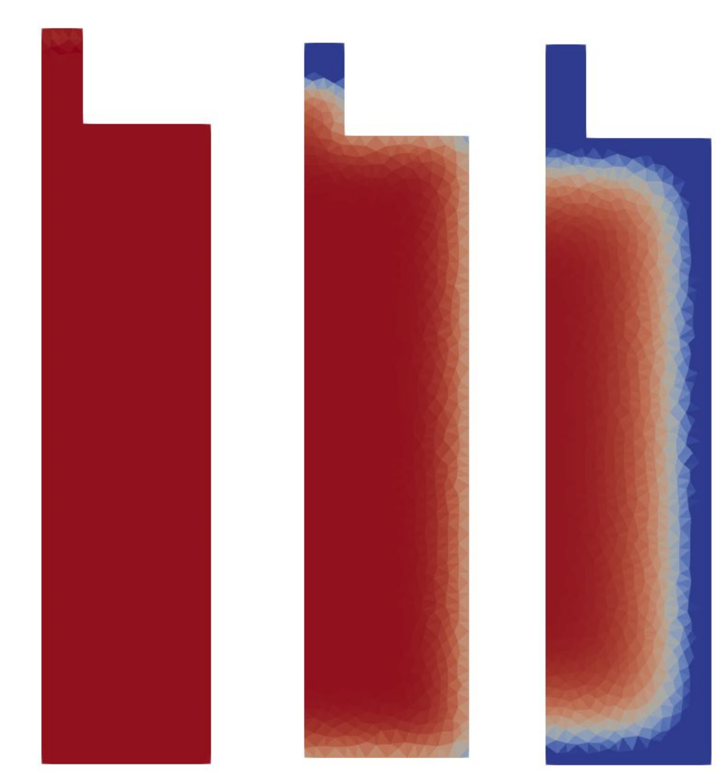
1) Maxwell Eucken equation

Results

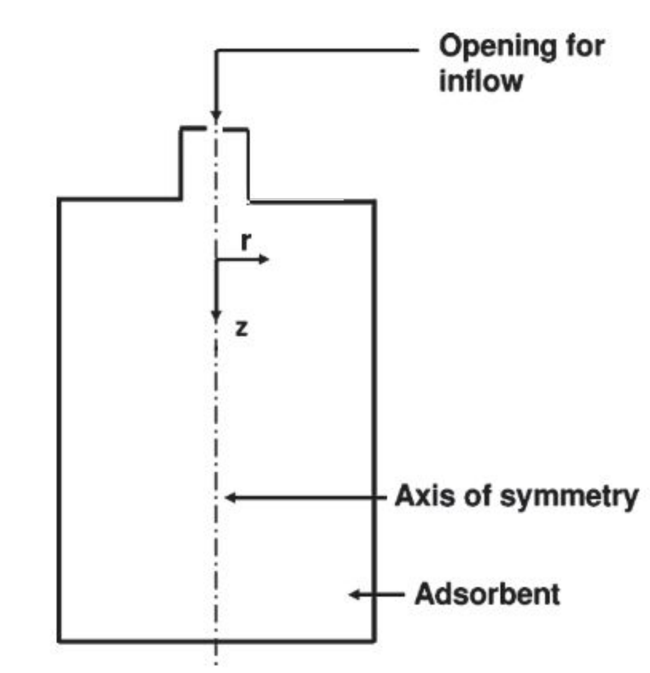
The mesh to the right shows our code generating a mesh and approximating adsorbate concentration at three timesteps.

Boundary conditions can be redefined according to experimental needs and iterative exploration of variable vessel designs can be automated.

The computational results can not answer our Research Question until computational investigations can be compared to experimental work.



Approximations for desorption at timstep = 0 seconds, 150 seconds, and 300 seconds.



Domain of computational interest is along r and z axis. An axisymmetric factor is included in output statistics to approximate real world atmospheric water collection.

Future Work

UTC undergraduate students and graduate students could participate in a wide variety of work on this project. The code is written symbolically allowing model reformulation and investigation of wide ranging parameters. Of particular interest are emerging Activation energy of surface diffusion, isosteric heat of adsorption, and adsorbed density models. The code has also been written to shape optimize for ideal condenser heat sink inclusion. Application of an shape fitting algorithm and proper characterization of the model should provide undergraduate research opportunities in the areas of atmospheric water harvesting, CO2 recapture and thermal heat pump optimization. Come join us!

References

1. Pradeepta Sahoo, Matthew John, Bharat Newalker, N.V. Choudhary, and K.G. Ayappa. "Filling Characteristics for an Activated Carbon Based Adsorbed Natural Gas Storage System."(2011)
2. Alina LaPotin, Hyunho Kim, Sameer R. Rao, Evelyn Wang, "Adsorption-Based Atmospheric Water Harvesting: Impact of Material and Component Properties on System-Level Performance." (2019)

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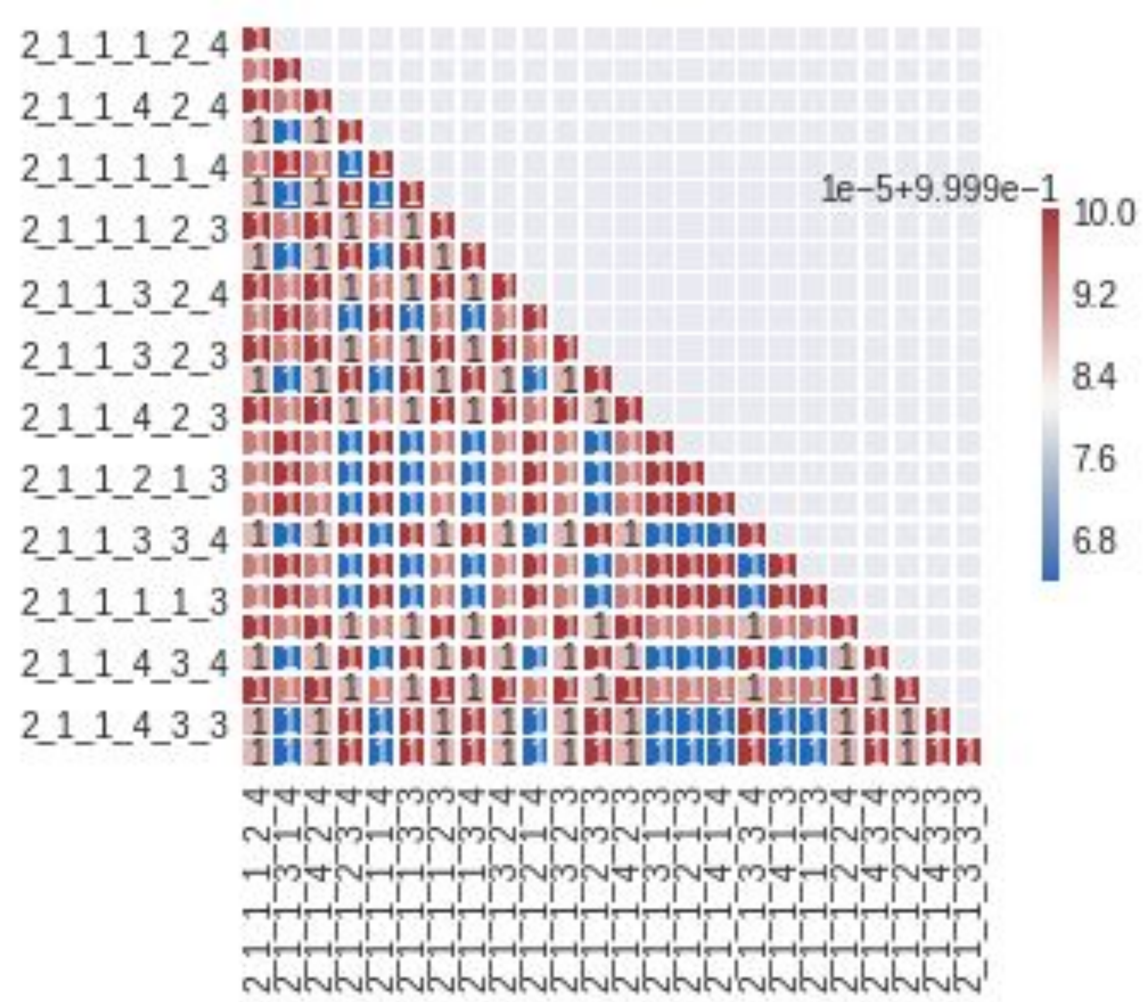
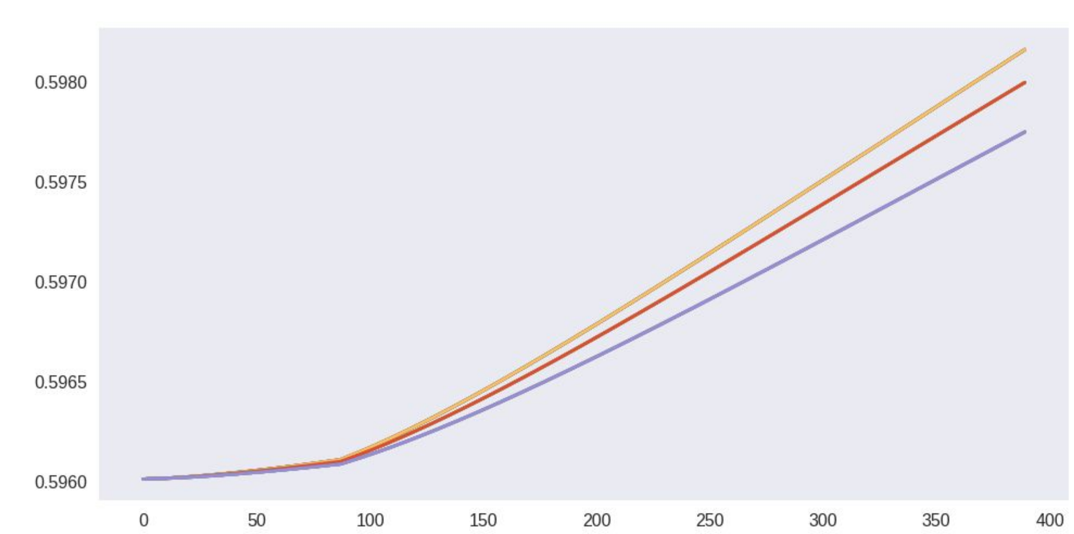
Toth Isotherm Studies

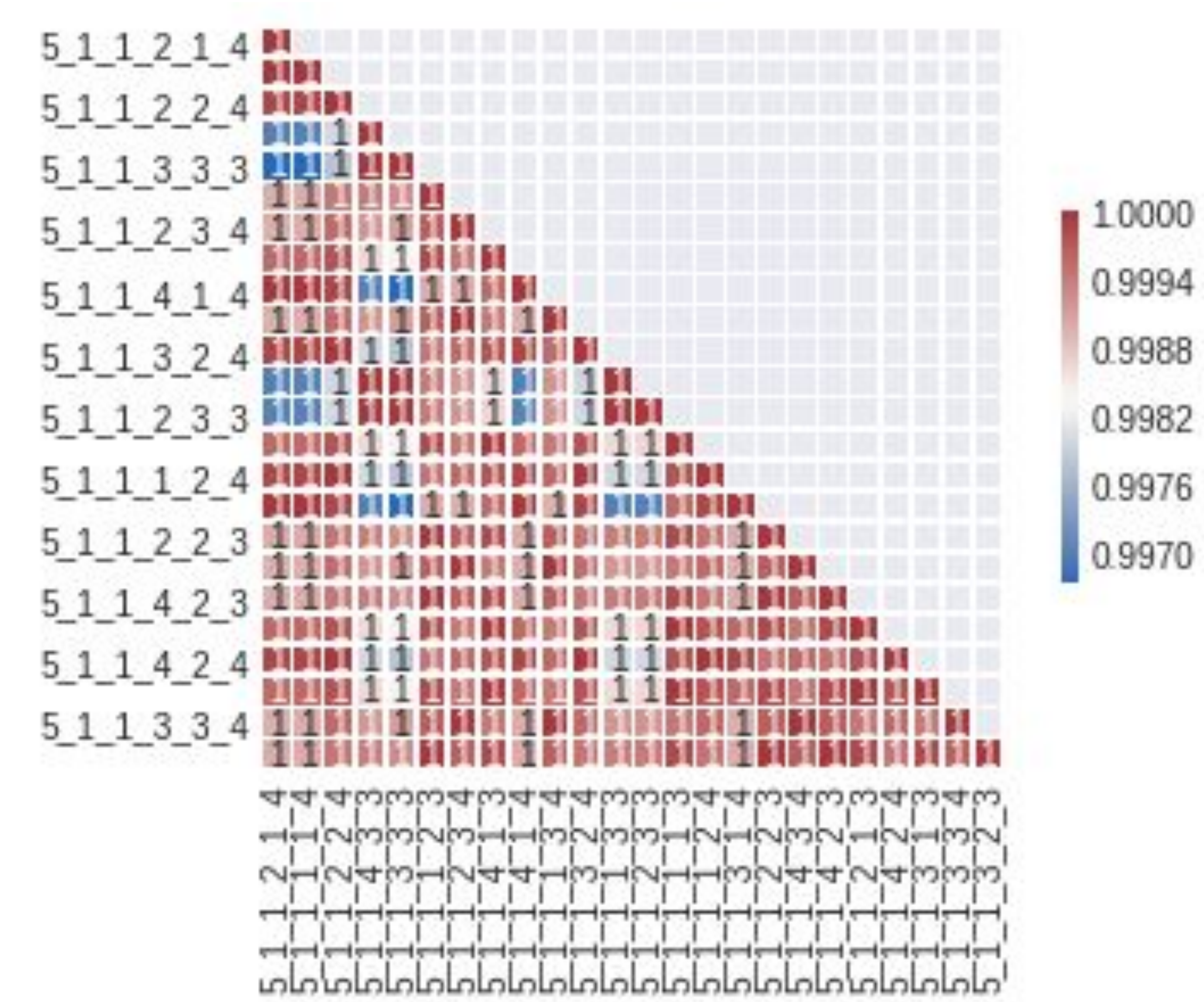


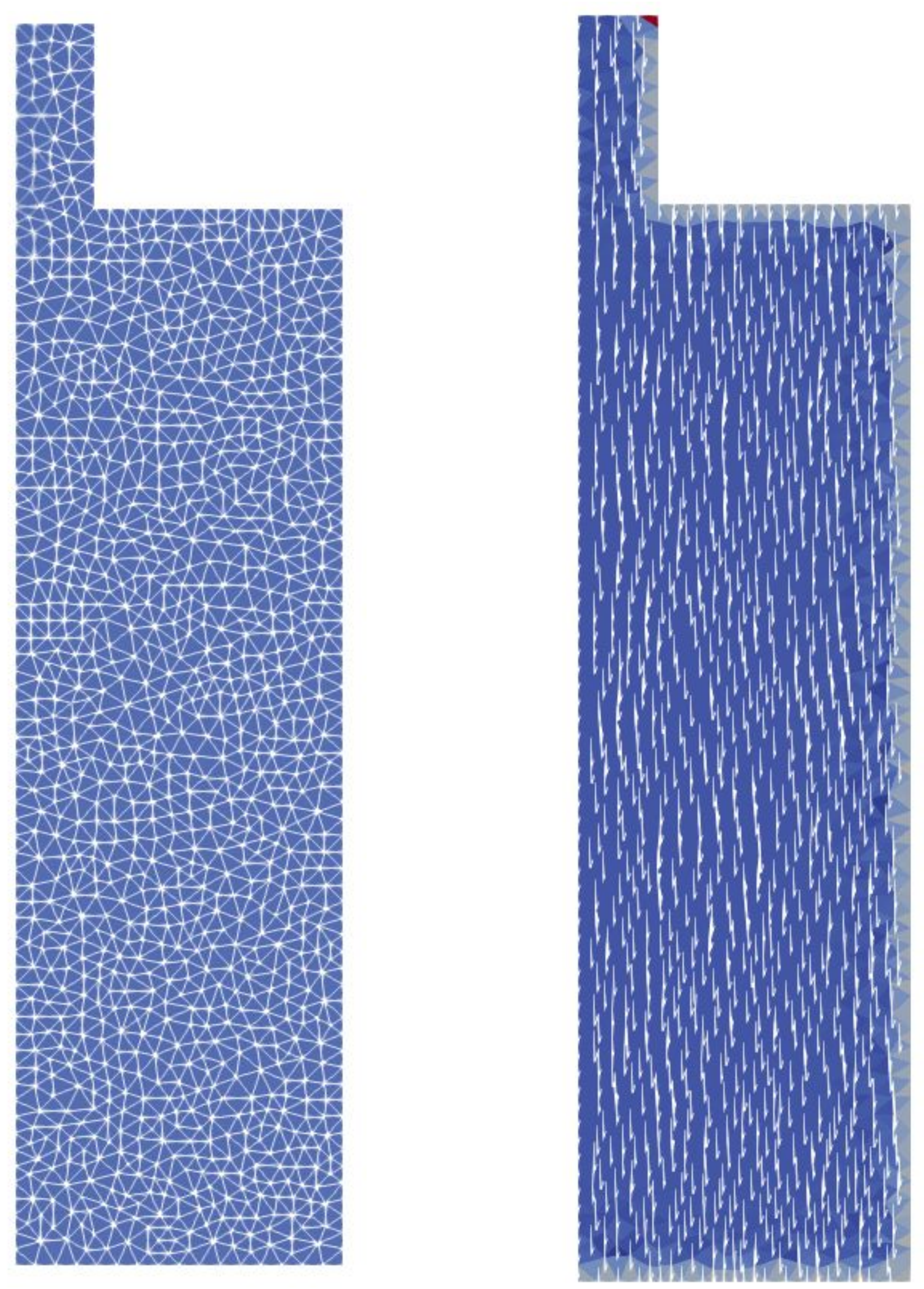


Code Index for Model Inputs [Qeq____DelH____Gvar____K____k____rhoadsT]

(Qeq) Adsorption Density Equilibrium: 1-Fitted 2-Toth-Narayanan 3- Toth-Ferreira 4-DA-Ferreira 5-DA Sahoo
(DelH) Heat of Adsorption: 1-Function of Uptake, 2-VantHoff
(Gvar) Mass Transfer Coefficients: 1-Vasilev , 2-Knudsen
(K) Permeability: 1-KozenyCarman Tortuosity, 2-KozenyCarman Tortuosity, Amigo, 3-K-C Effective Porosity Porosity,4-KozenyCarmanKozenyConstant
(k) Thermal Conductivities: 1-Sahoo, 2-MaxwellEucken, 3-ZehnderSchlunder
(rhoadsT) LocalAdsorbedGasDensity: 1-Mugele, 2-Hauer, 3-Osawa/Sahoo, 4 Ambrozek

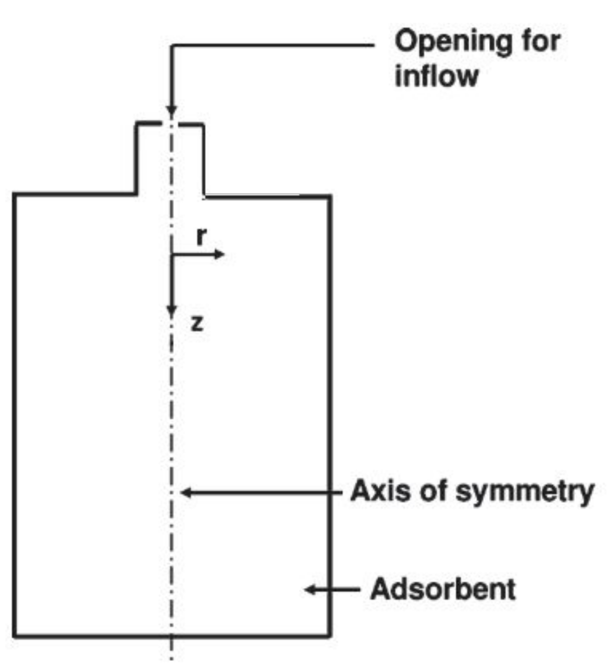
Dubinin-Astakhov Studies





300 s simulation using preferred inputs with pressure gradients represented as hooked arrows. .03 kg of water vapor estimated to be collected in a 1.82 Liter device.

Adsorbate Dimensional Optimization Study



These three computational designs differ only in dimensions. All other aspects of the code were held constant including the volume. The simulation progressed 300 seconds. The density of vapor is lower in the blue regions. The walls of the vessel are conducting heat away from the adsorbent allowing greater vapor uptake. These kinds of studies facilitate component level design.