Flow Analysis in a Radial Flow Fixed Bed Reactor

A Major Qualifying Project Report

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Abstract

When designing radial flow fixed bed reactors, one of the most prevalent design tasks is ensuring proper distribution through the catalyst bed. Utilizing COMSOL Multiphysics, a 2-d axis symmetric model was tested to evaluate the level of maldistribution of flow through the catalyst bed. Specifically, the effects of flow direction, catalyst size, overall and variable screen resistance, and the total amount of flow through the reactor. Maldistribution findings were based on a velocity profile through the catalyst bed.

Executive Summary

A major design task in radial flow fixed bed reactors is the effect of flow maldistribution in the catalyst bed of the reactor. In partnership with Cambridge Chemical Technologies, Inc. (CCTI) and a leading petrochemical company, a COMSOL Multiphysics model was created to simulate the flow patterns through a given reactor geometry. This executive summary reviews our process, as well as our findings and recommendations for future studies to be conducted by CCTI.

Methodology

Utilizing COMSOL Multiphysics, and the given geometry of the reactor, a 2-D axis symmetric model was created to simulate the reactor. From the provided flow data we attempted different physics systems before settling on a fully turbulent flow physics model. This included the implementation of varying flow resistances for each portion of the reactor as shown in Figure 1.

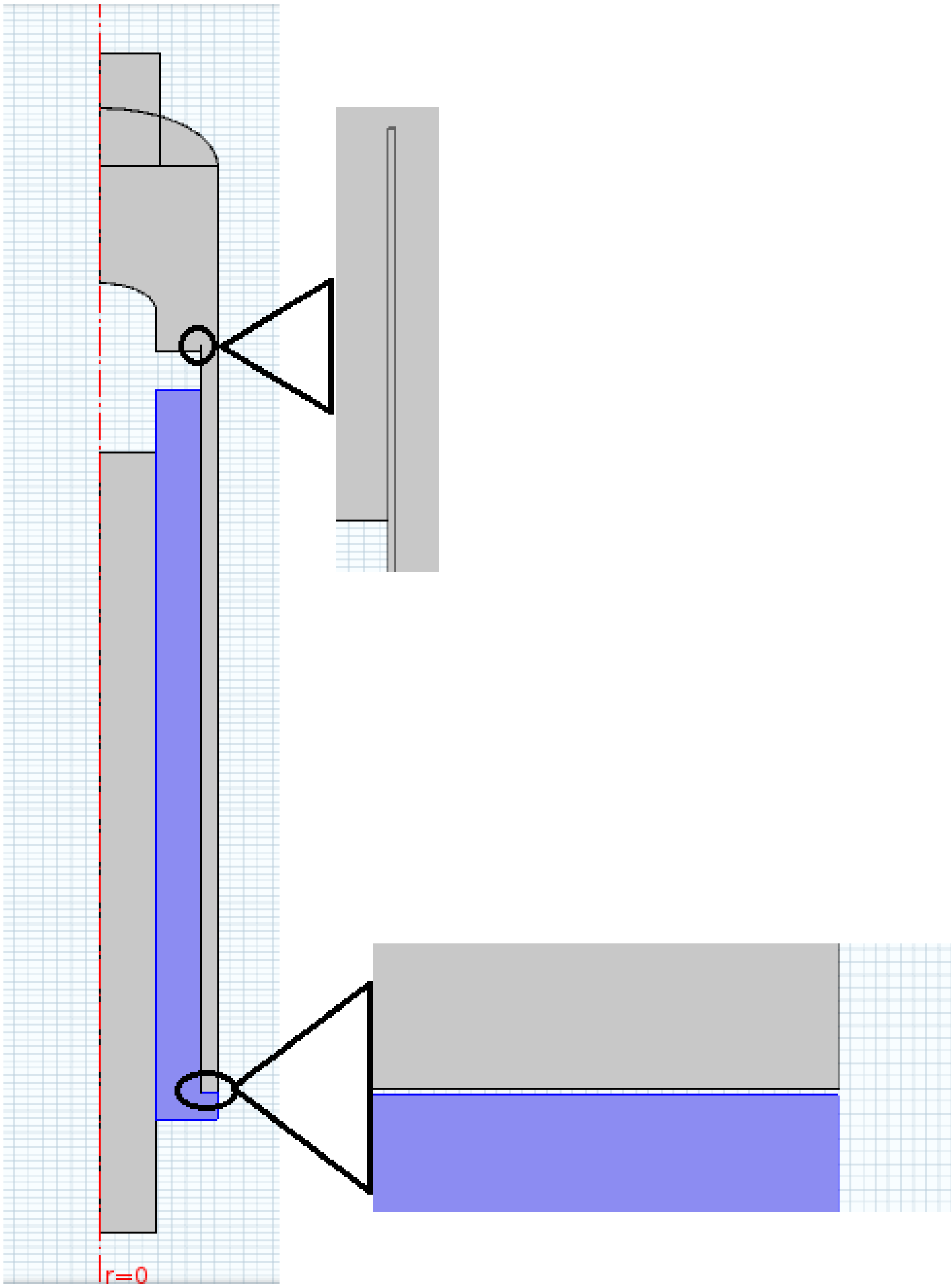

Figure 1: Reactor Geometry

Different variables were altered to determine their effect on the maldistribution through the catalyst bed. The variables studied were;

- Flow direction
- Catalyst size
- Overall screen resistance
- Amount of flow
- Variable screen resistance

From these models, velocity profiles through the catalyst bed were obtained and analyzed to determine the extent of the maldistribution in each reactor configuration, an example profile is shown in Figure 2.

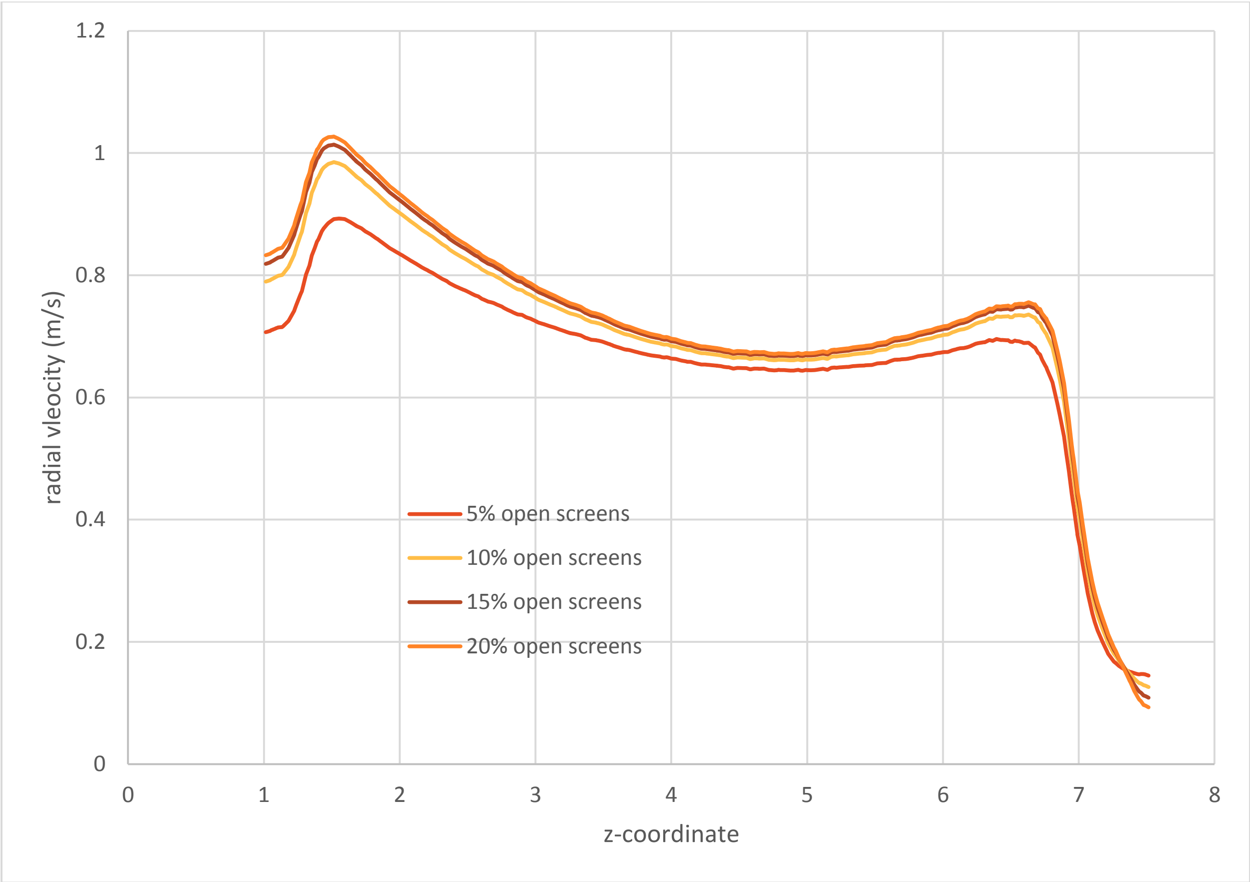

Figure 2: Example Velocity Profile

Results and Recommendations

After analyzing the data from the various simulations, we determined which configuration would give the least amount of maldistribution in the catalyst bed. That configuration is a normal flow direction with a 1/16" catalyst bed, utilizing a variable screen resistance. Upon completing our study, we made the following recommendation to CCTI in regards to future studies to further evaluate this particular reactor;

I. An additional simulation geometry should be created that makes use of a "dummy cone". This would involve a radially outward flowing design, where the inlet is directly above an inert cone that would direct the flow out radially. (Put in photo)

II. Conduct an in depth study of creating a screen with variable openness across it's length. This study could address the maldistribution in the reactor better than a single screen openness, which was largely used in this study.

III. The addition of Heat Transfer physics to the current model in COMSOL. This will provide a more comprehensive analysis for future use.

IV. Conducting an additional study on the reaction taking place within the reactor. This simulation will provide critical data that can be combined with the flow study for an overall reactor synopsis.

Acknowledgments

We would like to thank the following individuals and organizations for their support and contribution to the success of this project.

- Waheed Mukaddam, CEO of Cambridge Chemical Technologies for his great support of our project.
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- Professor Anthony Dixon for his efforts in challenging us to practice good engineering discipline and his excellent guidance and support through the project experience.
- Worcester Polytechnic Institute, who’s partnerships with companies like CCTI make project experiences like this possible.

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1. Introduction

Radial flow packed bed reactors are used to carry out large scale catalytic chemical reactions in the petroleum and chemical industries (Li, 2007). This specific type of reactor has strong advantages for catalytic processes such as ammonia synthesis, catalytic reforming, and dehydrogenation of ethyl benzene. The ability to operate at a low pressure drop compared to an axial flow reactor for the same volumetric flow creates opportunities for saving cost. Inside the radial flow reactor, a given volume flows radially throughout a catalyst bed. It is recommended to have a uniformly distributed flow over the bed to efficiently utilize the catalyst (Kareeri, Zughbi, Al-Ali, 2006). A flow distribution of processes can be studied using a computational fluid dynamics (CFD) model to understand the complicated system.

COMSOL Multiphysics ® is a modeling and simulation software that uses finite element methods for approximating partial differential equations (COMSOL , Inc, 2014). It can be used for analyzing sophisticated models involving electrical and mechanical applications, fluid flow and chemical reactions (COMSOL , Inc, 2014). One of the advantages of using this software is the flexibility in adding physics within the same model. For example, reactor geometry can be built to study a fluid flow and more features can be applied to the same geometry to expand the analysis on heat transfer or reaction physics of the system. Resources at Worcester Polytechnic Institute were utilized to conduct Major Qualifying Project (MQP) under a supervision of Professor Anthony Dixon. His scholarly work is in CFD studies of fluid flow through beds of particles, heat transfer in structured fixed-bed reactors and many more.

The goal of the project was to study the fluid maldistribution in a radial flow packed bed reactor keeping the low pressure drop, which was designed by a leading petrochemical company. By working with Cambridge Chemical Technologies, Inc (CCTI) and a leading petrochemical company, there were several objectives to accomplish this goal. First, three chemical engineering students from WPI formed a group with Professor Dixon to learn COMSOL, which was used to simulate the flow behavior in the reactor. Second, the group created reactor geometry and specified flow properties based on provided information from sponsors. Third, several simulations were ran varying flow configuration, total amount of flow, resistance in the reactor and catalyst size to find the best flow distribution condition. Lastly, the results were summarized in this report to provide detail analysis on findings, and COMSOL file was shared with appropriate group of people who were involved with this project.

2. Background

2.1 Radial Flow Reactors

Radial flow reactors differ from more commonly used axial flow reactors. In an axial flow reactor, feed enters at one end of the reactor, flows across the catalyst bed in the direction along the axis of the reactor, and exits from the other end. In comparison, a radial flow reactor is designed so that the feed is distributed along the length of the reactor. This technique is beneficial because a distance that feed travels through the reactor is longer, so it is useful for larger scale process. A flow passes through a catalyst bed in the radial direction, then exits the system. Figure 3 shows a simple schematic of the two types of reactors.

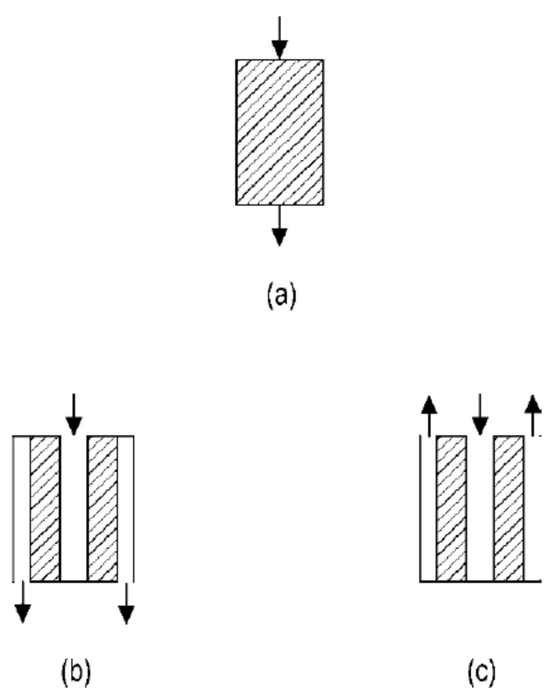

Figure 3: (a) Axial flow reactor, (b) Z-shaped and (c) Π-shaped radial flow reactors (Li, 2007)

In a Z – shaped reactor shown in Figure 3, the feed and the effluent flow in the same direction in the center pipe and the annulus, while the two flow move in the opposite directions in a Π – shaped reactor (Li, 2007).

Radial-flow reactors were developed to replace axial-flow reactors for large-scale chemical plants in the late 1960s and early 1970s (Li, 2007). To increase a plant capacity, a diameter needs to be increased for an axial flow reactor to keep the same pressure drop across the catalyst bed. This result in a thicker, heavier and more expensive reactor shell, and more risk to operate. There is also a limitation in a scale-up process because the ability to increase a diameter depends on capabilities of fabrication and transportation facilities. At some point, axial-flow reactors become impractically large so that multiple reactors are needed to install in parallel. In comparison, a capacity of a radial-flow reactor can be increased by increasing the length of the reactor instead of the diameter (Li, 2007). This is because a reactant is fed along the length of the reactor, so there is a larger cross sectional area available for the flow. The shallower catalyst bed also provides smaller pressure drop across the radial flow catalyst bed. Pressure drop plays an important role because smaller pressure drop allows a reduction in catalyst particle size to increase the productivity and effectiveness. It is also safer to operate under the lower pressure drop.

The design of the radial flow reactor is more complicated than that of the axial flow reactor (Li, 2007). There are some concerns that are unique to designing the radial flow reactor:

- The flow must be distributed uniformly along the length of the reactor to achieve a good conversion of the reaction (Kareeri, Zughbi, Al-Ali, 2006). If the flow is unevenly distributed throughout the bed, some part is used more than the other part, which could lead to corrosion.
- Over time, catalyst settling will create a void space at the top of a radial catalyst bed, which could allow a flow bypassing. About 5–15 % of extra catalyst is normally loaded in a radial-flow reactor to allow for settling (Li, 2007). This value depends on mechanical properties of the catalyst and the frequency of reactor startup and shutdown (Li, 2007).
- A radial flow reactor requires additional void space for distributing flow along the length of the reactor (Li, 2007). This space, called annulus, is used for distributing flow along the length of the reactor.
- The system efficiency and its cost-effectiveness are strongly influenced by the screen design (Johnson Screens, 2014). Screens are used to control the amount of flow goes through the bed by installing before and after the catalyst. They should be designed to withstand the thermal stresses that develop with each startup and shutdown process of the reactor (Li, 2007).

2.2 Applications of the Radial Flow Reactor

Some of the applications of the radial flow reactors are ammonia synthesis, ethyl benzene dehydrogenation and catalytic forming. Among others, the benefits of using the radial flow reactor were especially appealing for these processes.

2.2.1 Ammonia Synthesis

Converting from hydrogen and nitrogen is an exothermic reaction, where it is usually carried out at 400–500 C^{o} and 14 – 21 MPa (Li, 2007). The ammonia concentration in the reactor effluent is 12–22 %, which results in a large amount of the recycling of the synthesis gases (Li, 2007). In radial flow reactor, smaller compressor for the recycle gas can be used because of the smaller pressure drop, and also the efficiency can be improved by reduced catalyst particles.

2.2.2 Dehydrogenation of Ethylbenzene

Dehydrogenation of Ethylbenzene to styrene is an endothermic reaction carried out with steam dilution at 540 – 650 C^{o} and under low pressure or vacuum (Li, 2007). The reaction is limited by thermodynamic equilibrium, and the reactant must be reheated between the catalyst beds in order to achieve 60–70 % per-pass conversion (Li, 2007). Commercial styrene plants typically have two or three catalyst beds in series, each contained in individual vessels, with external or internal interstage reheaters (Li, 2007).

The radial flow reactor is preferred for this process because both the conversion and selectivity are favored by lower pressure (Li, 2007).

2.2.3 Catalytic Reforming

Catalytic Reforming is an important refining process for upgrading the octane number of naphtha for gasoline blending, where the endothermic reaction is carried out at a temperature range of 430 – 540 C^{o}, and the pressure of above 2.8 MPa to control catalyst deactivation caused by coking (Li, 2007). It is a major process for production of benzene, toluene, and xylenes for the petrochemical industry (Li, 2007). Several reactions take place in catalytic reforming: dehydrogenation, isomerization, dehydrocyclization, and hydrocracking. Using the radial flow reactor, providing the reduced pressure drop and the hydrogen recycle compressor, the newer generation of reformers operates below 700 kPa (Li, 2007).

2.2.4 Flow Distribution

Flow distribution along the length of the catalyst bed, catalyst basket design and catalyst settling are the important factors that must be considered for the mechanical design of a commercial reactor (Li, 2007). A low flow condition can affect the radial flow reactor, because it is more difficult to distribute the feed uniformly throughout the bed with low pressure drop. Longer the bed, larger the effect of flow maldistribution, resulting in an inefficient use of the catalyst bed. One way to solve this problem is to increase the pressure drop in the reactor. This will decrease the scale of maldistribution, but can also lead to increase in operational costs. Another way is to increase the resistance of the screens before and after the bed to control the amount of flow. By varying the hole size and location in the screens, flow can be designed to pass evenly through the bed. Johnson Screens is a leading company in screening technology in water treatment, food and beverage processing, pulp and paper, oil and gas, mineral and aggregate processing, and refining and petrochemical industries (Johnson Screens, 2014).

2.2.5 Screen Designs

Johnson Screens is the leading manufacturer of reactor internals and related assembles that are essential to produce high efficiency in radial flow system operations (Johnson Screens, 2014). Figure 4 below shows a Z – shaped radial flow reactor containing the screens before and after the catalyst bed. The process stream passes through the outer basket, across the catalyst bed and is collected in a center screen where it passes out the stream from the outlet.

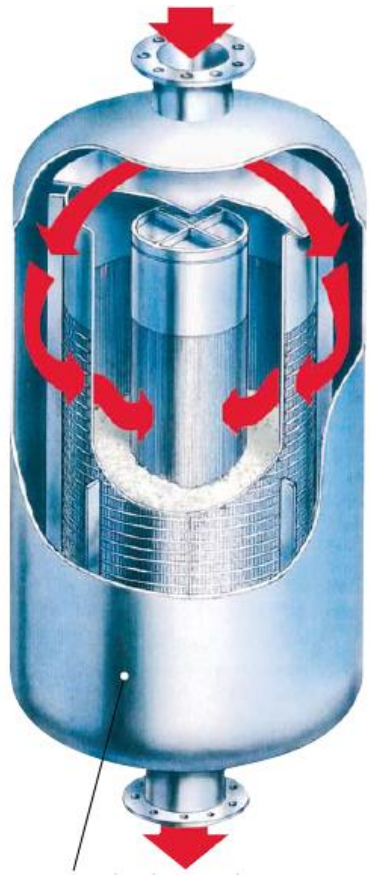

Figure 4: The inside of the Z – shaped radial flow reactor with screens (Johnson Screens, 2014)

There are several designs of the screens used in the catalyst basket, such as perforated sheet scallops that are standard in the industry, and Vee Wire screens that have inwardly enlarging slots which allow only two – point article contact shown in Figure 5 (Johnson Screens, 2014). The operating advantages of Vee Wire screens are that the vertical slots allow the catalyst to slide up and down smoothly without abrading, and each slot can be as narrow as 0.25mm to retain small size catalyst (Johnson Screens, 2014).

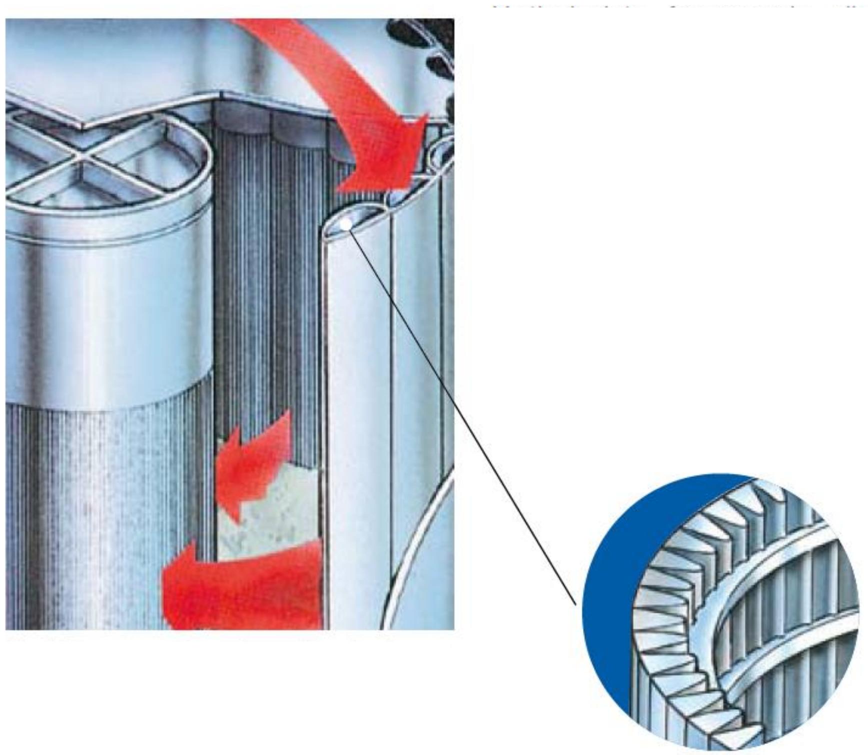

Figure 5: Vee Wire Scallops produced by Johnson Screens (Johnson Screens, 2014)

2.2.6 Catalyst Settling and Flow Bypassing

A critical feature in the design of a radial-flow reactor is to prevent bypass at the top of the catalyst bed (Li, 2007). This is because catalyst settles or slumps, physically drops in height, over time in a radial-flow reactor (Li, 2007). Catalyst shrinkage is a main reason why the radial-flow reactor is not as obvious a choice for methanol synthesis as for ammonia synthesis. The methanol synthesis catalyst is mechanically weaker than the ammonia synthesis catalyst, and it shrinks significantly during activation that takes place in the reactor (Li, 2007). The flow direction and distribution across a radial-flow reactor affect material selection and design of the catalyst bed, screens and catalyst settling.

2.3 Computational Fluid Dynamics

COMSOL Multiphysics ® is a modeling and simulation software that uses finite element methods for approximating partial differential equations (COMSOL , Inc, 2014). The computational fluid dynamics (CFD) module is a platform for simulating devices or systems that involve sophisticated models involving electrical and mechanical applications, fluid flow and chemical reactions (COMSOL , Inc, 2014). The CFD modules in COMSOL provide multiple physics interfaces to formulate equations. In fluid flow modules, particular physics can describe compressible, non-isothermal, non-Newtonian, two-phase, and porous media flows all in laminar and turbulent flow. One of the advantages of using COMSOL is that there is a flexibility in adding physics within the same model. Different features can be applied to the same geometry to expand the analysis on fluid flow, heat transfer and reaction physics of the system. There are necessary steps in modeling complex processes using the module:

- Selecting the description of the flow, such as single or two-phase, and laminar or turbulent flow.
- Creating the model geometry.
- Defining the fluid properties.
- Adding source and sink terms, or editing the underlying equations of the fluid model.
- Selecting mesh elements and controlling the density of the mesh at different positions.
- Selecting and tuning of solvers.

2.4 First Approach

The student group decided to use porous media flow module to model flow through catalyst bed. This module allows modeling the transport of single – phase and two – phase fluids in porous media (COMSOL, Inc. 2014). This is done by utilizing the combination of Darcy's Law and Brinkman's equations shown in Equation 1 and 2.

$$0 = \nabla \cdot \left[-\rho l + \frac{\mu}{\epsilon_p} (\nabla \mathrm{u} + (\nabla \mathrm{u})^T) - \frac{2\mu}{3\epsilon_p} (\nabla \cdot \mathrm{u}) l \right] - \left(\mu K^{-1} + \beta_F |\mathrm{u}| + \frac{Q_{br}}{\epsilon_p^2} \right) \mathrm{u} + \mathrm{F} \tag{1}$$

$$\rho \nabla \cdot \mathrm{u} = Q_{br} \tag{2}$$

Darcy's Law describes porous media where the pores are small enough to negate viscous effects, and so that the flow is driven by a pressure difference, which the Brinkman equations include terms accounting for viscous effects (COMSOL, Inc. 2014). This module was only appropriate for laminar flow, which lead the group to look for another solution as the given flow properties suggested the turbulent flow.

2.5 Second Approach

A single – phase flow module was selected to model turbulent flow. This module solves multiple variations of the Navier – Stokes equations to model flows in all velocity regimes including a low-velocity fluids, creeping flow (Stokes flow), laminar and weakly-compressible flow, and turbulent flow (COMSOL, Inc. 2014). Turbulent flow is modeled using the Reynolds – Averaged Navier-Stokes (RANS) approach and includes the k-ε, low-Reynolds k-ε, k-ω, SST (Shear Stress Transport), and Spalart – Allmaras turbulence models (COMSOL, Inc. 2014).

Navier-Stokes Equation (Equation 3) and Continuity Equation (Equation 4) were used to describe the incompressible turbulent flow in the radial flow reactor. These equations are used to describe a momentum balance and the relationship between fluid density, velocity, time, and the term F represents forces acting on the fluid per unit volume. This term was added to the system to provide the resistance in the screens.

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

$$\rho\nabla \cdot \mathrm{u} = 0 \qquad (4)$$

Reynolds-averaged Navier-Stokes (RANS) approach was used to describe the turbulence of the flow. Based on the Boussinesq hypothesis, Reynolds stresses can be modeled using an eddy (or turbulent) viscosity, μ_T, which includes two transport terms (Equation 5). Thus, the $k - \varepsilon$ model was selected to take two transport equations into account, the turbulent kinetic energy, k and dissipation ϵ shown in Equation 6 and 7 respectively. The k determines the energy in the turbulence, and ϵ determines the scale of the turbulence. Equations 6 and 7 describes the conservation of momentum in turbulence where starting volume flow is equal to the combination of the viscosity term and production term less the dissipation term. The production term P_k is shown in Equation 8, and necessary constant values, $C_\mu = 0.09, \sigma_k = 1.00, \sigma_\epsilon = 1.30, C_{1\epsilon} = 1.44\ and\ C_{2\epsilon} = 1.92$ were built in the COMSOL module.

$$\mu_T = \rho C_\mu \frac{k^2}{\epsilon} \tag{5}$$

$$\rho(\mathrm{u} \cdot \nabla)\mathrm{k} = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k}\right)\nabla_k\right] + P_k - \rho\epsilon \tag{6}$$

$$\rho(\mathrm{u} \cdot \nabla)\epsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_\epsilon}\right)\nabla_\epsilon\right] + C_{\epsilon 1}\frac{\epsilon}{k}P_k - C_{\epsilon 2}\rho\frac{\epsilon^2}{k} \tag{7}$$

$$P_k = \mu_T[\nabla\mathrm{u}: (\nabla\mathrm{u} + (\nabla\mathrm{u})^T)] \tag{8}$$

In addition to these built – In formulations, source or volume force terms can be introduced by customizing the variables. This is useful to take into account special material properties, and to define boundary conditions.

2.6 Sponsoring Organizations

This Major Qualifying Project (MQP) was sponsored by a leading petrochemical company and Cambridge Chemical Technologies, Inc (CCTI). The project was proposed from the company to simulate the pure component flow of the designed radial flow reactor, ignoring the reactions in the catalyst bed. This company contracted the research development to CCTI, with whom the student group worked together to understand the flow distribution in the radial flow fixed bed reactor with a given geometries. The pressure drop, flow rates and other necessary information for the simulation was provided by the sponsors. Located in Cambridge, Massachusetts, Cambridge Chemical Technologies, Inc. (CCTI) is a technology based process engineering firm with expertise in chemicals, petrochemicals, and alternative energy technologies (CCTI, 2014). CCTI was formed in 2004 as a client – centered and efficient, rigorous and creative thinking organization to offer services including technology transfer in diverse industries as synfuels, biofuels, agrochemicals, oleochemicals, alternative energy, and nuclear fuels (CCTI, 2014). CCTI engineers are especially recognized leaders in the application of fluid bed technology, with technically advanced designs in operation worldwide (CCTI, 2014).

3. Methodology

3.1 Geometry Creation

In order to perform a comprehensive study of the flow patterns through the catalyst bed in the reactor, it was important to develop an accurate geometry. A geometry was created based on a design with specified dimensions that was provided by the sponsor company. Since the design was a cylindrical model that had symmetry, the geometry was created using the 2-D axisymmetric modelling capabilities of COMSOL. The symmetry in the model allowed for the geometry to be drawn and simulated as a group of rectangular regions which could be rotated 360 degrees around a central axis to create a 3-D simulation. This allowed the model to be solved using less time and processing power than if it had been created with a 3-D geometry. The geometry was drawn in three sections to represent the three concentric regions of the reactor.

3.1.1 Inner Annulus and Inner Screen

The inner annulus was drawn as a rectangle with its left boundary on the line of symmetry. The rectangle had a length of 6.959 meters and a width of 0.5 meters to represent a cylinder with a length of 6.959 meters and a diameter of 1 meter. The bottom boundary of this rectangle was divided into two line segments. The first segment began at the bottom left corner of the rectangle and extended to the right 0.455 meters. The second segment extended the last 0.045 meters. This was done so that the eventual boundary condition could be only applied to one segment of the boundary in order to simulate the nozzle that was specified by the sponsor. The screen on the inside of the catalyst bed was drawn as a rectangle with a width of 0.001 meters and a length of 5.945 meters. The top of the screen was positioned so that it was level with the top of the first rectangle. The width of the rectangle was determined by looking at the screen thickness of standard screens manufactured for radial flow reactors by Johnson Screens (Johnson Screens, 2010).

3.1.2 Catalyst Bed and Outer Screen

The catalyst bed was drawn using the “Draw Line” function of COMSOL, allowing the creation of a unique shape. The shape began at the bottom right corner of the inside screen described previously. The first side extended up for 5.945 meters, then a line was drawn from that point going left for 0.001 meters. From there, a line was drawn going up 0.555 meters, then a line going right 0.499 meters, then a line going down 6.26 meters, a line going right 0.001 meters, a line going down 0.001 meters, a line going right 0.15 meters, a line going down 0.239 meters, and then a line connecting this point to the starting point. The screen on the outside of the catalyst bed was drawn as a rectangle with a width of 0.001 meters (Johnson Screens, 2010) and a length of 6.655 meters. The left side of this rectangle was touching the right side of the shape for the bed so that the two resembled an “L.”

3.1.3 Outer Shell

The outer shell region was drawn in three sections. The first section made up the outer annulus that ran adjacent to the catalyst bed. This section was again drawn using the "Draw Line" function. The starting point for the shape was at the bend in the "L" shape drawn previously. From this point, a line was drawn up 6.655 meters, then left 0.001 meters, down 0.05 meters, left 0.399 meters, up 0.357 meters, left 0.5 meters, up 1.289 meters, right 1.05 meters, down 8.251 meters, and then back to the starting point. An ellipse was then drawn with a width of 1 meter and a 2:1 width to height ratio. The top right quadrant of this ellipse was overlaying part of the shape so that when the "Difference" function in COMSOL was used, it cut that elliptical shape out from the geometry. The second section made up the inlet nozzle to the reactor. It was drawn as a rectangle that was 1.015 meters long and 0.535 meters wide. The third section was drawn as an ellipse with a width of 2.1 meters and a 2:1 width to height ratio. It was overlaying the two previous shapes so that a segment of the top-right quadrant would be added to the geometry after using the "Difference" function in COMSOL. These three shapes were then combined into one using the "Form Union" function. The "Form Union" function ensured the model would recognize the shapes as one continuous region rather than multiple different regions

3.1.4 Finished Model

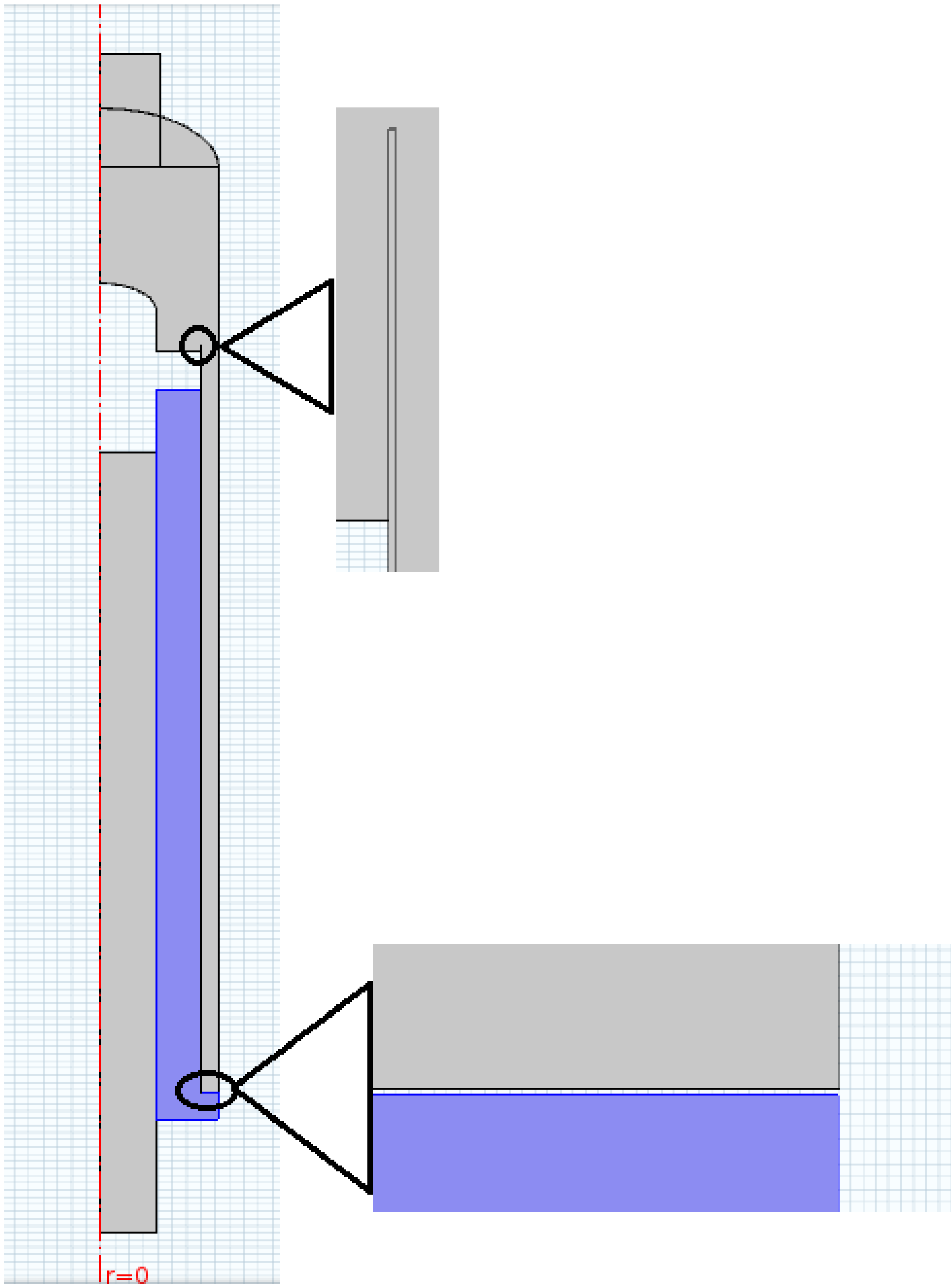

Figure 6: Finished Model Geometry

The final geometry for the flow model can be seen in Figure 6. The blue section represents the catalyst bed with its left and right borders containing the inner and outer screens respectively. In the real model, the empty space above the catalyst bed is filled by inert balls. However, since there was very little flow through the region, it was modelled as empty space so that it would contain no flow in the simulation. The inlay near the top of Figure 6 shows the area where the outer screen protrudes slightly into the open flow area. The inlay towards the bottom of Figure 6 shows that there is a 0.001 meter space between the bottom of the outer annulus and the catalyst bed so that there is no flow going downwards into the bed. Instead, all the flow is forced to turn and go through the bed in a radial direction. This geometry was used for all simulations in the study.

3.2 COMSOL Physics

This stationary study on the radial flow reactor used a single-phase turbulent flow model in order to accurately simulate the flow rate provided by the project sponsor, which had a Reynolds' number around 5 million at the reactor inlet and a Reynolds' number of 325 through the catalyst bed. In order to account for the resistance provided by the catalyst bed and both of the screens, source terms were added to the flow equations in those three regions (Ranade, 2006).

3.2.1 Free and Porous Media Flow

The initial COMSOL model utilized the "Free and Porous Media Flow" physics model. This particular physics setting was seen as optimal for the catalyst bed as it incorporated given data such as viscosity (μ) and density (ρ) into the model geometry. However, this particular model does not couple with the turbulent flow that is found in the outer annulus and center of the reactor, even though the flow through the bed is in a transitional phase. Therefore, a strictly turbulent model was developed to overcome this.

3.2.2 Turbulent Flow

The model applied a RANS type k-ε turbulence model to the entire geometry in order to simulate the fluid flow through the reactor. Both the fluid density (ρ) and dynamic viscosity (μ) were specified based on data supplied by the project sponsor. Even though it was a gas, the fluid was assumed to be incompressible because the pressure drop through the system was around 10 kPa, a reasonably low value. All walls in the system were specified to have a no-slip condition. The inlet and outlet pressures were specified as 466797 Pa and 453067 Pa respectively, based on the data provided by the project sponsor. The initial velocity for the entire geometry was specified as a velocity field with a radial component of 37 m/s and an axial component of 1 m/s. These values were chosen with the intent of helping the model simulate the first change of direction for the inlet flow.

3.2.3 Volume Force in Catalyst Bed and Screens

The resistances to flow found in both the catalyst bed and two screens were achieved by adding a source term to the flow model known as “Volume Force” in the COMSOL program (Ranade, 2002). The Volume Force is a source term (represented as F in COMSOL equations) that was calculated based on certain properties of the region and is given in units of N/m^3. It was dependent on the radial and axial velocity components calculated by the model at each coordinate.

The equation for the Volume Force in the catalyst bed was:

$$F = -\frac{\mu}{K} * v - \frac{C2B * \rho}{2} * |v| * \vec{v} \qquad (9)$$

With values specified in Table 1:

Parameter	Value/Equation	Description
v		Velocity
µ	0.0000194 Pa*s	Fluid Dynamic Viscosity
Dp	0.0042 m	Catalyst Particle Equivalent Diameter
ε	0.36	Catalyst Bed Void Fraction
K	(Dp^2*ε^3)/(150*(1-ε)^2)	Catalyst Bed Permeability
C2B	(3.5*(1-ε))/(Dp*ε^3)	Catalyst Bed Inertial Resistance

Table 1: Values used in Volume Force equation for Catalyst Bed

Equation 9 is essentially Darcy’s law, an equation utilized to describe single-phase laminar flow through a porous media. However, this version also includes a term to describe the inertial resistance, which comes from Forchheimer, making it the Darcy-Forchheimer Law. This inertial term must be added to help account for the non-linear flow created by the high velocity that the model was simulating. The equations used to calculate K and C2B are both based on equation 10, the Ergun equation.

$$\frac{\Delta P}{L} = \frac{\mu}{K} v + C_2 \left(\frac{\rho v^2}{2}\right) \qquad (10)$$

The equation for the Volume Force in the outer screen was:

$$F = -\frac{C2So * \rho}{2} * |v| * \vec{v} \qquad (11)$$

With values specified in Table 2:

Parameter	Value/Equation	Description
v		Velocity
ρ	2.42 kg/m^3	Fluid Density
Apo	37.6 m^2	Outer Screen Area
Afo	3.76 m^2	Combined Area of Holes in Outer Screen
C	0.62	Orifice Coefficient
Δx	0.001 m	Screen Thickness
C2So	((Apo/Afo)^2-1)/(C^2*Δx)	Outer Screen Inertial Resistance

Table 2: Values used in Volume Force equation for Outer Screen

The equation for the Volume Force in the inner screen was:

$$F = -\frac{C2Si * \rho}{2} * |v| * \vec{v} \qquad (12)$$

With values specified in Table 3:

Parameter	Value/Equation	Description
v		Velocity
ρ	2.42 kg/m^3	Fluid Density
Api	18.52 m^2	Inner Screen Area
Afi	1.85 m^2	Combined Area of Holes in Inner Screen
C	0.62	Orifice Coefficient
Δx	0.001 m	Screen Thickness
C2Si	((Api/Afi)^2-1)/(C^2*Δx)	Inner Screen Inertial Resistance

Table 3: Values used in Volume Force equation for Inner Screen

Equations 11 and 12 are both based on a simplified version of the Darcy-Forchheimer Law called the "porous jump" model. This model only includes the inertial term from the Darcy-Forchheimer Law and ignores the viscous term. This model was used because the fluid velocity was high enough through the screens so that the inertial term dominated the equation, making the viscous term irrelevant (Kareeri, 2006).

3.3 Changes Made for Each Set of Runs

Since the purpose of this study was to determine how changes in different aspects of the reactor would affect the velocity and flow distribution in the bed, multiple sets of runs were organized. For each set of runs, a single parameter was adjusted so that a comparison could be made on the effects of changing that parameter. Studies were done on the effects of changing the catalyst particle size, the direction of flow, the open area fraction of both of the screens, the amount of flow through the reactor, and the use of variable resistance screens.

3.3.1 Catalyst Particle Size

The first study was done on the effect of catalyst particle size on the velocity and distribution in the catalyst bed. The two catalysts that were used were a cylindrical particle with diameter of 1/8 inch and length of 3/16 inch. The other particle studied was also cylindrical, and it had a diameter of 1/16 inch and the same length of 3/16 inch. In order to reflect this change in catalyst particle size, the particle equivalent diameter that was used to calculate the Volume Force term in the catalyst bed was set as 0.0042 m for the 1/8 inch catalyst and 0.00262 m for the 1/16 inch catalyst. The equivalent diameter for each of the catalyst particles was calculated as the diameter of a sphere that had an equivalent volume to the cylindrical catalyst particle. This diameter was used because the flow resistance equation in the model was based on the Ergun equation, which is only accurate for spherical catalyst particles.

3.3.2 Normal Flow and Reverse Flow

The second study was used to determine the effects of changing the direction of flow. The “normal” flow pattern was simulated by setting the pressure boundary condition at the top port of the reactor to 466797 Pa. The pressure at the bottom port of the reactor was set to 453067 Pa, which satisfied the pressure drop that had been provided by the sponsor. This simulated a flow pattern that entered at the top of the reactor and exited out the bottom. The “reverse” flow pattern was simulated by switching the two boundary conditions. The higher pressure was set for the bottom port and the lower pressure was set for the top port so that the model would simulate flow entering the bottom and exiting the top of the reactor.

3.3.3 Different Screen Resistances

The next set of studies were done to understand the effects of using screens that had different resistances to flow. The study was done using the 1/8 inch catalyst in the normal flow configuration. The study consisted of four sets of data: one using inner and outer screens with an open fraction of 5%, one at 10% open, one at 15% open, and another at 20% open. These open fractions simulated changes in the amount and size of the holes in the screens used to hold the catalyst particles in place. This variable was controlled by changing the fraction of the open area to the total screen area for each of the screens (Afi to Api for the inner screen and Afo to Apo for the outer screen). Depending on the trial, the open area for each of the screens was either 6%, 10%, 15%, or 20% of that screen's total area. It is important to note that this study focused exclusively on screens with uniform resistance to flow.

3.3.4 Changing Total Flow through the Reactor

The fourth study focused on how changing the amount of flow through the reactor would affect the velocity and distribution in the bed. This study was performed on only the normal flow direction based on findings in previous studies, only utilized screens with an open area that was 10% of the total screen area, and included the catalyst of 1/16 inch diameter. Since the boundary conditions used in the model were based on pressure, the flow was changed by altering the pressure drop. The pressure drop was changed simply by changing the outlet pressure. Three trials were done: one with an outlet pressure of 453067 Pa, one with an outlet at 433067 Pa, and another with an outlet at 413067 Pa. Greater flow rates were unable to be studied because the thickness of the catalyst bed limited the pressure drop by design.

3.3.5 Variable Screen Resistance

The final study focused on creating screens that would improve the flow distribution in the reactor. Based on the inlet and outlet flow distributions from previous runs, it was determined that the outer screen should have more resistance at the bottom 0.5 meters than normal and that the inner screen should be more resistant at the top 0.5 meters and the bottom 2.5 meters. This was done by altering the geometry so that the rectangle representing the inner screen was broken into three rectangles and the outer screen was broken up into two rectangles. The screen resistances were adjusted so that the inner screen was 10% open at the bottom, 15% open in the middle section, and 5% open at the top. The outer screen was adjusted so that the bottom section was 5% open and the rest of the screen was 15% open. This was done by varying the fraction of Afi to Api for each of the inner screen sections and by changing Afo to Apo for both of the outer screen sections.

3.4 Data Analysis

3.4.1 Maldistribution Index

The maldistribution index is a measure of how non-uniform a flow distribution is. In some previous studies done on the distribution of flow through a radial flow reactor, the axial velocity just before the catalyst bed was used as a measure of uniform flow (Kaye, year unknown). For a uniform flow pattern, this axial flow would decrease linearly with the axial coordinate. Once the axial coordinate reached the bottom wall of the outer annulus, the axial velocity would be zero. The actual axial velocity profile would then be compared to this line and the area between the two was called the maldistribution index or maldistribution extent. However, since one aspect of our study utilized screens that had regions of varying resistance, this measure of uniform flow would not work. Instead, the average radial velocity at the radius being studied was used as a measure of a uniform flow pattern. This allowed the maldistribution index to be defined as the area between the average radial velocity and the radial velocity profile at whatever radial coordinate was being studied.

3.4.2 Velocity Profiles

Velocity profiles for the different studies were each taken from vertical cut lines when looking at the 2-D axisymmetric geometry. This meant that the data was from a constant radius while looking at the changes with the axial coordinate. This cut line was at one of three positions shown in Figure 7.

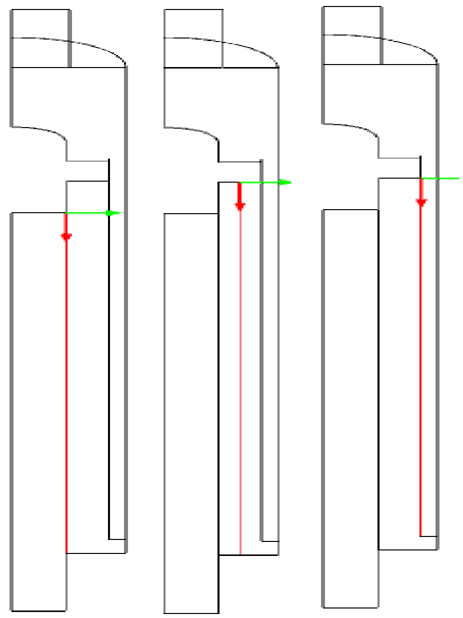

Figure 7: From left to right: bed outlet, bed middle, bed inlet

The names of each of the cut lines were based on the normal flow profile so that the inlet was at the right of the bed and the outlet was at the left of the bed when considering the 2-D axisymmetric model. In the bed inlet case, the line is .001 m to the left of the screen so that it gives an indication of flow in the bed just after the outer screen. However, the bottom of the line does not touch a wall, giving velocities that are not zero. The bed outlet line is .001 m right of the screen so that it gives an indication of flow in the catalyst bed just before the inside screen. The top of this line does not contact a wall, again giving velocities that are not equal to zero.

4. Results and Discussions

4.1 Flow Direction

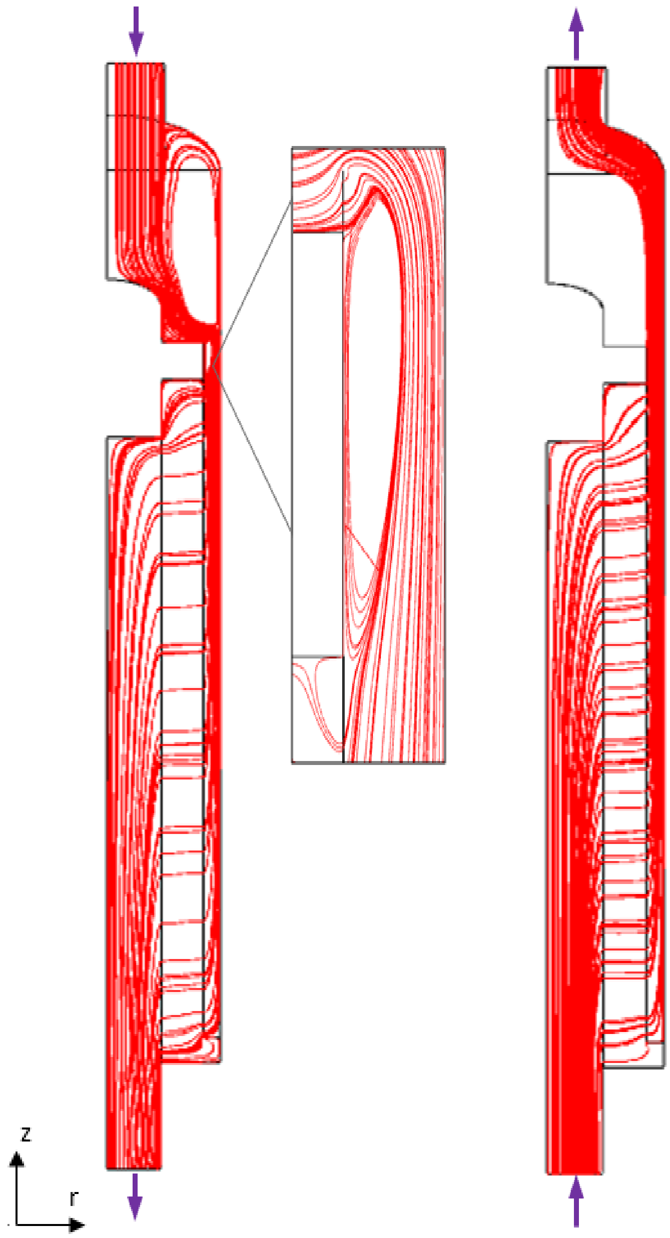

Figure 8: Velocity Streamline plots

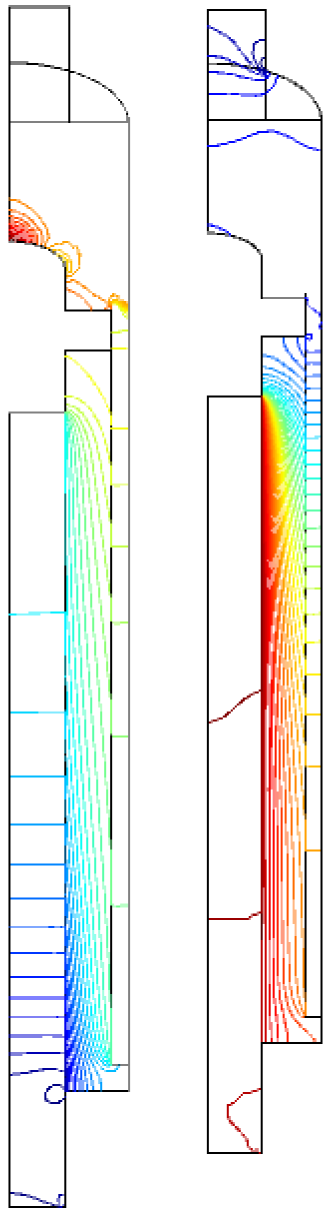

Figure 9: Pressure contour plots in which red represents high pressure and blue represents low. Normal Flow on the left, Reverse on the right

Figure 8 indicates that the normal flow model experienced fluid recirculation while the reverse flow model did not experience any significant recirculation. The normal flow model experienced recirculation in the top right region of the reactor, and also experienced a small pocket of recirculation at the top of the outer annulus and the top right of the catalyst bed. Although the reverse flow streamline does not show it, less significant recirculation patterns are expected to form in the empty space shown in the streamline near the top of the reactor. The consideration of recirculation patterns will be an important factor in determining which flow configuration to use. This recirculation could cause unexpected stress on some components of the reactor, most notably the portion of the outer screen that extends above the outer annulus into the open flow area, and could also cause some reactants to spend too much time in the catalyst bed, leading to unwanted reactions.

Figure 9 shows that the fluid in the normal flow model experiences a good deal of pressure drop before the fluid even reaches the catalyst bed. Once the fluid does enter the bed, the pressure drop is somewhat localized at the top of the bed outlet, and throughout the bottom of the catalyst bed. This localization of pressure drop illustrates maldistribution in the flow. The reverse flow model experiences the majority of its pressure drop in the catalyst bed, but the pressure drop is extremely localized. This is illustrated by the very close contour lines at the top of the catalyst bed. The maldistribution index values in Table 4 support this observation.

Flow Direction	**Inlet Flow (kg/hr)**	**Avg. Bed Velocity (m/s)**	**Maldistribution Index**
Normal	2.75×10^5	0.71	0.71
Reverse	2.35×10^5	0.80	1.05

Table 4: Inlet Flow and Bed Velocity values for each flow direction.

Another thing to consider when choosing the flow configuration is the flow rate and bed velocity. The values in Table 4 indicate that the normal flow configuration allows a higher flow rate than the reverse flow configuration at the given pressure drop. This means that more material can be sent through the reactor in a certain amount of time while keeping the same pressure drop. The fact that the normal flow model has a lower average bed velocity is also beneficial because it means the fluid will spend more time in the catalyst bed, allowing for a higher overall conversion in the reactor.

The final property to consider, which was briefly discussed with the pressure contours and maldistribution index values, is the distribution of the flow. The velocity profiles plot the velocity in the middle of the catalyst bed versus the z-coordinate in the bed so that the left side of the plot represents the bottom wall of the bed and the right side of the plot represents the top wall of the bed.

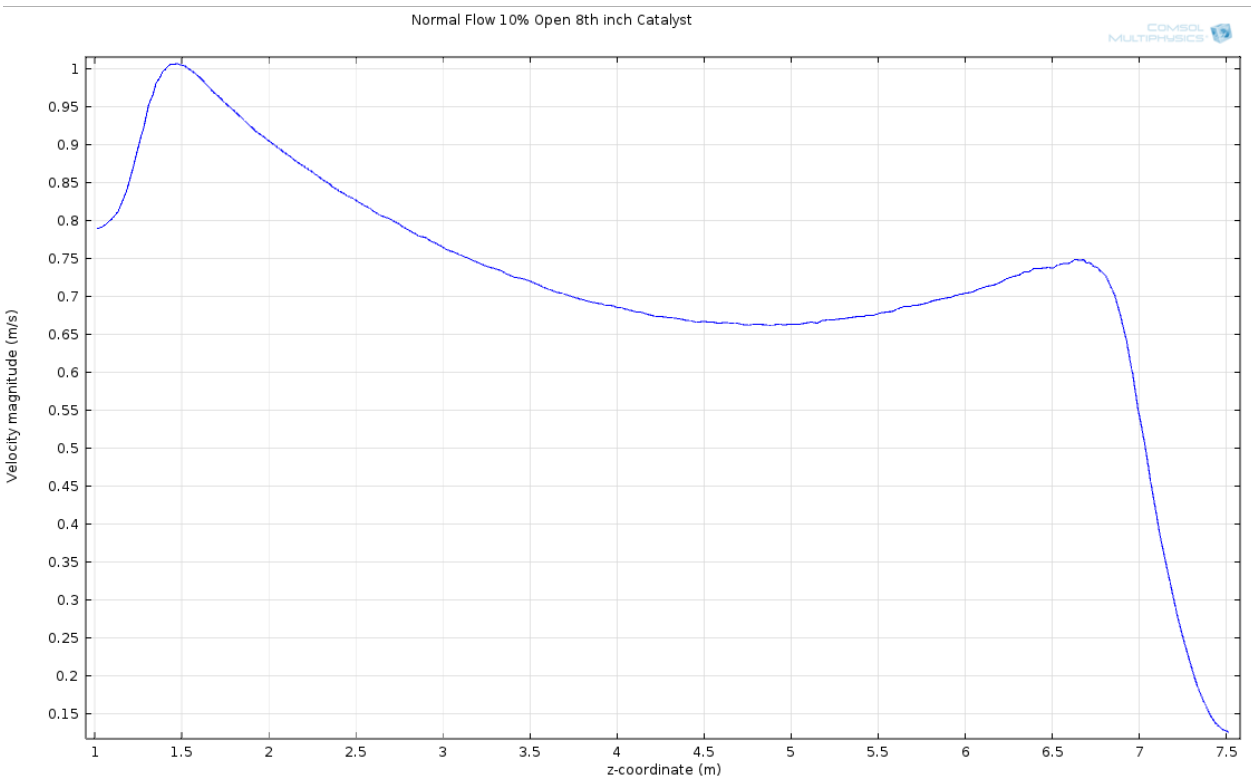

Figure 10: Flow Distribution in the middle of the catalyst bed for Normal Flow configuration

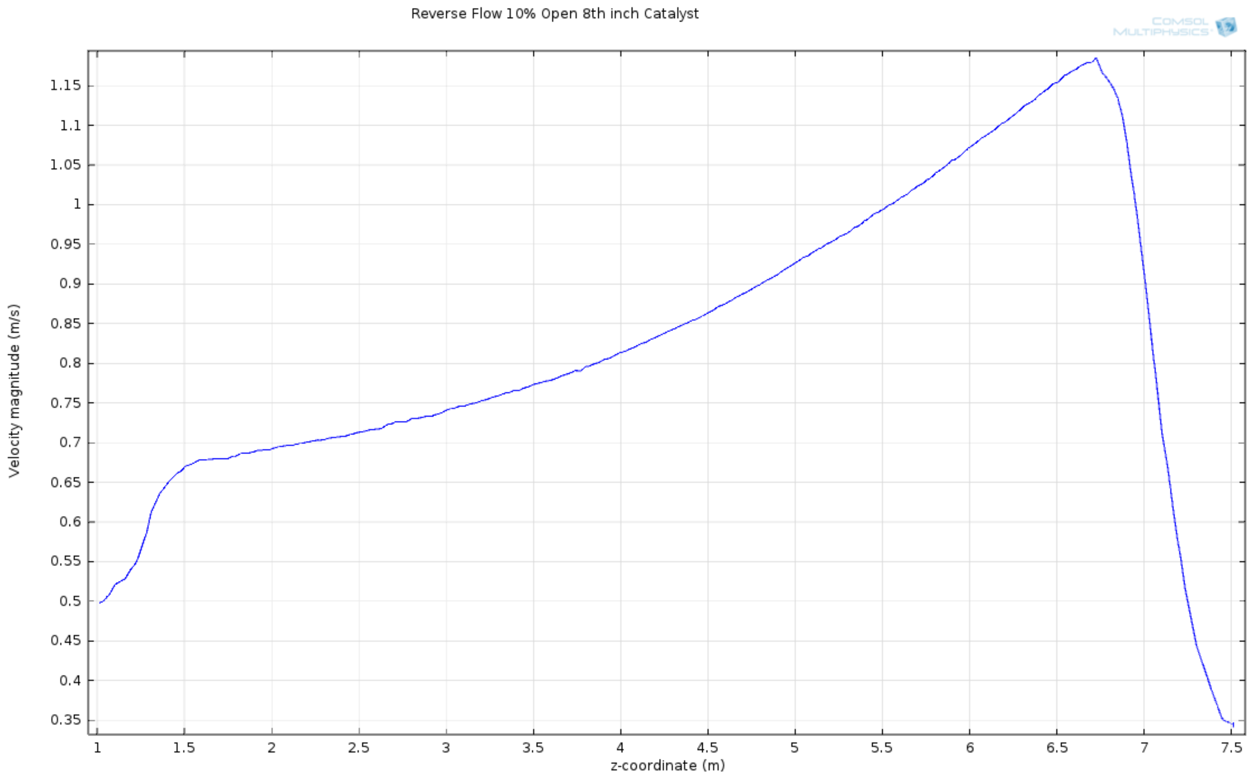

Figure 11: Flow Distribution in the middle of the catalyst bed for Reverse Flow configuration

Both Figure 10 and Figure 11 illustrate that the bed experiences low flow close to the top and bottom walls of the catalyst bed. This is most likely a result of the geometry having a bed inlet and outlet that are not level with one another, as well as the fact that the walls have a no-slip condition. The differences between Figures 10 and 11 are the more important aspect. As predicted by the maldistribution index values in Table 4, the reverse flow configuration has a much less uniform flow distribution through the catalyst bed than the normal flow model. Figure 10 shows that the normal flow configuration experiences higher flow near both the top and bottom walls of the catalyst bed. Figure 11 shows that the reverse flow configuration experiences most of its flow near the top wall of the bed, while the bottom of the bed experiences significantly less flow. The major problem with this fact is that the maldistribution in the reverse flow model may be too significant to be remedied by using higher resistance screens, which would increase pressure drop through the system. Since the maldistribution in the normal flow configuration is not as significant, and the fact that it allows a higher flow rate, it seems that the normal flow configuration would result in a more productive reactor.

4.2 Changing Catalyst Particle Size

This study focused on how changing the catalyst particle size would affect the reactor flow rate and velocity in the catalyst bed. It also took into account the effect on the flow distribution in the bed.

Catalyst Particle Diameter (inch)	Inlet Flow (kg/hr)	Avg. Bed Velocity (m/s)	Maldistribution Index
1/8	2.75×10^5	0.71	0.71
1/16	2.48×10^5	0.64	0.53

Table 5: Inlet Flow and Bed Velocity values for each catalyst size

The values in Table 5 reveal that the catalyst with a diameter of 1/8 inch allows both a higher flow rate and a higher bed velocity at the specified pressure drop. Although the higher flow rate could be beneficial, the higher bed velocity means that the fluid would spend less time in the catalyst bed, decreasing the reaction conversion. Table 5 also gives values for the maldistribution index that suggest the 1/16 inch catalyst provides better distribution in the bed.

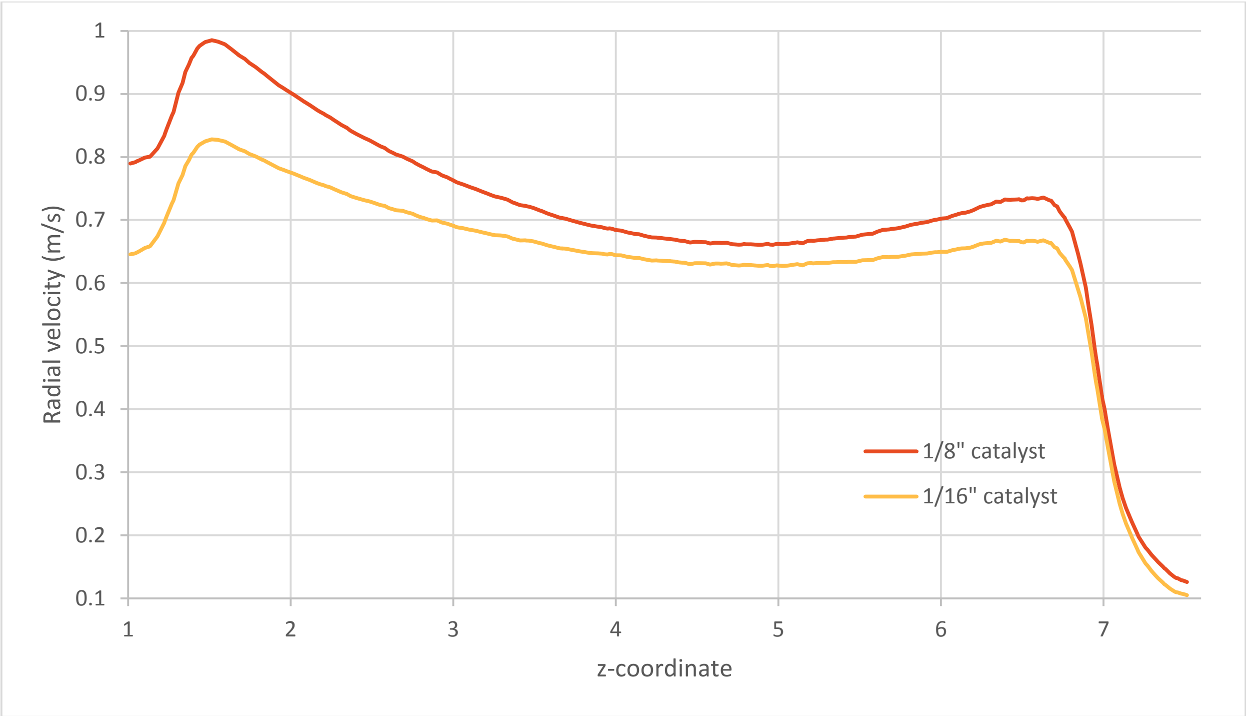

Figure 12: Bed velocity profile at bed middle using both catalyst sizes

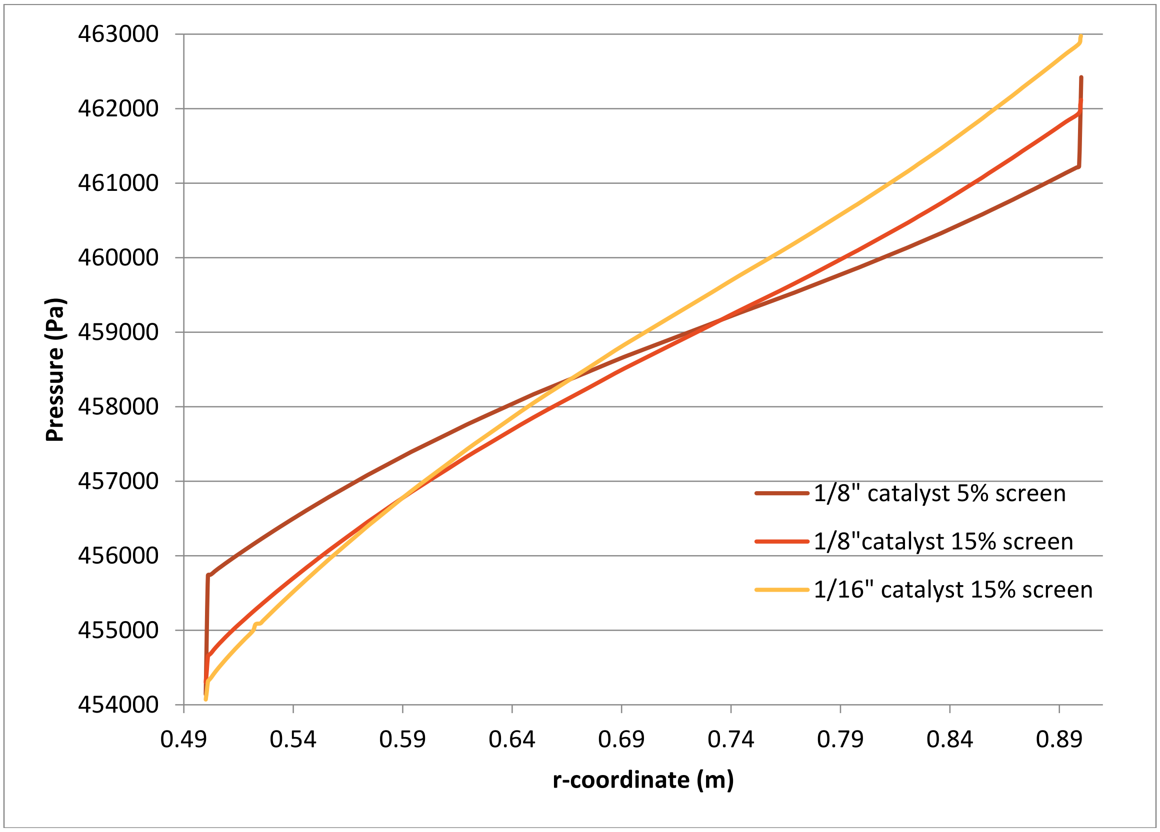

Figure 13: Pressure values vs. r-coordinate going radially outwards from the inner screen to the outer screen

Figure 12 shows that there is a difference in the flow distribution depending on which catalyst size is used. The locations of high flow are very similar between the two catalysts, suggesting that it is a result of the geometry. However, the 1/16 inch catalyst has a distribution that is much closer to a uniform flow than that of the 1/8 inch catalyst. This fact is significant because of the pressure drops shown in Figure 13. Even with the most resistant screens used in the study, the catalyst bed is still responsible for the majority of the pressure drop in the reactor. This indicates that the catalyst particle size will be the number one determining factor for the flow distribution in the center of the catalyst bed. A better distribution through the catalyst bed increases the reaction conversion and the efficiency of the reactor. In fact, this increased efficiency in the reactor using the 1/16 inch catalyst may be enough to overcome what it gives up in terms of the flow at the specified pressure drop. This indicates that the 1/16 inch catalyst would be more beneficial to use in the model reactor because it will create a more efficient reactor.

4.3 Changing Total Flow through Reactor

The purpose of this study was to see how bed velocity and distribution changed with total flow in an effort to optimize the flow rate. The first part of the study focused on how the average velocity in the bed changed with the amount of flow, and consequently pressure drop, in an effort to aid in optimizing the operating conditions for the reactor.

Pressure Drop (Pa)	Inlet Flow (kg/hr)	Avg. Velocity in Bed (m/s)	Maldistribution Index
13730	2.48×10^5	0.64	0.53
23730	3.29×10^5	0.85	0.71
33730	3.95×10^5	1.02	0.86
43730	4.50×10^5	1.16	0.99
53730	5.01×10^5	1.29	1.09

Table 6: Values for Inlet Flow and Average Velocity at each Pressure Drop for the model.

The data presented in Table 6 shows that increasing the pressure drop in the radial flow reactor does have benefits. An increase in pressure drop is caused by an increase in the flow through the reactor. This leads to an increase in the velocity going through the catalyst bed, which could both positively and negatively affect the reaction conversion. The increased fluid velocity in the bed could be beneficial because it would help overcome some of the mass transfer limitations found in every catalyst bed. However, if the bed velocity became too high, the reactants would be pulled from the catalyst before they finished reacting, which would decrease the conversion in the reactor. However, the values for the maldistribution index at each pressure drop show that this increased flow comes at a price. As the amount of flow through the reactor is increased, the flow distribution through the catalyst bed becomes significantly worse. This is studied further in Figure 14.

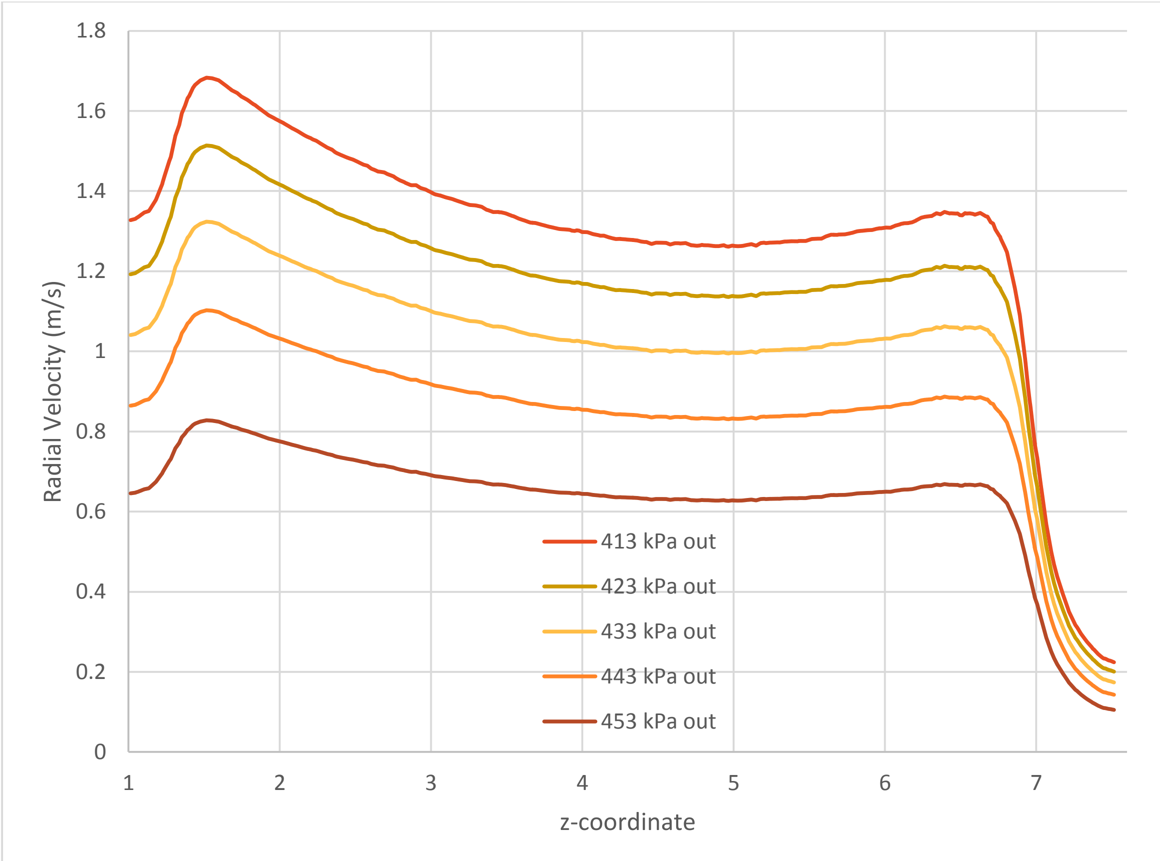

Figure 14: Velocity profile at outlet of catalyst bed for different pressure drops

As can be seen in Figure 14, the amount of flow through the reactor did affect the distribution of flow through the bed. The change in flow distribution is most evident by looking at the difference in velocity between the right side of the profile and the lowest point of the profile. The high values along the left and right of the plot indicate a larger amount of flow near the walls of the catalyst bed, which could lead to inefficient use of the catalyst or could create “hot spots” during the chemical reaction. This increased maldistribution within the catalyst bed, as well as the increased pressure drop through the reactor, would most likely outweigh any of the possible benefits received by increasing the flow rate.

4.4 Different Screen Resistances

This study was intended to determine how the bed velocity and flow distribution were affected by changing the resistance for the inner and outer screens. The first part of the study focused on how the flow rate and bed velocity changed with the screen resistance.

Screen Open Fraction	Inlet Flow (kg/hr)	Avg. Bed Velocity (m/s)	Maldistribution Index
5%	2.59×10^5	0.67	0.61
10%	2.75×10^5	0.71	0.71
15%	2.79×10^5	0.72	0.74
20%	2.81×10^5	0.73	0.76

Table 7: Values for Inlet Flow and Bed Velocity at each Screen Open Fraction

According to the data in Table 7, the inlet flow and average bed velocity are affected differently by the resistance of the screen. The average bed velocity increases almost linearly with the screen open fraction up to values over 15%. The inlet flow rate, on the other hand, experiences a reduction in flow two times that of the previous reduction for each incremental decrease in screen open fraction. This indicates that, if uniform resistance screens are used, they should be between 10% and 15% open because they will allow reasonable values for both inlet flow and bed velocity. The second part of the study focused on the changes in flow distribution.

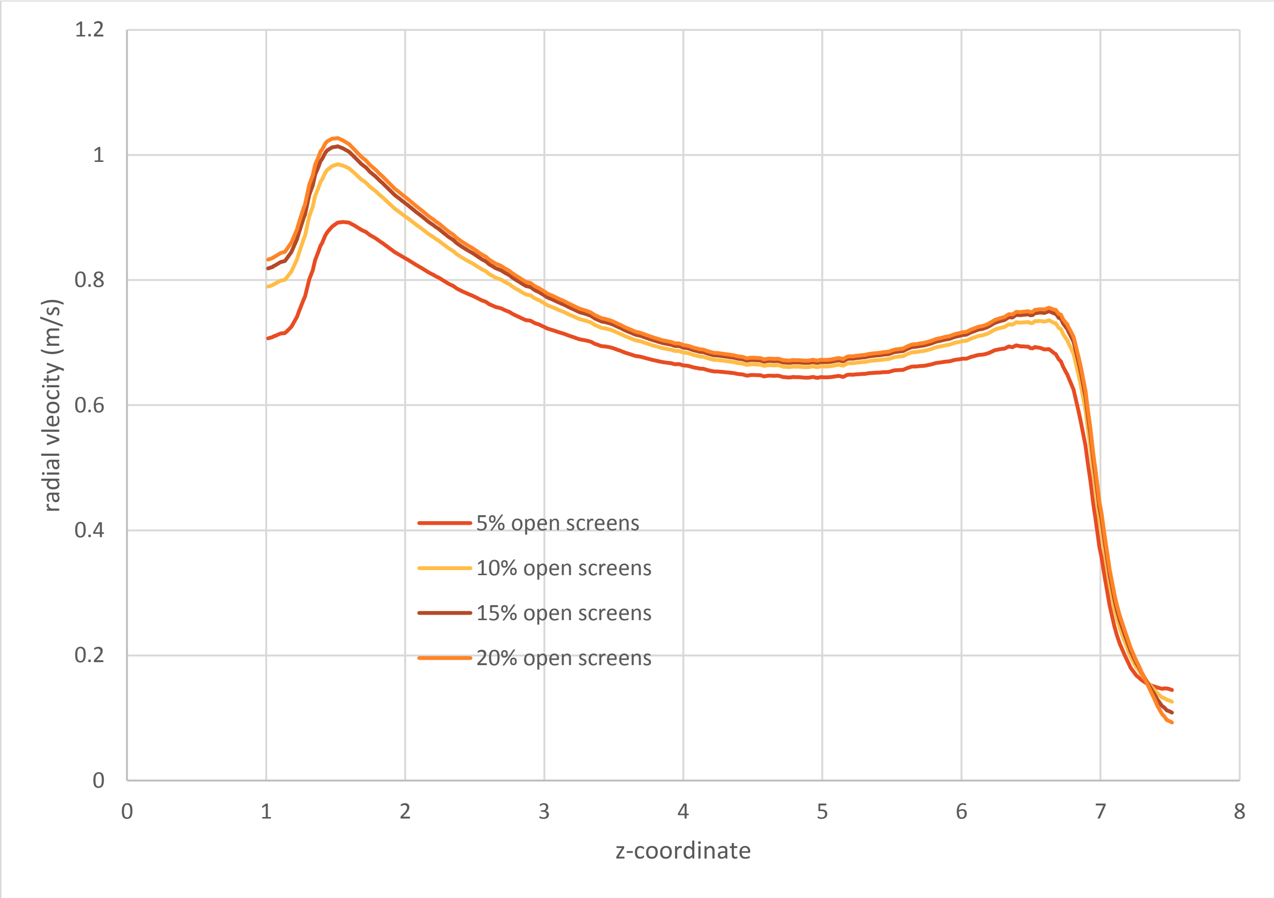

Figure 15: Velocity profile vs. z-coordinate in the middle of the bed

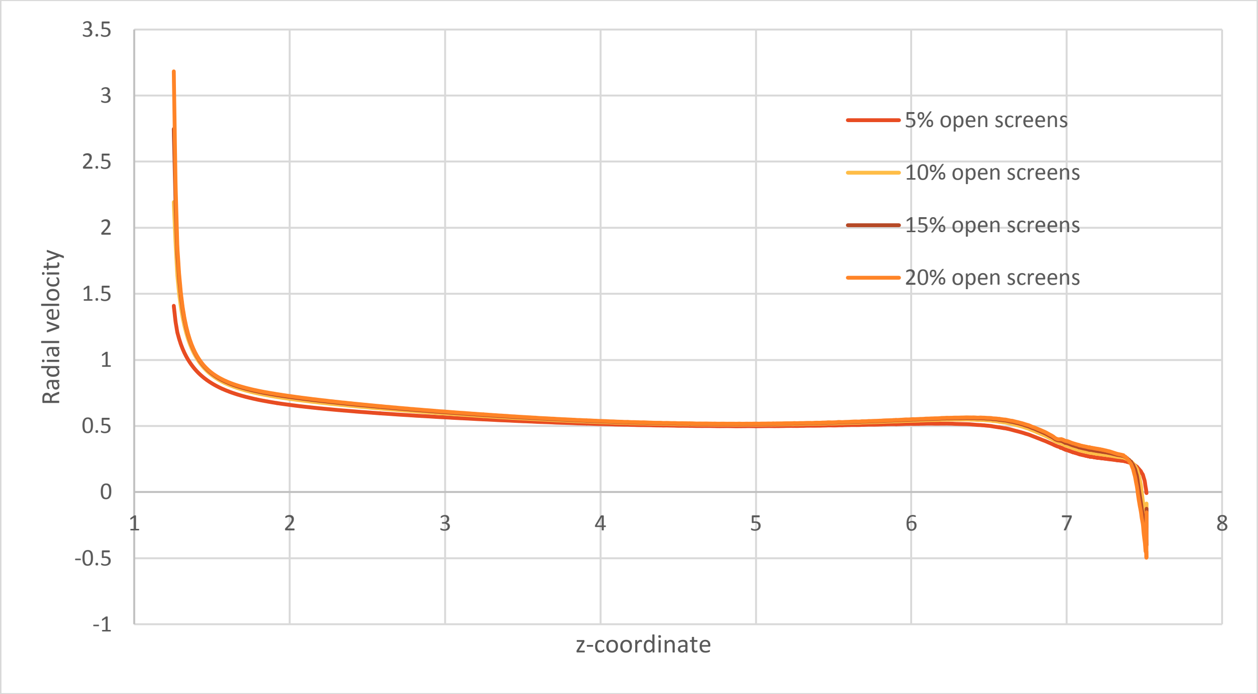

Figure 16: Velocity profile vs. z-coordinate at the bed inlet

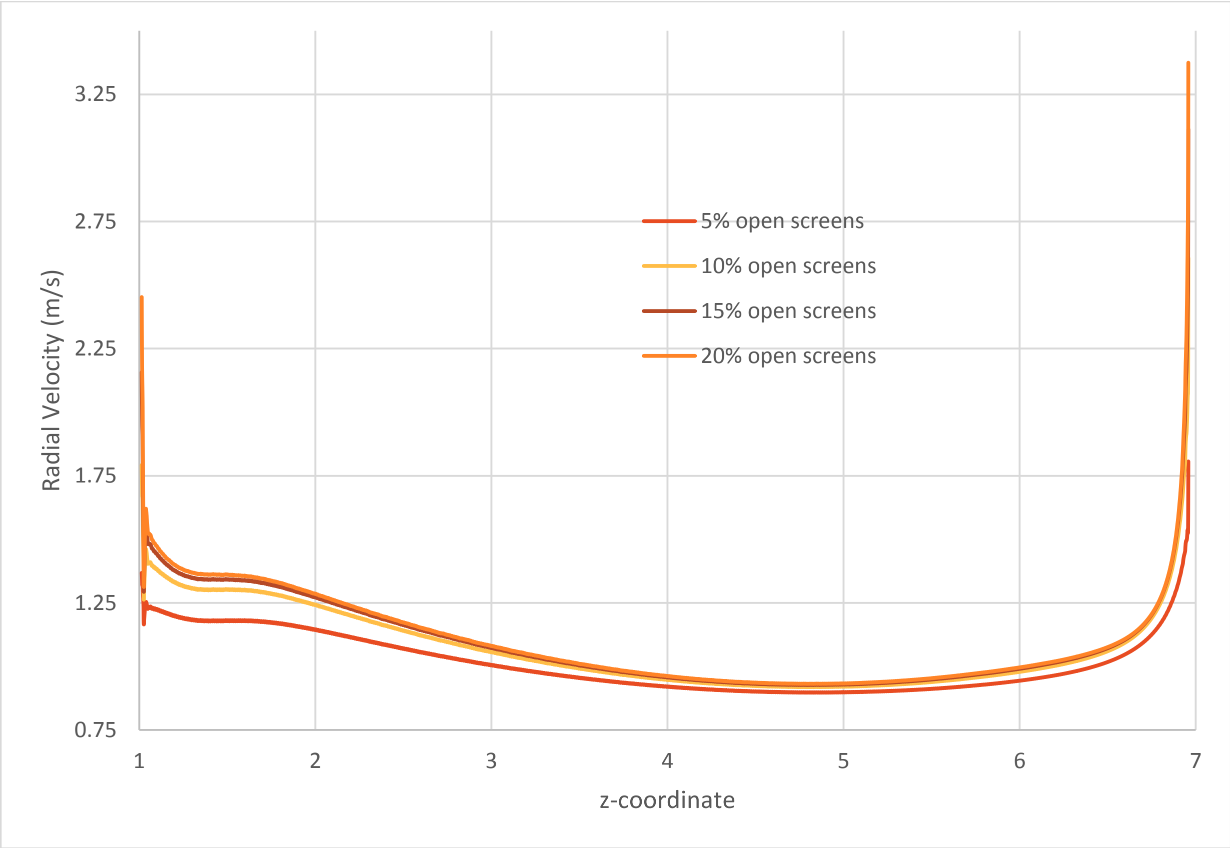

Figure 17: Velocity profile vs. z-coordinate at the bed outlet

Earlier in the reactor study, it was predicted that the screen resistance would not have a significant impact on the distribution in the middle of the bed. The maldistribution index values in Table 7 and the velocity profiles in Figure 15 further support this prediction. However, Figures 16 and 17 indicate that the open fraction of the uniform screens can partially affect the distribution near the bed inlet and outlet. Although the overall distribution profiles were essentially the same no matter what the screen resistance was, the velocities along the walls at the bed inlet and outlet did increase as the screens became more resistant. This indicates that the resistance of the screens can be used to limit the amount of flow in areas near both the bed inlet and outlet, leading into the final study.

4.5 Screens with Variable Resistance

In all previous studies, a trend was seen that there was flow maldistribution in the bed, especially at the walls of the bed inlet and outlet. In order to see if this could be fixed, screens with variable resistance were used so that the ends of the screens had different resistances to flow than the middle of the screen. The inlet flow rate was not analyzed in this study, only average bed velocity and the flow distribution at two points: the inlet to the bed and the outlet of the bed.

Screen Resistance	Avg. Bed Velocity (m/s)	Maldistribution Index
Uniform	0.58	0.70
Variable	0.58	0.66

Table 8: Comparison of average radial velocity in bed and maldistribution index at bed inlet

Screen Resistance	Avg. Bed Velocity (m/s)	Maldistribution Index
Uniform	1.09	0.84
Variable	1.09	0.62

Table 9: Comparison of average radial bed velocity and maldistribution index at bed outlet

The values in Tables 8 and 9 indicate that the variable resistance screens can improve flow distribution at the inlet and outlet without significantly impacting the pressure drop through the system. For both sides of the bed, the average velocities were identical while the maldistribution index for the variable resistance screens improved, especially at the bed outlet.

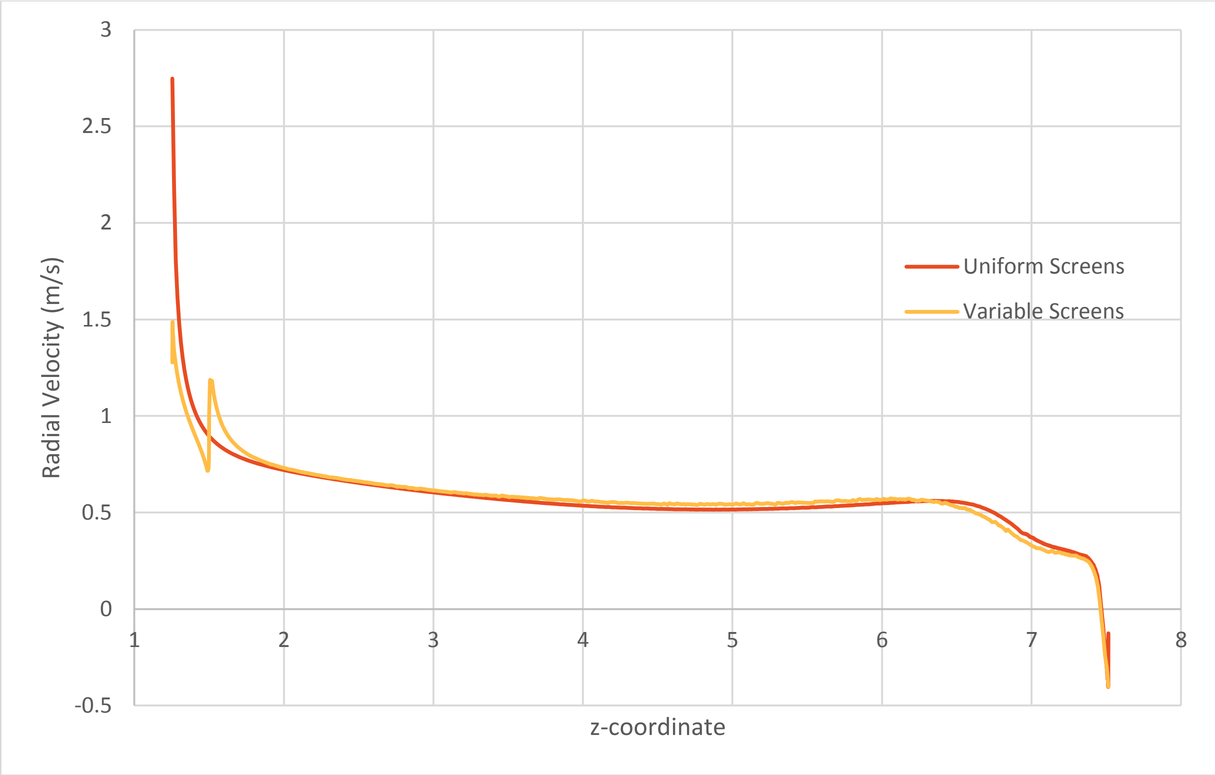

Figure 18: Velocity distributions at bed inlet for uniform and variable resistance screens

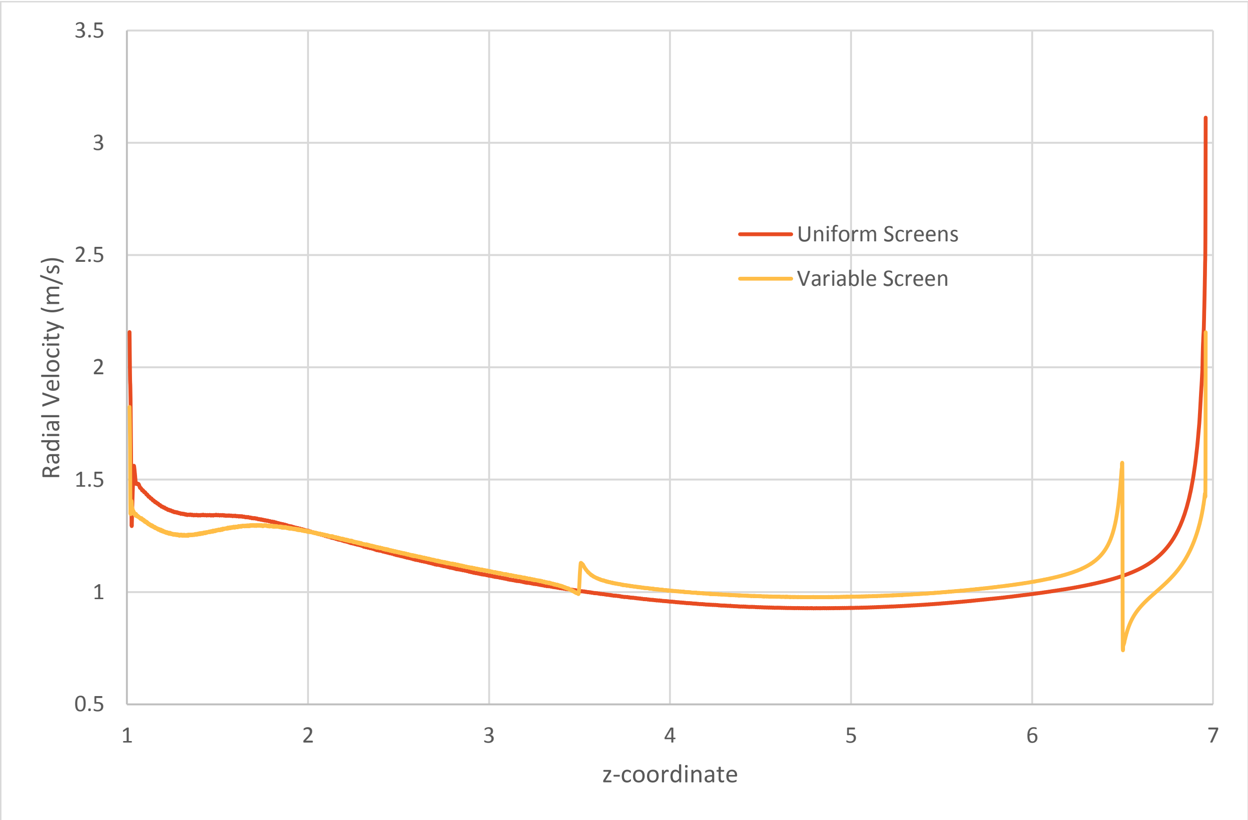

Figure 19: Velocity distributions at bed outlet using uniform and variable resistance screens

When analyzing Figures 18 and 19, it is important to focus on the velocities near the far left and far right of the graphs. Figure 18 shows these velocities at the bed inlet. At the bottom of the catalyst bed, this velocity was significantly reduced by the localized resistance in the variable screen. However, the flow at the top of the bed remained low for both screen types. This distribution may have to be accepted because the only way to fix it is to increase the overall resistance of the screen, which would also increase the pressure drop through the system. Figure 19 shows the velocity distribution at the bed outlet, which was significantly improved by the variable resistance screens. The high flow at the top and bottom of the screen was reduced by using the sections with higher resistance near the walls. In a real screen, this increase of resistance would occur gradually rather than the abrupt change in resistance used for simulation purposes, which causes the spikes in the graph. Based on these results, we recommend using screens with variable resistances to decrease maldistribution at the bed inlet and outlet. In future studies, the actual resistances used in each region could be refined to provide better results.

5. Conclusions and Recommendations

5.1 Recommendations

After completing the flow study, the group makes the following recommendations to CCTI for future projects on this reactor system.

I. An additional simulation geometry should be created that makes use of a “dummy cone”. This would involve a radially outward flowing design, where the inlet is directly above an inert cone that would direct the flow out radially. (Put in photo)

II. Conduct an in depth study of creating a screen with variable openness across it’s length. This study could address the maldistribution in the reactor better than a single screen openness, which was largely used in this study.

III. The addition of Heat Transfer physics to the current model in COMSOL. This will provide a more comprehensive analysis for future use.

IV. Conducting an additional study on the reaction taking place within the reactor. This simulation will provide critical data that can be combined with the flow study for an overall reactor synopsis

5.2 Conclusion

All variables studied did contribute in some part, to the overall maldistribution found in the catalyst bed. Starting with flow direction, assuming the reactor is to be run in one direction only, than normal flow is clearly the best choice in terms of maldistribution, as it rates a 0.71 versus the 1.05 of the reverse flow configuration. While only 0.09 m/s of bed velocity is sacrificed.

The favored catalyst size is the 1/16" versus the 1/8" option. The 1/16" allows for a greater surface area for the catalyst to react with the flow passing through the bed. It has a slightly lower bed velocity at 0.64 m/s, but a much better maldistribution rating at 0.53.

Changing the total overall flow through the reactor had an obvious effect on maldistribution as well as bed velocity. At the extremes, an increase of pressure drop by 4000 Pa more than doubled both bed velocity and maldistribution to 1.29 m/s and 1.09 respectively. While the initial case yielded a velocity of 0.64 m/s and a maldistribution rating of 0.53. So there is an obvious trade-off between the maldistribution found in the bed and a desired bed velocity.

Altering the screen resistances had an expected effect on the maldistribution. The higher the screen resistance, the better the overall distribution. While again it was observed that there is a trade off with overall velocity versus maldistribution when the different resistances were tested. The best maldistribution rating was 0.61, but that only had a bed velocity of 0.67 m/s.

Variable screen resistances provided better maldistribution ratings at the inlet and outlet areas of the bed, while having near identical numbers in the middle of the bed where the other studies were done. Having an inlet and outlet rating of 0.66 and 0.62 respectively.

Therefore, based on the information collected and data provided, our recommended reactor configuration is a normal flow, 1/16” catalyst bed, with a screen that can provide variable resistance across its length.

6. Works Cited

Benson, T. (2014). *Reynolds number.* Retrieved 11/12, 2014, from http://www.grc.nasa.gov/WWW/k-12/airplane/reynolds.html

C. Foias, O.Manley, R.Rosa, R.Teman. (2001). *Navier-stokes equations and turbulence*The Press Syndicate Of The University of Cambridge.

Cambridge Chemical Technologies, I. *About us.* Retrieved 11/27, 2014, from http://www.cambchemtech.com/

CFD Online. *K-epsilon models.* Retrieved 12/2, 2014, from http://www.cfd-online.com/Wiki/K-epsilon_models

Chang, H., & Calo, J. M. (1981). An analysis of radial flow packed bed reactors: How are they different? *ACS Symposium Series, 168*, 305-329.

COMSOL Inc. *CFD module.* Retrieved 10/13, 2014, from http://www.comsol.com/

Jeff C. H. LI. (2007). *Radial-flow packed-bed reactors*. Online: Ullmann's Encyclopedia Of Industrial Chemistry.

Johnson Screens. (2010). *Internals for radial flow reactors.* Retrieved 12/14, 2014, from http://www.johnsonscreens.com/sites/default/files/6/705/Internals%20for%20Radial%20Flow%20Reactors.pdf

Kareeri, A. A., Zughbi, H. D., & Al-Ali, H. H. (2006). Simulation of flow distribution in radial flow reactors. *Industrial & Engineering Chemistry Research, 45*(8), 2862-2874.

Kaye, L. A. In Exxon Research and Engineering Company (Ed.), *Fluid distribution in radial flow, vapor phase, fixed bed reactors*

Macdonald, I. F. Flow through porous media - the ergun equation revisited.*18*(3)

Pal, L., Joyce, M., & Fleming, P. (2006). *A simple method for calculation of the permeability coefficient of porous meida*Tappi Journal.

Ponzi, P. R., & Kaye, L. A. (1979). Effect of flow maldistribution on conversion and selectivity in radial flow fixed-bed reactors. *AIChe Journal, 25*(1), 100-108.

R. C. Givler and S. A. Altobelli. (1994). A determination of the effective viscosity for the Brinkman–Forchheimer flow model , , *Journal of Fluid Mechanics, 258*, pp 355-370.

Ranade, V. V. (2002). Fixed bed and other types of reactors. *Computational flow modeling for chemical reaction engineering vol. 5* (pp. 403-423). San Diego, CA: Academic Press.

Vafai, K. (2005). In Hadim H. (Ed.), *Handbook of porous media* Marcel Dekker.

Yoo, C. -., & Dixon, A. G. *Maldistribution in the radial-flow fixed bed reactor.* Unpublished Worcester Polytechnic Institute, Worcester, MA.

Yoo, C., & Dixon, A. G. (1988). Modelling and simulation of a mixed-flow reactor for ammonia and methanol synthesis. *Chemical Engineering Science, 43*(10), 2859-2865.