Simulation of Flow and Heat Transfer Through Packed Beds of Spheres

A Major Qualifying Project Report

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By

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Abstract

Fluid flow and heat transfer in fixed beds with tube to particle diameter ratios of N=3 and N=5.96 were simulated using COMSOL, a multiphysics program. The geometries of these models consisted of 55 and 400 spheres respectively. This type of study is traditionally done using a Computational Fluid Dynamics (CFD) software package, however, in this study it was desired to see how well a multiphysics package could compare. Results obtained from COMSOL were compared to data from published studies which performed similar simulations using a CFD package, and the data agreed relatively well. So COMSOL is a useful tool for simulating these types of models.

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Introduction

In this study, flow patterns and heat transfer within packed beds was examined. A packed bed is made up of a tube, which creates the outer shell of the bed, and packing material which can either be arranged or randomly dumped and packed within the tube. Packed beds are used quite extensively in the chemical production industry. They can be used in separation processes such as absorption, stripping, and distillation (Seader and Henly, 2006). A diagram of a packed tower used for absorption can be seen in Figure 1. Other applications of packed beds include reactors, in which the packing material acts as a catalyst on which reaction occurs (Fogler, 2006).

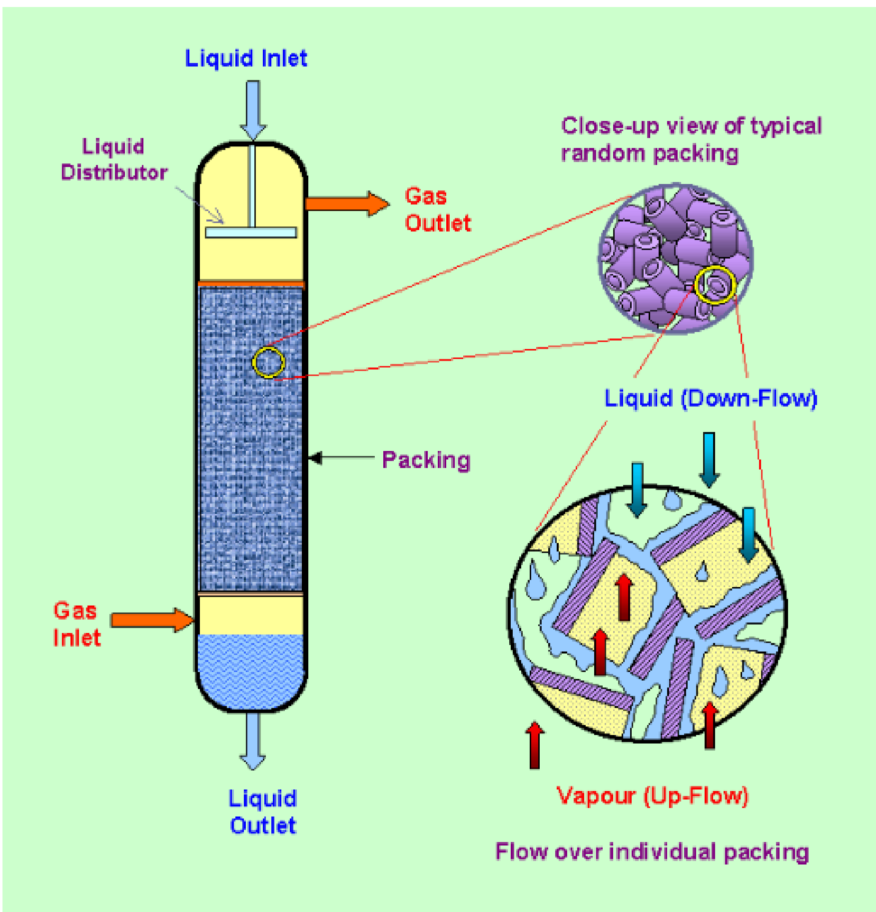

Figure 1 - Diagram of a Packed Bed (http://www.separationprocesses.com/Absorption/GA_Chp04.htm)

Since packed beds, in particular packed bed reactors are so common in the chemical processing industry it would be useful to have a good understanding of the flow patterns and heat transfer occurring within them. It is important to understand these phenomena so that a safe and optimal design of these reactors can occur. Some of the reactions that take place are highly endothermic or exothermic, so before lab scale experiments are made it is useful to try and simulate the processes with a computer program. According to Logtenberg and Dixon (1997) the area of particular importance is the low tube to particle diameter (N) range, due to the large number of reactors that use narrow tubes.   So in this study, two geometries were simulated; one with N=3, comprised of 55 spheres and one with N=5.96, comprised of 400 spheres. A diagram of these geometries can be seen in Figure 2.

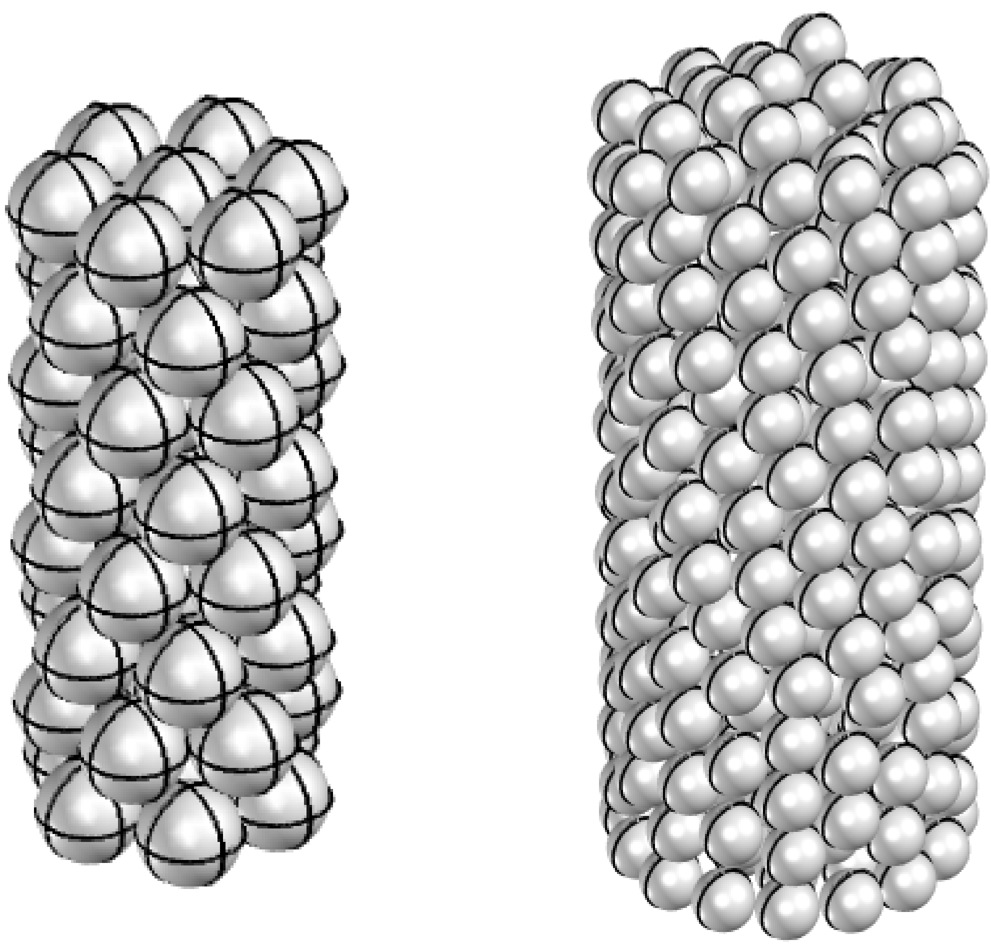

Figure 2 - Packed Bed Geometries: N=3 is on the left and N=5.96 is on the right

The purpose of this study was to simulate flow and heat transfer in packed beds with low N using COMSOL, a commercially available multiphysics computer program. Typically this type of study would be performed using a Computational Fluid Dynamics (CFD) software package such as Fluent, but it was desired to determine the feasibility of doing similar simulations on a multiphysics software package. COMSOL is designed to be able to handle many types of problems, from electricity and magnetism to structural mechanics and many other problems from different engineering disciplines, while CFD packages focus more specifically on fluid flow. CFD packages excel at modeling turbulence; have better 3D geometry set up, and better post processing features, however these types of programs struggle with conjugate heat problems and modeling of solid diffusion. It was unclear what the limitations would be for a program like COMSOL in simulating a packed bed, which is really a quite complex model. The three main areas of focus for the simulations were fluid flow, heat transfer, and diffusion, and the purpose of this study was to determine if COMSOL could simulate these phenomena in a packed bed in a way that is comparable, or even better, to that of a CFD program.

Background

Modeling Fluid Flow

The basis for almost all CFD and multiphysics fluid flow modeling are the Navier-Stokes equations. The Navier-Stokes equations are the basic equations for a viscous, heat conducting fluid. The term Navier-Stokes equations is used to describe three equations; the momentum equation, the continuity equation, and the energy equation. In particular cases the Navier-Stokes equations can be simplified dramatically. In all cases simulated in this study, simplification was applicable. When density is relatively constant and there is an incompressible, Newtonian fluid flow, the Navier-Stokes equations can be simplified into a continuity equation and a momentum equation. Equation 1 is the continuity equation and equation 2 is the momentum equation.

$$\nabla \cdot v = 0 \qquad (1)$$

$$\rho\left(\frac{\partial v}{\partial t} + v \cdot \nabla v\right) = -\nabla \rho + \mu \nabla^2 v \qquad (2)$$

Modeling Turbulence

Since it was desired to run several models at a high flow rate, with a Reynolds Number in the turbulent flow regime, it was necessary to use a special model that would be able to fully describe this flow pattern. COMSOL has several models that it can use to solve for turbulent flows; the approach used in this study was a Reynolds-averaged Navier-Stokes (RANS) equation. Typically when using a RANS equation it is necessary to refine the mesh and make it much finer at the boundary layers in order to allow the model to predict the transition from laminar to turbulent flow. However, one of the benefits of using a physics controlled mesh in COMSOL is that it will automatically refine the mesh near the boundary for flow models using a RANS equation. So no further mesh refinement is necessary on the user's part.

The particular RANS model used in this study was the k-ε model. This is one of the most common turbulence models. There are actually two formations of the k-ε model, the one used in this study is referred to as the "Standard" k-ε model and was developed by Launder and Sharma (1974). It is a two equation model, meaning that it takes into account two extra transport equations in order to account for the turbulent properties of the flow. Equation 3 takes into account the turbulent kinetic energy, k, and determines the energy of the turbulence. Equation 4 is called the turbulent dissipation, ε, and it is the variable that determines the scale of the turbulence.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k + P_b - \rho\varepsilon - Y_M + S_k \quad (3)$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}(P_k + C_{3\varepsilon}P_b) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon \quad (4)$$

This model for turbulence is not accurate for all situations; however, according to Bardina, Huang, and Coakley (1997) this model gives good agreement with experimental results for wall bounded flows with small mean pressure gradients. All of the flows in this study are wall bounded and have relatively low pressure gradients so this model was chosen to simulate all turbulent flows.

Pressure Drop

One of the most important parameters to have information about when designing a packed bed reactor is the pressure drop. This is important because the pressure drop determines the amount of energy the pumps or compressors need to supply to the system, and this directly correlates to how much the equipment will cost to run. The pressure drop of packed beds has long since been studied and general agreement has been reached on the influence of Reynolds Number in infinite beds (Eisfeld & Schnitzlein, 2001). However, in cases of low tube to particle diameter ratios, wall effects have a definite effect on the pressure drop, and there are several different equations and correlations which try to account for this effect.

There have been studies that suggest having a wall bounded packed bed would cause additional resistance due to wall friction (Carman, 1937). While others say that the wall forces particles to form in such a way that a void forms approximately half a particle diameter away from the walls (Benati & Brosilow, 1962). In order to determine what influence confining walls actually had on pressure drop Eisfeld & Schnitzlein (2001) performed a study on over 2000 different data points from the published literature and suggest that the best possible correlation available is that of Reichelt (1972). Equation 5 is the equation for dimensionless pressure drop, and equations 6 and 7 are the correction factors for the confining walls. Equation 6 accounts for the contribution of the confining walls to the hydraulic radius. Equation 7 described the porosity effect of the walls at high Reynolds Number.

$$\psi = \frac{K_1 A_W^2}{Re_{dp}} \frac{(1-\overline{\varepsilon})^2}{\overline{\varepsilon}^3} + \frac{A_w}{B_w} \frac{(1-\overline{\varepsilon})}{\overline{\varepsilon}^3} \qquad (5)$$

$$A_w = 1 + \frac{2}{3(\frac{D}{d_p})(1-\overline{\varepsilon})} \qquad (6)$$

$$B_w = [k_1 \left(\frac{d_p}{D}\right)^2 + k_2]^2 \quad (7)$$

Methodology

Geometric Modeling

When performing computational fluid dynamics a good geometric model is the first step to assure a successful simulation. In this study, two different geometric models were used for simulation. Both of the models are packed bed of spheres contained within a cylinder. The first bed was made up of 55 spheres with a tube to particle diameter ratio of N=3. This geometry was imported manually into COMSOL. The other bed was made up of 400 spheres with an N=5.96. This geometry was much too complex to be imported manually and thus was generated using Gambit, and then imported to COMSOL via the CAD import module.

Manual Geometry Input

The packed bed consisting of 55 spheres with an N=3 had its geometry inputted manually into COMSOL. The bed consists of several relatively simple geometric shapes that are arranged into a complex formation. After selecting what type of physics being used in the simulation, the geometry can be constructed. In the model builder on the left hand side of the COMSOL user interface, under the model heading, there is a geometry selection. Since the packed bed is made up of mainly spheres and a cylinder, the input of the geometry is relatively simple. The spheres were generated by right clicking on geometry and selecting the sphere option. When this was done a settings window popped up asking for information on the sphere. First, the sphere has to be designated as a solid object or just a surface, in this simulation spheres were generated as solid objects. Next, the radius had to be set. In this simulation the radius was set at 0.495 in. The reason for setting this radius at 0.495 inches and not 0.5 inches was because if the particles are contacting each other than the program has trouble running the simulation, so the radius was reduced to 99% of actual size to provide a small space at the boundary layers. The last remaining parameter that needed to be set was the coordinate of the spheres center. This procedure was repeated 55 times until all of the spheres in the bed had been generated.

Next, the cylinder containing all of the spheres was generated. This was done in a similar fashion to the spheres. The first step was to right click on geometry and then select cylinder. The cylinder was designated to be a surface, not a solid. Then all of the other necessary information was inputted; the radius, height, and center of the cylinder. The next step was then to cap off both ends of the cylinders. This was achieved by creating a work plane at both the top and bottom of the cylinder. This was achieved by right clicking on geometry and selecting work plane. Then it was specified that it was a xy-plane, and the z-coordinate for the top of the cylinder was inputted. This closed off the top portion of the cylinder. The same procedure was then repeated for the bottom portion of the cylinder, with the only difference being the specified z-coordinate. Since the cylinder was made up of three different surfaces, COMSOL did not recognize them as being part of one solid entity, so it was then necessary to form a union between these three surfaces. This was done by right clicking geometry and then selecting union under Boolean Operations. After all of the necessary data was inputted, the Build All option was selected and the entire geometry was constructed.

Importing with the CAD Import Module

The packed bed with 400 spheres with N=5.96 was much too complicated to be input manually so it was necessary to import the geometry from a separate program. Geometry can only be imported into COMSOL if the CAD Import Module is enabled. It is relatively easy to import a geometry using this module, so the more complex geometry of this bed was created using GAMBIT, which can create the geometry much faster and easier. Then this geometry was imported over to COMSOL. The geometry is imported into COMSOL by right clicking on geometry and selecting import. Then under the import settings window there is an option to browse for an import file. After selecting the file it was necessary to ensure that the relative tolerance of the import file matched that of the tolerance defined in COMSOL. After that the Build All option was selected and the geometry was generated in the COMSOL Graphics window.

Meshing and Model Verification

In order to verify that the type of mesh that was used in these simulations was adequate, a mesh verification was performed. This verification consisted of running the same simulation with several different kinds of meshes to determine what, if any, effect it would have on the results. All of the meshes were created using COMSOL's physics based meshing option. In this fashion, three meshes were created; these meshes are designated by COMSOL to be Normal, Coarse, and Coarser. Figure 3 depicts all three of these meshes.

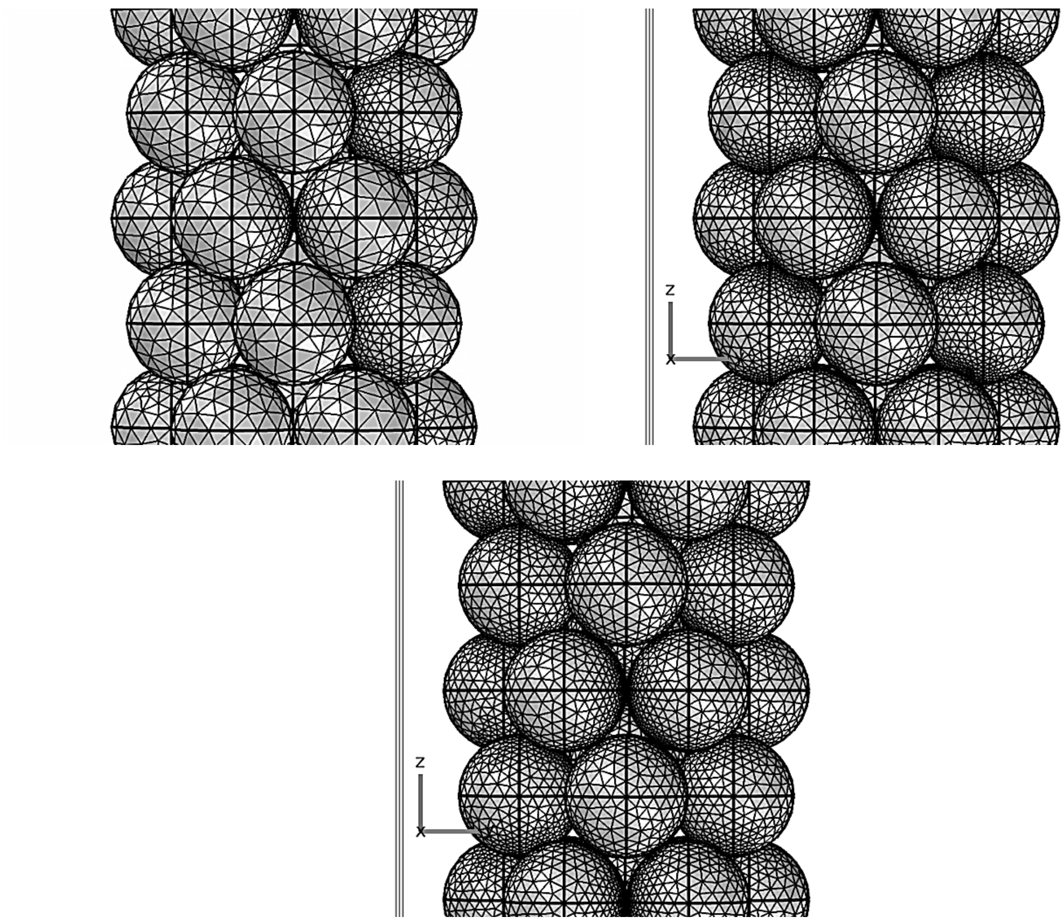

Figure 3 - Meshed Geometries: Coarser is on Top Left, Coarse on Top Right, Normal on Bottom

These meshes were used for the simulation of a laminar flow run with a Reynold's Number of ten. The results obtained for these simulations were compiled into plots of velocity profiles, which were constructed in excel with data points obtained from COMSOL. Then the plots for each mesh were compared as seen in Figure 4. It can be seen that the results obtained for both the coarse and normal mesh agreed with each other quite well, while data from the coarser mesh was more inconsistent. This led to the conclusion that both a coarse or normal mesh would be adequate enough for all future simulations, and a coarser mesh should no longer be used.

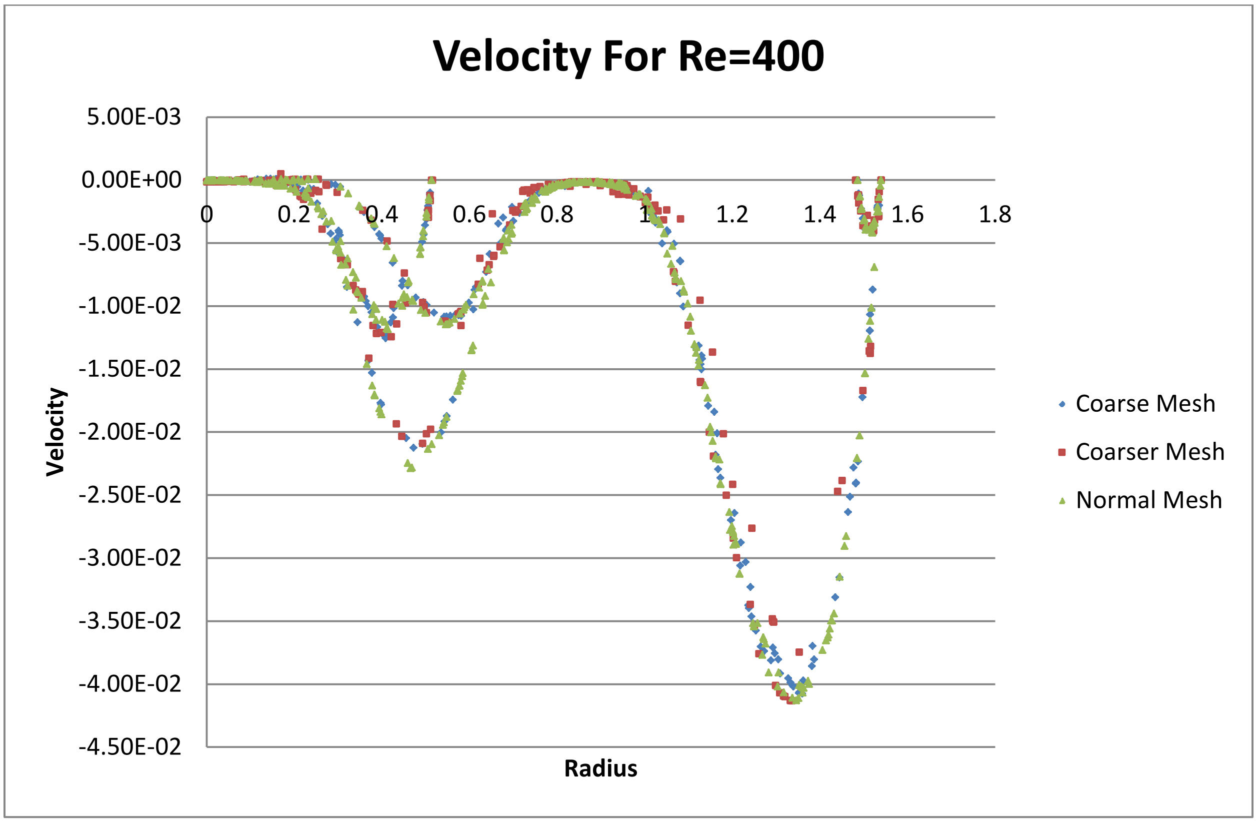

Figure 4 - Laminar Flow at Re=400 for Different Meshes

COMSOL Setup

Laminar Flow Models

Laminar flow simulations were done on both the N=3 geometry and the N=5.96 geometry. Two simulations were performed on each of the geometries, a model run at a Reynold's Number of 10 and a Reynold's Number of 100. All of the simulations had almost the exact same setup, the only real difference being the inputs for fluid velocity.

The first step to running a laminar model, after opening COMSOL, was to select the correct physics for the model. Since laminar flow was being modeled, the fluid flow menu was selected. Under fluid flow, single-phase flow, and then subsequently laminar flow were selected. After moving on to the next menu screen, a stationary study was chosen, and then the model was added into the COMSOL model builder.

The next step necessary was to set up the correct domains and input all of the required boundary conditions. The domain for the fluid flow was set by clicking on Laminar Flow in the Model Builder and then doing a manual selection in the Settings window. It was necessary to define the domain of the fluid to be the area within the cylinder that was not made up of the solid spheres. To do this, the cylinder was selected as the domain and all of the spheres were left un-selected. Also in this same window the flow was set to be incompressible. COMSOL has several default boundary conditions; Fluid Properties, Wall, and Initial Values. Fluid Properties allowed for the input of the desired density and viscosity of the fluid, which in this case was air. Next the no slip boundary condition was set under the Wall menu for all surfaces except the inlet and outlet of the cylinder. The Initial Values menu allowed for the input of a velocity field and pressure, pressure was set at atmospheric for all of the simulations, but the velocity field depended on the desired Reynold's Number of the flow, the Initial Values do not actually define simulation parameters they are the values that get the iterations for the solver started. It was then necessary to add a boundary condition for the inlet of the cylinder. This was done by right clicking on

Laminar Flow then adding the Inlet condition. Then in the settings window for the inlet, the top of the cylinder was selected as the boundary and then the velocity was set, depending on which Reynold's Number was desired. Then the outlet was set in a similar fashion, however the boundary condition chosen was, "pressure, no viscous stress" then p_0 was set. After all of the boundary conditions were successfully inputted, the final step was to mesh, all of the meshes created in COMSOL were physics controlled and automatically generated. The meshes varied in size ranging from a coarser mesh all the way up to a normal mesh.

Turbulent Flow Models

COMSOL has several different models at its disposal to simulate turbulent flow. In this study the k-ε approach was used. Setting this as the model for these simulations was done similar to the laminar runs. The k-ε model was located under fluid flow, then single phase flow, then turbulent flow. After selecting this for the physics of the model, again a stationary study was chosen and then was added into the COMSOL model builder.

The next steps were to correctly set the domain for the fluid and the boundary and flow conditions. The domain was set in the settings window under the turbulent flow header. The cylinder was selected as the domain for the fluid and, again, the spheres were left unselected. This ensured that the flow was going through only the part of the cylinder not occupied by the spheres. Since it was desired to model incompressible flow, this option was also selected in this window. There were only a few differences between the boundary and flow conditions from the laminar runs described above. These differences include only the condition at the wall and adding information about the turbulence under the inlet option. For a turbulent model, the No Slip boundary condition cannot be used at the wall; so instead, the Wall Functions condition was used. The other difference is made under the Inlet settings, where it is necessary to input values for turbulent intensity and turbulence length scale values for these were 0.05

and 6.5*10-3 respectively. After all the conditions were set, the model was then meshed using a physics controlled mesh and then solved.

Heat Transfer Models

After running all of the simulations for fluid flow successfully it was then desired to couple both heat transfer and flow into a single simulation. This of course made the problem much more sophisticated and harder to do. There are several ways in which this coupling of two different physics could have been accomplished, but the simplest of them will be described.

The first step, as always, was to input what kind of physics would be used in the simulation. This could have been done several ways, however, it was decided that using a non-isothermal flow model was the best way to couple a fluid flow problem with a heat transfer problem. The Non-isothermal module was located under the Fluid Flow heading. Non-isothermal flow could be run with either a laminar or turbulent flow and simulations were completed for each. A stationary study was then again chosen and then was added into the COMSOL model builder.

The setup for these simulations is a quite deal more difficult than the simulations that were run with flow only. One of the most important steps in this simulation was the correct setup of domains. This was difficult because for these kinds of problems, there was fluid flow in one of the domains, heat transfer in the fluid domain, and then heat transfer in the solid spheres. The solution for correctly setting the domains is not obvious and will be described below.

In the settings window, under iso-thermal flow, there was an option to choose the default heat transfer model, either fluid or solid can be chosen, in this case it was taken to be fluid. In the area where the domain can be set, all of the domains must be chosen, even the solid spheres where there will be no fluid. Then under non iso-thermal flow a fluid properties menu now appeared, and all of the necessary physical properties of the fluid was input, again the fluid in these simulations was air. Then the wall conditions and initial values were input in the exact same fashion as the flow problems. Then in order to get COMSOL to also model solid heat transfer within the spheres it was necessary to add another setting under the non-isothermal flow. This was done by right clicking on non-isothermal flow and then selecting Heat Transfer in Solids. In the solid heat transfer settings the spheres were set as the domain for solid heat transfer. Doing this caused COMSOL to go back and override the spheres as a domain in the fluid heat transfer, and now all of the domains were correctly set. Then solid properties were also set, our solid in this case being Alumina. The physical properties of both air and alumina can be seen in Table 1. The inlet and outlet for flow were then set in the same way as before. Temperature for both the wall and the inlet were set by right clicking on non-isothermal flow and adding them in. And then the outflow condition was set on the same boundary as the flow outlet.

Table 1 - Physical Properties of Air and Alumina

	Air	Alumina
Thermal Conductivity (k)	0.45 W/m*K	1 W/m*K
Heat Capacity (C_p)	1 kJ/kg*K	1000 kJ/kg*K
Density (ρ)	1.225 kg/m^3	1947 kg/m^3

Results and Discussion

Laminar Flow Models

Laminar flow models were run on a packed bed geometry with a tube to particle diameter ratio of N=3 and N=5.96. Several runs were performed to see if there was a discernable difference between flow patterns based on the Reynold's Number of the flow. The first run that was performed was at a Re=400 and a diagram of the flow patterns created in this geometry is shown in Figure 5.

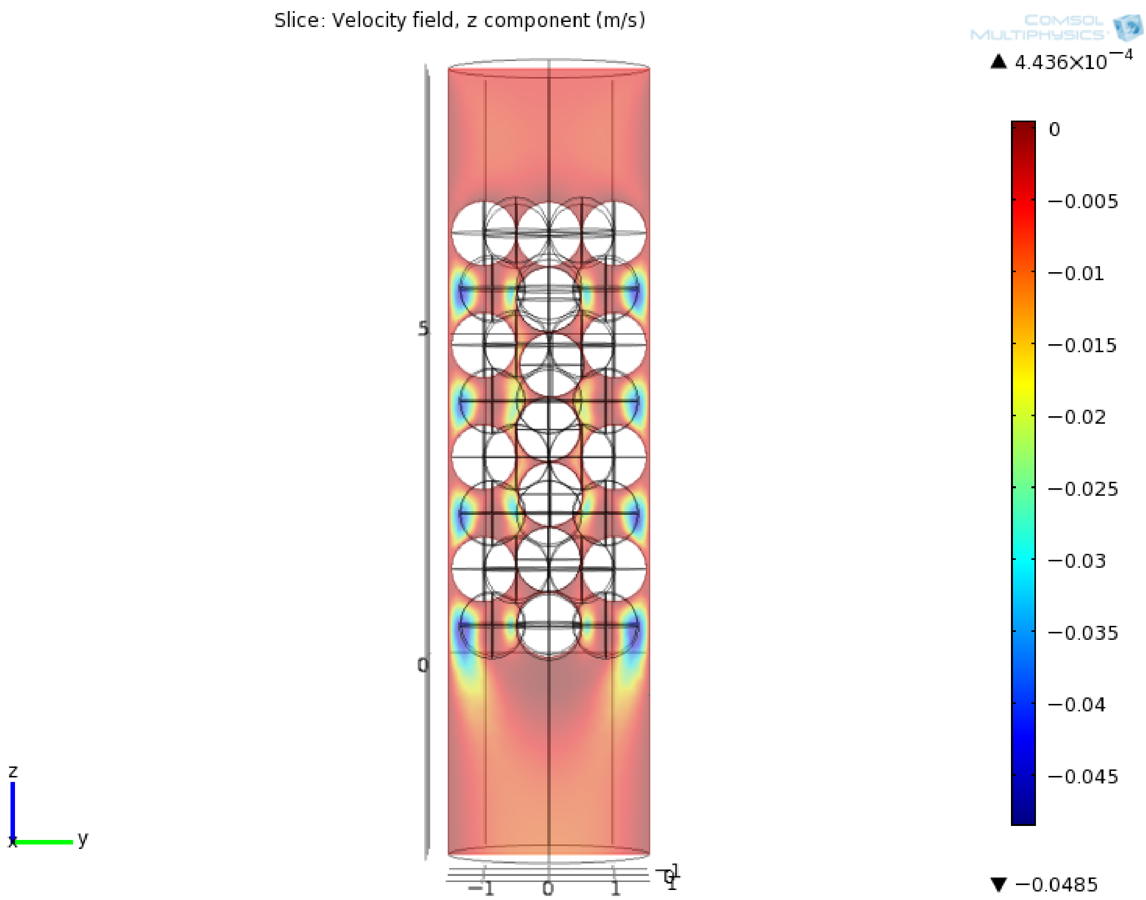

Figure 5 - Vertical Cross Section of N=3 Geometry with a Re=400 Laminar Flow

It can be seen here that the fluid velocity is greatest in the narrow spaces that occur in between particle to particle contacts and the particle to wall contacts. This happens because the fluid is forced to flow through a relatively smaller space, forcing it to accelerate. This causes several areas of local maximum velocity in this type of geometry. So if a plot of velocity versus tube radius was to be created, it would be expected to see two peaks. The first peak would be expected to be seen at the contact occurring between the particle on the centerline and its neighboring particle. The second peak would be expected to be seen at the area where the outer most particle is contacting the tube wall. This plot was created and it can be seen in Figure 6 that these are in fact the two areas that created local maximum velocities.

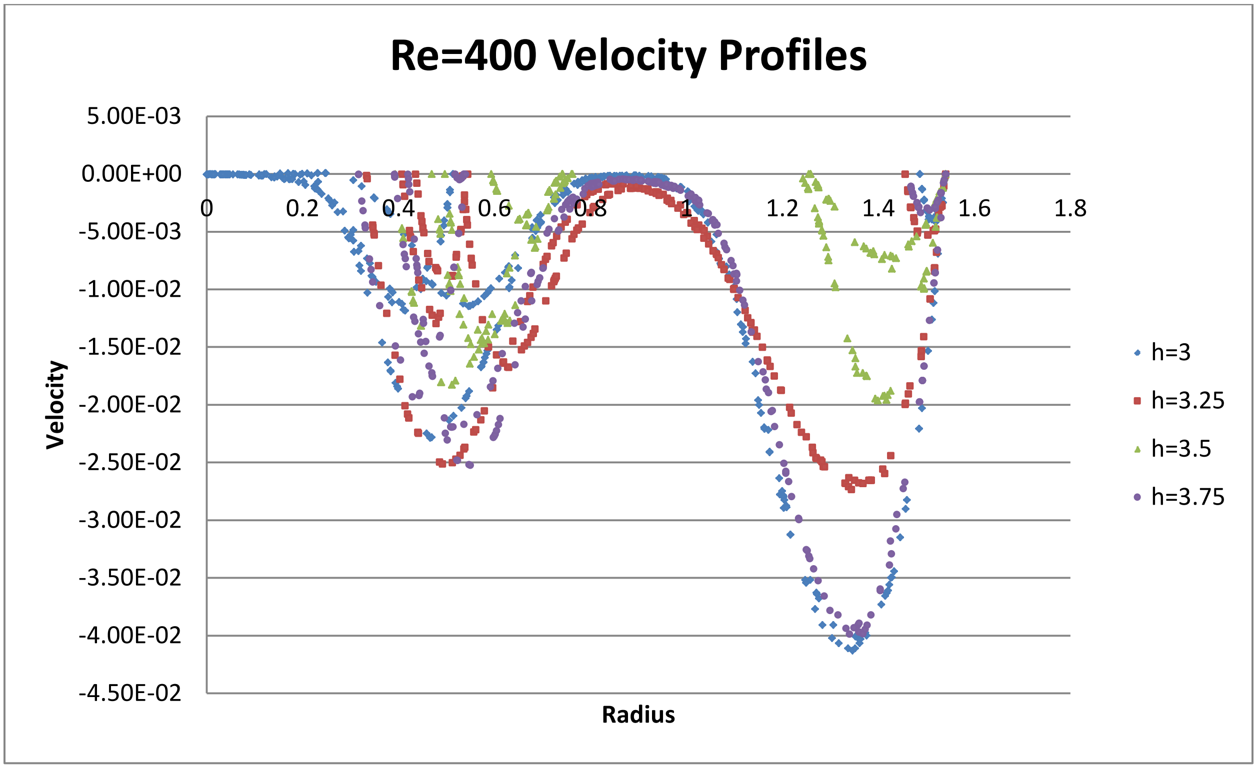

Figure 6 - Velocity Profiles at Various Bed Heights for Re=400

This plot shows the velocity profile of the fluid flow at several different heights in the bed. At each height, four different radii were examined and the velocities along each of these radii were plotted. It can be seen that bed height affects the velocity of the flow. This has to do with the bed geometry, it can be seen that areas with the highest maximum velocity are occurring at bed heights of 3 inches and 3.75 inches. These areas are caused because at these bed heights, the distance between neighboring particles and the wall are smallest. The centerlines of several spheres are located at a bed height of three inches, and the spheres are widest at this point which creates very narrow gaps between them, which is why on the plot the velocity is highest at a height of three inches. Moving away from the centerline of the spheres causes an increasingly larger space for fluid to flow through and thus causes a smaller local maximum at these bed heights.

In order to determine if flow pattern would be influenced by Reynold's Number another simulation within the laminar flow regime was performed. This simulation was run at a Reynold's Number of 100. Velocity profiles for the same exact bed heights previously obtained were plotted in Figure 7. It can be seen that while the magnitude of the velocity does change, the flow pattern itself does not. This led to the conclusion that flow pattern in the laminar flow regime will remain unchanged with respect to a differing Reynold's Number.

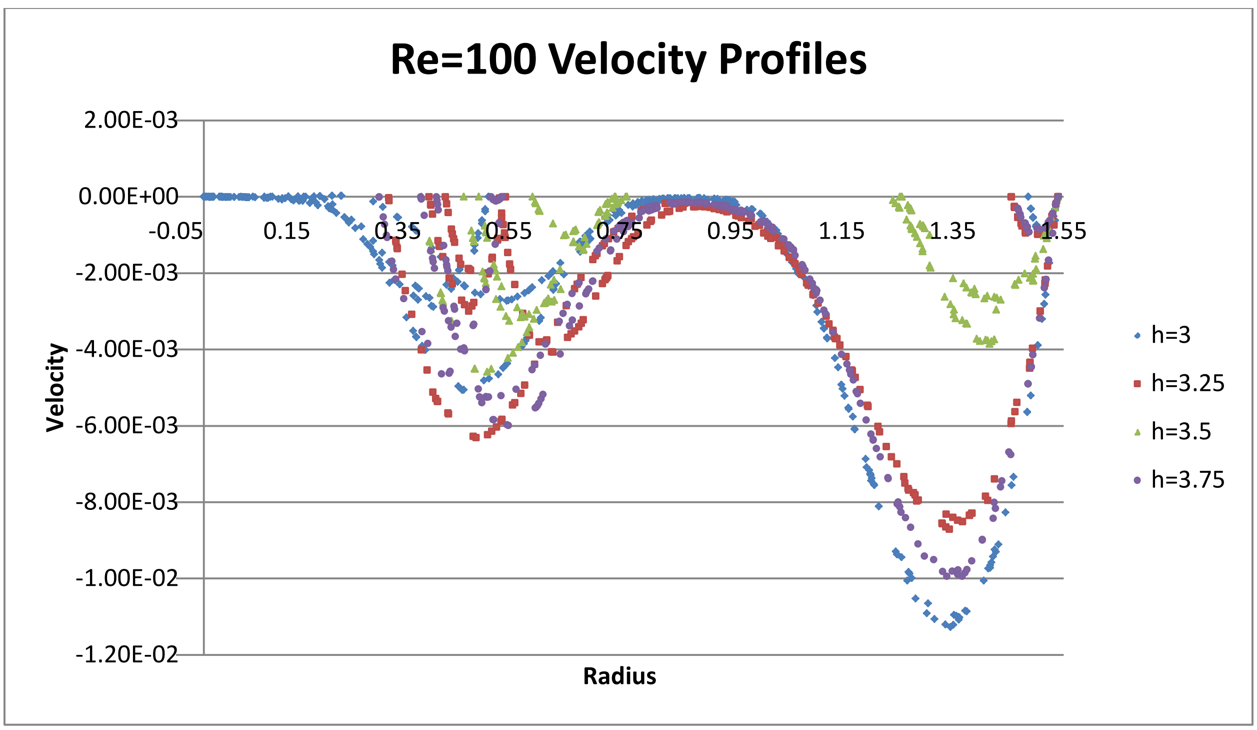

Figure 7 - Velocity Profile at Various Bed Heights for Re=100

In order to see how different bed geometries affect flow patterns, the model was scaled up and made into a more complex geometry, consisting of much more particles and with a tube to particle diameter ratio of N=5.96. Since bed geometry almost exclusively dictates what type of flow pattern is formed it was expected to differ wildly from that of the simpler geometry presented in the N=3 model.

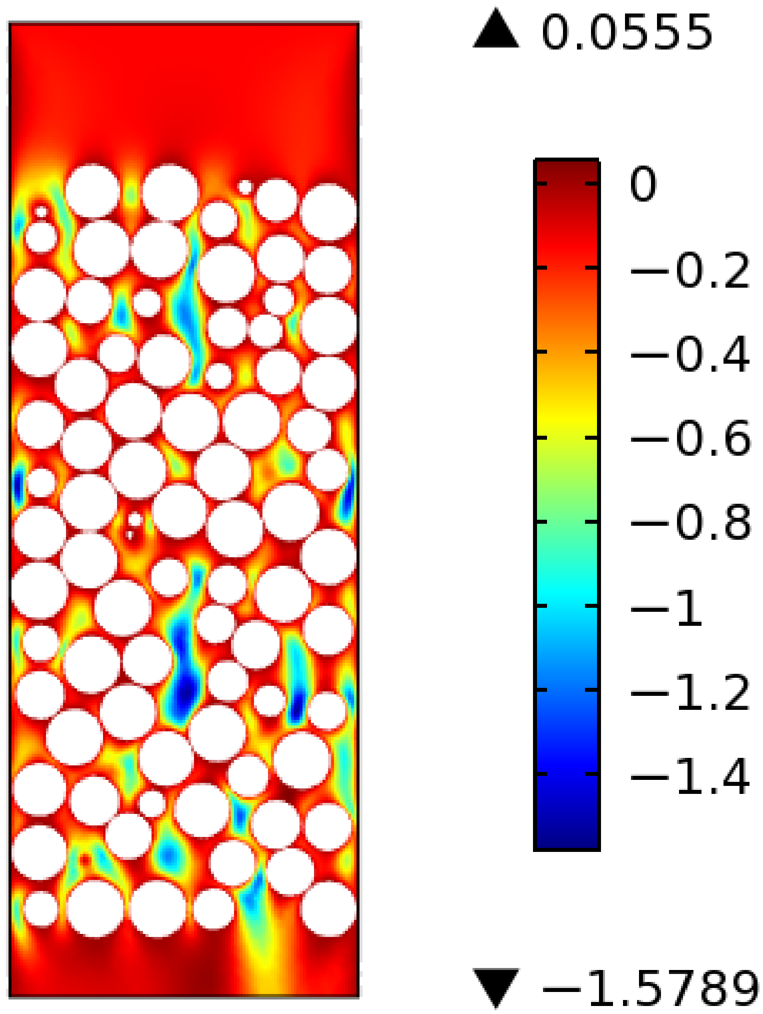

Figure 8 - Vertical Cross Section of N=5.96 Geometry for a Re=100 Laminar Flow

Depicted above in Figure 8 is the centerline view of the z-component velocity in a bed with N=5.96 and a flow with Reynolds number of 100. As predicted the flow pattern is completely different from that of the N=3 bed. Also it appears that with a bed of this complexity there is no real way to predict areas of local maximum velocity with any reliability. The fluid sometimes finds its way into channels, and in these channels, areas of higher velocity occur, but there is no real way to predict where the channels will occur because of the irregular bed geometry.

Turbulent Flow Models

In order to determine the effect of turbulence on the flow pattern in packed beds, several simulations were performed on the same geometries described above, but with a flow in the turbulent regime. The first simulation that was performed was for a flow corresponding to a Reynold's Number of 1000. As seen in Figure 9 below, the major difference is that the velocity along the walls of the particles no longer goes to zero. This is because the turbulence caused by the high flow makes it impossible for a no slip boundary condition to occur.

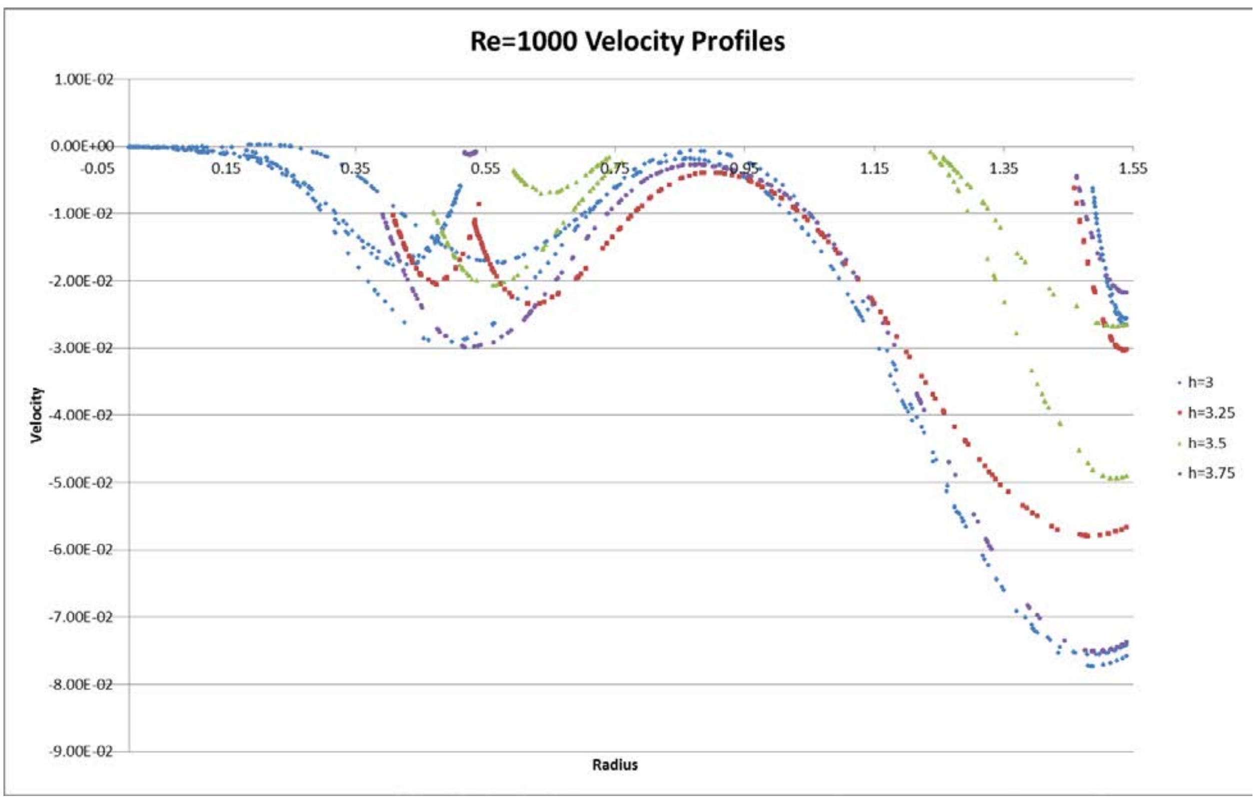

Figure 9 - Velocity Profile at Various Bed Heights for a Re=1000 Turbulent Flow

Other than this slight difference, there are not really many other things that set the flow pattern of the turbulent model apart from that of the laminar model. The major velocity peaks are still occurring at relatively the same location along the radius of the tube. Even the relative intensity of the two peaks is comparable to that of the laminar runs. This result led to the belief that flow pattern is not affected tremendously by Reynold's Number.

Just to reaffirm this assumption, another run was performed with a Re=5000. As expected the flow pattern remained ultimately unchanged, the only difference being the magnitude of the velocity peaks. The plot for this simulation can be seen in Figure 10.

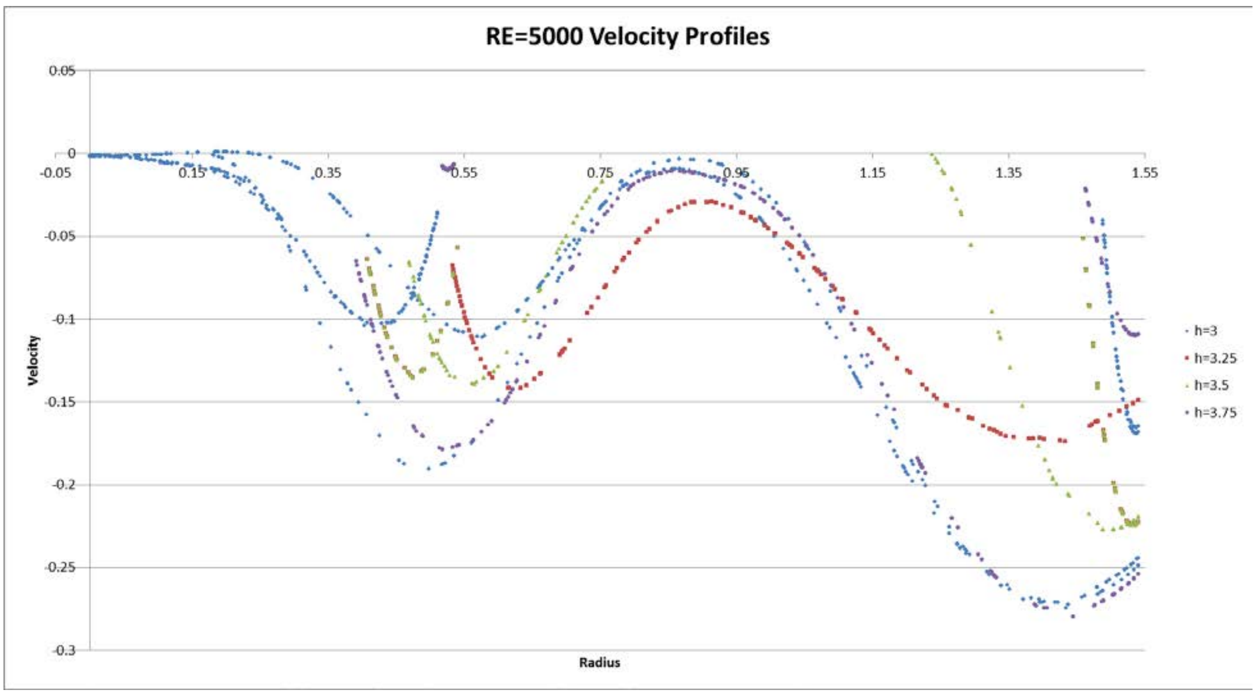

Figure 10 - Velocity Profile at Various Bed Heights for a Re=5000 Turbulent Flow

Heat Transfer Models

After successfully simulating both laminar and turbulent flow in COMSOL, the next step was to introduce heat transfer into that flow. All of the variables that were set for flow in previous runs were exactly the same and produced identical flow patterns and velocity profiles. What were introduced in this model were heat transfer properties for the fluid and spheres, and temperatures for the inlet and walls. These runs were completed to determine how well heat would transfer within the beds.

In these heat simulations the walls were set at a hot temperature and the inlet was set at a lower temperature. It was expected that the temperature be greatest at the walls and the fluid and spheres would become hotter along the length of the bed. As seen in Figure 11 this is in fact what does occur.

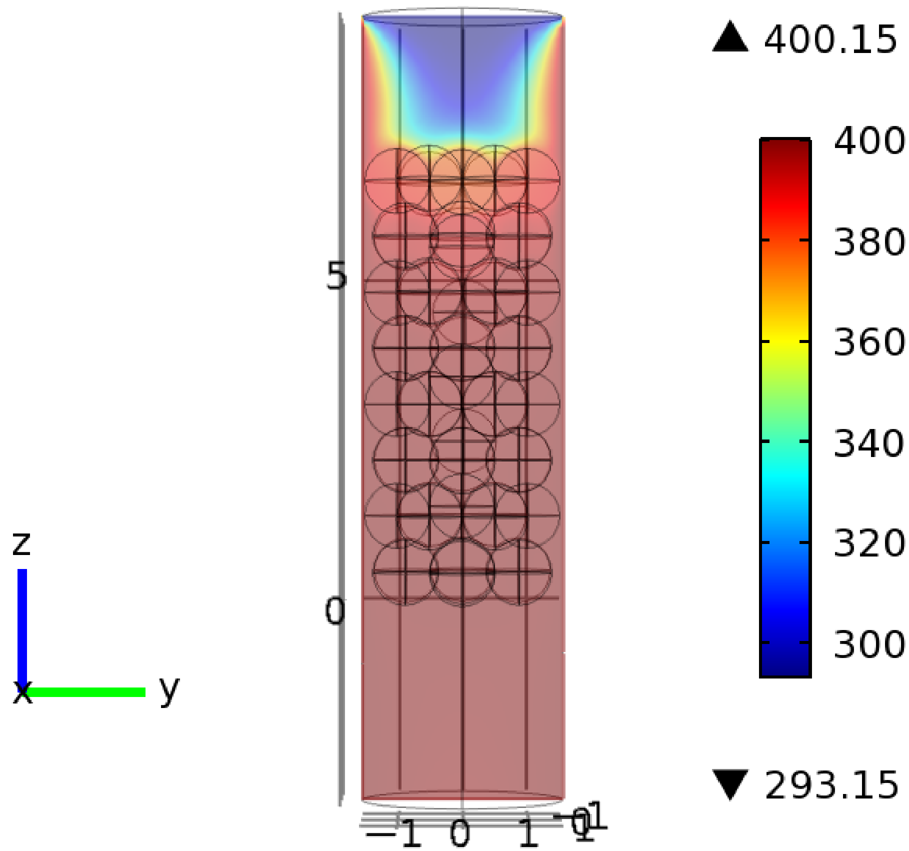

Figure 11 - Vertical Cross Section of N=3 Geometry with Re=400 Flow and Conjugate Heat Transfer

The temperature forms a parabolic looking curve, with the colder temperature persisting near the center of the bed, while the higher temperatures exist on the outer edges. Because this is a simulation of a low Reynolds Number flow, the low temperature from the inlet does not persist very far down the bed.

When examining a cross section of this bed as seen in Figure 12 it can be seen that the spherical particles off up some resistance to heat transfer that allows the center spheres to remain cooler than there outermost counterparts. The material of the spheres was set to be Alumina, which has a relatively low thermal conductivity. This made the outer spheres act almost like an insulator and kept the center spheres from heating up as much. Also seen in this figure is that the temperature differs from 380 K to 400 K at his bed height, which is only 2.5 inches from the inlet to the bed.

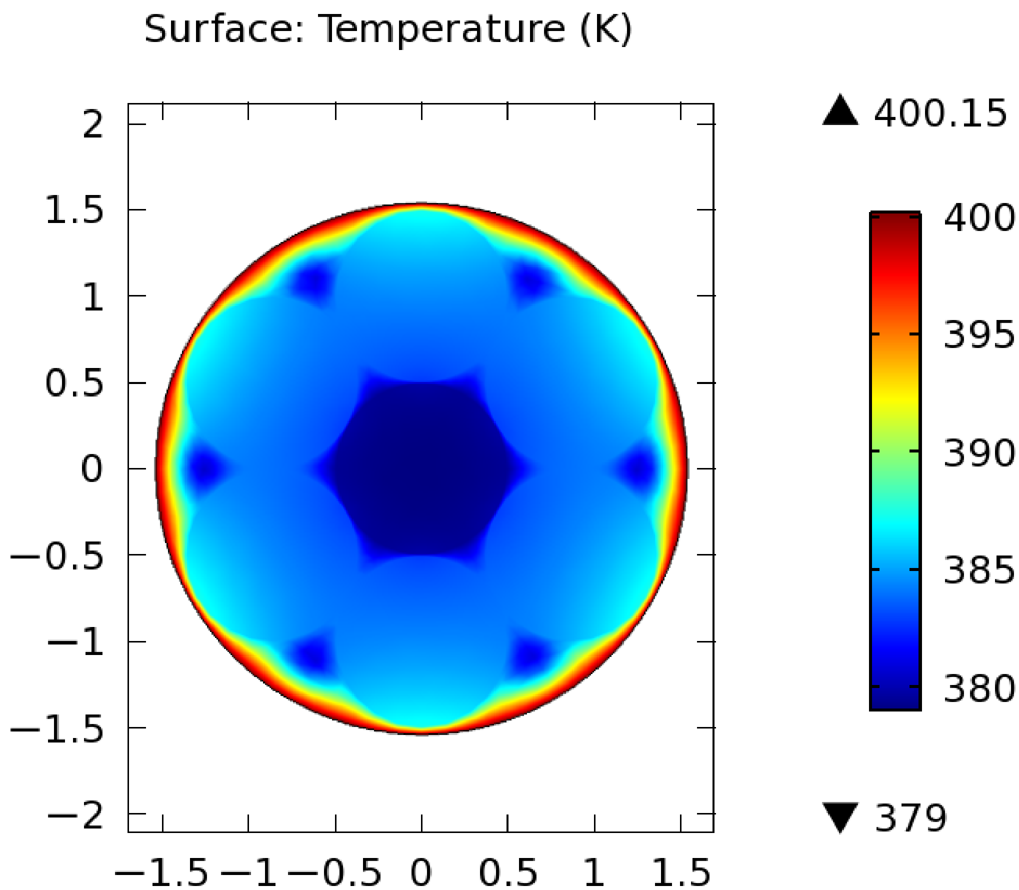

Figure 12 - Cross Section of N=3 Geometry 3.5 Inches From Inlet

As the flow progresses along the bed the spheres quickly approach the temperature of the walls. Figures 13 and 14 depict bed heights 6 inches and 8 inches away from the inlet respectively, and it can be seen that the temperatures start to become almost uniform across the bed. In the cross section 6 inches from the inlet, which is only half way through the packing material the temperature of the center sphere only differs from the temperature of the wall by about 2 degrees. And moving further down to the bottom of the packing as seen in the cross section 8 inches from the inlet, the temperature varies by little more than one degree. This occurs because as the fluid travels down the bed, the flow pattern caused by the spheres provides very good mixing of the fluid and allows for a great deal more heat transfer.

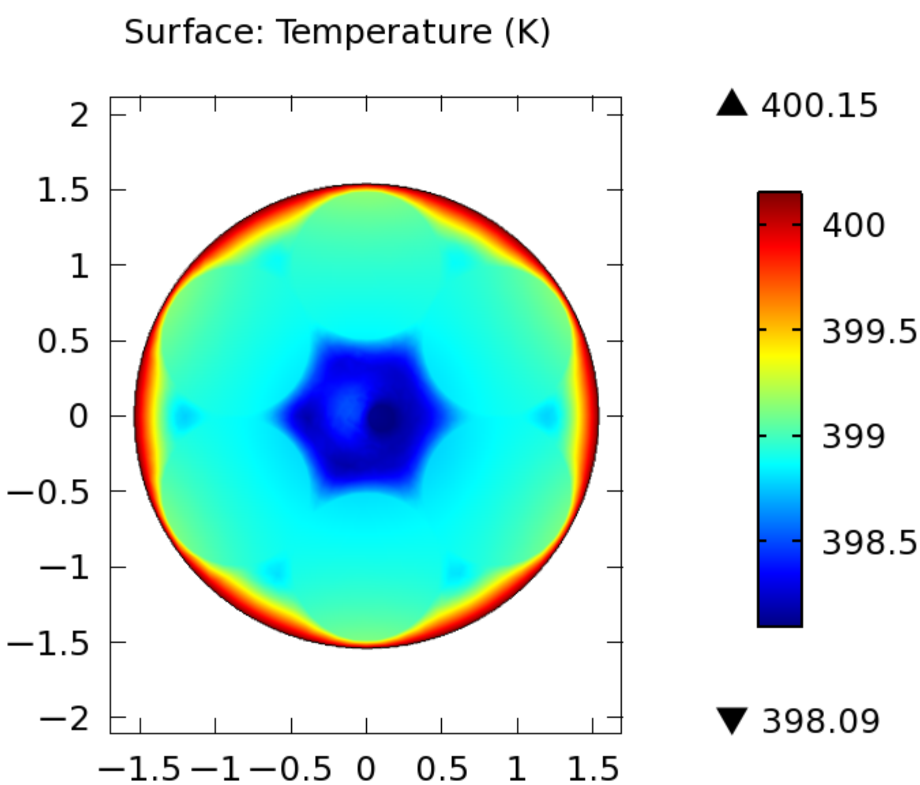

Figure 13 - Cross Section of N=3 Geometry 6 Inches From Inlet

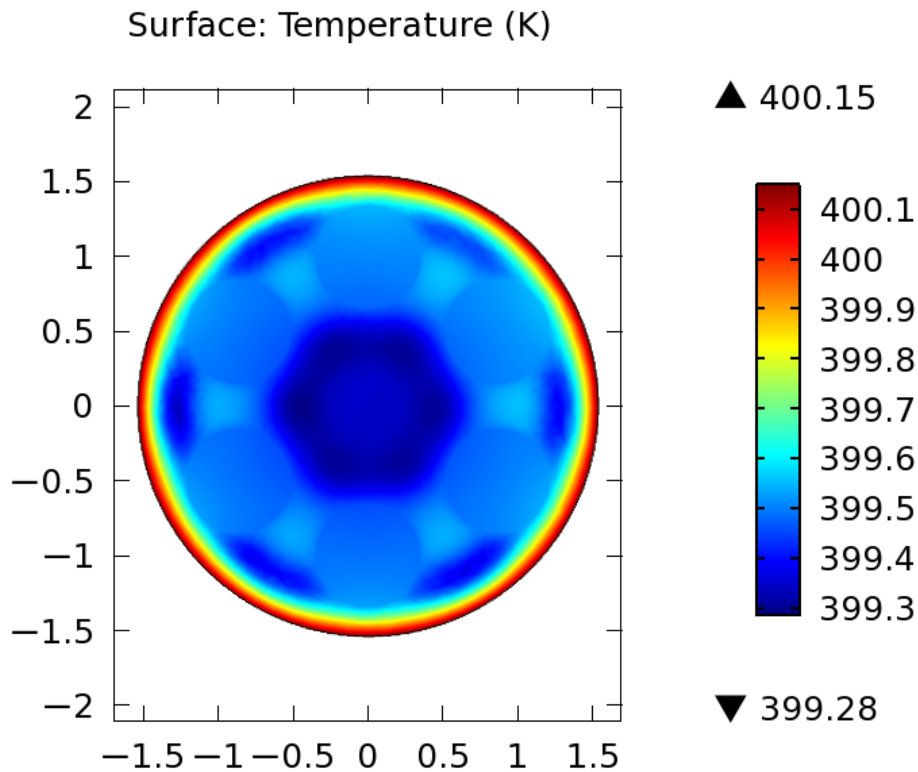

Figure 14 - Cross Section of N=3 Geometry 9 Inches From Inlet

Several runs were completed with varying Reynolds Number without much change in result, so plots for these runs can be found in Appendix A.

Pressure Drop

For all of the models one additional property was examined, pressure drop across the bed. Results for pressure drop were obtained for flows of Re= 100, 400, 1000, and 5000. These values were then compared with values obtained through calculation using the Reichelt correlation and tabulated. Results of these calculations as well as data obtained from COMSOL can be seen below in Table 2. This area seemed to have a great deal of difference between expected results and actual results. So it appears that COMSOL may not be the best tool to use for modeling of pressure drop in these packed beds.

Table 2 - Pressure Drop Data for Re= 100, 400, 1000, 5000

Re	K1	k1	k2	ε	D	d	A	B	ψ from Calculation	Press Drop from COMSOL	ψ actual
100	154	1.15	0.87	0.4	0.0762	0.0251	1.365996	0.989582	2502.158108	0.005	266.3502
400	154	1.15	0.87	0.4	0.0762	0.0251	1.365996	0.989582	635.245303	0.0235	80.71949
1000	154	1.15	0.87	0.3	0.0762	0.0251	1.313711	0.989582	777.2201256	0.1015	54.06908
5000	154	1.15	0.87	0.4	0.0762	0.0251	1.365996	0.989582	62.72537628	0.7051	16.01063

Conclusions and Recommendations

In conclusion COMSOL is a useful tool for modeling laminar and turbulent flows as well as heat transfer; however COMSOL does have some difficulty with simulating diffusion as well as predicting pressure drop. CFD programs are also very good at modeling flows and have better capabilities for modeling turbulence, along with better post processing features. Both programs seem to have trouble with simulating diffusion.

The conjugate heat transfer module for COMSOL is relatively good, so it is recommended to use this feature when attempting to simulate a conjugate heat problem. However, if simulating flows or turbulence, a CFD program excels in this area and should be preferred over COMSOL. One area of interest it is recommended to be examined further is diffusion with COMSOL. COMSOL will allow for diffusion in solid objects, something CFD struggles with, but is very difficult to set up in COMSOL, so this is one area that it would be beneficial to examine a little bit further.

References

Bardina, J. E. and Huang, P. G. and Coakley, T. J. and Ames Research Center. *Turbulence modeling validation, testing, and development [microform] / J.E. Bardina, P.G. Huang, T.J. Coakley* National Aeronautics and Space Administration, Ames Research Center ; National Technical Information Service, distributor, Moffett Field, Calif. : [Springfield, Va. : 1997.

Benenati, R.F. and Brosilow, C.B., 1962. Void fraction distribution in beds of spheres. *A.I.Ch.E. Journal* 8, pp. 359–361.

Carman, P.C., 1937. Fluid flow through granular beds. *Transactions of the Institution of Chemical Engineers (London)* 15, pp. 150–166.

Eisfeld, B. and Schnitzlein, K. The influence of confining walls on the pressure drop in packed beds. *Chemical Engineering Science*, *Volume 56, Issue 14*, *July 2001*, *Pages 4321-4329.*

Fogler, H. Scott (2006). *Elements of Chemical Reaction Engineering* (4th Edition ed.). Prentice Hall.

Launder, B. E., and Sharma, B. I. (1974), "Application of the Energy Dissipation Model of Turbulence to the Calculation of Flow Near a Spinning Disc", Letters in Heat and Mass Transfer, vol. 1, no. 2, pp. 131-138.

Logtenberg, Simon A and Dixon, Anthony G. Computational fluid dynamics studies of fixed bed heat transfer. *Chemical Engineering and Processing*, *Volume 37, Issue 1*, *January 1998*, *Pages 7-21.*

Reichelt, W. Calculation of Pressure Drop in Spherical and Cylindrical Packings for Single-Phase Flow. (1972) Chemie-Ingenieur-Technik, 44 (18), pp. 1068-1071.

Seader, J.D. and Henley, Ernest J. (2006). *Separation Process Principles* (2nd Edition ed.). John Wiley & Sons.

Appendix

Appendix A: Miscellaneous Heat Transfer Plots

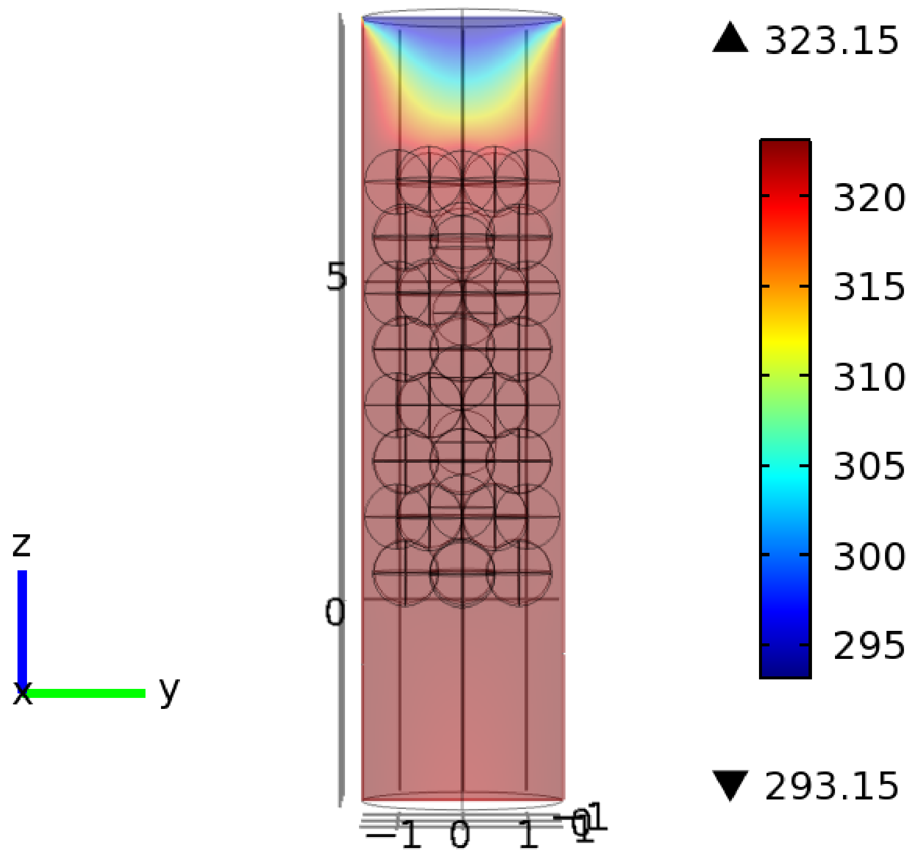

Figure 15 - Verticle Slice for Re=100 Heat Transfer Simulation

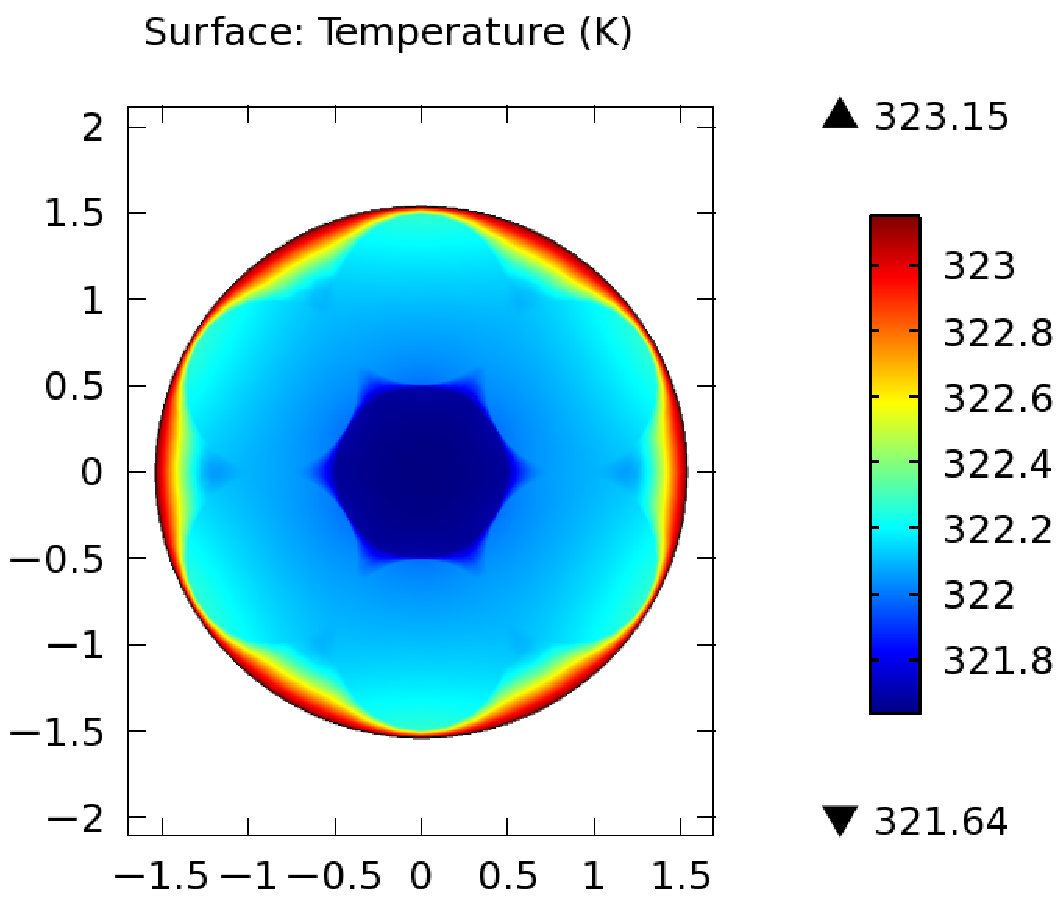

Figure 16 - Cross Section of N=3 Geometry 3.5 Inches from Inlet

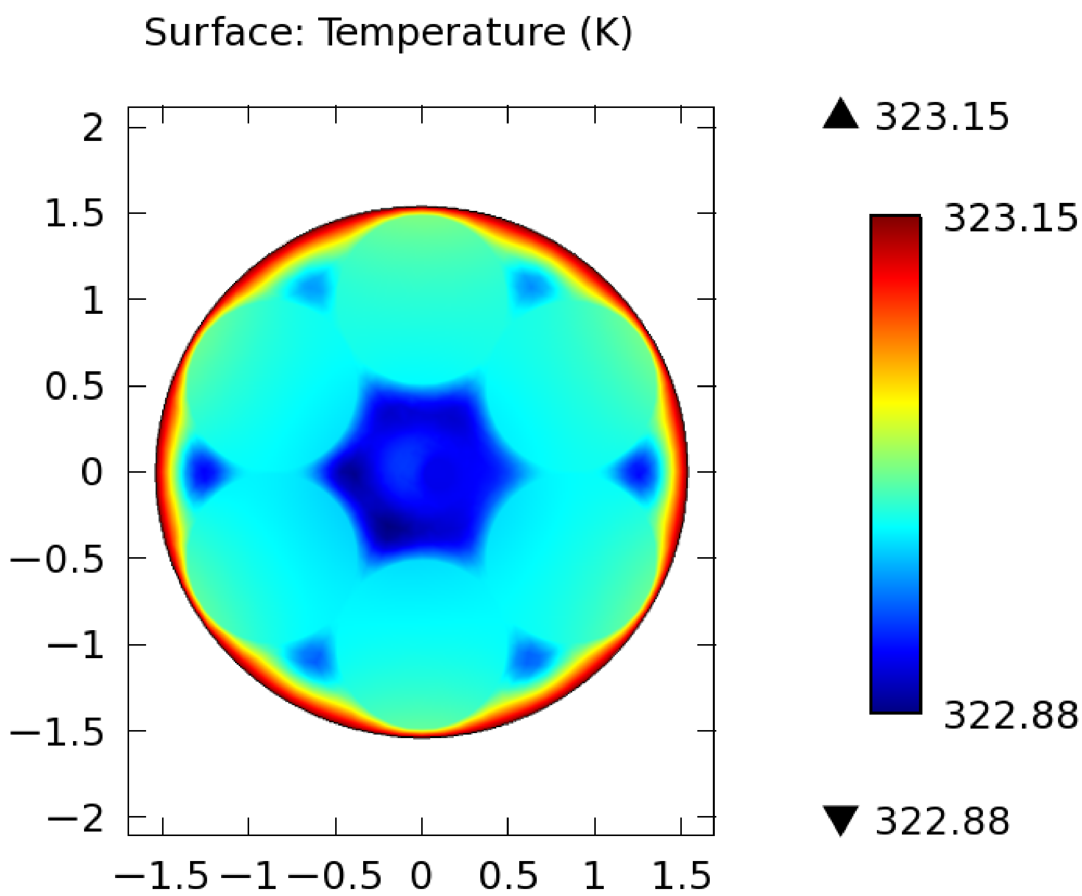

Figure 17 - Cross Section of N=3 Geometry 6 Inches from Inlet

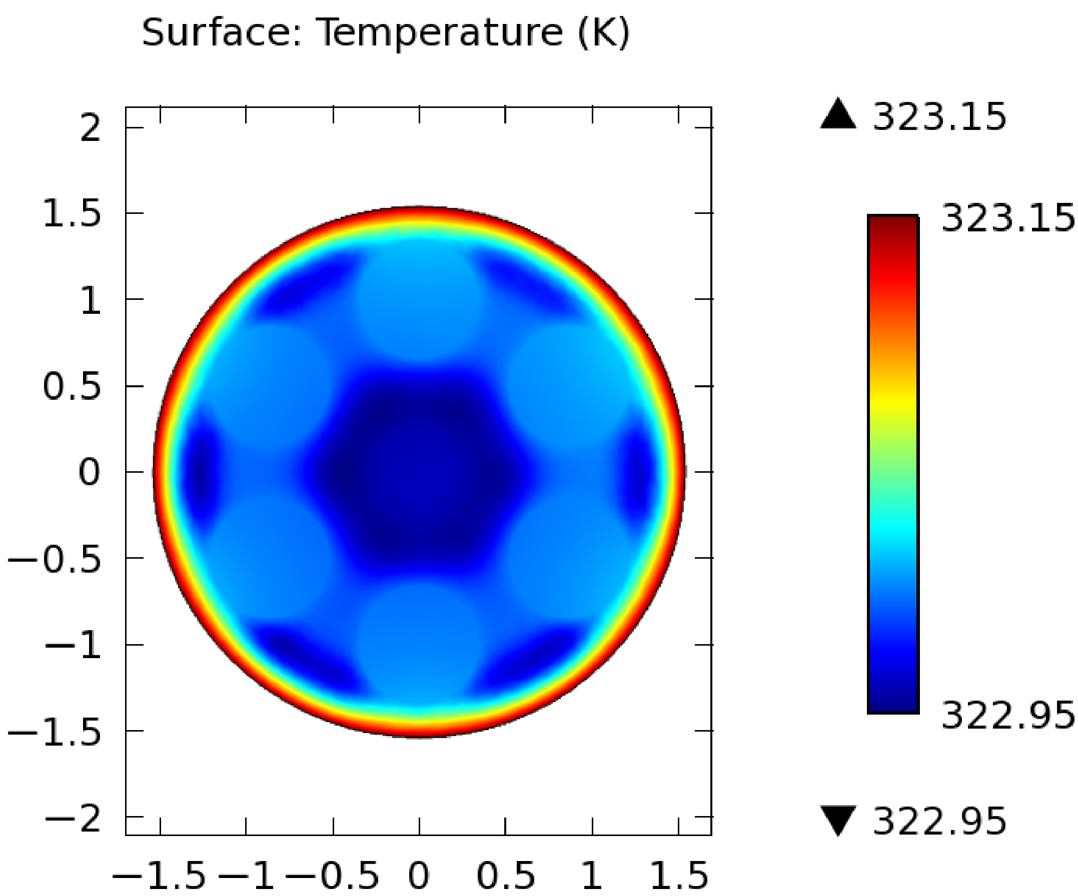

Figure 18 - Cross Section of N=3 Geometry 9 Inches from Inlet