Modeling and Simulation of Single Phase Fluid Flow and Heat Transfer in Packed Beds

by:-
Balaaji Mahadevan || Shaurya Sachdev|| Subhanshu Pareek ||Amol Deshpande
Birla Institute of Technology and Science, Pilani – K.K. Birla Goa Campus

COMSOL CONFERENCE INDIA 2012

BITS Pilani
K K Birla Goa Campus

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Outline

1. Introduction to Packed Beds
2. Background
3. Scope and Objective
4. Governing equations
5. Modeling – COMSOL Multiphysics
6. Analysis of results

Packed Beds

In chemical processing a Packed Bed is a hollow tube, pipe or other vessel that is filled with a packing material. The purpose of a packed bed is typically to improve contact between two phases in a chemical or similar process.

Application In Industries

1. Chemical Reactor
2. Distillation
3. Gas Absorption and Stripping
4. Separation and Ion-Exchangers

Background

- Dalman et al, 1986.2-D, Axisymmetric radial plane
- Lloyd and Bohem, 1994, 2-D in commercial FE packaged FIDAP, 8 spheres in a line instead of 2
- Derkx and Dixon, 1996, 3-D 3 sphere model
- Logtneberg and Dixon,1998, 3-D 8 sphere model
- Logtenberg et al, 1999, 3-D 10 sphere model
- Michiel Nijemeisland and Anthony G. Dixon, 2004 for N=2 and N=4 in Fluent

Scope and Objectives

- With modern CFD codes and growth of technology it is now possible to obtain detailed flow fields and temperature profiles in packed beds.
- From fluid mechanical perspective, the most important issue is that of the pressure drop.
- Our study not only includes pressure drop but also encompasses velocity fields of fluids and heat transfer in packed beds.
- Pressure drop, velocity fields and temperature profiles obtained by simulating above models on COMSOL Multiphysics help us understand the packed bed and also estimate various fluid flow and heat transfer parameters.
- Models have been developed for N=4 and N=8 which are more closer to reality but there is scope of developing higher N models which are more in agreement with actual packed beds

Governing Equations

- Ergun Equation
- Continuity Equation
- Navier Stokes Equation
- Heat transfer equation- conductive and convective
- Turbulence Equation (k-ϵ model)

Ergun Equation

Explains pressure drop across packed beds.

$$\frac{\Delta p}{L} = \frac{150\overline{V}_0\mu}{\Phi_s^2 D_p^2}\frac{(1-\varepsilon)^2}{\varepsilon^3} + \frac{1.75\rho\overline{V}_0^2}{\Phi_s D_p}\frac{(1-\varepsilon)}{\varepsilon^3}$$

$$\frac{\Delta p}{L} = \frac{150\overline{V}_0\mu}{\Phi_s^2 D_p^2}\frac{(1-\varepsilon)^2}{\varepsilon^3}$$

Kozeny-Carman

Re<1

$$\frac{\Delta p}{L} = \frac{1.75\rho\overline{V}_0^2}{\Phi_s D_p}\frac{(1-\varepsilon)}{\varepsilon^3}$$

Burke Plummer

Re>1000

Continuity Equation

Conservation of Mass equation(general case):

$$\nabla . \rho \vec{V} + \frac{\partial \rho}{\partial t} = 0$$

1. Incompressible fluids and Steady flow

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = \nabla . \vec{V} = 0$$

2. Steady Flow processes

$$\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = \nabla . \rho \vec{V} = 0$$

Navier Stokes Equation

The equations of motion. (Momentum Equation)

(Newtonian, Incompressible flow and constant viscosity)

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}+w\frac{\partial u}{\partial z}\right)=\rho g_x-\frac{\partial p}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)$$

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}+w\frac{\partial v}{\partial z}\right)=\rho g_y-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}+\frac{\partial^2 v}{\partial z^2}\right)$$

$$\rho\left(\frac{\partial w}{\partial t}+u\frac{\partial w}{\partial x}+v\frac{\partial w}{\partial y}+w\frac{\partial w}{\partial z}\right)=\rho g_z-\frac{\partial p}{\partial z}+\mu\left(\frac{\partial^2 w}{\partial x^2}+\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial z^2}\right)$$

K-Ɛ Turbulence Model

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + (\mu+\mu_T)\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) - \frac{2}{3}\rho k\mathbf{I}\right] + \mathbf{F}$$

$$\rho\nabla\cdot\mathbf{u} = 0$$

$$\rho(\mathbf{u}\cdot\nabla)k = \nabla\cdot\left[\left(\mu + \frac{\mu_T}{\sigma_k}\right)\nabla k\right] + P_k - \rho\epsilon$$

$$\rho(\mathbf{u}\cdot\nabla)\epsilon = \nabla\cdot\left[\left(\mu + \frac{\mu_T}{\sigma_\epsilon}\right)\nabla\epsilon\right] + C_{\epsilon 1}\frac{\epsilon}{k}P_k - C_{\epsilon 2}\rho\frac{\epsilon^2}{k}, \quad \epsilon = \mathrm{ep}$$

$$\mu_T = \rho C_\mu\frac{k^2}{\epsilon}, \quad P_k = \mu_T\left[\nabla\mathbf{u} : \left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\right]$$

C_μ , σ_ϵ , $C_{2\epsilon}$, $C_{1\epsilon}$, σ_k are all taken as constants.

Heat Transfer Equation

$$\nabla \cdot (-k\nabla T) = Q - \rho C_p \mathbf{u} \cdot \nabla T$$

Conductive heat Transfer term

External heat term

Convective heat Transfer term

Basic Methodology(CFD)

Problem Identification

1. Define goals
2. Identify domain

Pre-Processing

3. Geometry 4. Mesh
5. Physics 6. Solver Settings

Solve

7. Compute solution

Post Processing

8. Examine Results

Update Model

Packed Bed Modeling in COMSOL Multiphysics

Model Specifications

For both N=4 and N=8

- Space Dimension – 3D
- Physics – Turbulent Flow with Standard k-ε Model
- Study Type – Stationary
- Sub-domain – Air at 293.15K and 1atm

Geometry

N=4

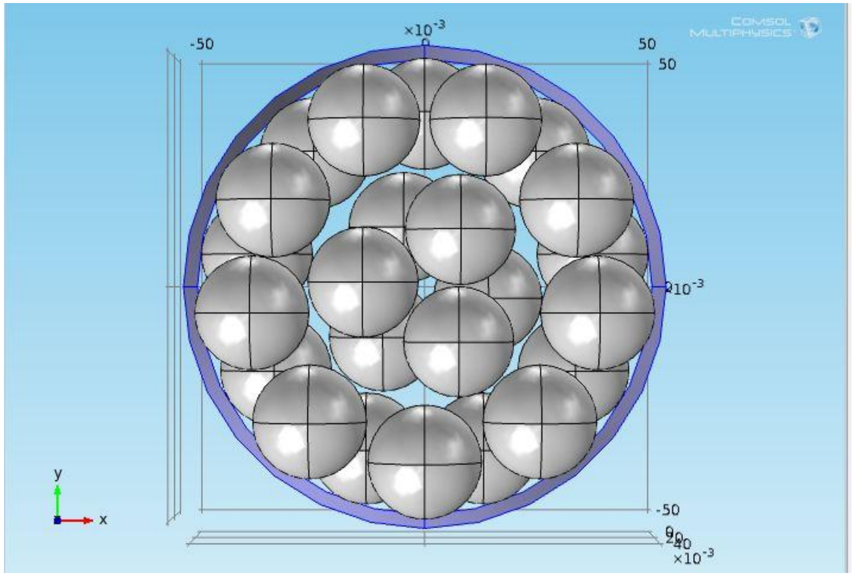
- Packing = Spherical
- Bed Length = 4.75 cm
- Bed Diameter = 10.16 cm
- Packing Diameter = 2.5 cm
- Spheres per layer = 12

N=8

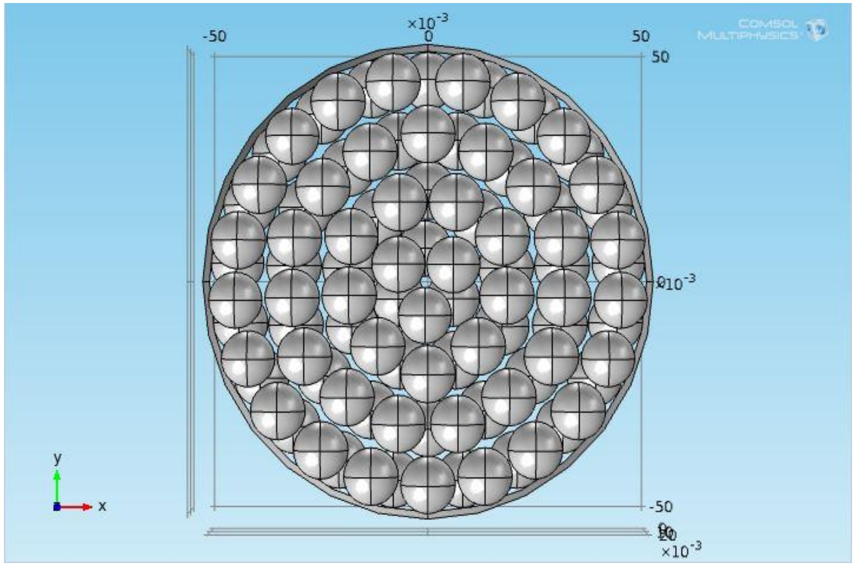
- Packing = Spherical
- Bed Length = 2.5 cm
- Bed Diameter = 10.16 cm
- Packing Diameter = 1.27 cm
- Spheres per layer = 47

Geometry

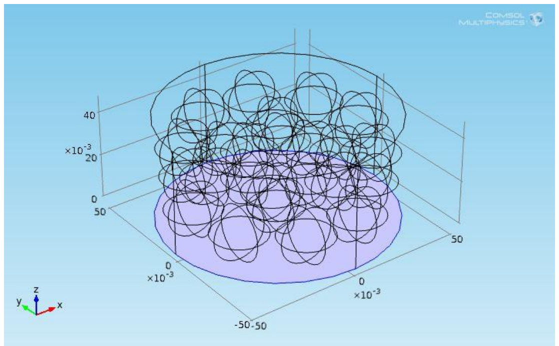
N=4



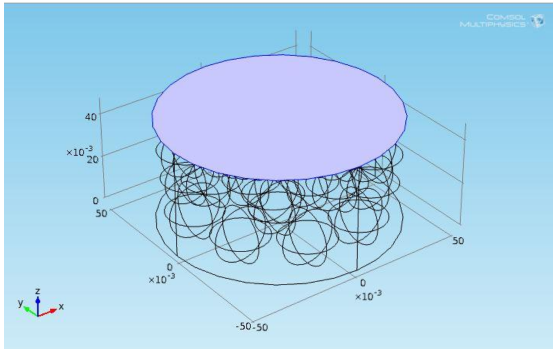
N=8



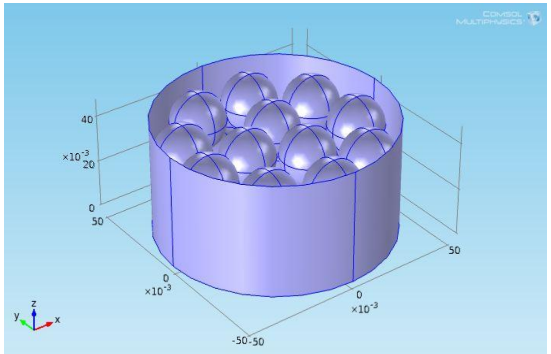
Boundary Conditions (N=4)



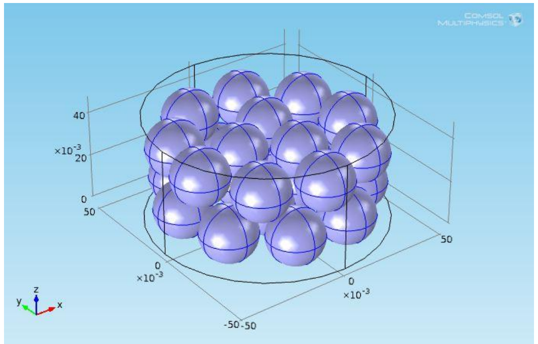
Inlet
Velocity = 1.0624m/s
Temperature = 300k



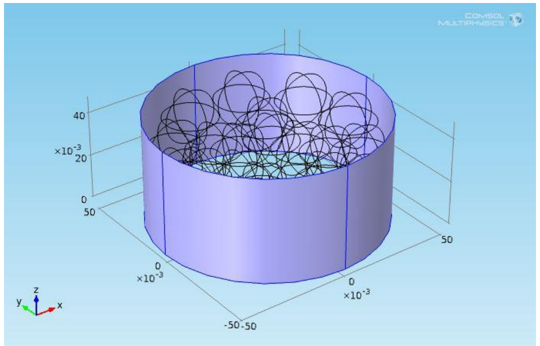
Outlet
Pressure = 0 atm (gauge)
Thermal Insulation



Wall
Wall Function

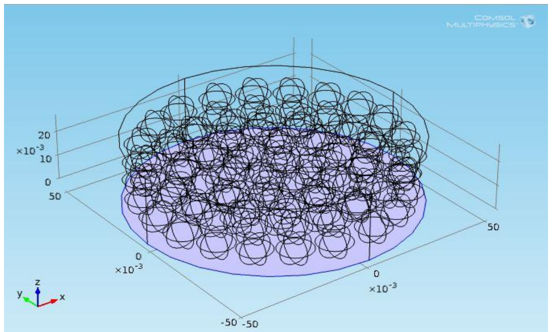


Wall
Temperature = 300K

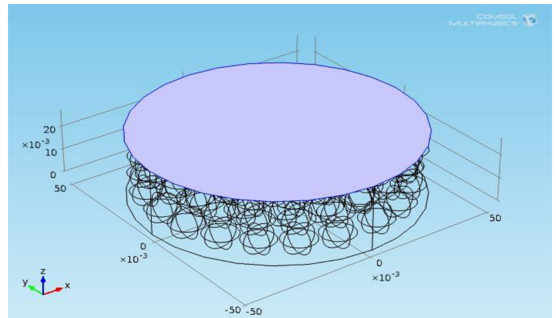


Wall
Temperature = 400K

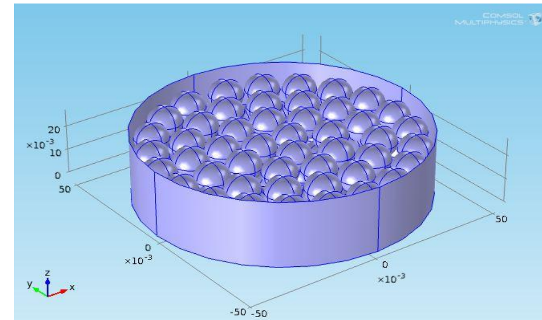
Boundary Conditions (N=8)



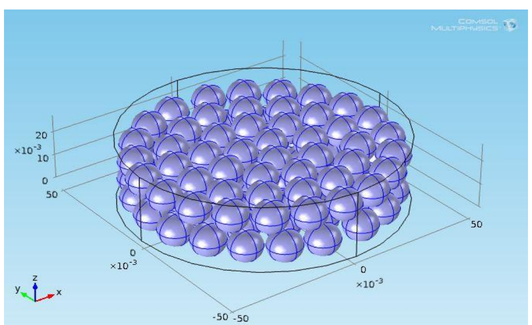
Inlet
Velocity = 1.0624m/s
Temperature = 300k



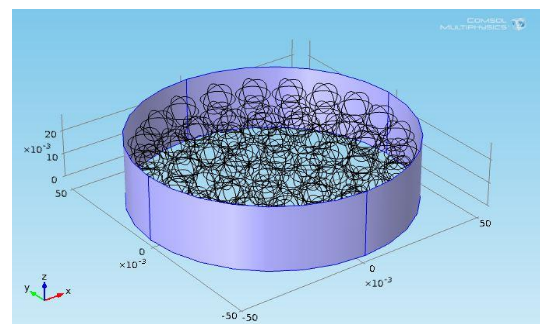
Outlet
Pressure = 0 atm (gauge)
Thermal Insulation



Wall
Wall Function



Wall
Temperature = 300K

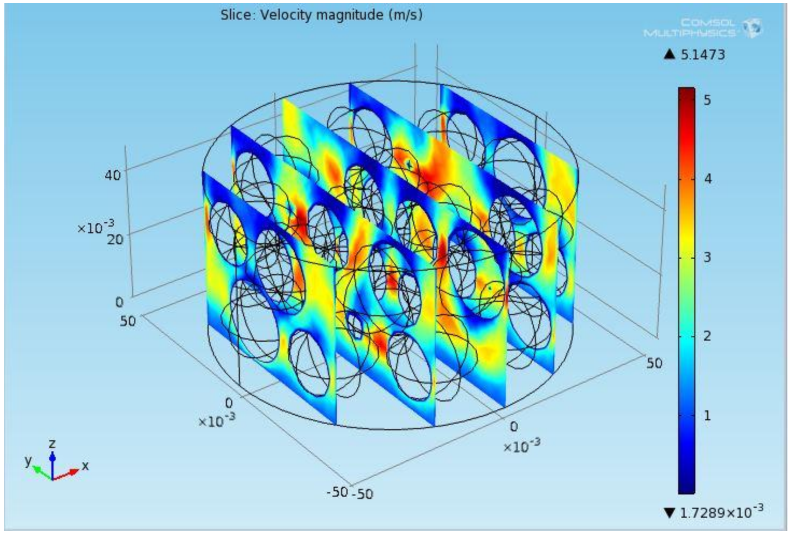


Wall
Temperature = 400K

Results and Discussion

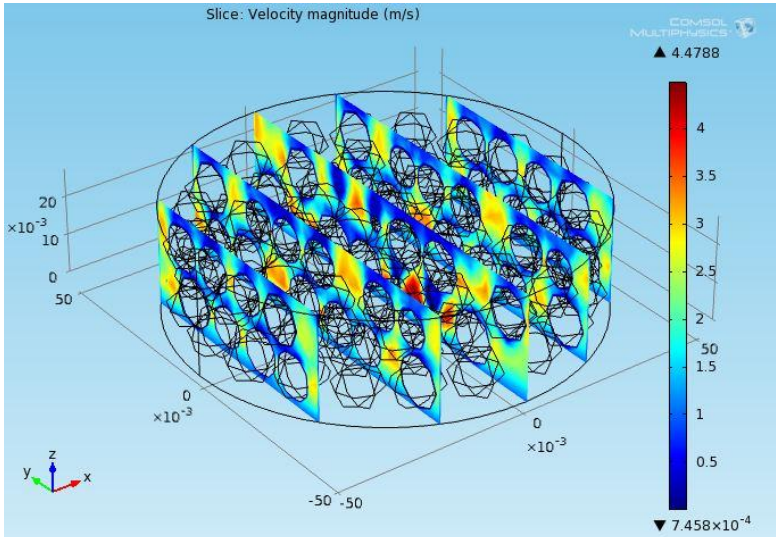
Velocity Field

N=4



Max Velocity = 5.1473 m/s

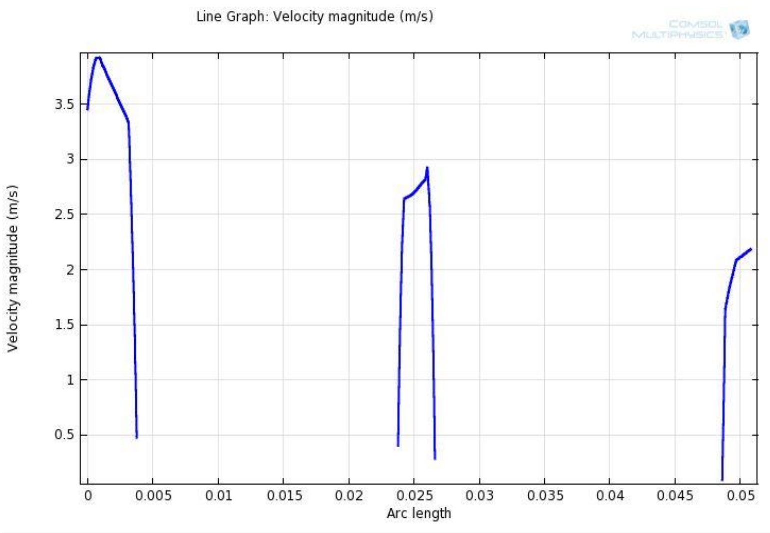
N=8



Max Velocity = 4.4788 m/s

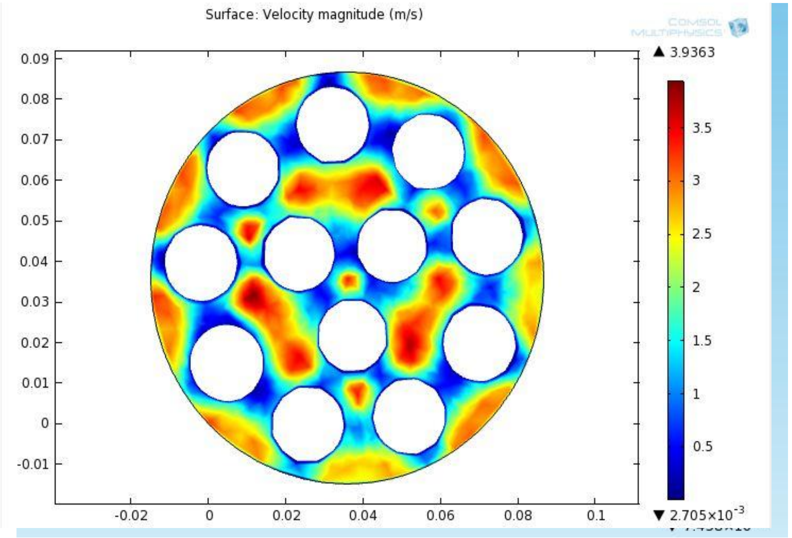
Velocity Field (N=4) - Detailed

Line Plot



Coordinates
(-5.08, 0, 3.4):(0, 0, 3.4)

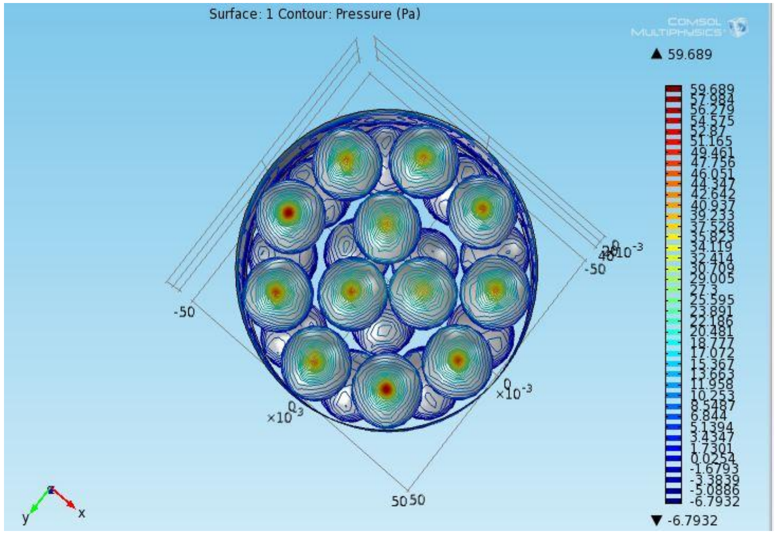
Area Plot



Coordinates
(-5.08, 0, 2.3):(0, -5.08, 2.3): (5.08, 0, 2.3)
Max Velocity = 3.9363 m/s

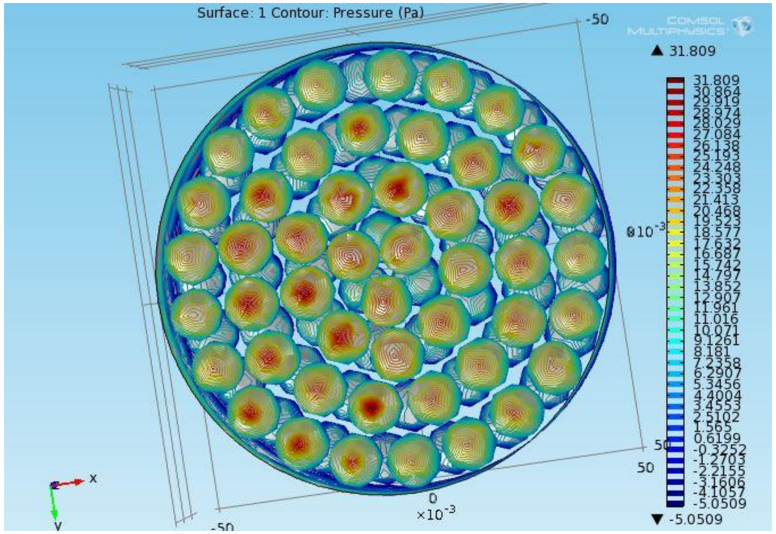
Pressure Field

N=4



Max Pressure = 59.589 Pa

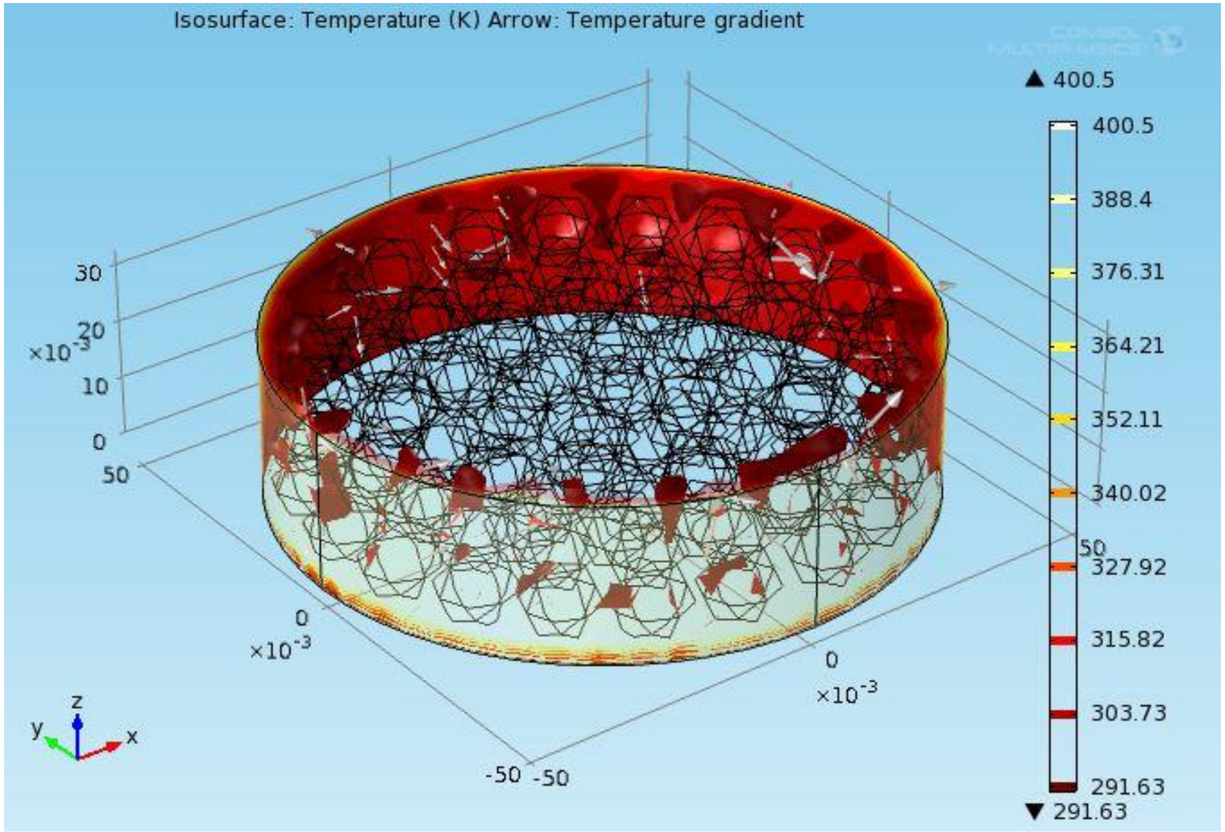
N=8



Max Pressure = 31.809 Pa

Temperature Profile

N=8



Max Temperature =400.5 K

Conclusion

- Flow of air through packed beds with spherical packing for N=4 and N=8 geometries (3D models) were analyzed
- Plots for velocity field, pressure contours, and temperature profiles were obtained and were validated with literature data
- The nature of results for N=4 and N=8 models were similar but the values obtained for N=8 model are more practical because its packing arrangement is closer to reality
- Developing models for even higher N values which are closer to reality is possible but their modelling is difficult because of complicated geometry and presence of wall effects across the entire radius of the bed

Thank You