EFFECT OF THE MICROCHANNEL CONFIGURATIONS ON MIXING PERFORMANCE

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LIST OF ABBREVIATION

CFD	Computational Fluid Dynamics
LF	Laminar Flow
PDB	Pengiraan Dinamik Bendalir
TDS	Transport of Diluted Species

LIST OF SYMBOLS

Symbol	**Description**	**Unit**
C	Concentration	Mol/dm^3
D	Diffusion Coefficient	m^2/s
D_h	Hydraulic Diameter	M
P	Pressure	Pa
L	Length	Mm
R	Radius	Mm
Re	Reynolds Number	
Pe	Peclet Number	
T	Absolute Temperature	K
V	Velocity	m/s
μ	Dynamic Viscosity	
ρ	Density	Kg/m^3
μm	Micrometer	
Å	Angstrom	

KESAN REKA BENTUK SALURAN MIKRO KEPADA PRESTASI CAMPURAN

ABSTRAK

Dengan perkembangan teknologi dalam dekad ini, teknologi mikrosaluran telah menjadi salah satu alat yang paling penting dalam sintesis kimia kerana manfaat dalam menyediakan banyak percampuran dalam masa yang singkat. Ia juga terkenal kerana keupayaannya dalam melaksanakan proses intensifikasi selari dengan trend dalam industri. Dengan kebolehan dalam mengurangkan saiz, kos rendah, produktiviti yang tinggi dan meningkatkan keselamatan, membuat reaktor mikro sebagai salah satu alat yang berguna untuk masa depan kejuruteraan kimia. Kualiti pencampuran dalam peranti bendalir mikro disiasat dengan lebih mendalam untuk menaik tarafkan kajian-kajian yang telah dikaji oleh penulis lain. Dalam kajian ini, tiga dimensi Pengiraan Dinamik Bendalir (PDB) dengan keratan rentas bulat telah dibangunkan untuk menyiasat kualiti pencampuran dalam konfigurasi saluran mikro yang berbeza dengan halaju masuk yang berbeza, pekali resapan dan jenis bersirat. Keputusan telah menunjukkan bahawa halaju masuk mempunyai kesan yang besar kepada prestasi pencampuran. Prestasi pencampuran yang lebih cepat dapat dilihat apabila halaju masuk yang rendah dan pekali resapan yang tinggi telah digunakan. Jenis bersirat denda menunjukkan kualiti pencampuran lebih perlahan daripada jenis bersirat biasa kerana ia mengambil banyak masa walaupun ia adalah lebih baik dalam menyelesaikan masalah dalam perisian PBD. Mikrosaluran berbentuk Y menunjukkan kualiti pencampuran lebih baik daripada microchannels berbentuk T dan Arrow berbentuk.

EFFECT OF THE MICROCHANNEL CONFIGURATIONS ON MIXING PERFORMANCE

ABSTRACT

With the technology development in this decade, microchannel technology has became one of the most important tool in chemical synthesis because of its benefit in providing greatly enhanced mixing in short time. It is also widely known because of its ability in performing the process intensification which significantly catching up with the trend in the industry. With the abilities in reducing the size, low cost, high productivity and enhance safety, make microreactor as one of those useful tools to the future of chemical engineering. The mixing quality in the microfluidic device is further investigated in order to improve the one that have been studied by other authors. In this study, three-dimensional Computational Fluid Dynamics (CFD) model with circular cross section have been developed to investigate the mixing quality in different microchannel configurations with different inlet velocity, diffusion coefficient and type of meshing. The results have shown that inlet velocity has a great impact on the mixing performance. The faster mixing performance can be seen when low inlet velocity and high diffusion coefficient have been used. The fine type of meshing shows slower mixing quality than normal type of meshing because it takes a lot of time even though it is better in solving the problem in CFD software. Y-shaped microchannel shows better mixing quality than T-shaped and Arrow-shaped microchannels.

CHAPTER ONE

INTRODUCTION

1.1 Research background

Microreactor technology has came into spotlight by most of researchers as one of the most useful tool in the industries in the last few decades. It has shown that the microscale device is more beneficial than macroscale device because of its potential in replacing batch synthesis of a chemical to continuous reaction from lab-on-a-chip biotech devices to industrial applications since more than 10 years (Falk and Commenge, 2010). The microscale device is popular not just because of its ability in replacing large-scale conventional laboratory instrumentation, with the advantages include reduced hardware costs, low reagent consumption, faster analysis speeds, low weight, low size, highpower characteristics and the capability of operating in a massively parallel scale can make it as one of the most needed tool in the industries (Sudarsan, 2006, Kashid, 2007). The microchannels are widely used in pharmaceutical researching, microreactors in refineries and the energy industry, chemical microreactors, chemical and biological analyzers, drug delivery systems, and a lot more.

The microchannels have been known by most of chemical industries investors because of its potential in performing the process intensification. They are several important factors to achieve the process intensification; to lower the cost, optimize the energy, environmentally friendly, safety benefits, compactness and reaction time. The microreactor systems have been chosen as the most suitable and efficient tool in fulfilling the requirements of the process intensification because of its abilities in size reduction, low equipment and energy costs, precise process control, high productivity, inherent safety, enhanced reaction selectivity, well-defined flow patterns and very high interfacial area (Kashid, 2007, Lü et al., 2016). It provides the beneficial in equipments development and techniques in order to achieve the aim of the process of intensification. Process intensification has been considered as one of revolutionary development in chemical industry as it can achieve by revisiting fundamentals of fluid dynamics, heat and mass transfer (Kashid, 2007).

The microchannel systems are mostly focused on fluid mixing as it is the main process in the system (Capretto et al., 2011). Under microchannel group, there are micromixers which are designed for mixing purpose. The mixing process depends solely on both geometric structure and operating conditions. The operating conditions such as flow analysis, velocity profile, concentration profile and mixing quality are necessary to be investigated to provide better insights in the microchannel (Lü et al., 2016). In micro-scale mixing, the process relies mainly on diffusion due to the laminar behaviour of the flow with low Reynolds number. The flow is specified as laminar flow because of Reynolds number is small in the microfluidic systems. Re is typically smaller than 100. Thus, it cannot be turbulent. Microchannels are generally classified into two basic principles in order to influence mixing at the microscale; active and passive. The active mixers depend on external energy source while passive mixers depend on pumping energy (Capretto et al., 2011).

There are two methods for characterizing the mixing performance; by experimental method and simulation method. For this research, the simulation method has been chosen (Lü et al., 2016). For simulation method, computational fluid dynamics (CFD) can be used because it provides the details understanding on the physical events in which involving the flow of fluids around and within designated objects by using the applied mathematics, physics and computational software. It is also used to know how the gas or liquid affects the objects as it flows past. The explanation on CFD simulation will be further discussed on section 2.2. The examples of CFD that can be used in this project are Solid Work, AutoCAD, ANSYS and COMSOL Multiphysics (version 5.2). The COMSOL Multiphysics has been chosen.

1.2 Problem statement

Microchannel system comes into spotlight by most of researchers as one of the most useful tool in process industries. It is widely used in pharmaceutical researching, microreactors in refineries and the energy industry, chemical microreactors, chemical and biological analyzers, drug delivery systems, and a lot more. With all of these applications, it has shown clearly that the microchannel played a big role and the concept of microfluidic system is needed to be understand thoroughly. Mixing is one of important process that occured in the microchannel system and the most discussed topic by most of the authors.

Thus, it is needed to modify the current configurations in order to enhance the mixing. The study on the mixing via Y-shaped (120°), and T-shaped (180°) with rectangular cross section have been done recently by the researchers. Nevertheless, the simulation of Y-shaped and T-shaped with circular cross section especially the simulation of arrow-shaped (260°) are not widely studied by the authors. Owing to this lack of informations, it becomes the main objective of this research.

This research mainly focused on mixing performance as it is the main process in the microscale devices. The research was done by constructing different geometries with circular cross section in CFD software. The mixing performance was observed in every geometry configurations with different inlet velocity, diffusion coefficient and type of meshing.

1.3 Research objectives

The objectives for this research are:

I. To contruct the geometry configurations of microchannels with different inlet angle (120°, 180°, 260°)

II. To evaluate mixing performance at different inlet velocities, diffusion coefficients and different types of meshing in order to make comparison between the geometry configurations

III. To estimate mixing quality via CFD visualization and numerical analysis

CHAPTER TWO

LITERATURE REVIEW

This chapter described the study on microchannel in general. The next section is the classification of microchannel. This is then followed by microfluidic environment and mixing in microchannel. In addition, a brief description on computational fluid dynamics (CFD) is also given in this chapter.

2.1 Microchannel

Microreactor systems are a very small-scale device which are made from stainless steel, and resins that have microchannels on the order of micrometers. It allowed the chemical reactions and continuous flow reactions to take place and perform in the system. The continuous flow reactions can be occured by using microfabrication modules. The continuous flow in microchannels allow reaction processes to be monitored, controlled, analyzed and intermediate storage to be minimized (Asano et al., 2010). The characteristics dimension of internal structure of microchannels like fluid channels typically range from sub-micro meter to the sub-milimeter range (Ehrfeld et al., 2000).

The microchannels have attracted a lot of chemical industries investors as one of their main tool because of its potential in performing the process intensification. Process intensification has been considered as one of revolutionary development in chemical industry as it can be achieved by revisiting fundamentals of fluid dynamics, heat and mass transfer (Kashid, 2007). The important criteria to achieve process intensification are mainly focused on lowering the cost, optimizing the energy, environmentally friendly, safety benefits, compactness and reaction time (Stankiewicz and Moulijn, 2002). The microchannel systems have been chosen as the most suitable in fulfilling the requirements of the process intensification because of their abilities in size reduction, low equipment and energy costs, precise process control, high productivity, inherent safety, enhanced reaction selectivity, well-defined flow patterns and very high interfacial area (Kashid, 2007, Lü et al., 2016). It is considered as cheaper processes because of these factors. With the development of equipments and techniques provided by the microscale devices, the aim of the process of intensification can be achieved successfully.

2.1.1 Classification of microchannel

Microchannels are generally classified into two basic principles in order to influence mixing at the microscale system; active and passive. The active mixer depends solely on external energy source whilst the passive mixer depends on pumping energy. Substantively, active microchannels can perform higher mixing efficiency but the undesirable limitations occured in practical applications. The limitations included the complex and expensive fabrication process, the demand to integrate peripheral devices such as the actuator for the external power source into the microscale device and higher temperature that can damage biological fluids (Capretto et al., 2011).

The passive mixer has been chosen as the most suitable for the microscale devices because of its simple process in achieving a great mixing performance by only designing the geometry of microchannel systems (Charpenteir, 2003). As a result, the mixing efficiency can be enhanced, the diffusion length can be reduced and the contact surface area can be maximized. In addition, the passive mixer required low production cost, and can be easily integrated into more complex devices. Thus, passive micromixers are more favorable fabrication than active micromixers (Capretto et al., 2011).

The examples of passive mixer are parallel lamination micromixer, standard slit interdigital micromixer (SSIMM), droplet micromixer, T-shaped and Y-shaped micromixers. Since the microchannels used in this study is categorized into passive mixer, there are three different geometries take part for this research; T-shaped microchannels (180° inlet channels), Y-shaped microchannels (120° inlet channels) and Arrow-shaped microchannels (260° inlet channels).

2.1.2 Microfluidic environment

The microchannel systems are not merely the transformation of macrodevice system to microdevice system because their environment conditions are totally different from each other such as diffusion, surface tension and surface area-to-volume ratio. Both microscale and macroscale have different environmental conditions. It was found that the major advantage of microscale device is it has high area-to-volume ratio. Owing to this advantage, microchannel systems have better yield and selectivity than the conventional reactors (macroscale devices). It can also increase the rates of mass transfer and heat transfer significantly (Termizi and Shukor, 2014).

The geometrical configurations of microscale devices have a great effects on fluid flow, inlet velocity of the fluid, pressure and temperature (Jyh-tong Teng et al., 2012). The fluid flow in microchannels is divided into two types of flow; laminar and turbulent (Capretto et al., 2011). For microchannel system, the fluid flow is categorized as laminar flow because of low Reynolds number. The Reynolds number for the passive micromixers is less than 100 (Itomlenskis et al., 2008). The Reynolds number (Re) formula is defined as,

$$Re = \frac{\rho u D_h}{\mu}$$

(2.1.2.1)

Where, where ρ and μ are the fluid density (kg/m^3) and viscosity (kg/m.s) respectively; u is the velocity of the fluid (m/s) and D_h is the hydraulic diameter of the channels (m). The hydraulic diameter for circular cross section can be calculated as,

$$D_h = \frac{4\pi r^2}{2\pi r} = 2r$$

(2.1.2.2)

Where r is defined as the radius of cross section of the geometric configurations used in this research.

Besides the low Reynolds number, the flow can not also be turbulent because of the hydrodynamic instability does not develop in the microreactor system (Capretto et al., 2011). The laminar flow is parallel to each other and the velocity is unsteady with time at any locations when the boundary conditions are constant. From this point of view, the convective mass transfer can be presented and mixing can be achieved solely by molecular diffusion.

Aside from determining the type of flow in microchannel system, Re is giving a great impact on the prediction of inlet velocities in microchannels. The chosen of inlet velocities depend on Re. The chosen of higher velocity is not suggested in the microscale device because it will be decreased the contact time between two phases. As a result, the efficiency of the transport phenomena will be decreased if the contact time decreased. The higher velocity is not just affected the transport phenomena, it is also caused an increase in the hydrodynamic force and in the same time, affected the surface tension. The hydrodynamic force and interfacial tension force are the factors that we need to take into account while doing the research on microchannel systems (Capretto et al., 2011).

It was found that inlet pressure would be also gave an impact to the velocity and concentration profile. However, it has a very little effect on the velocity profile and no effect on the concentration profile. Thus, the inlet pressure is not considered as important as the inlet velocity because it does not have significant effects towards the concentration profile as the line intersected with each other (Termizi and Shukor, 2014).

2.1.3 Mixing in microchannel

Mixing is one of important process that occured in the microchannel system and the most discussed topic by most of the authors. Mixing is the process of the reduction of inhomogeneities which is relating to the chemical composition. Basically, the mixing in the liquid can be occured by combining two or more types of liquid to form desired homogenisation (Bothe et al., 2008).

There are two principles which are important for the mixing process; diffusion and convection. Diffusion is the net movement of particles from high concentration to low concentration while advection is the motion of particles along the bulk flow. The combination of both diffusion and advection will be formed convection which is the collective motion of particles in a fluid (Benke, 2014, McCabe et al., 2005). The convective effects can improve the quality of mixing which is associated with the transversal flows employed by the asymmetric ridges (Itomlenskis et al., 2008). The relationship between these two mechanisms can be characterized by dimensionless number, Peclet number (Capretto et al., 2011). The Peclet number can be defined as;

$$\mathrm{Pe} = \frac{\mathrm{vL}}{\mathrm{D}}$$

(2.1.3)

Where v is the velocity (m/s), L is the characteristic hydraulic dimension (m) and D is the diffusion coefficient (m^2/s). The Peclet number is used to define the ratio of advection versus diffusion mixing.

Other authors have suggested another ways to increase the mixing efficiency in microchannel systems by adding the obstacles or roughening the channel walls. The aim of this study is to determine a simple channel structure where secondary flows can be produced to improve the mixing with low flow rates and pressure losses. The basic design of the new channel configuration was created from the intuitive idea of a geometry that can promote flow circulations at different flow rates and not solely because of the presence of obstacles in the microchannels (Johnson et al., 2002).

Other than focusing on the mixing performance, we are also needed to consider the unfavorable effects of imperfect mixing on conversion and selectivity. It can be avoided by reducing the total mixing time. The total mixing time should be below the time-scale of chemical reaction (Bothe et al., 2008). The mixing time can also be reduced by dividing the fluid stream using serial or parallel lamination. In the passive mixing, the fluid has to be continuously divide and recombine, forming reqular-sized fluid embodiments because of high viscous force (Wolfgang Ehrfeld et al., 2000).

2.2 CFD simulation

Computational Fluid Dynamics (CFD) is the software in the computer which is used to solve the governing differential equations numerically. It provided the details understanding on the physical events in which involving the flow of fluids around and within designated objects by using the applied mathematics, physics and computational software. The examples of the physical events are diffusion, convection, boundary layers, slip surfaces, turbulence and shock waves which can be classified and related to the action and interaction of phenomena (Lomax et al., 1999). The CFD has came to the spotlight by most of the engineers as one of the easiest way to obtain the solutions to the governing equations for most of engineering problems (Bhaskaran and Collins). The examples of CFD available are Solid Work, AutoCAD, ANSYS, and COMSOL Multiphysics. The COMSOL Multiphysics (version 5.2) has been chosen for this research.

There are two methods can be used for this research; by experimental method and simulation method (Lü et al., 2016). CFD simulation has been considered as the most beneficial technique as compared to the experimental method because it gives an insight into flow patterns that are difficult, expensive or impossible to study.

CFD is widely used in variety of applications in industries. It is widely used in aerospace, automobile, building HVAC (heating, ventilation and air conditioning), petrochemicals, process engineering and etc. For building HVAC, CFD is employed to provide more accurate and fast predictions of building performance such as air flow, pressure, temperature and similar parameters (Bhaskaran and Collins). CFD is considered as the most efficient way to simulate full picture of the real fluid flows in the building (Lomax et al., 1999).

2.2.1 Advantages of CFD

There are a lot of advantages of CFD aside from its ability in solving governing differential equations. Firstly, simulating in the CFD software is not just a helping tool in solving the equations to the user but also a good cost and time reduction. Eventhough experimental method gave more accurate and useful data to the user, it is expensive and time-consuming. The probabilities of the flow to get disturbed excessively, poor safety and incorrect parameters scaling may be high by using experimental method. Owing to this problems, CFD simulation is the most suggested way to use. It gives an insight into flow patterns that are difficult, expensive or impossible to study. In addition, CFD can give more specific data, visualized and detailed information about the velocity field, pressure, temperature, etc. The safety can also be ensured to the user by CFD simulation (Lomax et al., 1999, Craft)

2.2.2 Limitation and error of CFD

Aside from its advantages in simulation, the limitation and errors are needed to take into account. We should be noted that the solution in CFD is not totally correct because the solutions will have some error associated with them. There are three sources of errors; modelling errors, discretization errors and interation errors. Because of the presence of modelling errors, the result of the simulation results and reality will be totally different. But the errors were small and can be neglected. For discretization errors, it can occur with approximating the differential equations by a set of algebraic ones relating variable values at the grid nodes. While for iteration errors, it is usually observed how far the current estimate from the exact solution of the set of discretized, algebraic, and equations. Despite the fact that the iteration can be reduced by performing more iterations of the solver, it will cause a huge computational cost (Craft, Lomax et al., 1999).

The user needs to analyze thoroughly and fully understand the concept of the software in order to get the accuracy of a CFD solution.

CHAPTER THREE

METHODOLOGY

In this section, it will be explained more details about the methodology used in simulating the geometry configurations of the microscale devices in the CFD software. There are six main topics included in this section; project flow chart, simulation of microchannel, Computational Fluid Dynamics (CFD), parameter study, data collection and result analysis and verification and validation of result. All the topics will be discussed further in this section.

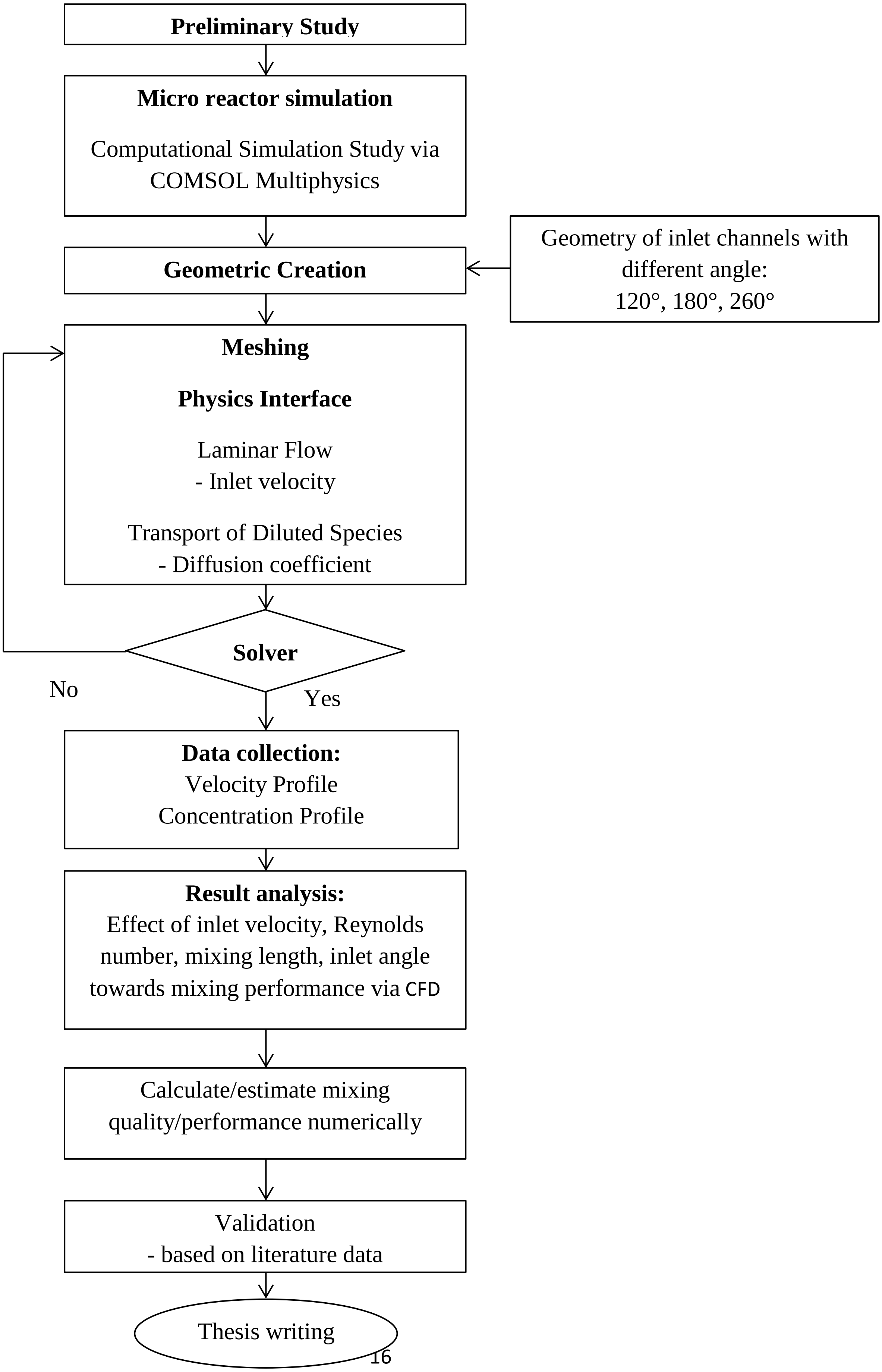
3.1 Project flow chart

The project starts with preliminary study and followed by the simulation of microchannel. The simulation of microchannel is mainly simulated in COMSOL Multiphysics (Version 5.2). COMSOL Multiphysics is the main simulation software used in this research. The geometries of inlet are created at different angle; 120°, 180° and 260°. By using the available simulation software, the geometries of the microchannels are created with different angles. The geometries are then meshed in order for simulation to be done. The detail part was discussed in Section 3.3.2.

Next, after the geometries have done, the process proceeded to the next step; the selection of the physics interface. In the physics interface, the Partial Differential Equation (PDE) has been chosen. In the research study, Laminar Flow (LF) and Transport of Diluted Species (TDS) physics interface were utilized to study on the mixing behavior in microchannel. Laminar flow is chosen because this research is only in one-phase. The solver will be solving the PDE. The laminar flow interface solved for velocity while the transport of diluted species was used to solve for the concentration. The velocity and concentration profiles are then evaluated and recorded.

The result is analyzed by observing the effect of inlet velocity, Reynolds number, mixing length and the angle of inlet channel towards the mixing performance via CFD. The mixing quality and performance can be calculated and estimated numerically. After the analysis of the result was done, it will be compared with the literature data to validate the simulation results. Finally, the research will be continued with the thesis writing. The full processes of the research can be seen clearly in the project flow chart below in Figure 3.1.

Figure 3.1 : Project flow chart



3.2 Simulation of microchannel

The simulations were done by drawing the geometry configurations in the COMSOL Multiphysics (version 5.2). The simulation of microchannel configurations are constructed with different angles of inlet channels; 180° (T-shaped), 120° (Y-shaped) and 260° (Arrow-shaped). For this simulation, water is considered as the fluid flows in the microchannel system. The choice of fluid dynamics must be correct because microchannel devices involve micron dimension. The molecular diameter for the water is 1.9 Å, which is the result in Knudsen number of 9.5×10^{-8}. As a consequence, the fluid can be treated as continuum and classical fluid dynamics can be used for this study (Harley, 2012).

3.3 Computational fluid dynamics

The main objective of the project is to investigate the mixing performance in different microchannel configurations. The CFD simulation has played an important role in this research as it is the main tool in the project. The examples of available tools that can be used in this study are Solid Work, AutoCAD, ANSYS and COMSOL Multiphysics (version 5.2). The COMSOL Multiphysics has been chosen as the main tool for geometric creation.

After deciding the dimension for T-shaped, Y-shaped and Arrow-shaped microchannel configurations, the process is proceeded to meshing. In meshing, it will be transformed the geometry into multigrid for partial different equation solving procedures. After meshing has done, the step followed by the physical model interface. In physics interface, the physics of the study have been chosen according to the project's requirement. In the physics interface, the Partial Differential Equation (PDE) has been chosen. Next, the solver will be solving the PDE. Finally, the data collection from the simulations was done (COMSOL, 2012).

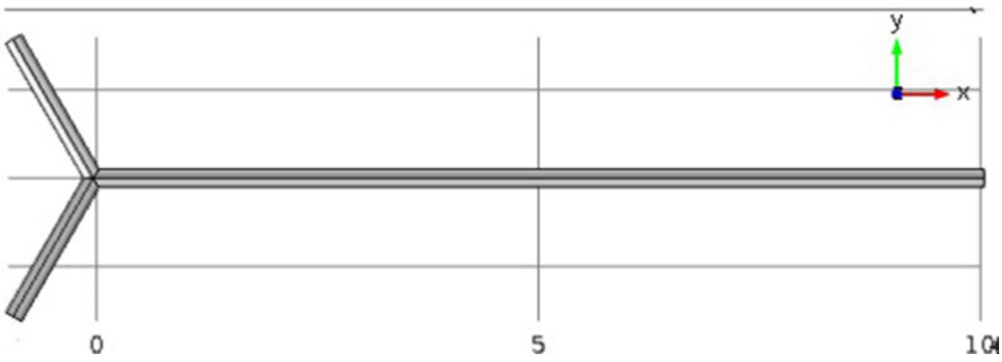
3.3.1 Geometry creation

The CFD simulation has played an important role in this research as it is the main tool for this research. The examples of available tools that can be used in this project are Solid Work, AutoCAD, ANSYS and COMSOL Multiphysics (version 5.2). The COMSOL Multiphysics has been chosen for this research.

The microchannels constructed in the simulation software have two inlets and an outlet. The inlet channels were designed with different angle; 120°, 180° and 260°. This research was done to study the effect of different angles of inlet channels on mixing performance. The angle of inlet channels was changed for each microchannel designs in order to know which one performed better in mixing.

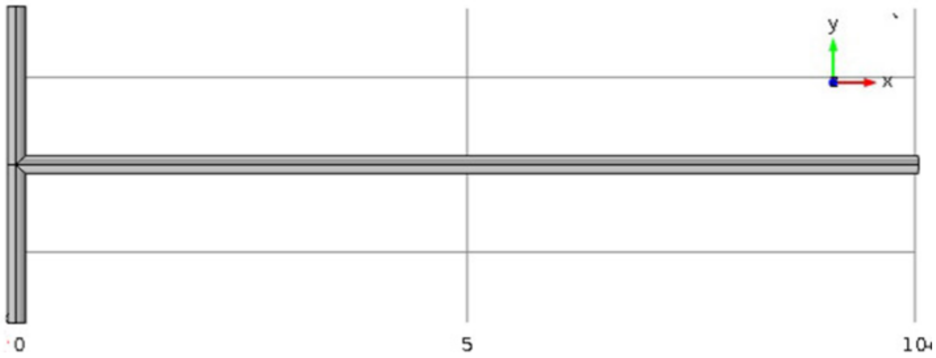
Aside from setting up different angle of inlet channels, the boundary conditions also played an important role for the requirement of the simulation. The boundary conditions consist of inflow, outflow boundaries, solid wall, symmetric boundaries and etc. After setting up all of these according to the research's requirements, the step continues to meshing. In meshing, geometry simulation is divided into small grids or element which is called meshed cell (Lomax et al., 1999). The meshing part will be discussed further in the next section.

There are an important parameters that should be considered for the research which is important in inlet and outlet channels. The examples of parameters that should be considered for this research are velocity, pressure, material properties and etc. In inlet channels, the important parameters are different values of velocity and diffusion coefficient. In outlet channel, the important parameter is pressure. The figures below have shown the geometric creation for Y-shaped (120°), T-shaped (180°) and Arrow-shaped (260°) microchannel configurations.



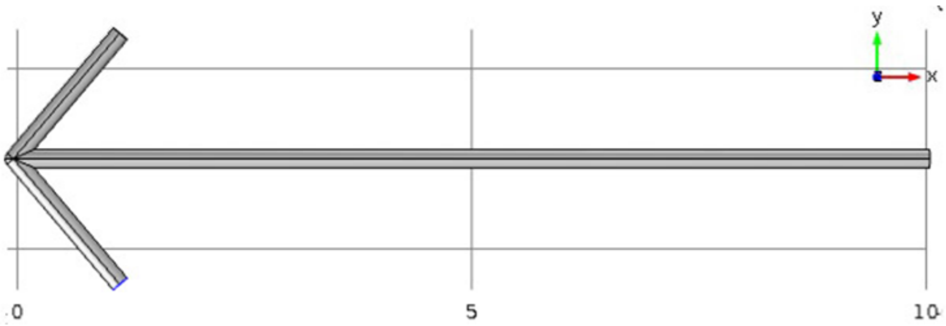
(unit = mm)

Figure 3.2 : Y-shaped (120°) of inlet channels



(unit = mm)

Figure 3.3 : T-shaped (180°) of inlet channels



(unit = mm)

Figure 3.4 : Arrow-shaped (260°) of inlet channel

3.3.2 Meshing

There are two purposes of meshing. Firstly, it subdivides the model of geometry simulation in software into smaller pieces, or elements, over which it is possible to write a set of equations describing the solution to the governing equation. Secondly, it is used to represent the solution field to the physics being solved. Meshing was done for the solution to become more accurate and to solve the flow physics within the domain.

There are three elements available in COMSOL Multiphysics; 1D, 2D and 3D. For this research, the element has been considered is 3D. The Mesh elements enable the discretization of the geometry model into small units of simple shapes. There are four types of 3D mesh elements as shown in Figure 3.5; tetrahedral, hexahedral, prism, and pyramid.

Tetrahedral elements are widely used for most physics within COMSOL Multiphysics. It is the only mesh element that can be used with adaptive mesh refinement and it can mesh any kind of 3D volume, regardless of shape or topology. The pyramid type of mesh element is only used when producing a transition in the mesh between bricks and tetrahedral. Bricks, prisms, and pyramids are used when it is motivated to use regarding to the condition of geometry simulation.

In the software used for this research, there are two options provided for type of sequence; physics-controlled mesh and user-controlled mesh. For this research, physics-controlled mesh with normal size and fine size were chosen. The software sets up the meshing sequences automatically and it fits the physical setting of the simulation the best. While for the user-controlled mesh, the mesh was created according to the user own input of size, element type and etc (COMSOL, 2012).

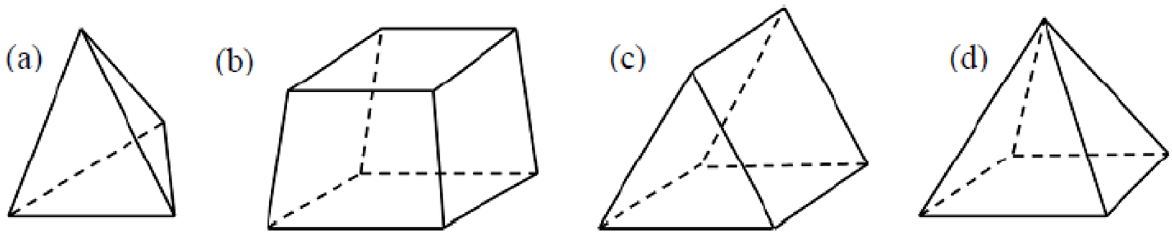


Figure 3.5 : 3D mesh elements; (a) tetrahedral (b) bricks (c) prisms (d) pyramid

3.3.3 Physics interface

The user has been provided with two types of physics interfaces. It contained user interfaces with already given equations and variables for specific area of physics interfaces and predefined templates. The multiphysics models occured when the user used more than one type of physics or equations. The physics interfaces involved in this research are Laminar Flow (LF) and Transport of Diluted Species (TDS).

Laminar flow interface is used in order to compute the velocity and pressure fields for the flow of a single-phase fluid in the laminar flow regime and incompressible fluids by using Navier-Stokes equation. The flow is specified as laminar flow because of Reynolds number is small in the microreactors systems. Re is typically smaller than 100. Thus, it cannot be turbulent. The Navier-Stokes equation for incompressible flow is given as (COMSOL, 2012):

$$\rho\frac{\partial v}{\partial t}+\rho(v.\nabla)v = \nabla.[-pl+\mu(\nabla v+(\nabla v)^T)]+F \tag{3.1}$$

$$\rho\nabla.v = 0 \tag{3.2}$$

Where,

v is velocity vector (SI unit : m/s)

p is the pressure (SI unit: Pa)

F is the volume force factor (SI unit: N/m^3)

ρ is the density (SI unit: kg/m^3)

μ is the dynamic viscosity (SI unit: Pa.s)

T is the absolute temperature (SI unit: K)

(The density and the viscosity data for the water ρ = 1000 kg/m^3 and μ = 0.001 Pa.s)

The driving force for the fluid to flow through the mixing slot to the outlet is the applied inlet velocity boundary conditions on the inputs whilst the pressure boundary condition is assumed to be equal to zero. Meanwhile, the chamber wall is assumed to have non-slip boundary condition. Mixing is obtained by diffusion of the various species in the fluid. The species are diluted in the water, thus having material properties like water. The transfer equation with a reaction term as shown below (COMSOL, 2012):

$$\frac{\partial c}{\partial t} + v.\nabla c = \nabla.(D\nabla c) + R \tag{3.3}$$

Where,

c is the concentration of the species (SI unit: mol/ m^3)

D is the diffusion coefficient (SI unit: m^2/s)

R is a reaction rate expression for the species (SI unit: mol/ m^{3}s)

v is velocity vector (SI unit : m/s)

In this model, R=0 because there is no reaction occurred. The species is introduced at different concentration from the range of 0 to 1 mol/m^3 where one species is at concentration of 1 mol/m^3 on one of the input boundary while the other is at zero concentration. At the output boundary, the substance flows through the boundary by convection (Termizi and Shukor, 2014).

3.3.4 Study and solver

In this section, it allows the user to choose their type of study according to what theer simulation needed. There are a lot of available study types provided in COMSOL Multiphysics. For instance, AC Impedance Stationary, AC Impedance Time Dependent, Eigenfrequency, Boundary Mode Analysis, and etc. Basically, there are two types of study that frequently used by the user; Stationary and Time dependent. In Stationary, it generates the equations without time derivatives whilst the time dependent study generates the equations for time-dependent (transient) simulations.

For the study and solver part, there are three types of basic parts included. Firstly, study step which is allowed the user to choose, according to the project. After the study type has been chosen, the process proceeds to the next part, solver configuration. The solver configuration provided user with related configurations for dependent variables to solve for, intermediate storage of solutions, and specific solver settings. Last part in study and solver features is job configuration which is contained the batch jobs, parametric jobs and cluster computing. In solver configuration, the solution will be computed after all the study types, parameters, geometry configurations and boundary condition have been inserted in the software. Just then, the job configurations will be functioned in examining the derivative value (COMSOL, 2012).

3.4 Parameter study

The parameters are decided before starting the simulation in CFD software. Table 3.1 has shown the parameters used in this research. The inlet velocities have been decided by using Reynolds number. The Reynolds number (Re) is defined as,

$$Re = \frac{\rho u D_h}{\mu}$$

(3.4)

Where, where ρ and μ are the fluid density (kg/m^3) and viscosity (kg/m.s) respectively; u is the velocity of the fluid (m/s) and D_h is the hydraulic diameter of the channels (m). The hydraulic diameter for circular cross section can be calculated as,

$$D_h = \frac{4\pi r^2}{2\pi r} = 2r$$

(3.5)

Where r is defined as the radius of cross section of the geometric configurations used in this research.

The Reynolds number range for microscale device is in the range of 0.01 to 100. Basically, it must be less than 100 because it is laminar flow. The diffusion coefficients are determined for this research by using the values for the binary diffusion coefficient. The values of diffusion coefficients for small particles in liquid is $10^{-9} - 10^{-11}$m^2/s and the value of diffusion coefficient for self-diffusion for liquid is in the range of $10^{-8} - 10^{-9}$ m^2/s.