Modelling and Simulation of Flow Behavior through Millichannel Reactor for Biodiesel Production Using CFD

by

Nurul Fatinah Bt Sapuan

13676

Dissertation submitted in partial fulfillment of
requirements for the
Bachelor of Engineering (Hons)
(Chemical)

MAY 2014

Universiti Teknologi PETRONAS
Bandar Seri Iskandar
31750 Tronoh
Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

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Approved by,

…….
Dr Bawadi Abdullah

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

May 2014

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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NURUL FATINAH BT SAPUAN

ABSTRACT

This paper describes the numerical study of the fluid flow behavior at the inlet of millichannel reactor for biodiesel production. A computer simulation study was conducted to understand the behavior of the fluid flow in different parameters; velocity and pressure inside the millichannel reactor using Computational Fluid Dynamic (CFD)-ANSYS Fluent software. Palm oil and methanol are fed into a small channel reactor where the diameter is 1.62mm with length of 1000mm. The mixture of the feed is reacted with Potassium Hydroxide as the catalyst through transesterification method.

The results show when the inlet velocity is varied, there were significant changes happened to the fluid flow behavior. While, when outlet pressure is varied, there were no significant changes observed. From the results analysis, it can be used for finding an optimal design for biodiesel production.

ACKNOWLEDGMENT

In the name of Allah, the Most Gracious and the Most Merciful. Praise to Him the Almighty that in His will and given strength, the final year project is successfully completed within the allocated eight months period. Upon completing the project, I owe a great thanks to many people for their help and support, as well as their contribution in time, effort, advice, supervise, discuss and help during the period.

First of all, special thanks to my supervisor, Dr Bawadi Abdullah. The supervision and support that he gave truly helped the progression and smoothness throughout the project period. His willingness to guide and assist gave an opportunity to me in achieving the goals of the project. Besides, he was always sharing his knowledge and experiences with me. The co-operation is much indeed appreciated.

I would like to express my gratitude to the master students who helped me a lot; Wan Norita and Mr Ehsan in understanding the software. They are willing to help me as I am not expert in the Fluent software. I am truly appreciated with their kindness.

Last but not least, endless thanks to those who helped me to finish up my project directly or indirectly for their guidance, sharing and support throughout the entire two semesters. In short, I feel blessed to have completed my final year project and for all help that all parties involved had given to me.

TABLE OF CONTENT

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1: INTRODUCTION

1.1 Background of Study

This study is part of a larger project that makes renewable fuel (biodiesel) from palm oil in milli scale chemical processing systems. Normally, a millichannel reactor consists of milli-sized pipes or channels in which fluid flows and undergoes a chemical reaction. For this project, feed (palm oil and methanol) flows into a small channel, which then reacts with a presence of homogenous catalyst, potassium hydroxide and produces two important products: glycerin and biodiesel fuel. The purpose of this project is to study the behavior of fluid flow in the milli-sized channel at the inlet of the channel by using Computational Fluid Dynamic (CFD)-ANSYS Fluent software. When the behavior of the fluid is known, then an optimal design of any production can be designed for better quality of the product.

Micro and milli size units have features like small volumes, large surface area, small size, and low energy consumption (Sankarshana, Kalyan, Virendra, & Alamayehul, 2012). Millichannel reactor has many advantages such as high volume/surface ratio, higher transport (e.g., heat and mass transfer) rates, short diffusion distance, simplify process control and other used in the industrial process (Rahimi, Aghel, Alitabar, Sepahvand, & Ghasempour, 2013).

The large surface area to volume ratios help with rapid heat and mass transfer. The small-scale system has great benefits when compared to typical industrial scale devices. It will produce purer product faster. This should result in biodiesel fuel that is much less expensive than made by conventional techniques.

In order to study the behavior of the fluid flow in the millichannel reactor, a computer simulation is used as mentioned, which is the CFD-ANSYS Fluent. It is known as world-class software for reacting flows. Computational Fluid Dynamics (CFD) is a method that is becoming more and more popular in the modeling of flow systems in many fields; including reaction engineering (Ranade & Harris et al., 1995). CFD makes it possible to numerically solve flow and energy balances in

complicated geometries. The results show specific flow and heat transfer patterns that are hard to obtain with conventional modeling methods (Nijemeisland, 2000).

The CFD approach uses Navier Stokes equations and energy balances over control volumes, small volumes within the geometry at a defined location representing the reactor internals. After boundary conditions have been introduced in the system, the flow and energy balances are solved numerically. Hence, to decreases the error in the solution, an iteration process is conducted until a satisfactory result has been reached (Nijemeisland, 2000).

1.2 Problem Statement

Many methods were employed to design the experiments and find out optimum condition in the process. Design improvements are necessary to increase the reactor's ability to create product efficiently and affordably. Hence, it is important to know what is happening inside the reactor. But physical experiments are not feasible to know the behavior of the fluid flow as fabrication and physical experiments are expensive and time consuming. Besides, not all parameters can be measured or analyzed by conducting experiments. Hence, for this project, CFD-ANSYS Fluent software will be used for the modelling and simulation for the process.

1.3 Objective

The objective of the project is to study the behavior of fluid flow at the inlet of the millichannel reactor using CFD-ANSYS Fluent software.

1.4 Scope of study

To achieve the objective, there are two scopes that have been identified:

I. To conduct analysis by using CFD-ANSYS fluent software to investigate the behavior of the fluid flow in the millichannel reactor from various parameters. The parameters are:
    - Velocity
    - Pressure

II. To study on transesterification method of producing biodiesel

1.5 Relevancy and feasibility of project

This project is important, as it is useful for finding an optimal design for biodiesel production. We know that, biodiesel is an alternative and renewable fuels for diesel and other fuels used which pollute the environment. Biodiesel does not pollute the environment as it reduces the emission of carbon monoxide, carbon dioxide and other hydrocarbon. By knowing the optimal design, global warming issue can be solved and reduced. Hence, by using computer simulation, it provides the results that can be used to monitor the process of biofuel by analyzing the fluid flow behavior.

This project is feasible as it can be finished within two semester (FYP I & FYP II) timeframe and the availability of licensed Computational Fluid Dynamic (CFD) software provide in the university. As for the simulation, CFD software is proven viable to stimulate any fluid flow in various conditions.

CHAPTER 2: LITERATURE REVIEW

2.1 Biodiesel Fuel

Recent increases in liquid fossil fuel prices and uncertainties in its availability have stimulated interest in renewable liquid fuels. One of these attractive fuels is biodiesel, which can be made from triglycerides of various biomass sources such as plant oils (e.g., corn, palm) (Rathore & Madras, 2007) and microalgae oil (Demirbas, 2007). The chemical process to produce biodiesel is called transesterification in which triglycerides are reacted with methanol or ethanol to give methyl or ethyl esters of fatty acids and glycerol.

Commercial biodiesel is currently produced through transesterification reactions using acid or alkali solutions as catalysts. However, these conventional processes require a high purity of feedstock with very low free fatty acid and water content. Furthermore, the complexity of separation steps to remove catalyst, glycerol and excess alcohol from biodiesel drives up biodiesel cost (Warabi, Saka, & Kusdiana, 2004). The type of catalyst used must be chosen appropriately as the free fatty acid in the feedstock oil affect the purity of the production. In order to prevent any formation of soap, the maximum amount of free fatty acids acceptable in an alkali- catalyzed system is below 3 wt.% of FFA (Ribeiro, Castro, & Carvalho, 2011).

Converting vegetable oils or animal fats into esters of methyl and ethyl alcohols is known as Biodiesel. Esters can be produced from oils and fats by 3 methods:

I) Base catalyzed transesterification of oil with alcohol.
II) Direct acid catalyzed esterification of oil with methanol.
III) Conversion of oil to fatty acids and then to alkyl esters with acid catalysts.

The first method is preferred because it is economical which is the conversion of vegetable oil or animal fats (Triglyceride Esters) to methyl esters through transesterification process. Besides that, base catalyzed transesterification requires only low temperature and pressure and producing over 98% conversion yield.

2.2 Transesterification process

Transesterification of natural glycerides with methanol to methyl esters is a technically important reaction that has been used extensively in the soap and detergent manufacturing industry worldwide for many years. Almost all biodiesel is produced in a similar chemical process using base catalyzed transesterification as it is the most economical process, requiring only low temperatures and pressures while producing a 98% conversion yield (Biodiesel Production). The transesterification process is the reaction of a triglyceride (fat/oil) with an alcohol to form esters and glycerol. A triglyceride has a glycerine molecule as its base with three long chain fatty acids attached. The characteristics of the fat are determined by the nature of the fatty acids attached to the glycerine. The nature of the fatty acids can, in turn, affect the characteristics of the biodiesel.

The equation below shows the chemical process for methyl ester biodiesel (FAME) (Biodiesel Transesterification, 2008-2012). The reaction between the fat or oil and the alcohol is a reversible reaction, so the alcohol must be added in excess to drive the reaction towards the right and ensure complete conversion.

$$C_3H_5(RCOOH)_3 + CH_3OH \underset{KOH}{\longleftrightarrow} 3RCOCH_3O + C_3H_5(OH)_3$$

(Triglyceride) (Methanol) (FAME) (Glycerol)

The experimental setup is shown in below figure.

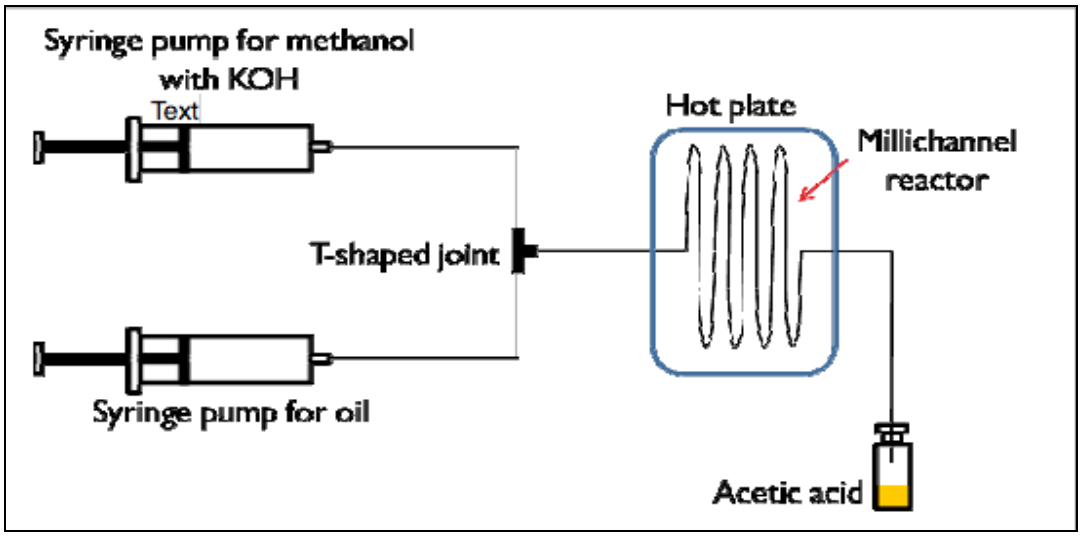


Figure 1: Experimental setup for Biodiesel production

2.3 Millichannel reactors

As there were still in researching of using millichannel reactor to produce biodiesel, hence microchannel reactors characteristic is used in explaining about millichannel reactor because there is no major difference in the productivity when comparing to the macroreactors (batch; conventional reactor system).

A millichannel reactor can be made from the micromachining of silicon, glass, ceramics, and wafer bonding. The most common method of construction involves etching a pattern on the bottom surface of the substrate. The pattern can be serpentine (shown in Figure 3) or straight. The pattern is etched down only a portion of the total depth. Figure 2 shows the example of the channel configuration: a serpentine configuration with resistance heaters for optimal heat transfer (Lewis, 2010).

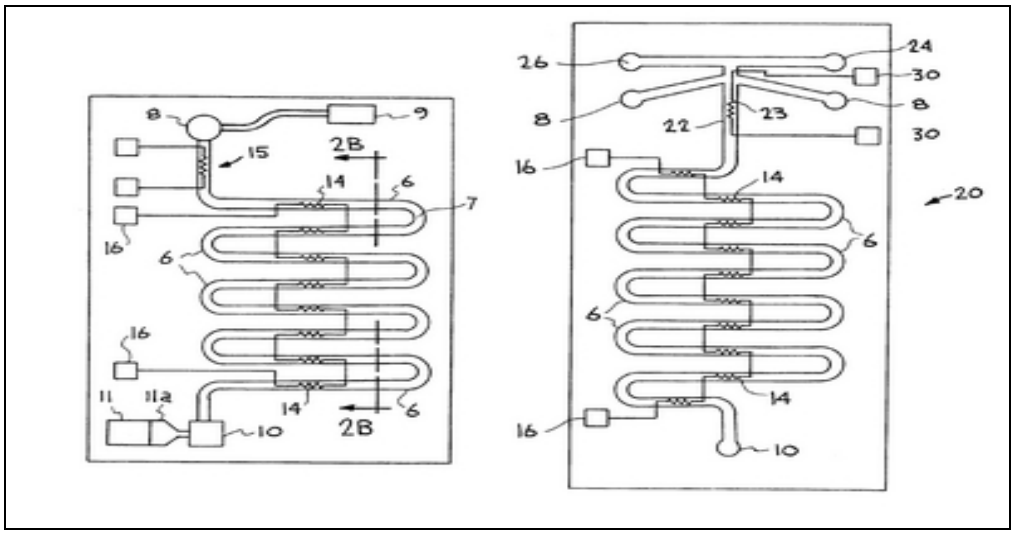


Figure 2: Cross Sectional View and Top View of a micro/millireactor, respectively (Lewis, 2010)

Millireactors are defined as miniaturized reaction systems fabricated by using, at least partially, methods of micro-technology and precision engineering. The term "millireactor" is the name that is generally used to describe a number of devices that have small dimensions. Reducing dimensions of the reaction system they exploit rapid reaction rates and minimize heat and mass transport limitations that usually present a problem in conventional reactor systems (Ehrfeld, Hessel, & Lowe, 2005).

Millireactors exhibit numerous practical and performance advantages when compared to batch reactors. The small dimensions of millichannel allow usage of minimal amounts of reagent under precisely controlled conditions and make it possible to rapidly screen reaction conditions and improve the overall safety of the process (Gerey, Codee, & Seeberger, 2008). Besides that, excellent mass and heat transfer, shorter residence time, smaller amount of reagents, catalyst and waste products comparing to macro-scale reactors, lightweight and compact system design, laminar flow, effective mixing, short molecular diffusion distance and better process control, and small energy consumption are just some of the millisystem advantages (Ehrfeld, Hessel, & Lowe, 2005). Furthermore, they could be easily coupled with numerous detection techniques together with the pretreatment of the samples on the one single chip. Having in mind all those benefits one of the main motivations for the use of millireactor technology is the gain in the yield and safety.

Because of the high surface to volume ratio of microreactors, heat transfer is very efficient and reaction temperatures in microreactors can be regulated by very effective heat removal or application (Pohar & Plazl, 2009). As a result, heat transfer coefficient measured in microreactor goes up to 25,000 W/(m^2K). This exceeds heat transfer coefficients of conventional heath exchangers by at least one order of magnitude (Ehrfeld, Hessel, & Lowe, 2005). The excellent heat transfer characteristics of micro-fabricated devices also avoid the risk of potential significant industrial accidents caused by thermal runaway (Chovan & Guttman, 2002). Comparison between micro-/milli and macro- heat exchanger systems is presented in Table 1. Below is the millichannel reactor used to produce biodiesel.

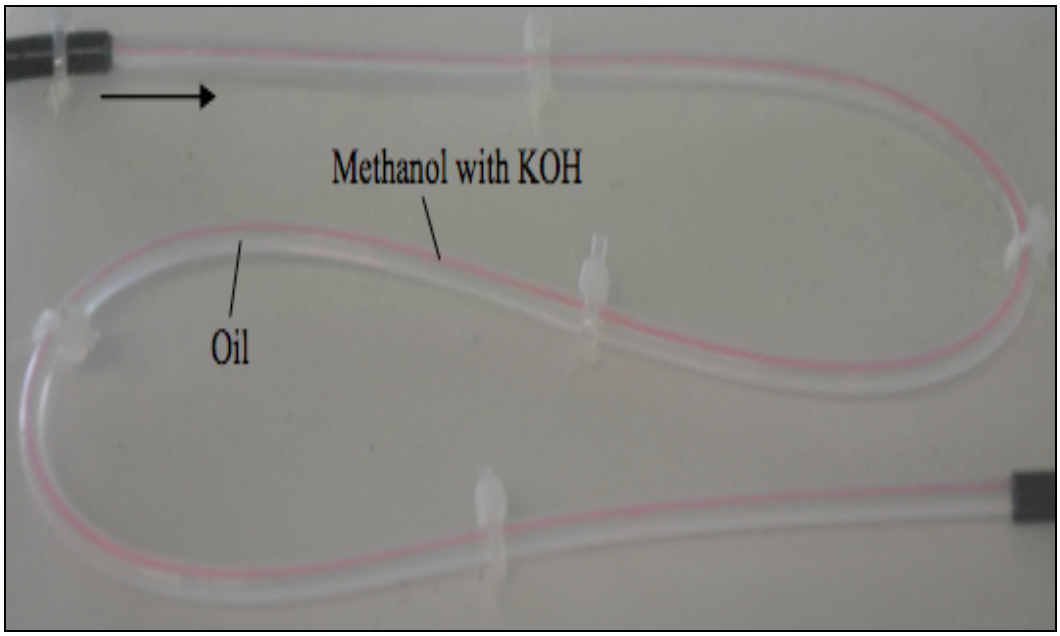


Figure 3: Millichannel reactor

Parameter	Shell and tube heat exchanger	Compact heat exchanger	Microchannel heat exchanger
Surface to volume ratio, m^2/m^3	50 - 100	850 - 1500	> 1500
Heat transfer coefficient, $W/(m^2 K)$ (liquid)	~ 5000 (tube side)	3000 - 7000	> 7000
Heat transfer coefficient, $W/m^2 K$ (gas)	20 - 100	50 - 300	400 - 2000
Approach temperature, °C	~ 20 °C	~ 10 °C	< 10 °C
Flow regime	Turbulent	Turbulent	Laminar

Table 1: Comparison of Macro- and Micro-Heat Exchanger System

2.4 Theory (Computational Fluid Dynamic, CFD)

Computational Fluid Dynamics (CFD) provides a qualitative (and sometimes even quantitative) prediction of fluid flows by means of

- Mathematical modeling (partial differential equations)
- Numerical methods (discretization and solution techniques)
- Software tools (solvers, pre- and post processing utilities)

CFD enables scientists and engineers to perform 'numerical experiments' (i.e. computer simulations) in a 'virtual flow laboratory'.

Solutions in CFD are obtained by numerically solving a number of balances over a large number of control volumes or elements. The numerical solution is obtained by supplying boundary conditions to the model boundaries and iteration of an initially guessed solution (Nijemeisland, 2000).

The balances, dealing with fluid flow, are based on the Navier Stokes equations for conservation of mass (continuity) and momentum. These equations are modified per case to solve a specific problem. The control volumes or elements, the mesh, are designed to fill a large-scale geometry, described in a Computer-Aided Design (CAD) file.

Typically, a CFD software package consists of three main groups of software; a pre-processor, a solver and post-processor.

i. Pre-Processing

Pre-processing includes geometry and mesh generation, flow specification, and setting solver control parameters. Once the geometry has been generated and meshed, the fluid properties, flow models and solver control parameters are specified and boundary and initial conditions applied. These steps are usually carried out through graphical interface.

ii. Solver

All the data defined in the pre-processing step are fed into the solver program. The solver is a specialized program that solves numerical equations based on the selected model and data specified. The results obtained by the solver are written to a results file for examination using the post-processor software.

iii. Post-Processing

In this software, the data obtained by the solver can be visualized and displayed using a variety of graphical methods such as contour, plane, vector and line plots. Calculations can also be made to obtain the values of scalar and vector variables, such as pressure and velocity, at different locations.

2.4.1 Mesh Topology

One of the most important parts of CFD modeling is the construction of the mesh topology. The mesh establishes the accuracy of the simulation. It has to be chosen with enough detail to describe the processes accurately and with a degree of coarseness that enables solution within an acceptable amount of time. There are three basic schemes for mesh methods; Smoothing (Spring analogy), Local remeshing and Layering. Table below describes the differences between the three schemes.

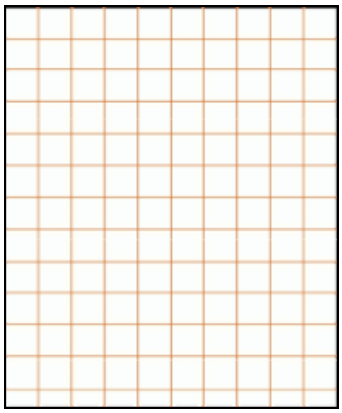
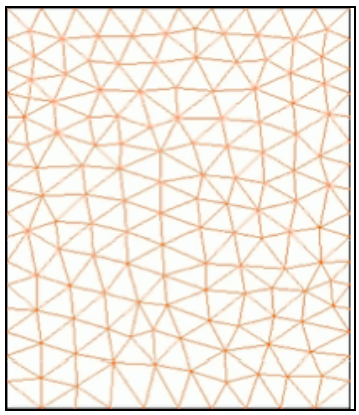
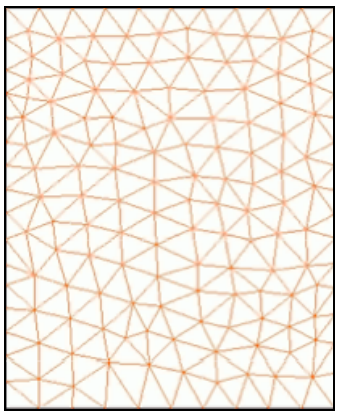
LAYERING	LOCAL REMESHING	SPRING ANALOGY
		
• Layers of cells are generated and collapsed as they are overrun by the moving boundary. • Layering is appropriate for qua/hex/prism meshes with linear or rotational motion and can tolerate small or large boundary deflections.	• In local remeshing, as cells become skewed due to moving boundaries, cells are collapsed and the skewed region is remeshed. • Local remeshing is appropriate for tri/tetra meshes with large range of boundary motion.	• Spring analogy is useful when there are small boundary deformations. The connectivity and cell count is unchanged during motion. • Spring analogy is appropriate for tri/tetra meshes with small deformations.

Table 2: Comparison between the three basic schemes for mesh methods

2.4.2 Multiphase Models Available in Fluent

When attempting to model a multiphase flow, the selection of the most appropriate modelling approach is very important. Fluent contains four distinct multiphase modelling approaches:

- Discrete Phase Model (DPM)
- Volume of Fluid Model (VOF)
- Eulerian Model
- Mixture Model

The selection is depending on whether the flow is stratified or disperse and also the Stokes number. The Eulerian Model and Mixture Model were selected as the model for this project because these two models are more suitable because of the mixture model applicability and application, which can be related to the project. Either one of them can be used and will show nearly the same results.

The Eulerian multiphase model is a multi-fluid model, which means that all phases are assumed to exist simultaneously. The model contains conservation equations for each phase contain single-phase terms and also interfacial terms such as drag, lift and mass transfer. While, Mixture Model is a simplified Eulerian approach, based on the assumption of small Stokes number. This model solves the mixture momentum equation and a volume fraction transport equation. The equations involve in calculating the results are discussed in the following sub topic (ANSYS, 2010).

2.4.3 Fluid Flow Fundamentals

For iteration CFD solvers use generalized fluid flow and energy balances based on the Navier Stokes equations. The balances are generalized so the user can influence which elements are added in the balance and which are not. The number of balances to be solved is also user defined; it can be advantageous to not solve all balances initially. The generalized balances that are used by the Fluent commercial CFD package are the Navier Stokes equations for conservation of mass and momentum, when it is set to calculate laminar flow without heat transfer (Nijemeisland, 2000).

There are equations in CFD-ANSYS Fluent that are used to model surface and volume conditions. These equations are used in conjunction with boundary conditions to model the reactor. When the assumptions listed below were introduced the equations were significantly simplified.

- The density and viscosity of the inlet fluid are constant and has been represented by the properties of the oil due to the complexity of the multi-phase process fluid.
- The fluid flow is in steady state condition and incompressible.
- The inlet fluid is pure reactant and therefore contains no product.

With the above assumptions made the Navier-Stokes Momentum Equation and the Mass Conservation Equation can be simplified to the following expressions. These equations are solved to find the pressure gradient and velocities within the microchannel.

Navier-Stokes Momentum Equation:

$$\nabla \cdot \mathbf{V} = 0$$

$$\rho \mathbf{V} \cdot \nabla \mathbf{V} = -\nabla p + \mu(\nabla^2 \mathbf{V}) + \rho \mathbf{g}$$

Where ρ = bulk mixture density (kg/m^3), $\mathbf{V}$ = Cartesian velocity vector (m/s), p =

pressure (Pa), μ = bulk mixture absolute viscosity (N•s/m^2), and **g** = gravitational acceleration vector (m/s^2).

Mass Conservation Equation:

$$\mathbf{V} \cdot \nabla C_i - D_i \cdot \nabla^2 C_i = 0$$

Where i = species indicator (one equation for each species), C_i = concentration of species i, and D_i = diffusivity of species i in solvent (m^2/s).

Arrhenius Equation:

$$k = Ae^{-E_a/RT}$$

Where k = rate constant (s^{-1}), A = pre-exponential factor (s^{-1}),
E_a = activation energy (J/mol), R = gas constant (8.314 J/mol*K), and T = temperature (K).

The equations are solved numerically using the computational software. As with all finite-volume methods, two major approximations are applied.

1. The physical domain is broken down into a series of very small control volumes or cells. The resulting collection of cells is called the computational grid.
2. The second approximation is the differential equations are replaced by a set of finite-difference equations that will approximate the differential equations in each cell.

As the equations show, the velocity, pressure, and concentration fields are linked. The variables are calculated iteratively to find the velocities and pressures based on the focus of the project.

CHAPTER 3: METHODOLOGY/PROJECT WORK

3.1 Flow of running the simulation

The research methodology is divided into four stages; problem identification, pre-processing, solver, and post processing.

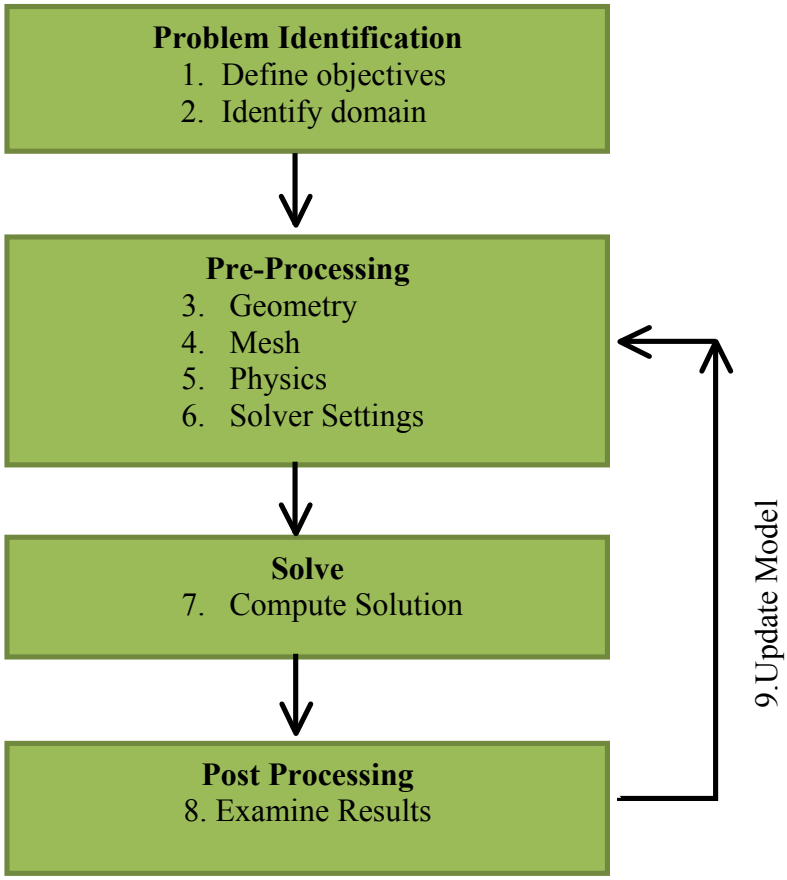


Figure 4: Flow Chart of CFD Analysis

3.1.1 Problem Identification

First step is to define the problem and understand the purpose of the simulation. At this stage, all necessary data required for running the simulation are gathered including geometry specification, fluid properties, flow details and boundary and initial conditions.

3.1.2 Pre-processing Phase

Geometry development, meshing, physics and solver settings were done at this stage. The geometry model for the reactor has been developed using ICEM software as the base case model for simulation purpose.

The process continues with meshing generation. At this stage, the domain is discretized into finite set control volumes or cells. The discretized domain is called "grid" or the "mesh".

The completed mesh generation was then will be imported into the ANSYS Fluent workbench for simulation. At this stage, physics such as the fluid properties and boundaries condition were specified, selection of model and prescribe operating conditions. Then solver control will be set up with convergence criteria and number of iteration for the simulation will be specified.

3.1.3 Solver

In this section, the CFD software performs iterative calculations to find a solution to the numerical equations representing the flow inside the reactor. The simulation continues the domain until a converged solution is obtained.

3.1.4 Post Processing

Once the solution converged, the results are analyzed through different type of methods such as contour, vector or line plots to check the satisfactory of the solution. If the result is unsatisfactory, the error needs to be identified. Then, CFD analysis is repeated several times with different types of model to choose the best flow model or check on the boundary/operating conditions.

3.2 Fluent Simulation

3.2.1 Geometry and Mesh (Base Case Model)

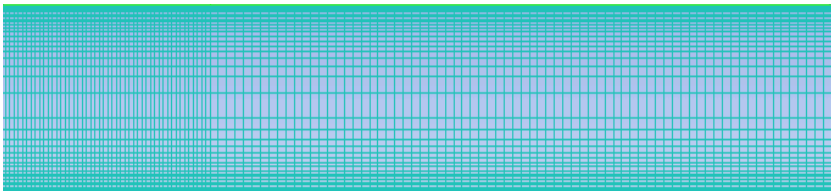


Figure 5: Geometry with Complete Mesh Generation

Figure 5 shows a 2D base case model used for the simulation. The geometry is meshed into smaller cells. At the inlet part of the reactor, the meshing is close to each other because it can give more accurate results. Structured meshing method is used for meshing the geometry. It is meshed into 4960 nodes and 5125 elements.

3.2.2 Boundary and Initial Conditions

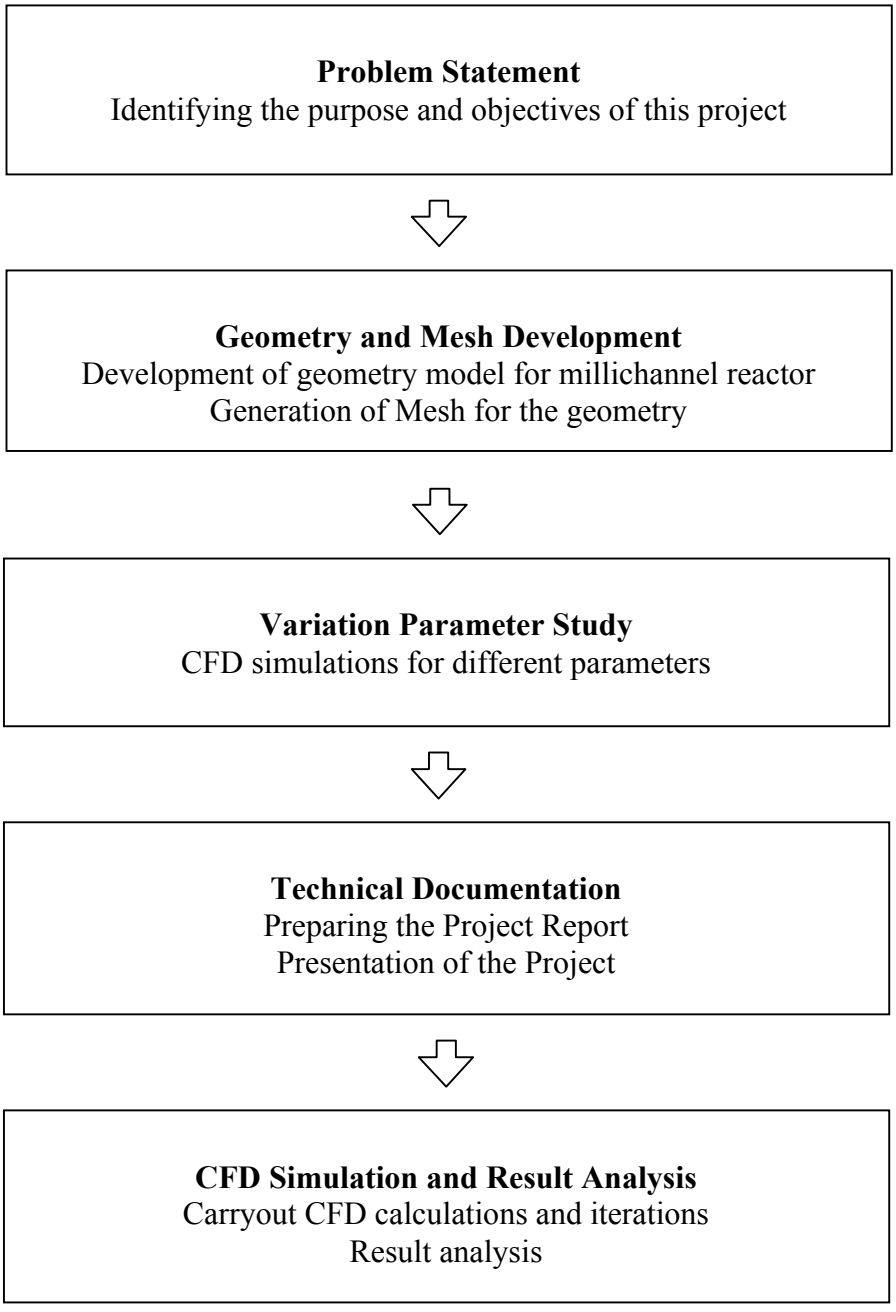
In order to obtain a well-posed system of equation, appropriate boundary conditions for the computational domain have to be implemented such as the inlet velocity of the species and pressure are specified. Slip boundary condition is specified at the interface.

3.2.3 Solution Techniques

In the Fluent's solver, it is set as segregated which solves the equation individually. Steady state simulation has been formulated and pressure based solver is used. The species transport model is considered. Mixture model is used to predict the reaction behavior. The discretization scheme for momentum, turbulent dissipation rate, turbulent kinetic energy and all has been taken as first order upwind.

3.3 Key Milestone

Below are several key milestones for this project that must be achieved in order to meet the objective of this project.



3.4 Gantt Chart

Activities	WEEK																													
	FYP I JAN 2014															FYP II MAY 2014														
	1	2	3	4	5	6	7	8	9	10	11	12	13	14		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Confirmation of Project Title																														
Literature Review																														
Submission of Extended Proposal																														
Proposal Defense																														
Project Continues																														
Submission of Interim Draft Report															S															
Submission of Interim Report															E															
CFD Simulation															M															
Project Work Continues															E															
Submission of Progress Report															S															
Pre-SEDEX															T															
Submission of Draft Report															E															
Submission of Dissertation (soft bound)															R															
Submission of Technical Paper															B															
Oral Presentation															R															
Submission of Project Dissertation (Hard Bound)															E															
															A															
															K															

CHAPTER 4: RESULTS AND DISCUSSION

In this section, steady state simulation results of velocity and pressure distribution of the flow behavior are discussed and analyzed. The results are in the form of contour plot where each colors represents the specific magnitude of the fluid flow. From the magnitude, the flow behavior can be analyzed. Here, the changes happen inside the reactor can be seen for changing in velocity and pressure.

Velocity Distribution

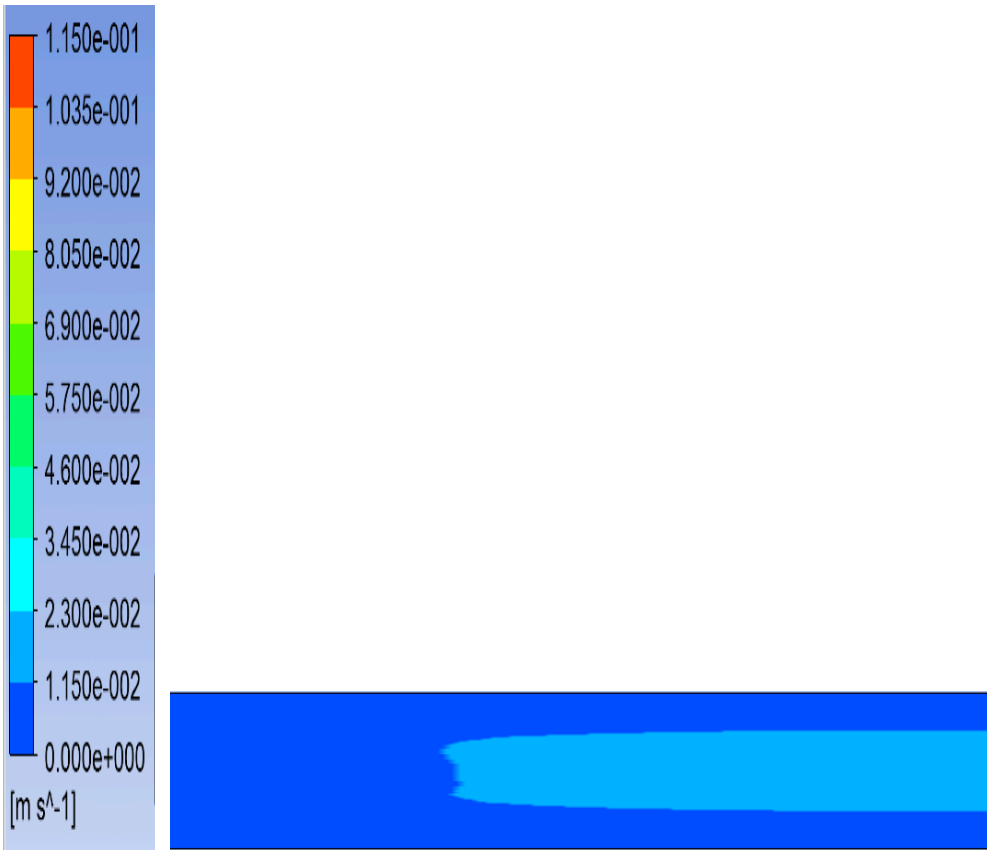


Figure 6: Velocity contour plot at 0.01 m/s at the inlet

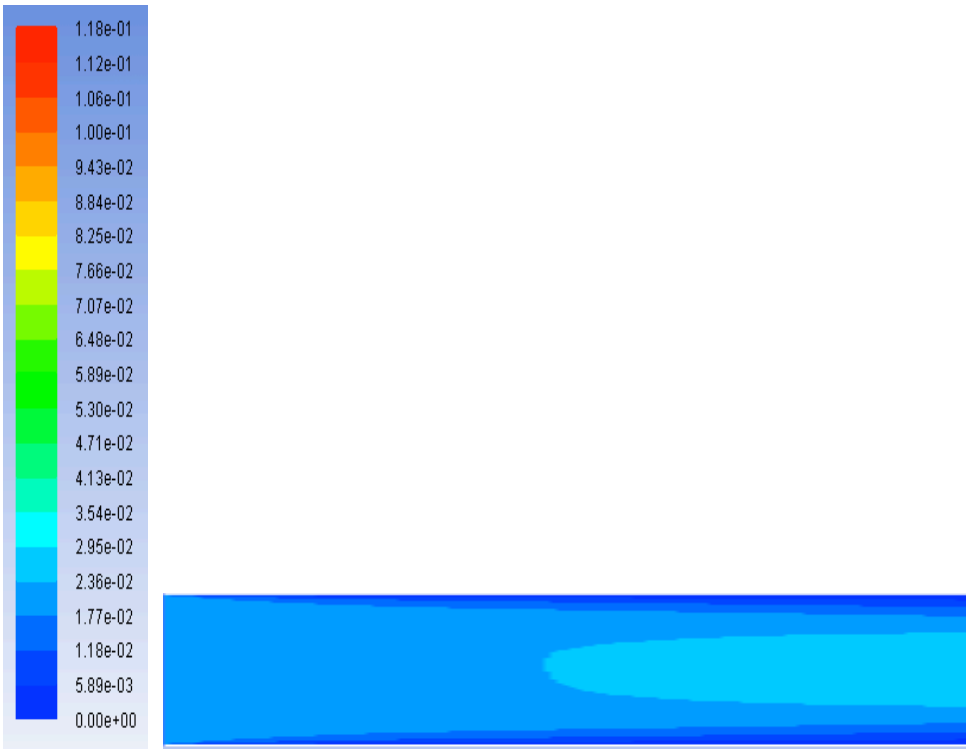


Figure 7: Velocity contour plot at 0.02 m/s at the inlet

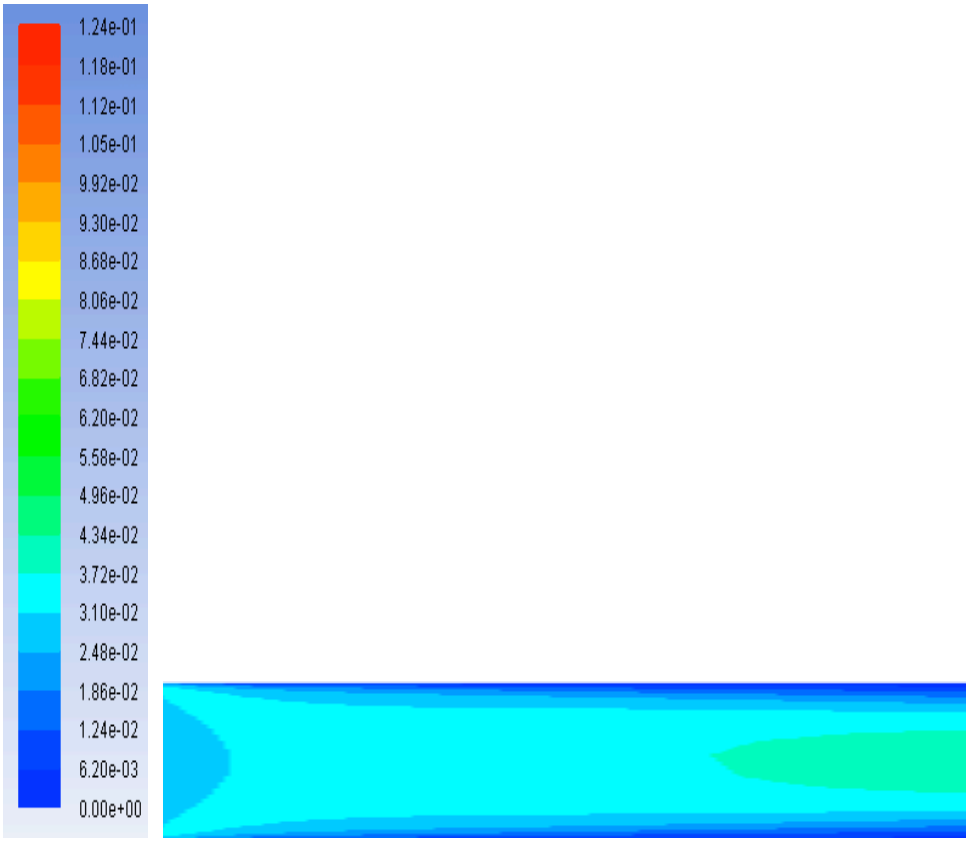


Figure 8: Velocity contour plot at 0.03 m/s at the inlet

Based on figure 6, 7 and 8, it shows the results generated with different inlet velocity. There were significant changes in the flow behavior when the inlet velocity is changing. It can be seen that, laminar flow is developed at the inlet part of the reactor because the velocity is varied from the lowest at the walls to the maximum along the cross-sectional center of the reactor. Hence, increase in inlet velocity affects the entrance length to get fully developed velocity profile and the entrance length is as expected increase with increase in Reynolds number. Besides that, the thickness of the zone with maximum velocity shrinks with increase in Reynolds number.

Pressure Distribution

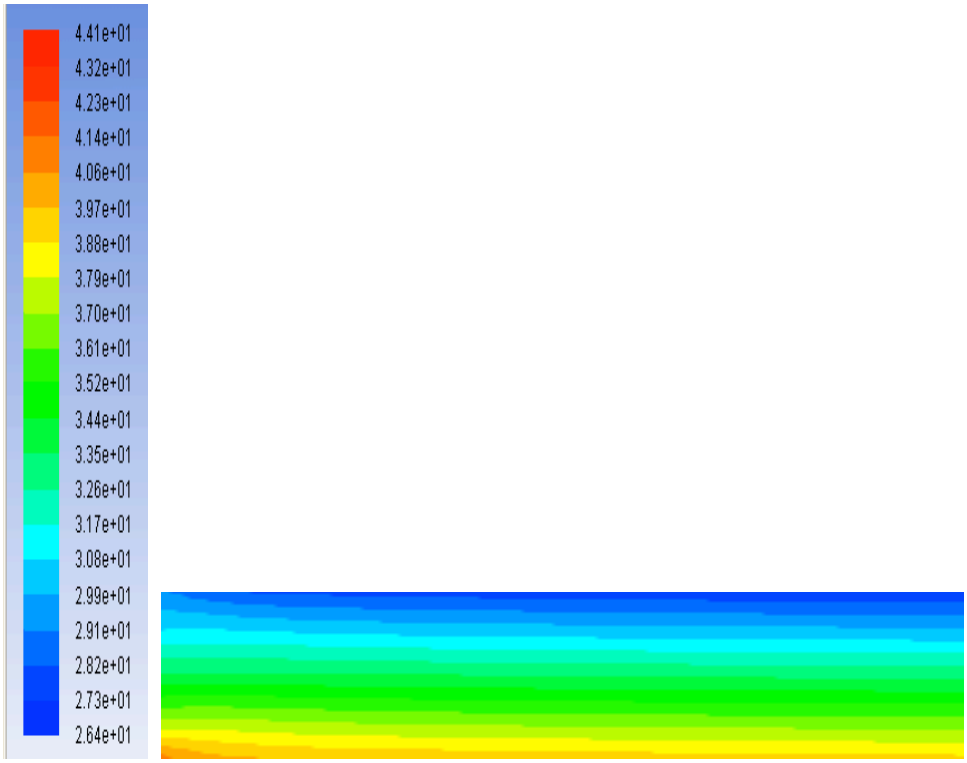


Figure 9: Pressure contour plot at 30 Pa

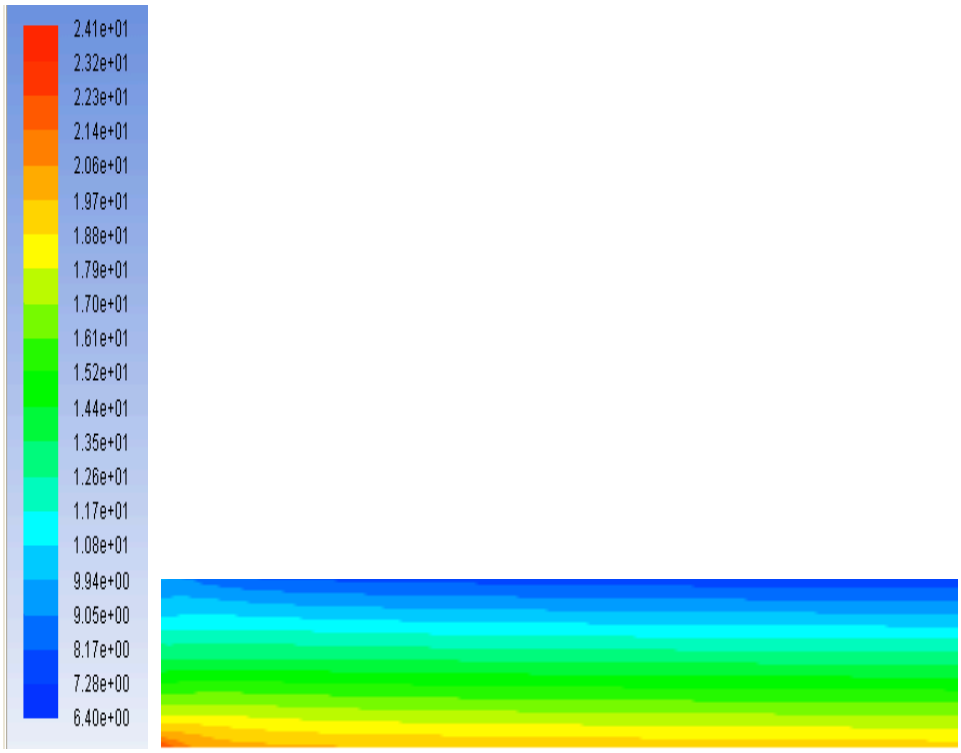


Figure 10: Pressure contour plot at 10 Pa

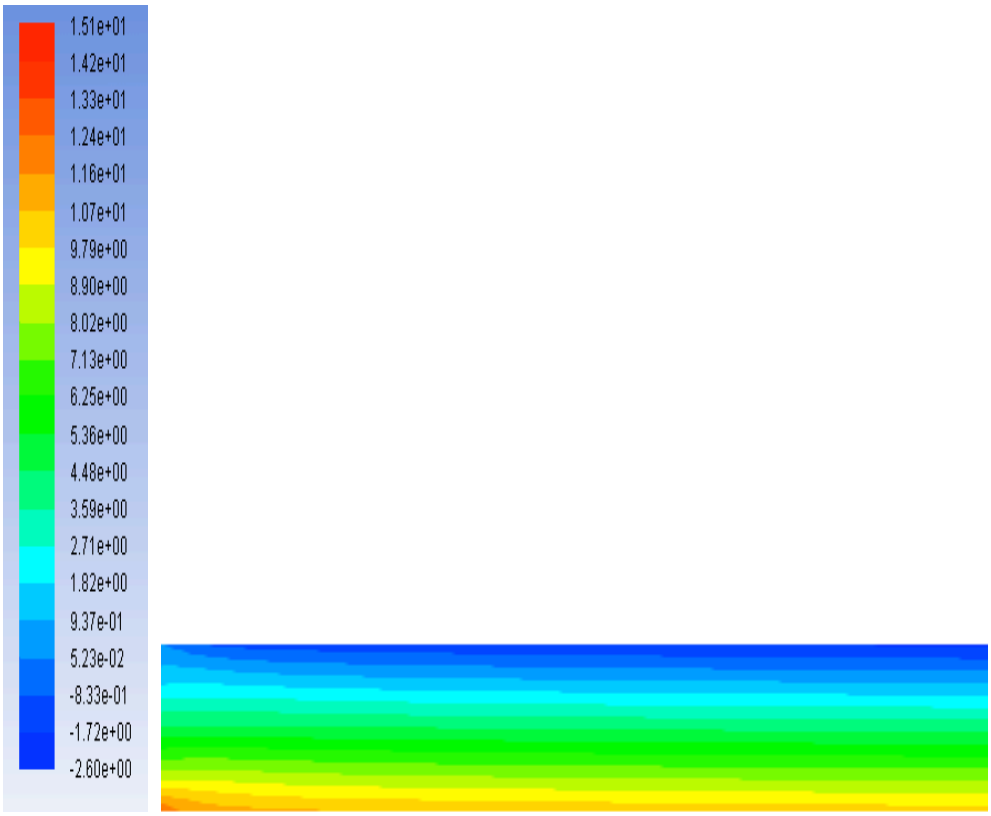


Figure 11: Pressure contour plot at 1 Pa

For the pressure distribution, outlet pressure was varied for 30 Pa, 10 Pa and 1 Pa. There were no significant change observed from figure 9, 10 and 11. As the outlet pressure varied, the flow is layering onto another and it is calculated that the Reynolds number is in the range of laminar flow. Hence, changing in the outlet pressure does not give significant changes on the flow behavior.

CHAPTER 5: CONCLUSION & RECOMMENDATION

As a conclusion, this project is important as it deals with alternative ways of producing biodiesel. Based on the results generated, it is believed that, by modelling and simulating method, the behavior of the fluid flow in the millichannel reactor can be known and analyzed for further optimization and design. For variation of inlet velocity, the flow behavior is changing with different value of Reynolds number but there were no significant change observed for variation of outlet pressure.

As a recommendation, simulation of millichannel reactor for model can be created with well-designed 3D geometry. By using 3D, the geometry can be drawn with more details for every corner or edge required. Hence, more accurate results will be obtained. Furthermore, assessment in variation of other parameters can be simulated and analyzed for further application use.

CHAPTER 6: REFERENCES

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