Modeling a fixed bed using Comsol Multiphysics and CFD

A Major Qualifying Project Report
Submitted to the faculty of

Worcester Polytechnic Institute

In partial fulfillment of the requirements for the
Degree of Bachelor of Science

By

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Abstract

For the conduction mode of heat transfer in a fixed bed, an evaluation of whether one of the most widely used equations for the stagnant overall thermal conductivity k_e^0, the Zehner-Schlunder cell model, is the most accurate and most efficient model in literature, was conducted. The equation was compared to a similar equation the Van Antwerpen. Multiple 1D Comsol Multiphysics models were constructed and analyzed for both set of equations. This data was compared to data from a three-dimensional computational fluid dynamics model or CFD model. These comparisons and data analyses established at least for now that the Zehner-Schlunder is still the best option when studying heat transfer in a bed, however further testing using other parameters is suggested.

Section 1 Introduction

Fixed beds have many uses in the industrial world, many of which where heat transfer is a very important process. Some of the uses in industry for fixed beds would be catalytic reactions, gas cooled nuclear reactors, absorbers and energy storage systems. To ultimately understand a fixed bed reactor and the heat transfer that goes on inside it, modeling software such as Comsol Multiphysics should be used. The basic mechanism that should be modeled using Comsol along with other modeling programs is thermal conduction under stagnant flow conditions, through an assembly in the model of randomly packed particles and the surrounding fluid.

The most applicable approach to modeling this conduction through fixed beds would be to replace the complex discrete packed structure of the bed with a continuous porous medium, known as a pseudo-continuum approach. In this approach, it can be seen that the mechanisms of heat transfer are lumped into an effective thermal conductivity, *k*. It is known that *k* depends on the position in the bed. Despite this fact, the thermal conductivity of *k* is often placed as a constant throughout the bed radius. Also despite that fact all increases in thermal resistance near the tube wall are lumped into a heat transfer coefficient *h* at the wall. In most recent years there have been a couple of models that are more physically realistic and can represent the variation of the thermal conductivity in the fixed bed reactor.

Zehner and Schlunder (1970) a set of formulas, which is the most commonly used and the basis for this project, for stagnant effective thermal conductivity. They developed this set of formulas using a unit cell model and relating the effective conductivity to the fluid and sold, which in the case of the models would be k_f and k_s respectively and the bed void fraction of epsilon, ε. These formulas were later extended and extensively compared to data by Bauer and Schlunder [5]. Despite publications [1] that point out discrepancies in the equations and have modified the existing equations, partially or entirely, they are still in widespread use among the scientific community.

The second set of formulas used to study this modeling procedure and the one that is being compared to the *Zehner-Schlunder* formulas would be that of *Van Antwerpen* [1]. This specific set of formulas has been compared to those works of Zehner, Schlunder and Bauer due to the increased accuracy claimed by the formulas

and their creators. For this model in particular and what makes it supposedly more accurate then the former is the fact that by accounting for the porous structure when calculating effective thermal conductivity and also using the empirical correlations set down in Du Toit [4], this set of formulas is able to simulate the effective thermal conductivity with more accuracy in the bulk region as well as in the near wall region of the randomly packed annular bed. Along with that change it can also be seen that existing thermal resistance models for point contact and particle roughness developed by Bahrami[2] and other newly developed thermal resistance models for other defined regions in the unit cell have been used. Finally a newly developed multi sphere unit cell is constructed which accounts for porous structure in a more accurate manner.

For this project an analysis of both of these formula models has been conducted for stagnant fluid beds with tube to particle diameter ratio N in the range 3.5-9.5. With the data from the CFD analysis a comparison is to be made of both of the formula sets to see which one is truly better in the sense of modeling effective thermal conductivity throughout a fixed bed reactor.

Section 2 : Methodology

2.1 : Comsol Simulation - Setup

The main area of research within this project is that of electronic computer simulations run on the software Comsol Multiphysics. The running of the CFD was done on a higher-powered computer with the ability to take the equations and run them for more complex 3D models than Comsol. The simulation run in the CFD was

3D and simulated annular beds of spheres. The running of the CFD allowed for temperature and voidage points, T(r) and $\varepsilon(r)$ respectively, to be provided as companion points to those collected for this project. For Comsol there was a detailed methodology put into place, when setting up the program to run both of the formula sets mentioned the previous section.

To start out the Comsol Multiphyics program was initialized and the main set up screen launched. After that the dimensions of the simulation had to be chosen from a list that included 1D, 1D axisymmetric, 2D, 2D axisymmetric, 3D and 3D axisymmetric. For the purpose of this project, the Comsol simulations run for the two formula sets had to be run in the 1D axisymmetric form. This axisymmetric geometry allowed for axial symmetry in the bed, which could then be used when the two temperatures, mentioned at a later time, to be evenly distributed between their sides of the reactor bed. After the dimensions of the simulation were chosen, the physics at which the simulation had to be run were selected. For this particular case, since heat transfer is the main focus of this project, Heat Transfer in Solids is the only physics that is selected for the running of these formula groups. The main equation for this physics is stated below

$$\frac{d}{dr}\left(rk(r)\frac{dT}{dr}\right) = 0$$

For this equation the temperature values set would be those of $T(r_i)=300$ and $T(r_0)=700$. This physics allows for the set up of heat transfer through the bed reactor and all parameters to be set within the reactor such as heat flux, density and heat capacity at a constant pressure. In this case the heat flux is defined as kec,

whose equation is stated above, the density is $8700\,\frac{kg}{m^3}$ and the heat capacity is defined as $385\,\frac{J}{kg*K}$. Along with those parameters, for all the runs completed, there is also the parameter of *ks* and *kf* or *kg*. These variables are respectively the thermal conductivity of solid, the thermal conductivity of fluid or gas phase and the thermal conductivity of the gas phase. Now for the Zehner-Schlunder run of Comsol, ks and kf were used as parameters for the simulation with values of $1\,\frac{W}{m*K}$ and $0.0242\,\frac{W}{m*K}$ respectively. For the W van Antwerpen formula, ks was also used along with kg which has a value of $0.0242\,\frac{W}{m*K}$ as it is the same as kf from the previous formula set.

After these parameters are set up, the model is then given an interpolation to run, In this case that interpolation would be values of epsilon to be run with the equations given. Epsilon is the void fraction for the fluid bed reactor. A void fraction is the measure of the void or empty spaces in a material and is a fraction of the volume of voids over the total volume. All of these values for epsilon lie between zero and one.

After this these interpolations are set up then the geometry of the model was designed. The geometry of the model is a line due to the 1D selection made previously in the setup of the model. This line has two points a starting point and an end point. The starting point for all of the modeling in the Comsol simulations, both for the Zehner-Schlunder and W van Antwerpen is the same. This starting point is one half of the diameter of the inner tube in the bed reactor, which is a value of 0.00127 meters. For the end value of the model, one half of the tube to particle

diameter ratio or the N value is used. The values for N range from 3.5 – 9.5 with a step of 1 for each model run.

After the geometry is set up the physics in the model needs to be developed. As stated above the parameters for the heat transfer in solids has already been set up, however boundary conditions need to be established for the model. For the boundary conditions on all of the models run, there are two temperature values. The first value is that of 300K and that applies to the starting point for the geometry of the model. The second value is that of 700K and that applies to the end point of the geometry. After the boundary conditions are applied, there is a normal mesh that is set up for the model. This mesh is composed of 15 elements. With all of the information entered into Comsol the model can then be run to completion.

2.2: Comsol Simulation - Post-Processing

After the running of the Comsol Modol, post-processing must be done to allow for data to be collected to be analyzed later in the results section of the paper. To start out the post-processing the results section of the Comsol model is opened. Under this results section a section that is classed data sets appears in a subsection underneath. Under data sets right clicking on data sets and selecting that option adds a 1D cut point. In the cut point 1D setting it can be seen that there is a point data subsection. Under this subsection there is an entry method, which is kept at coordinates, and under that there is a r-value which is the range of the cut point. The range of the cut point is a range from the starting point of the geometry to the ending point of that same geometry. There is also a middle number for this range and that is the split for the number of temperature points that is to be recorded to

the Comsol Simulation. This split number for this specific running of the models ends up being $2.54 * 10^{-4}$ for the jump between each recording of temperature data along the line of the graph created when the simulation was run. After this is done a subcategory under derived values is created called Point Evaluation. For this point evaluation, for the data set, the new cut point from above should be selected and the expression should be for temperature with units of Kelvin. After this is done evaluate is selected at the top of the settings menu for the point evaluation. This calculates all of the temperature values for the range selected before and puts them all into a table at the bottom of the comsol running screen. Going to the table and selecting the export icon extract this data. This allows for the data to be put into a text file and in turn be copied and pasted into excel for further analysis.

2.3: Equation Development

Both the Zehner-Schlunder and the Van Antwerpen formulas have many different equations that help construct their entirety. For this project each set of equations for each formula set needed to be analyzed and simplified so when they were put into comsol they would run in the correct manner and develop the correct results. The first set of equations analyzed was that of Zehner-Schlunder. To start out the main equation, stated below for this formula needed to be studied.

$$k_e^0 = kf\left[1 - \sqrt{1-\varepsilon} + \sqrt{1-\varepsilon} * \frac{2}{(N-M)^2}\left(\frac{B}{(N-M)^2} * \frac{kp-1}{kp} * ln\frac{kp}{B} - \frac{B+1}{2} - \frac{B-1}{N-M}\right)\right]$$

For this specific equation the only simplification that needed to be done, was for the equation to be split into different parts, instead of comsol trying to analyze such a large equation. The first variable defined when separating this equation was

that of *kp*. This variable is defined as ratio between the solid thermal conductivity and the fluid thermal conductivity or in equation terms $\frac{ks}{kf}$ with ks and kf being defined later on in the paper. After that is defined, next is the variable epsilon. This variable is defined below when the actual set up of the comsol model is explained. After epsilon is entered into comsol, then the variable B must be set as the equation given below.

$$B = 1.25 * \frac{1 - \varepsilon^{10/9}}{\varepsilon}$$

After B is defined then the variables of N and M must be defined. For N the equation is given below and for M it is defined as 0 for this specific running of the formula set

$$N = \frac{1 - B}{kp}$$

To help further simplify for the $\sqrt{1 - \varepsilon}$ sections of the equations a variable is created and defined as Sq. For the final sections of the equation they are defined as a,b,c,d,e,f respectively. These variables and their equations are defined below.

$$a = \frac{2}{N}$$

$$b = \frac{B}{N^2}$$

$$c = \frac{(-1+kp)}{kp}$$

$$d = log\left(\frac{kp}{B}\right)$$

$$e = 0.5 * (1 + B)$$

$$f = \frac{(-1 + B)}{N}$$

The second set of equations analyzed and simplified were those of Van Antwerpen. To start out the main equation given below was analyzed to determine what variables or sections of the equations were needed for this particular iteration.

$$Rm = \frac{(2 * R_j)}{N_c}$$

This particular equation stands for the thermal resistance of multi sphere unit cell. The use of this is perfect of analyzing the packed bed reactor since it is made up of multiple spheres packed up next to one another while the reactor is running. After the main equation has been determined the parts of it require analysis of their own. The first variable that needs to be analyzed is that of N_c. This variable for this equation stands for the coordination number for the packed bed. The equation that makes it up can be seen below which is made up of epsilon values that have been pre-determined as stated below and can only include a range of epsilon values of 0.2398 to 0.54 for these particular coordination numbers for the runs of these models.

$$N_c = (25.952 * \varepsilon^2) - (62.364 * \varepsilon^2) + (39.724 * \varepsilon) - 2.0233$$

The next variable that needs to be analyzed and is the largest part of the main equation is R_j. This variable is defined as the thermal resistance of unit cell or the contact between two particles in the reactor bed. The equation for this variable is stated below.

$$Rj = \left(\frac{1}{R_{in12} + R_L + \left(\frac{1}{R_g} + \frac{1}{R_s}\right)} + \frac{1}{R_{mid12} + R_\lambda} + \frac{1}{R_{out12} + R_G} \right)^{-1}$$

For this particular iteration or running of this type of formulas in Comsol only macro gaps were analyzed when looking at the fixed reactor bed. The reasoning behind only looking at the macro gaps and discarding he micro gaps is the fact that when this simulation is run in Comsol there are no micro gaps to be recorded and the only gaps that would appear would be those of macro description. Since there is a decision to not recognize macro gaps for this type of simulation the variables that would be omitted would be every variable except for $R_{out12}$and R_G so the simplified equation would be the one given below.

$$Rj = \frac{1}{R_{out12} + R_G}^{-1}$$

After this simplification is made, both of the variables that make up this main equation must be analyzed a simplified in their own right. The first variable to be analyzed would be R_{out12}. This variable is defined as the outer solid thermal resistance of the bed. To start out the main equation for the outer solid thermal resistance of the bed is given below.

$$R_{out12} = \frac{\frac{log(Ao + Bo)}{(Ao + Bo)}}{(ks * \pi * Bo)}$$

Now for this equation the value of ks has been defined in an earlier part of this paper and the value of pi is known to be 3.14159. For the value of Ao and Bo two different equations must be used to get values for these variables. These equations can be seen below.

$$Ao = rp - 0.5 * (\omega + \lambda)$$

$$Bo = \sqrt{(rp^2 - r_\lambda{}^2)}$$

Looking at the equation for Ao it can be seen that there are three undefined variables in the equation. The first of these variables rp is the particle radius and is given a value of 0.0127 for all the runs of this set of equations. The second is omega, which is this case, can be omitted due to the conditions given for the bed reactor. The third and last variable is the mean free path of the gas molecules in meters. The equation for the mean free path is given below.

$$\lambda = \frac{k_g * T_g}{\sqrt{2} * \pi * P_g * {D_m}^2}$$

For this equation kg has a value of $0.0454 \frac{W}{m*K}$, T_g is the gas temperature, P_g is the gas pressure and D_m is the diameter of the gas molecule. The gas being used for all of these value would just be air at constant temperature and pressure. The value calculated after plugging in all of the values for the variables above would be $68 * 10^{-9}$.

Going back to the Ao and Bo equation above the only other variables left to define would be those of rp and r_λ. The variable rp has already been defined abover and the variable r_λ is the radius-indicating end of Knudsen regime conduction in meters. The equation for this variable is stated below.

$$r_\lambda = \sqrt{rp^2 - (rp - 0.5 * \omega - 5 * \lambda)^2}$$

Since all of the variables are now defined for R_{out12} it can now be calculated when plugged into Comsol with all of its part.

Going back to the original main equation there is still one variable that needs to be defined into order to complete the equation, R_G. This variable is the thermal

resistance of the interstitial gas in the macro-gap between each particle in the reactor bed. The equation for this variable is given below.

$$R_G = \frac{2}{\pi * k_g \left(A_G * ln\left(\frac{A_G}{A_G - 2 * \mathrm{B}_G}\right) - 2 * \mathrm{B}_G \right)}$$

In terms of this equation there are two variables that have not been formally defined in the paper and those variables are A_G and B_G. The equations for both of these variables are given below.

$$A_G = 2 * \mathrm{rp}$$

$$\mathrm{B}_G = \sqrt{rp^2 - r_\lambda{}^2}$$

Since the two variables that are included in both of these equations have been previously defined the values can be calculated for both of these variables. With both of these variables formally defined the value of R_G can be found allowing for the value of Rj to be determined.

Now that Rj can be calculated the main equation stated formally can be found for the entirety of the model.

There is also one more variable that needs to be defined for the comsol model that is very important to the running of the Comsol model. This variable is k_e^c and it is the effective thermal conductivity of the multi-sphere unit cell. The equation for the variable is stated below.

$$k_e^c = \frac{4 * \mathrm{dp}}{(\pi * (dp^2) * R_m)} * \sin(\theta)_c$$

For this equation the variables that need to be formally defined are those of $(\theta)_c$and dp. The variable dp is defined as the diameter of a sphere and is given a value of

0.0254 meters. The variable $(\theta)_c$ has a more formal equation and it is defined below

$$(\theta)_c = -6.1248 * Nc^2 + 73.419 * Nc - 186.68$$

Since Nc has been defined formally above, the variable can be calculated and thus so can the value of k_e^c. This value of k_e^c as stated in the comsol setup section of the paper is used under heat transfer in solid as the thermal conductivity of the bed. With this variable formally defined all variables have been defined to allow for placement in the Comsol model.

Section 3: Results and Discussion

After all the models have been run there is temperature data that has been extracted from all the Comsol models for both the Zehner-Schlunder and Van Antwerpen formulas. First looking at the Zehner-Schlunder graphs in the appendix something very apparent can be seen. The Comsol data collected for the temperature value of a certain range of tube to particle radiuses is close to exactly even with that of the CFD data collected for the same parameters. For all of the graphs for this particular formula it can be seen that they all are very similar. This is due to the fact that the data collected for each of them follows the same trend. However for each of them it can be seen that there are slight bumps on the lower N values and as the N value increases the lines smooth out. Also what cannot be seen by the graph but is also important is the fact that as the N number increases the number of data points for each graph increases. For example, for N=3.5 the amount

of data point was around 100 and for N=9.5 the amount of data points was around 400.

When looking at the Van Antwerpen formula graphs we see a different trend of temperature data at least for the beginning sections of the graph itself. It can be seen, instead of following the CFD trend line like the Zehner-Schlunder, this formula has a sharp jump at the beginning of the temperature recordings and then slowly lowers back down and eventually follows the trend line of the CFD perfectly. It can also be seen that as the N value increases so does the height of the peak at the beginning of the graph. For example when looking at the N=3.5 graph in the appendix it can be seen that the peak is somewhere around 650 K, however when looking at the N=8.5 graph it can be seen that the peak for the graph reaches over 1000 K. The graphs for the 5.5, 7.5 and 9.5 data runs of this formula were excluded due to data that was not useable in the case of this project. For all of those runs, the data did not follow the typical trend line that was formed for the other runs of the data set. Instead they had many steep peaks and valley and even in some cases temperature values that were too high to even be reasonable in the case of this experiment.

The reasoning that can be determined for the differnces in the graphs for the Zehner-Schlunder and the Van Antwerpen formulas could be the fact that the Antwerpen equation pays more attention to the packing structure based on coordination number and contact angles. Due to this there is a more rigorous differentiation of the effective thermal conductivity in the bulk of the reactor and near the bed walls. This would allow for more heat to be present in this model than

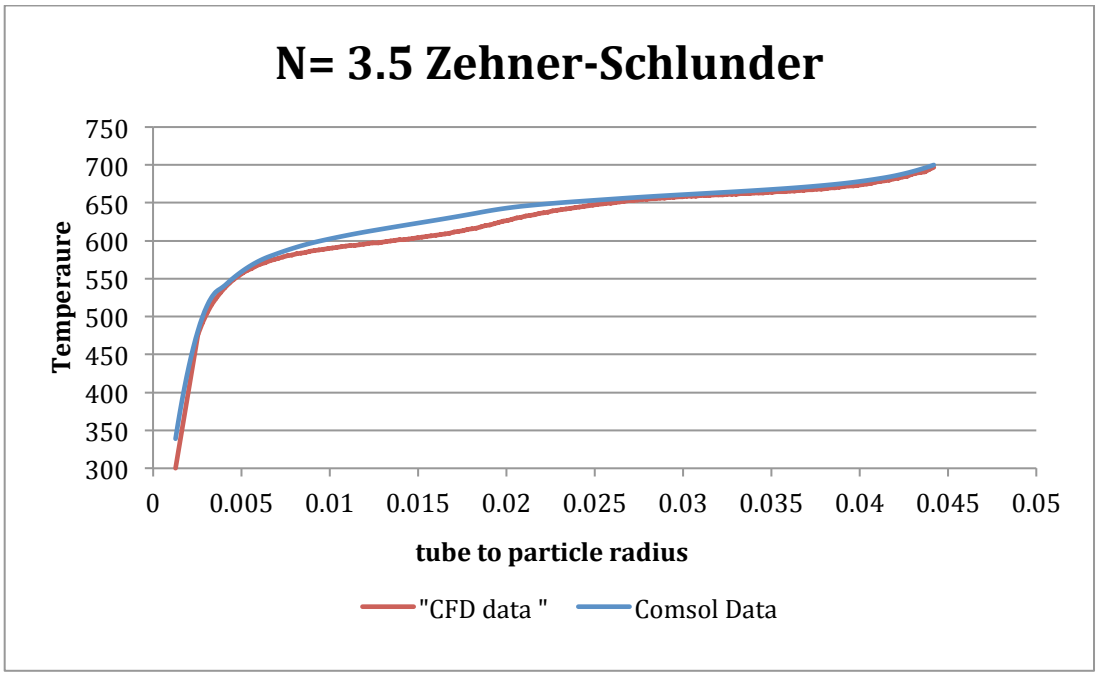
the other, allowing for higher temperature spikes and larger temperature values. Another reason that could account for the difference is the fact that maybe for the variable Nc in the Van Antwerpen equation some of the epsilon values given do not run well because they are out of the range for the equation of that variable.

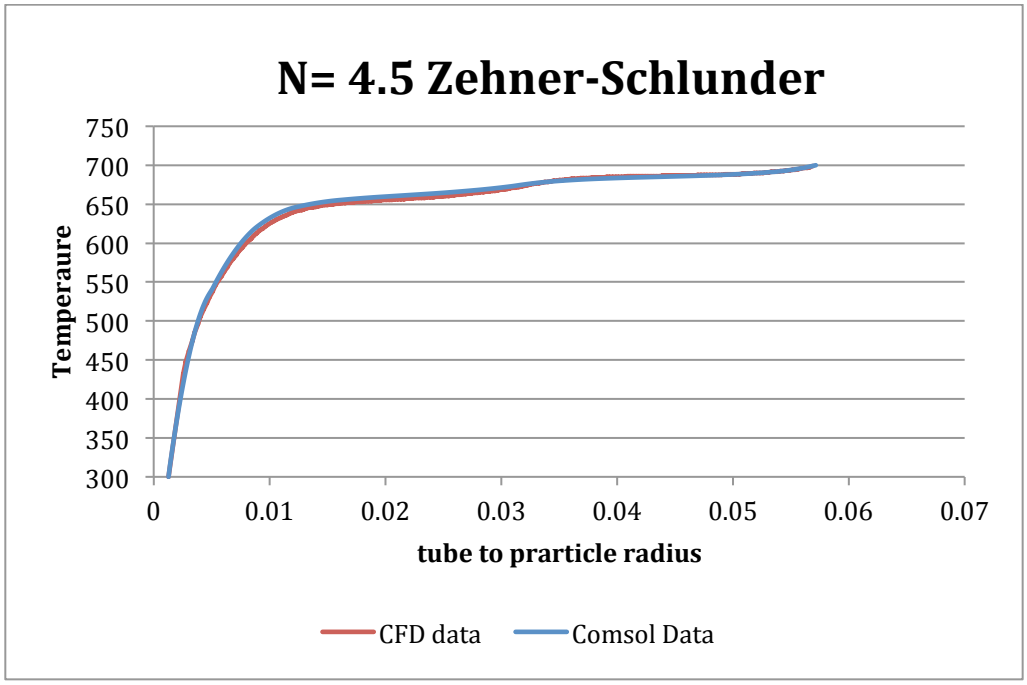
Section 4 : Conclusions

The main object of this project was to compare both the Zehner-Schlunder and the Van Antwerpen formulas to see if the claim made by Van Antwerpen on whether his formula was more accurate was correct. It can be seen from the data collected that he indeed was more accurate in some respects. His formula takes into account more parameters than his competitors such as solid conduction, gas conduction, and surface contacts. This allows for the temperature reading collected from this formulas set of models to be more accurate as to predicting what the actual temperature values running across the fixed bed reactor will be. This study doe need more data to be confirmed however. It can be suggested that for future projects radiation should be introduced into the bed using equations given by both formula sets, that way the data collected from those runs could be collected and a larger set of data be available for comparison in this matter

Section 5 : Appendix

5.1 - Zehner-Schlunder Formula Graphs




N= 4.5 Zehner-Schlunder
Temperaure
750
700
650
600
550
500
450
400
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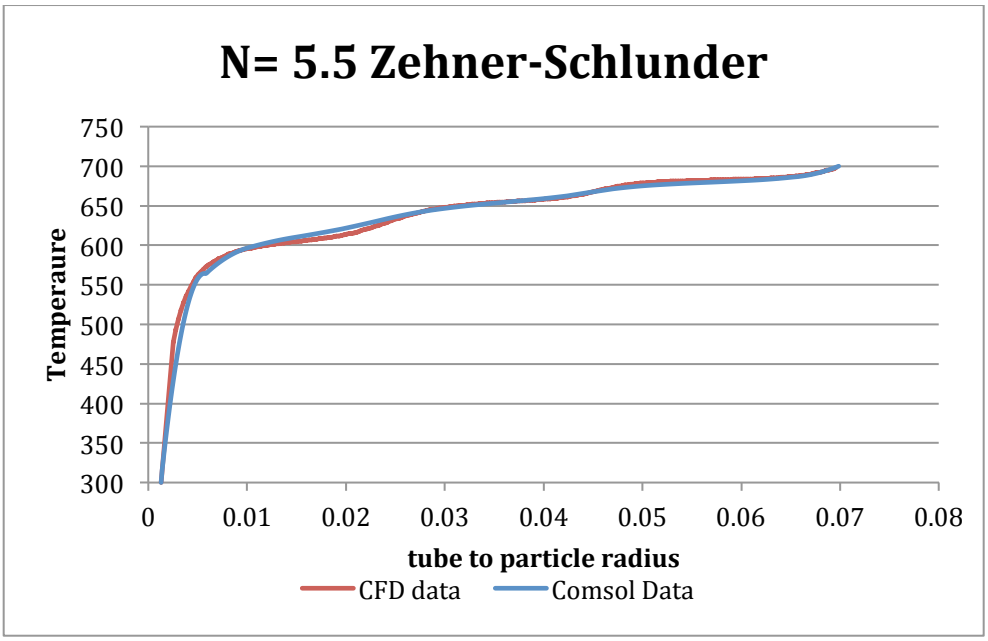
0.07
tube to prarticle radius
CFD data
Comsol Data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Temperaure
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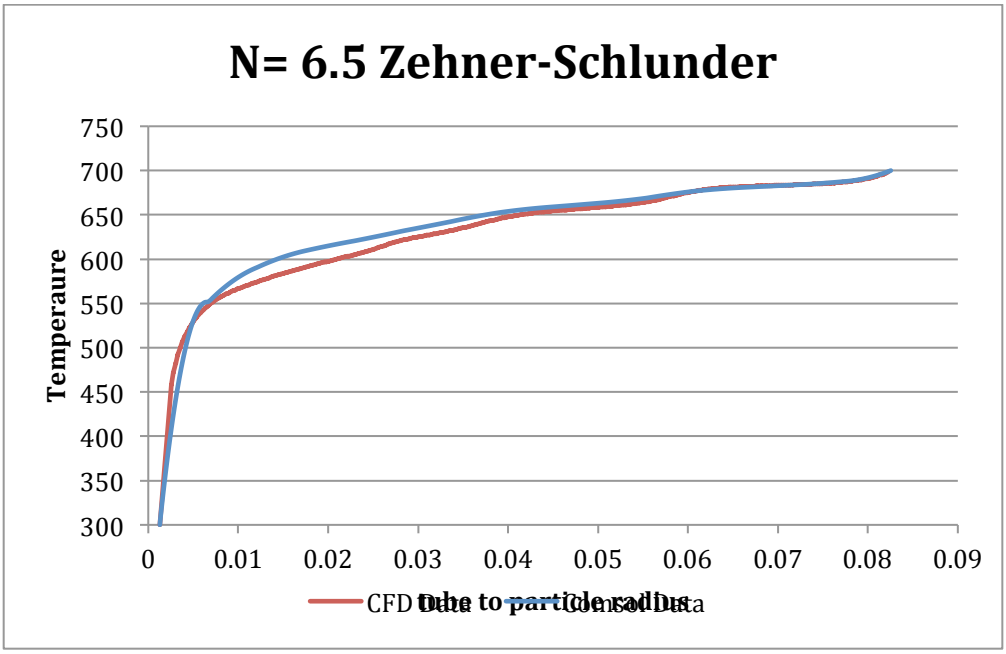
tube to particle radius
CFD data
Comsol Data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Temperaure
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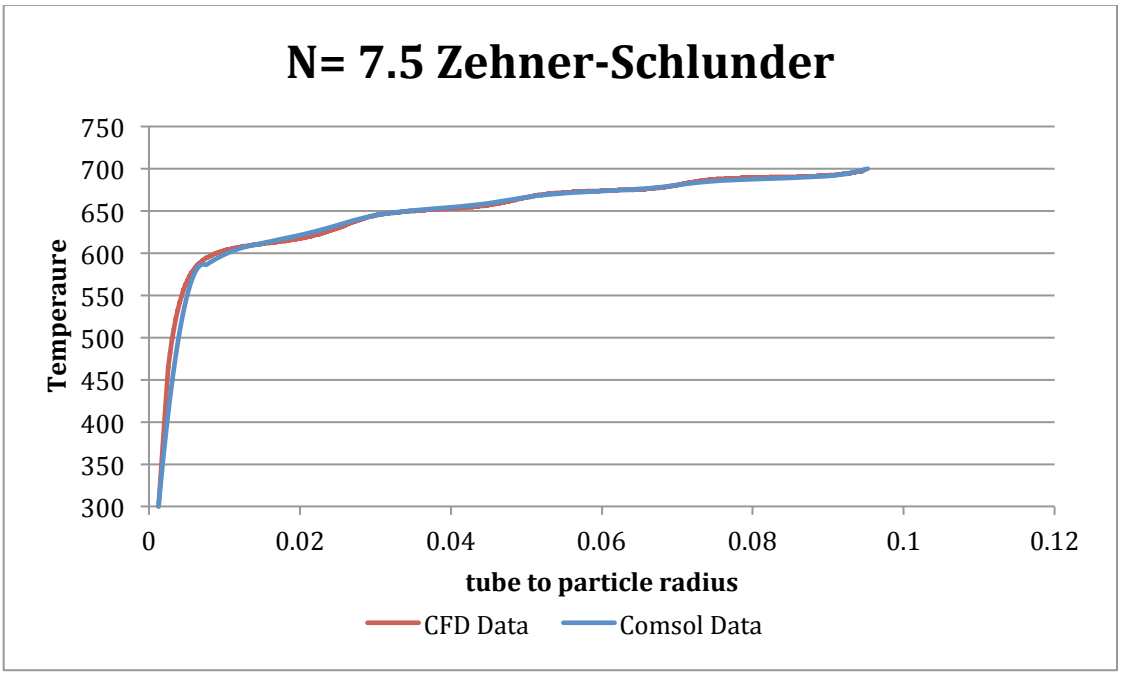
0.09
CFD Data
Comsol Data


N= 7.5 Zehner-Schlunder
Temperaure
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700
650
600
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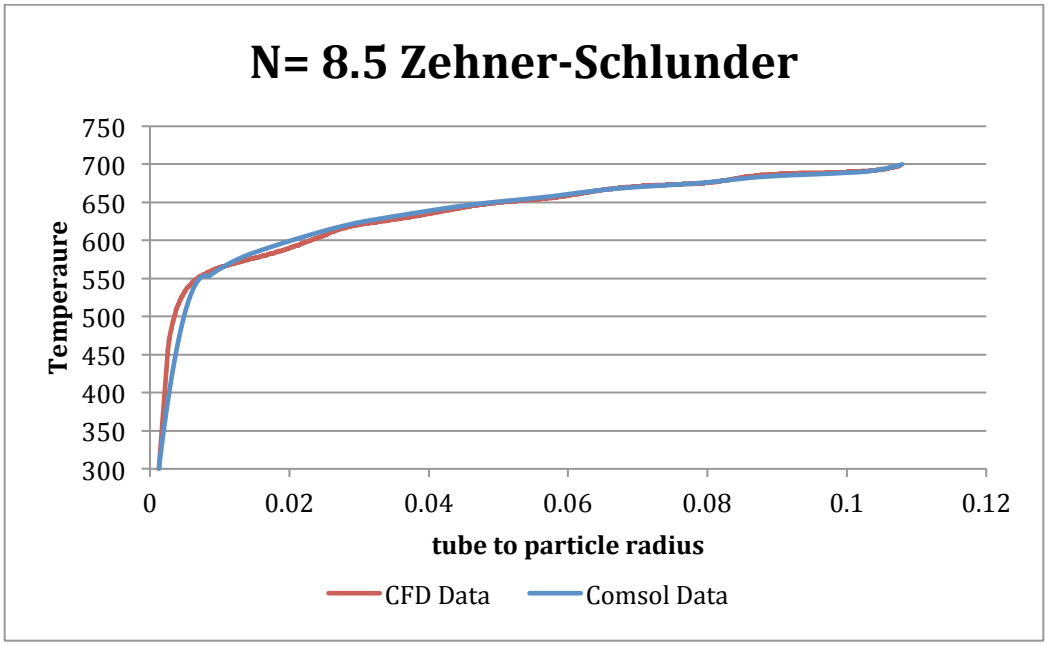
0.06
0.08
0.1
0.12
tube to particle radius
CFD Data
Comsol Data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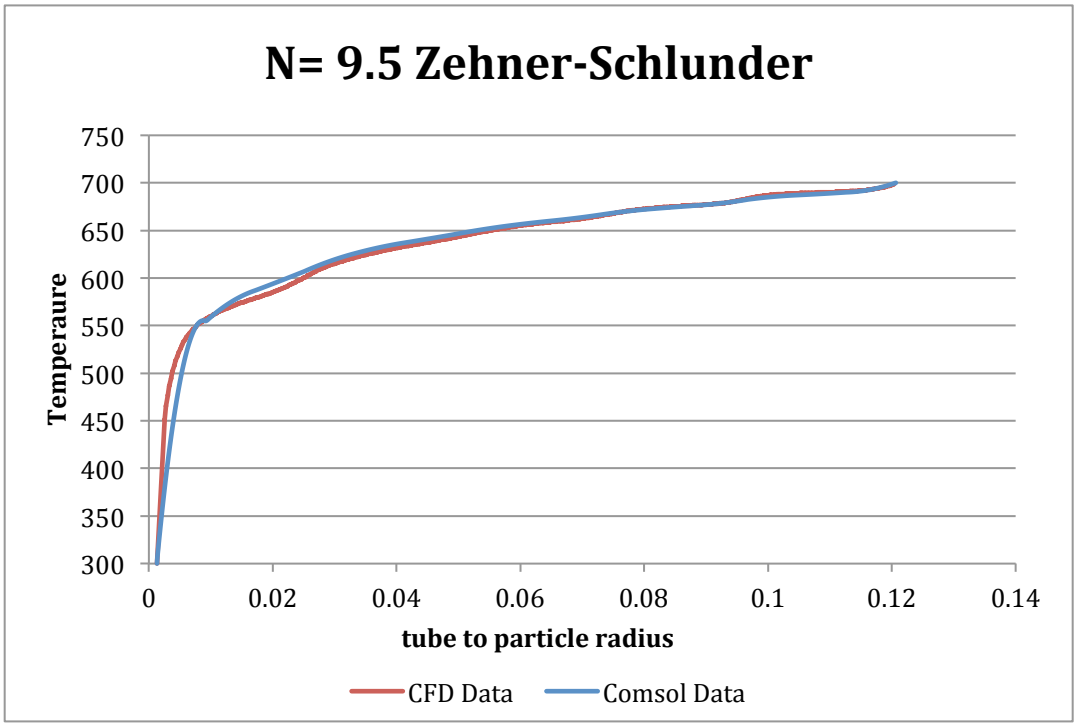
0.1
0.12
tube to particle radius
CFD Data
Comsol Data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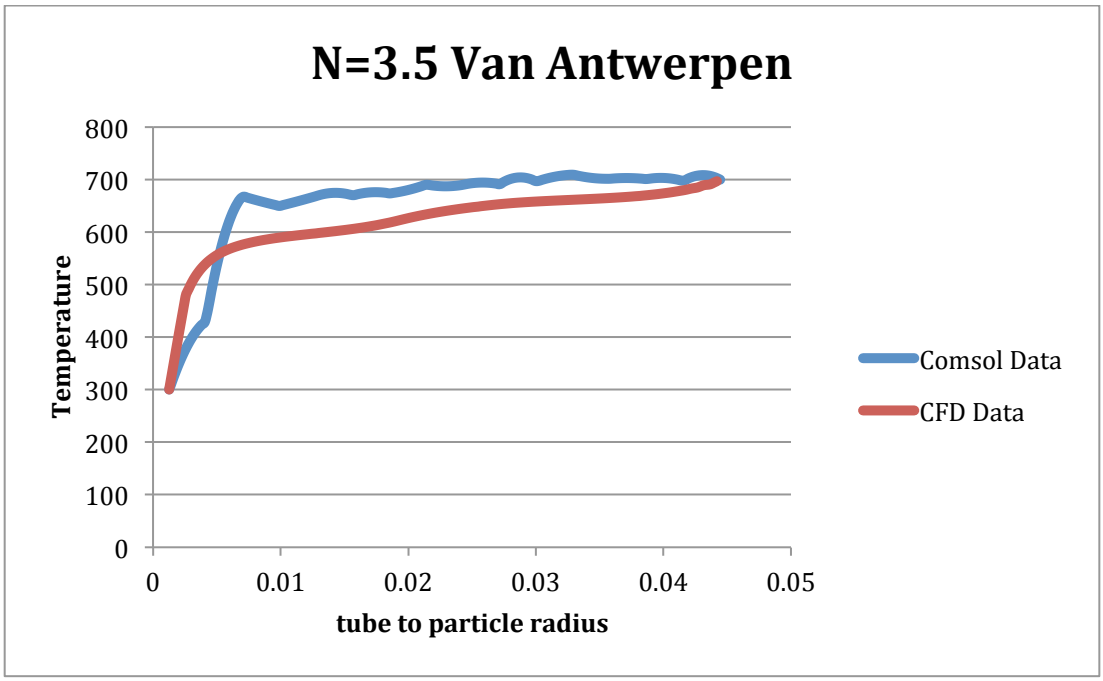
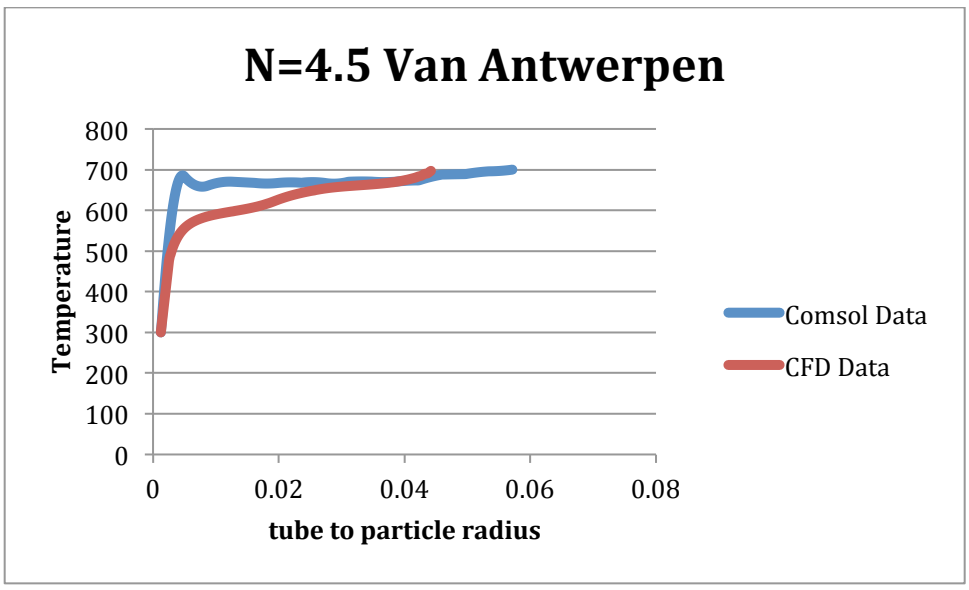
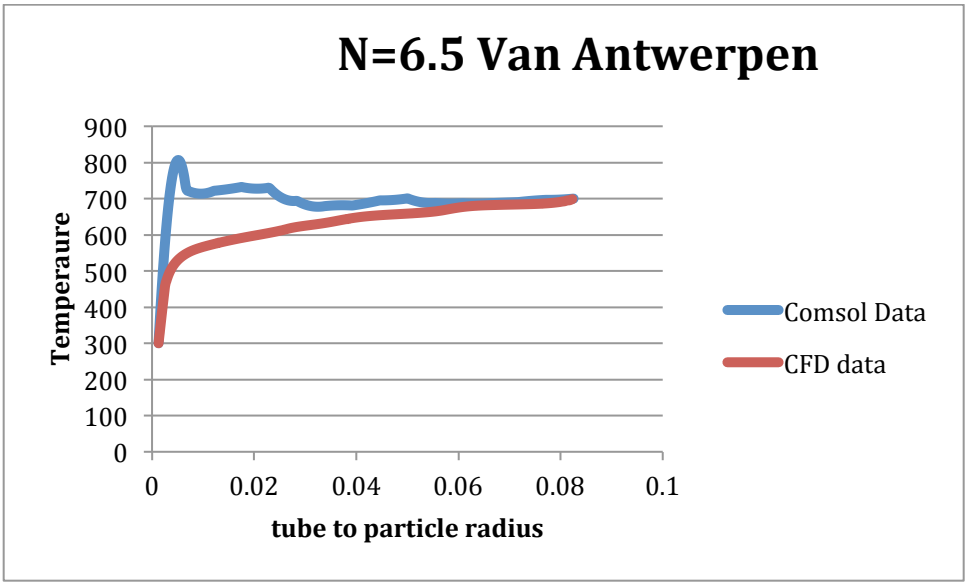
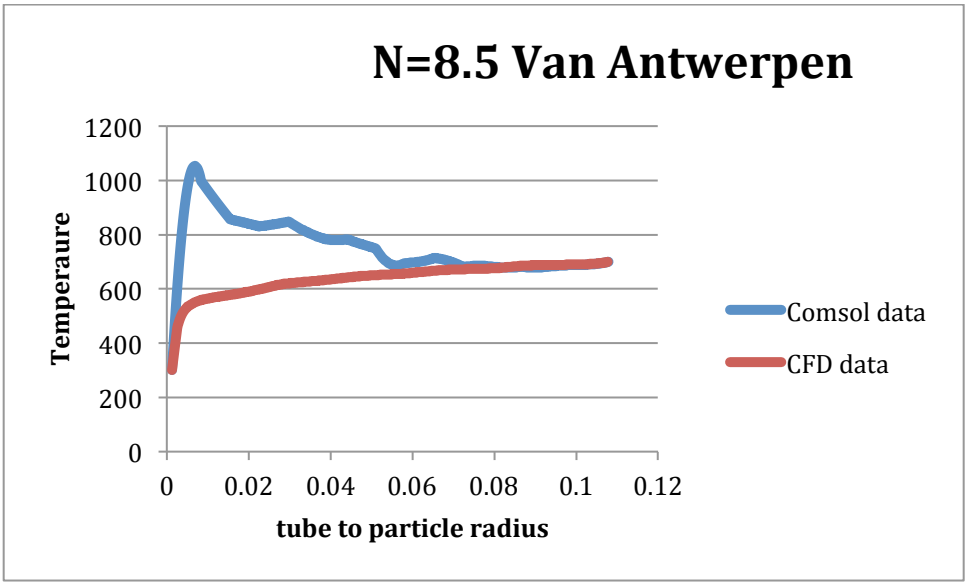
0.14
tube to particle radius
CFD Data
Comsol Data

5.2 - Van Antwerpen Formula Graphs









Section 6: References

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