Investigation of the Flow Behavioral Dynamics of Ammonia Component Gases in a Microreactor via Computational Fluid Dynamics (CFD) Approach

by

Ivan Liaw SheanYik

Dissertation submitted in partial fulfillment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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Approved by,

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(Mr. Mohd. Zamri bin Abdullah)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH PERAK

May 2013

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 reference and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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IVAN LIAW SHEAN YIK

ABSTRACT

Ammonia (NH_3) synthesis has been among the most favorable production process in the industry, especially for its application as synthetic urea. As the current conventional system of synthesizing NH_3 poses some disadvantages in terms of its operating conditions and production cost, yet producing low conversion and product yield; this project offers a new technique to enhance NH_3 synthesis through channeling the reactants in a microreactor consisting of supported catalyst at ambient operating condition. Prior to the process of constructing the rigs for experimental work to investigate NH_3 production in the said condition, a computer simulation via the utilization of computational fluid dynamics (CFD) approach will be conducted. This is to examine the flow behavior of the reactant gases in a microfluidic environment, particularly their mixing characteristics, which would assist in optimizing the localization of the catalyst for the reaction to take place. The results of the simulation will lead to the design of the overall microreactor itself, which will be used in the experimental approach of the NH_3 synthesis in the next step of the project. CFD is preferred as parametric studies in determining optimal design could be varied without the need to construct the real rig, which thus could reduce cost, time and material wastage.

ACKNOWLEDGEMENT

First and foremost, I would like to express my gratitude to my supervisor, **Mr. Mohd. Zamri bin Abdullah** for giving me the opportunity to carry out my bachelor thesis under his supervision. His invaluable guidance and advice throughout my Final Year Project period has tremendously contribute to the completion of this project. Besides that he always spend time through his busy working schedule to meet and discuss and explain to me the theory and procedure to carry out this project study. Without his kind encouragement, I believe I would not have been able to complete this project smoothly. It was indeed a pleasure working with him throughout this project study.

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CHAPTER 1

INTRODUCTION

Synthetic ammonia (NH_3) refers to ammonia that has been synthesized from natural gas. According to market research done by Ceresana (2012), the total ammonia production in year 2012 was 198 million tons, an increment of 35% over the global estimated output in year 2006. As of today, approximately 80% of ammonia produced worldwide is applied in agricultural field as fertilizers, with some other applications such as precursor to nitrogenous compound, cleaning agent, fermentation agent etc.

Together with carbon dioxide, it has found its importance in the chemical industries as a source for the production of synthetic urea. The most widely practiced ammonia (NH_3) production process, the Haber-Bosch process, was discovered by the German chemist Fritz Haber along with Carl Bosch dated back to early twentieth century. The highly pressurized synthesis was successfully commercialized in 1913, by which NH_3 is produced by the reaction of two gases i.e. nitrogen (N_2) and hydrogen (H_2). However, the reaction does not proceed at ambient temperature. At gas phase, N_2 requires a lot of energy to dissociate at around 3000^oC; while hydrogen which has a weaker molecular bond dissociates at temperature above 1000 ^oC. Improvement with an iron based catalyst towards the process will only lowered the reacting temperature to approximately 250-400^oC, with the reacting pressure remains high in the range of 150-200 atm. (Modak, 2011). Although NH_3 is one of the most highly produced inorganic chemicals, the

technique of Haber-Bosch process imposes some disadvantages. Low conversion of product yield is usually obtained while the high operating temperature and pressure causes the production process to be costly as high energy consumption is therefore required.

In order to improve the production of ammonia considering its high market demand especially in the agricultural sector, OneBAJA program introduces a new method of NH_3 synthesis, where the reaction process will be carried out in a redesigned reactor that can help to enhance the process and performance respectively. In this project, H_2 and N_2 gases will be channeled through a microreactor consisting of supported catalyst, where the reaction producing NH_3 takes place at ambient operating conditions by the means of magnetic induction zone. Besides generating higher conversion and yield efficiency, this new method offers advantages such as lowering the risk of the overall system due to its ambient operating conditions, which thus reducing the operating cost as well as saving spaces and energy due to its high surface-to-volume ratios, which makes them an attractive alternative to the any current conventional system.

Nevertheless, cases of ineffective mixing in a microreactor could also occur. That is mainly contributed by the laminar flow behavior of the fluids in the microfluidic device. Current researches involve in the field of micro reaction engineering have found the key interest in the issue arises from the said mixing process. Various simulation tools have been applied in order to assist the field experts and researches in their experimental work and theoretical studies. (Salim, 2011) As for the OneBAJA program, the experimental modeling and simulation tests for the said microreactor will be conducted through the utilization of Computational Fluid Dynamics (CFD) approach.

CFD has been the choice of researches to assist in modeling mixing problems in the recent years. The reactor and its system are simulated through a computational grid and the governing equations are discretized using numerical methods. (Marchisio & Barresi, 2003). It is stated that usually the physical design of a microreactor is based upon trial and error technique, resulted in inefficiency and suboptimal design. (Falk & Commenge,

2010). Without accurate theoretical knowledge with proper test methods and support of modeling, it is very costly for the industry to apply the said technique on a new product within a commercial industry. Therefore CFD modeling is significant as it could predict mixing characteristics prior to the real process designation. Through the simulation and modeling, the mixing process can then be optimized through trial and error method, by substituting various parametric values of the system.

In this project, CFD simulation using ANSYS CFX 14.5 will be conducted to determine the optimum parameter for the design of a microreactor in the synthesis of NH_3 from N_2 and H_2 at ambient temperature and pressure. At this stage, reaction between N_2 and H_2 will not be considered, whereby the simulation will look into determining the hydrodynamics of the mixing behavior of the two component gases in the microfluidic environment. Design parameters of the microreactor will be varied such as its diameter, the number of cyclic turns and the amplitude of the cyclic channel. It is expected that through the hydrodynamics study the optimum design will be achieved, which will be applied in the localization of catalyst into the microreactor for the reaction producing NH_3 to take place in the next step of the project.

CHAPTER 2

LITERATURE REVIEW

2.1 Microtechnologies

In 1959, Richard Feynman's thought-provoking speech "There's Plenty of Room at the Bottom" (Feynman, 1992), has witnessed the most rapid technology development in the history of humanity- the miniaturization of electronic devices. As for development of miniaturized non-electronic devices, the early stage of microfluidics was first applied on micro-flow sensors, micro-pumps, and micro-valves in the late 1980s. During the 5th International Conference on Solid-State Sensor and Actuators, Manz et al. (1990) indicated that life sciences and chemistry are the main application fields of microfluidics. Since then, the field of micro-fluidics has appeared to be the new research discipline dealing with transport phenomena and fluid-based devices at microscopic length scales.

Microfluidics has an advantage of utilizing scaling laws for new effects and better performance. These advantages are derived from the microscopic amount of fluid a microfluidic device can handle. By shrinking down the device size, the fluid behavior also changes, some of which are beneficial. (Nguyen & Wereley, 2006)

The field of micro-chemical engineering has a significant importance in chemical engineering studies as the replication of micro-reactors to those conventional facilities

used in the industries has advantages particularly on the high surface area to volume ratio. Besides, fast alterations of the operating conditions can be done with minimal time demand to reach its equilibrium states. (Cengel, 1997)

With the exploration of its new effects, microfluidics today is looking for further application beyond the conventional field such as flow control, chemical analysis, biomedical diagnostics, and drug discovery. New applications such as distributed energy supply and distributed thermal management has shown promising aspects, especially in chemical production using distributed microreactor to make new products. The large-scale production can be realized easily by running multiple identical micro-reactors in parallel. Thus it is shown that the concept of micro-reactor has a promising future, at the same time bringing forward the trend of nanotechnology in which technology imitates nature. (Nguyen & Wereley, 2006)

2.2 Micromixing

According to Paul et al. (2004), mixing is a transport process for species, temperature and phases to reduce inhomogeneity which leads to secondary effects such as reaction and change in properties. Three established terminology for mixing techniques has been defined as macromixing, mesomixing, and micromixing. Macromixing refers to mixing process which governs by the largest scale of fluid motion, for example the scale of macromixing corresponds to the diameter of the mixing tank. Micromixing refers to the mixing process at the smallest scale of fluid motion and molecular motion, while mesomixing is in the scale between macromixing and micromixing. Although micromixing may have dimension on the order of micrometers, transport process in micromixers may still be classified as mesomixing process.

The objective of micromixing is to obtain a uniform distribution of the components being mixed down to the smallest scale and quickly as possible. Many different methods of mixing have been reported by Nguyen (2008), such as molecular diffusion, eddy diffusion, advection, and Taylor dispersion. However due to small dimensions of the internal structures in micromixers (Aubin & Xuereb, 2009) and the dominant viscous effect in microscale, the flow is predominantly laminar in such divices. Therefore eddy diffusion mixing is not relevant for micromixing process. Thus, the main transport phenomena in micromixers are molecular diffusion, advection and Taylor dispersion.

Molecular diffusion is caused by the random motion of molecule which is characterized by the molecular diffusion coefficient. On the other hand, advection is explained as transport phenomena caused by fluid motion, where a simple Eulerian velocity can lead to chaotic advection. Thus, chaotic advection would be ideal for the laminar flow condition in micromixers. (Nguyen, 2008)

Meanwhile, Taylor dispersion is an advection caused by a velocity gradient. Even though mixing based on Taylor dispersion can be two or three orders faster than mixing based on pure molecular diffusion, in this project the velocity is set constant throughout the mixing process. Hence the fluidic mixing of the project will be based on both molecular diffusion and advection only.

Micromixing has found its superiority over the conventional mixing processes in the industry today. Due to its miniature size, micromixers allow the control over a number of parameters of production process in chemistry and pharmaceutical industry. Reaction conditions that are unusual in conventional mixing process are becoming technically possible in micromixers. Among the advantage of reaction in micromixers are the small thermal inertia, uniform temperature, and high gradient of different physical fields. Besides, a micromixer also reported to have a short residence time and the high volume to surface ratio as compared to a macroscale mixer. (Nguyen, 2008)

As a micromixer has a small thermal inertia, it allows fast and precise temperature control during the micromixing process. Furthermore, its miniaturization will leads to the

higher rates of heat and mass transfer. Compared to their macroscale counterparts, micromixers can offer a more aggressive reaction conditions. Its large surface to volume ratio allows effective suppression of homogenous side reactions in heterogeneously catalyzed gas phase reactions. In addition, the small size of micromixers makes the reaction safer because of the suppression of flames and explosions. Lowe et al. (2002) suggest that explosion can be suppressed by using mixing channels with hydraulic diameter less than the quenching distance.

Moreover, the slow mass and heat transfer in conventional macroscale reactor causes the reaction time for fine chemicals becomes much longer than needed for reaction kinetics. Through replacement of a batch-based conventional macroscale reactor by a continuous-flow microreactor, the reaction time can be significantly reduced, although the reactor volume is smaller but the total throughput per unit time is higher. Additionally, the large surface-to-volume ratio of micromixers provide more surface for catalyst incorporation compared to its conventional macroscale counterparts. Nguyen (2008) states that the amount of catalyst needed in a microreactor can be decreased by a factor of 1000.

Micromixing has found its importance in chemistry production, drug discovery and proteomics. Mixing is necessary in lab-on-a-chip (LOC) platforms for complex chemical reactions. Micromixers can also be integrated in a microfluidic system or work as a stand-alone device. (Nguyen & Wu, 2005) It is reported that Kamholz et al. (1999) use the basic T-mixer to measure analyte concentration of a continuous flow, while Hinsmann et al. (2001) used micromixer to study the rapid chemical reactions in solution with stopped-flow time-resolved Fourier transform infrared spectroscopy (TR-FTIR). Similarly, Wu et al. (2004) used Y-mixer to investigate the nonlinear diffusive behavior of a fluorescein. Besides sensing and analysis applications, micromixers were used as toll for dispersing immiscible liquids and forming micro droplets (Haverkamp, et al., 1999) In above all, micromixer can also works as a separator for particles based on their different diffusion coefficients (Brody & Yager, 1997) or as a generator of concentration gradients (Burke & Regnier, 2003).

In this project study, attention is paid to a number of operating parameters such as Reynolds number, Re, and Knudsen number, Kn.

$$Re = \frac{\rho \bar{u} L_{ch}}{\mu} = \frac{\bar{u} L_{ch}}{\upsilon}$$

[Equation 2.1]

Where

ρ = density

ū = mean velocity

L_{ch} = characteristic length (usually refers to hydraulic diameter)

μ = dynamic viscosity

υ = kinematic viscosity

Reynolds number represents the ratio between the advective mass transport and momentum transport, which can be further explained as ratio of momentum and viscous friction. Reynolds number above a critical value of around 2300 indicates a turbulent flow. In most cases of microfluidics, a low Reynolds number and a laminar flow is expected. Due to the micro-scale dimensions of the design, the Reynolds number is generally less than 100 (Re <100) or may even approach to 1, where in this case the flow is fully laminar and no turbulence within it.

$$K_n = \frac{\lambda}{D_h}$$

[Equation 2.2]

Where

λ = mean free path

D_h = hydraulic diameter of channel structure

The dimensionless Knudsen number is the ratio between the distance of molecules and the channel size. Generally, fast mixing can be achieved with smaller mixing path and larger interfacial area. If the channel geometry is small, the fluid molecules collide most often with the wall and not the other molecules. In this case, the diffusion process is called Knudsen diffusion. (Cussler, 1997)

All the further consideration concerning micromixing in this project study are valid for single phase systems, either gas or liquid. This is due to the specificity of gases in microchannels lies in the hypothesis of continuity of the fluid. Moreover, the distance between two molecules in the gas phase can be on the order of magnitude of the channel width (for Knudsen number, Kn > 0.1) (Aubin & Xuereb, 2009).

2.3 Micromixer

In this study, the term “microreactor” or “micromixer” is used interchangeably, as both are referring to the present invention of device that comprise of microfluidic channels at micrometer dimension.

Micro-reactor is a miniaturized reaction system fabricated using methods of micro technology. With its mini-plant functionality, chemical reactions are carried out in three-dimensional structures with the inner dimensions in the range of micrometers. The enhancement of the micro-reactor technology in mass transport and its accurate control of relevant process parameters like temperature, pressure, and flow rate and residence time

make the micro technology to be more outstanding than the conventional reactor system, where its operation can also be conducted under challenging conditions with its compact space-saving physical. Yield improvement and cost saving while operating in safe operating condition is also reported. (Hsu et al., 2007)

Nguyen & Wu (2005) and Hessel (2005) categorised micromixers as passive micromixers and active micromixers. The former stated that passive micromixers do not require external energy, while Hessel (2005) further explained that mixing process relies on the energy of the flow and the geometry of the mixer in order to manipulate the fluid. As simple passive structures are robust, it is more stable in operation and easily integrated in a more complex system.

Meanwhile, an active micromixer operates through the disturbance generated by an external field for the mixing process, such as ultrasound, vibrations, pulse flow rates etc. (Hessel, 2005). With the inclusion of external disturbance, the structure of the active micromixers are more complicated as compared to passive micromixers. In addition to the requirement of complex fabrication process and external power sources, Hessel (2005) also states that its integration into microfluidic system is challenging and expensive.

Classification of both passive and active micromixers are presented in TABLE 2.1 below:

TABLE 2.1: Means for Inducing Active and Passive Mixing (Aubin & Xuereb, 2009)

Passive Mixing Methods	Active Mixing Methods
Lamination	Electrokinetic instabilities
Multilamination	Periodic flow perturbations
Hydrodynamic focusing	Acoustic vibrations
Flow splitting and recombination	Magnet hydrodynamic force
Structured channel geometries	Ultrasound
Chaotic advection	Piezoelectric actuators
Micronozzle injection	Micropumps and valves
Impinging jets	Mechanical impellers

Due to the dominating laminar flow on microscale, mixing in passive micromixers relies mainly on molecular diffusion and chaotic advection. Increasing the contact surface between the different fluids and decreasing the diffusion path between them could improve molecular diffusion. Conversely, chaotic advection can be realized by manipulating the laminar flow in microchannels. Thus, resulting flow pattern will shorten the diffusion path and thus improves the mixing process. (Nguyen & Wu, 2005)

A simple method to reduce the mixing path is to make a narrow mixing channel (Veenstra, 1999), or realizing lamination with multiple streams. (Jackman, 2001) Since external power source is not available in passive mixing, the flow stream can be controlled by adjusting its dimensions such as the height, length and width (Bhagat, 2007). Lamination is a manipulation technique whereby the inlet stream of a micromixer splits into *n* sub streams and then joined into a stream as laminae.

The basic design is a long microchannel with two inlets to its geometry, often called the T- and Y-type micromixer. (Kamholz et al., 1999, 2002; Ismagilov et al., 2000) T- and Y-type micromixers are extremely simple contactors and relatively efficient micromixer if it is correctly designed. According to Aubin & Xuereb (2009), if the dimension of the microchannels is sufficiently small, mixing process by molecular diffusion can occur at very fast rate due to the minute size of characteristic length scale of the system. FIGURE 2.1 below shows a T-type and Y-type micromixers:

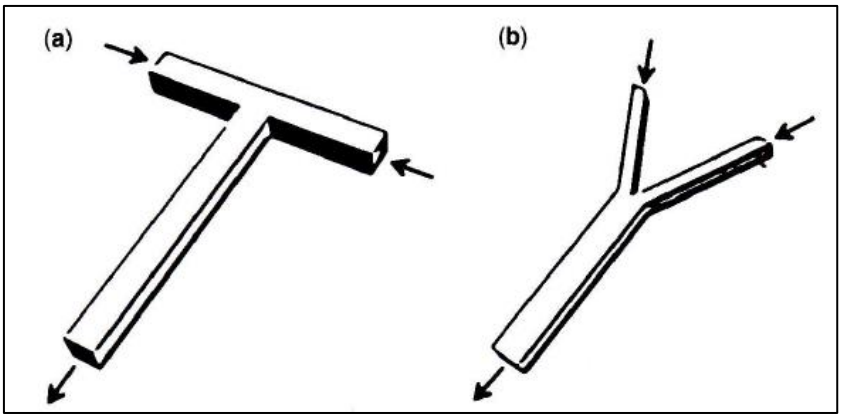


FIGURE 2.1: (a) T-type and, (b) Y-type micromixers (Aubin & Xuereb, 2009)

In order to reduce the mixing path, the inlet streams of a T-type micromixer (FIGURE 2.1a) can be twisted and laminated as two thin liquid sheets, with a chaotic

flow is expected with the induced vortices. As a basic design a T-type micromixer is ideal for investigation of basic transport phenomena on microscale, such as scaling law, butterfly effect and other non-linear effects. Nevertheless, a T-type micromixer depends entirely on molecular diffusion only, therefore a longer mixing channel is usually needed. (Hinsmann et al., 2001)

Experimental work conducted by Yi & Bau (2003) using a Y-type micromixer (FIGURE 2.1b) is reported to be able to generate vortices at Reynolds number of above 10 (Re >10), while at Reynolds number higher than 30, the mixing process is achieved right after the bend.

Another concept of reducing the mixing path for lamination micromixers is hydrodynamic focusing. The basic design is a long microchannel with three inlets, where the middle inlet is of sample flow, while the solvent streams join through the two inlets and work as the sheath flows. Hydrodynamic focusing is observed when the split and recombination occurs in the horizontal and vertical plants respectively. (Knight et al., 1998)

Besides molecular diffusion, advection is another important form of mass transfer in flows with a low Reynolds number. Generally chaotic advection can improve mixing significantly. It can be generated by special geometries in the mixing channel or induced by external force. Other than that, chaotic advection can be used on both passive and active micromixers. But in this project, only chaotic advection in passive micromixers will be discussed.

FIGURE 2.2 below shows the designs for mixing with chaotic advection at high Reynolds number. At high Reynolds number (Re > 100), the simplest method to achieve chaotic advection is by inserting obstacle structures into the mixing channel (Figure 2.2a and 2.2b). On the contrary, at low Reynolds number (Re <10) obstacles are reported to be unable to generate eddies or recirculation even though improvement on mixing performance is achieved at high Reynolds number. (Wang et al., 2002)

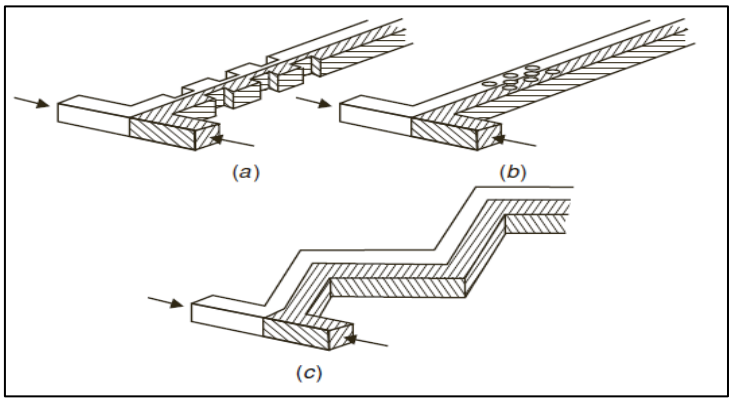


FIGURE 2.2: Design for mixing with chaotic advection at high Reynolds numbers: (a) obstacles on wall (Wong, Ward, & Wharton, Micro T-mixer as a rapid mixing micro-mixer, 2004), (b) obstacles in the channel (Wang, Iovenitti, & Masood, 2002), (c) zigzag shaped channel (Mengeaud et al, 2002)

Another method to generate chaotic advection is by using a zigzag microchannel (FIGURE 2.2c) to produce recirculation around the turns at high Reynolds number. Mengeaud et al. (2002) have discussed the periodic steps of the zigzag shap as the optimizing parameter in their work.

Conversely at low Reynolds number, as similar to the inner structure of conventional macromixers, ribs (FIGURE 2.3a) and grooves (FIGURE 2.3b) on a channel wall can produce chaotic advection. Johnson et al., (2002) were among the first to investigate this phenomena by creating grooves on the bottom wall of the microchannel using a laser. At the same time, investigation of the groove effect was carried out by considering two groove patterns (FIGURE 2.3b and FIGURE 2.3c), where the so called staggered-herringbone micromixer is reported to work well at Reynolds number ranging from 1 to 100. (Strook et al., 2002)

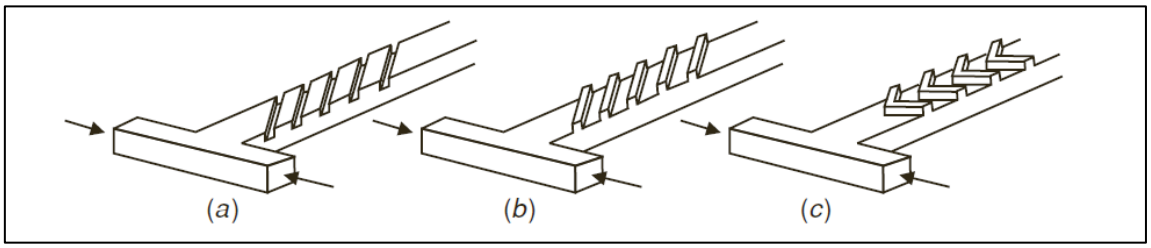


FIGURE 2.3: Modification of mixing channel for chaotic advection at low Reynolds numbers: (a) Slanted ribs (b) Slanted grooves, (c) staggered-herringbone grooves. (Strook et al, 2002)

In this project, a passive micromixer will be applied for the study of flow behavioral dynamics of ammonia synthesis process since it is more stable and less complex in its geometry design with addition to its operation as compared to an active micromixer. The choice of micromixer is based on the studies done by Rosli (2012) and Azeman (2012), therefore as a continuation of their work, a similar micromixer but without the Y-shaped inlet will be adopted into this study.

2.4 Design of Micromixer

Existing designs in conventional macroscale micromixers cannot be simply scaled down for microscale applications. One of the main challenges related to miniaturization is the dominance of surface effects over volume effects. Actuation concepts based on volume forces working well in macroscale may have problems in its microscale counterparts. Moreover, a surface force-based actuation concept would allow scaling down because the ratio between the driving force and friction force would remain unchanged. Other than

that, the laminar flow condition is another challenge for the designs, which is similar to problem faced by macroscale laminar mixers (Nguyen, 2008).

Nguyen (2008) also states that the mixing process for gas is even shorter than liquid mixing as the diffusion coefficient is around 1000 times larger than that of liquid. Therefore the design of microdevice and the type of contacting fluid employed are the determining factors for micromixer performance.

Generally, the transport of molecular diffusion obeys Fick's Law. A large interfacial area, gradient and diffusion coefficient can lead to high diffusive flux. Since diffusion coefficient is material constant and improvement based on temperature and viscosity is not significant, thus the mixing in micromixer based on molecular diffusion can only be optimized by geometrical design to decrease the striation thickness.

Rearranging Fick's Law, the mixing time is actually proportional to the characteristic diffusional path and diffusion coefficient:

$$t_{md} \propto \frac{l^2}{D}$$

[Equation 2.3]

Where

l = characteristic diffusional path

D = diffusion coefficient

From Equation 2.3 above, it is shown that the mixing time is highly dependent on the characteristic length of the system, which is determined by the dimension of the microchannels (Aubin & Xuereb, 2009).

Because most micromixers used for analysis work has relatively low flowrates, the Reynolds number would be expecting to be high enough for flow stability. Since inertial force is not applicable, flow instability at low Reynolds number can be achieved by stretching and recoiling of the fluid molecules against the viscous forces to induce instable chaotic advection as proposed by Aubin & Xuereb (2009).

Lin et al. (2011) proposed a novel passive micromixer (FIGURE 2.4) which can induce flow stretching by combining square-wave-shaped channel structure with periodic cubic grooves, in order to facilitate laminar flow recirculation and further enhancing the mixing process. However this geometric design with grooves is not necessary for this project study as the rate of diffusivity between the component gases is expected to be higher as compare to basic liquid flow used in most experimental study, including in the proposal by the authors .

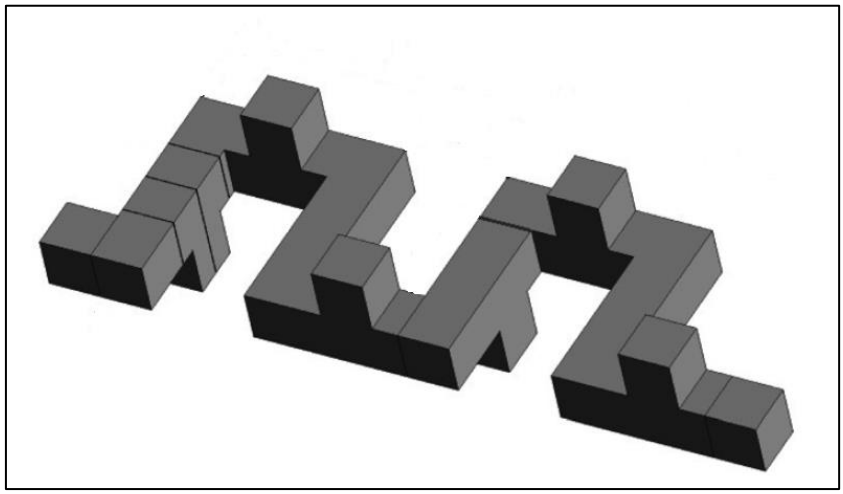


FIGURE 2.4: Schematic of the micromixer proposed by Lin, Yu, Wang, Tu & Wang (2011)

Groisman and Steinberg (2001) used a mixer design with repeated circular turns to induce viscoelastic stability. Because of the turns, instability is caused by complex interplay between inertial, viscous, centrifugal and viscoelastic forces. Good mixing result was reported in their work.

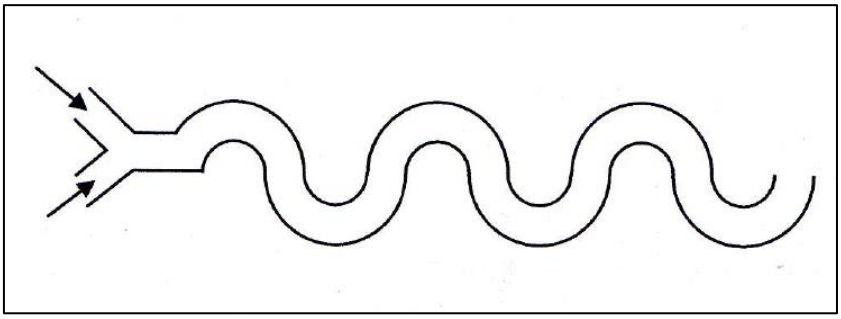


FIGURE 2.5: Micromixer based on viscoelastic instability.(Nguyen, 2008)

Nguyen and Wu (2005) stated that typical dimension of micromixers are defined as a function of the desired performance of the mixer. The fluid flow of micromixers with channel widths in the range of 10 to 1000 micrometers is expected to be at the range of milliliters per hour to liters per hour. The most common dimensions fall in the range of 100 to 500 micrometers or 50 to 300 micrometers. (Wong et al., 2003) For simplicity, the boundary condition for the inner walls of the microchannels was usually defined as the no slip condition. (Yamaguchi, et al., 2004)

Through manipulation of the geometry variables of the micro-reactor to induce the mixing phenomenon, synthesis of ammonia via the reaction of nitrogen and hydrogen gases in the microfluidic system will be investigated. A passive Y-type micromixer with geometric design similar to Groisman and Steinberg (2001), as shown in FIGURE 2.5 will be applied to study the fluid dynamics of ammonia synthesis in microscale. Geometric reference will be made based on previous work done by Rosli (2012) and

Azeman (2012), where the horizontal length of micromixer is fixed constant at 10 cm excluding the length of both inlet and outlet. The length of the inlet and outlet is measured at 1.00 cm each, which sums up the total horizontal length of 11.00 cm. At a pitch height of 0.15 cm and 5 cyclic turns, the velocity of fluid along the microchannel is observed to be very stable compared to other geometric dimensions. (Rosli, 2012). However the number of cyclic turns will be further study in this project, as the studied parameter of both Rosli (2012) and Azeman (2012) was closed to the range of nano-scale instead of micro-scale.

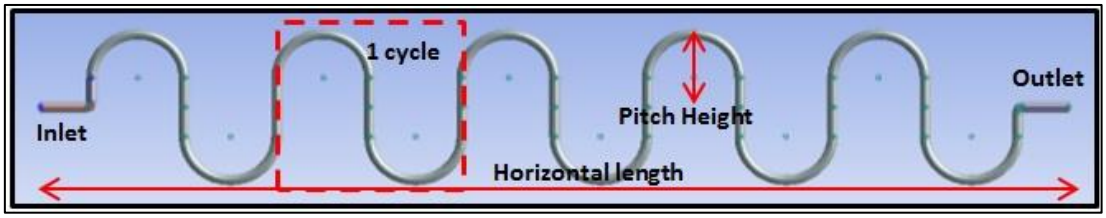


FIGURE 2.6: Microreactor geometry (Rosli M. , 2012)

In addition, Azeman (2012) has found that an inlet design of 30˚ angle, as shown in FIGURE 2.7 below, with component hydrogen in the main stream resulted in best mixing performance among the other designs and component setups. Nevertheless, the Y-type inlet will not be apply onto this study, with the result obtained by Azeman (2012) being referred to as reference purpose only.

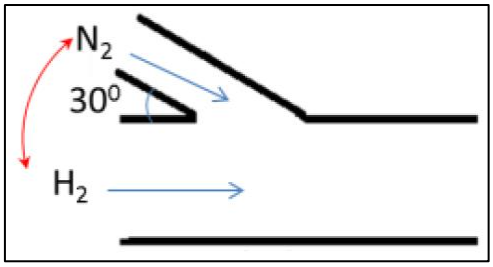


FIGURE 2.7: Inlet geometry of 30° with hydrogen in the mainstream (Azeman M. K., 2012)

2.5 Micromixer Performance Evaluation

Further evaluation of the choice of micromixer has to be done other than based on their respective technical aspects and the given applications. Various performance characteristics of the device can be determine, such as pressure drops, hydrodynamics, mixing efficiency, residence time distribution and presence of dead zones. (Aubin & Xuereb, 2009)

Aubin & Xuereb (2009) mentioned that the evaluation can be done either experimentally or virtually via the numerical simulation of the flow. Experiment testing of a wide range of micromixers could be time consuming and costly, moreover it may requires specific equipment that is most often found only in research laboratories. Numerical simulation method such as computational fluid dynamics (CFD) of flow within micromixer is an attractive alternative, enabling different geometries to be quickly designed and tested in a virtual manner. Besides that, user can design the most suitable geometry of the micromixer for application and then evaluate their performance experimentally.

Through CFD simulation, pressure field of micromixer can be solved using the Navier-Stokes equation for flow simulations, velocity components of the flow within the

micromixer in all three directions throughout the entire volume of the device could be determined using CFD, enabling a better understanding of the flow patterns created in the micromixer. In addition, by applying Langarian approach the residence time distribution (RTD) of the micromixer can be found through this simulation method. (Aubin et al., 2005)

CFD simulation will be used as the tool to assist the design of geometric development of the microreactor system in this study, so as to identify the optimum hydrodynamics condition of the mixing process and at the same time to trace the suitable location for catalyst insertion, for further improvement of the ammonia synthesis process.

Hsieh & Huang (2008) proposed that the mixing efficiency of a micromixer can be evaluated at different positions, from the upper to lower locations. The mixing efficiency is defined as:

$$m_{eff} = \left(1 - \frac{\int_0^w |v - v_\infty| dx}{\int_0^w |v_0 - v_\infty| dx}\right) \times 100\%$$

[Equation 2.4]

Where

v = volume fraction of distribution across the transverse direction at the outlets

v_∞ = volume fraction of complete mixing

v_o = initial distribution of the volume fraction before mixing

W = width of micromixer

CHAPTER 3

METHODOLOGY

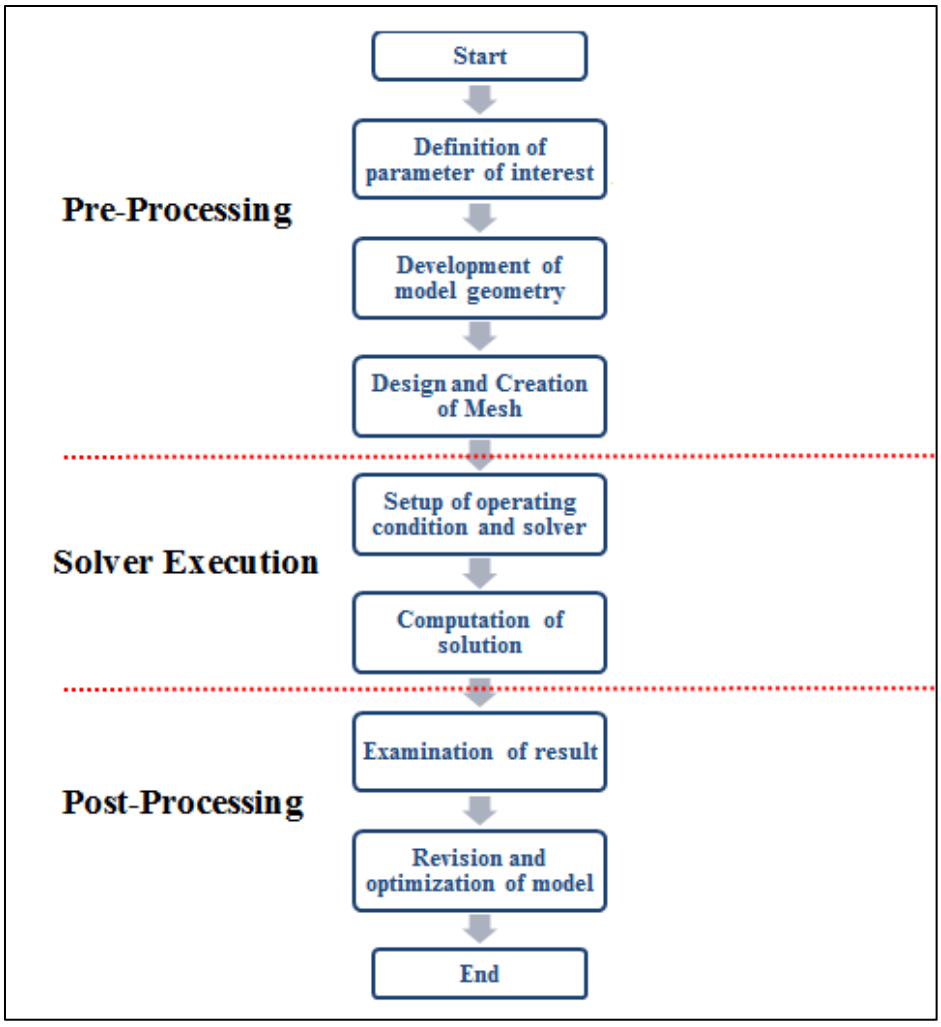


FIGURE 3.1: CFD Modeling Process Flow

This project utilized ANSYS CFX 14.5 to investigate the hydrodynamics of fluid for the ammonia synthesis process under microfluidic system. Three major phases are expected in the CFD modeling processes which are illustrated in FIGURE 3.1: pre-processing, solver execution and post-processing.

3.1 Pre-Processing

Pre-processing is the phase where the parameter of interest is being defined based on the objective of project study. This is then followed by the development of the geometries and meshing of the geometries. In order to investigate the hydrodynamics of fluid for ammonia synthesis in microreactor system, mesh sensitivity is being identified as the parameter of study, where three different meshes will be tested.

3.1.1 Development of Geometry

In the design phase, the geometry of the system is produced in the computer-aided design (CAD) system. ANSYS Design Modeler will be connected to the CAD system to transfer data including the parameters from the CAD software. With the assist from the software, updates and manipulation of the parameters and the geometry design can be done according to the requirement of the study from time to time. In this study, at least three different configurations of meshes will be tested. Based on the proposed geometry done by Rosli (2012) and Azeman (2012), specific geometric condition of the system i.e. pitch

height, angle of the inlet and the inflow configuration, will be used as reference for the design of this project study.

The geometry designed for the proposed microreactor to be is shown as in FIGURE 3.2 as in ZX-plane. Several parameters of the design such as the pitch height of 0.15cm, internal diameter of 0.01 cm, and total length of 11.00cm for the microreactor including both its inlet and outlet, are kept constant throughout the project study. Meanwhile through 10 cyclic turns of the microreactor its hydrodynamics of the fluid flow are to be observed.

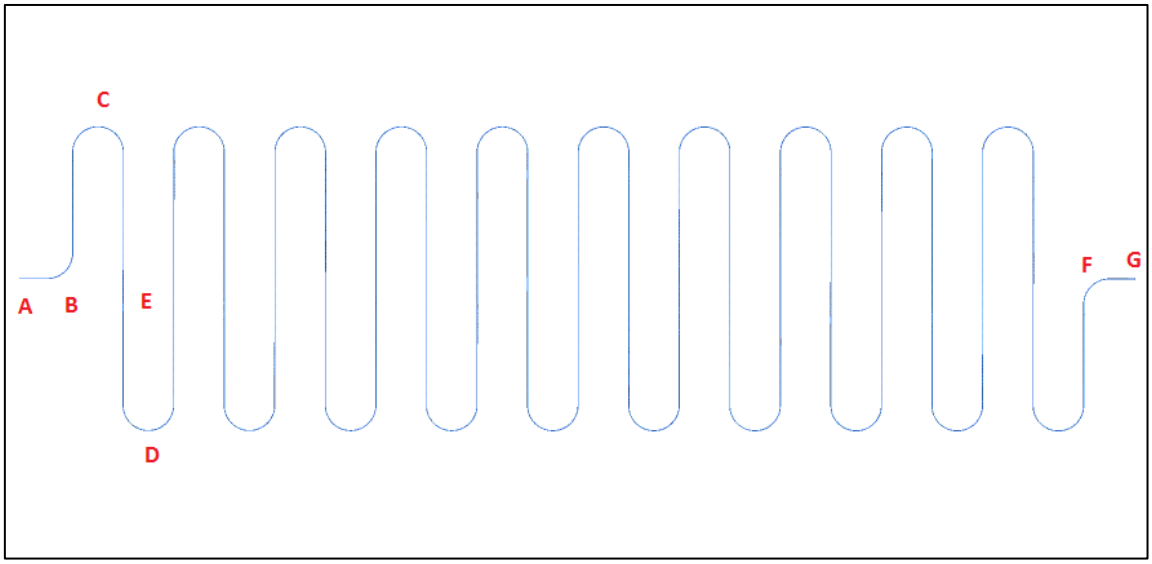


FIGURE 3.2: Geometry Design

Total length of geometry = A to G

Radius of turns = B, C and D

Inlet/Outlet length = A to B and F to G

Pitch height = C to E or E to D

Total height of geometry = C to D

The detail dimensions for 10 cyclic turns are stated in TABLE 3.1 below.

TABLE 3.1: Specification of Geometry Design

No. of cyclic turns	Total length (cm)	Length of inlet/outlet (cm)	Pitch height (cm)	Radius of turns (cm)	Diameter of microreactor (cm)
10	11.00	0.50	1.50	0.25	0.01

3.1.2 Creation of Mesh

In order to ensure the accuracy of the simulation, the discretization of the flow geometry will be carried out. This is done through the creation of mesh or grid for the system. A generated mesh with too many cells will take a longer duration to for the solver to solve; while a mesh generated with too few cells may give an inaccuracy to the final result. Therefore, various meshing properties can be manipulated to obtain the most appropriate mesh quality for a result with high accuracy.

To ensure the mesh created is of high quality, grid sensitivity analysis is being carried out. There are many meshing properties that need to be considered, however in this project study, only the number of nodes, elements and its orthogonal quality will be taken into interpretation. The orthogonal quality is considered as to see the grid quality in terms of the angle at the point of intersection between cells. An angle of nearing to 90 degrees

between the cells will ensure a better distribution among the cells in the grid. While the orthogonal quality calculated is between 0 and 1, the best cells will have an orthogonal quality of converging towards value of 1. (Azeman M. K., 2012)

In this context, three different meshes are being generated for grid sensitivity analysis, based on the geometry design of microreactor with ten cyclic turns. The numbers of nodes generated are ranging between 3,700,000 nodes to 4,200,000 nodes for analysis. Through the analysis, the selected meshing property is then used for other simulations of the proposed microreactor with different number of cyclic turns.

FIGURE 3.3 below shows the detail of the meshing parameters of one of the mesh generated. The mesh properties are inputted before meshing is done. The curvature normal angle is set to default (12.0˚) for all meshes, while the “min size”, “max face size”, and “max size” are adjusted to acquire the desired number of nodes and elements.

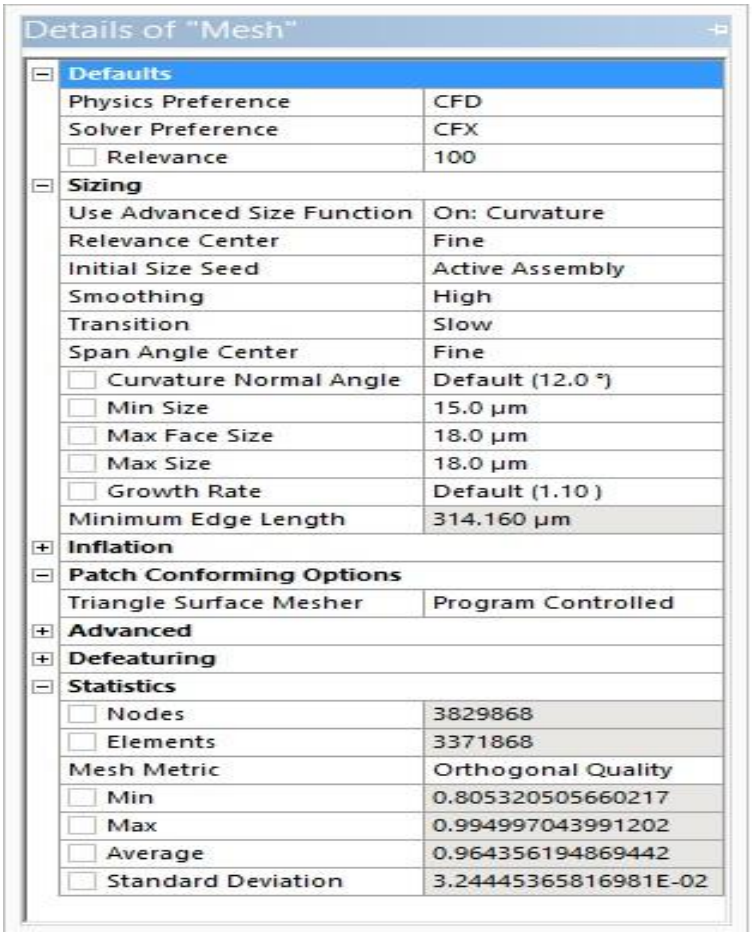


FIGURE 3.3: Mesh properties

3.2 Solver Execution

In this phase, the properties of the study material will be defined before it is simulated. Appropriate physical models and operating conditions will be prescribed as well as the boundary conditions at all boundary zones. Through ANSYS CFX 14.5 solver, the computation of the flow occurs where it will solves the discretized conservation equation in an iterative manner until appropriate convergence is obtained.

3.2.1 Setup of Operating Condition and Solver

The setup defines the study material, in this case are the N_2 and H_2. The materials will be defined as "fluid", and the physical model parameters such as boundary condition, meshing domain physics, boundary physics, turbulence, volume fractions, flow regime, etc. will be determined, besides the operating condition of the microreactor system.

The settings for all the parameters and controls are as shown in FIGURE 3.4, TABLE 3.2, TABLE 3.3 and TABLE 3.4 below:

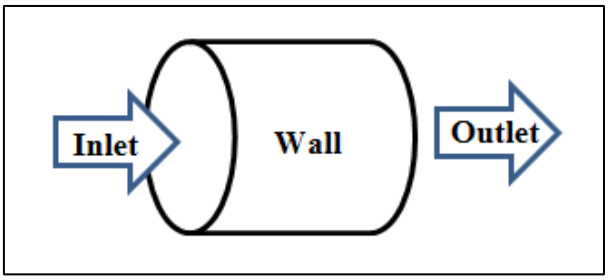


FIGURE 3.4: Boundary Conditions

TABLE 3.2: Domain Physics for CFX

DEFAULT DOMAIN	
Domain Type	Fluid Domain
MATERIALS	
H_2 at STP	

Fluid Definition	Material Library
Morphology	Continuous Fluid
Minimum Volume Fraction	0.75
N_2 at STP	
Fluid Definition	Material Library
Morphology	Continuous Fluid
Minimum Volume Fraction	0.25
BASIC SETTINGS	
Buoyancy Model	Non Buoyant
Domain Motion	Stationary
Reference Pressure	1 [atm]
Heat Transfer Model	Isothermal
Homogeneous Model	On
Fluid Temperature	25 [C]
Turbulence Model	Shear Stress Transport
Wall Functions	Automatic

TABLE 3.3: Physics Boundaries

BOUNDARY: INLET	
Boundary Type	Inlet
Location	Inlet
Boundary Details	

Flow Regime Option	Subsonic
Mass and Momentum	Normal Speed
Normal Speed	3.33 [m s ^ -1]
Turbulence Option	Medium (Intensity = 5%)
Fluid Values	
Hydrogen Volume Fraction	0.75
Nitrogen Volume Fraction	0.25
BOUNDARY: OUTLET	
Boundary Type	Outlet
Location	Outlet
Boundary Details	
Flow Regime Option	Subsonic
Mass and Momentum	Static Pressure
Relative Pressure	0 [Pa]
BOUNDARY: WALL	
Boundary Type	Wall
Location	Wall
Boundary Details	
Mass and Momentum	Non Slip Wall
Wall Roughness	Smooth Wall
Wall Contact Model	Use Volume Fraction

TABLE 3.4: Solver Control

SOLVER CONTROL	
Advection Setting	High Resolution
Turbulence Numeric	First Order
Convergence Control	
Min. Iterations	1
Max. Iterations	100
Fluid Timescale Control	
Timescale Control	Auto Timescale
Length Scale Option	Conservative
Timescale Factor	0.0001
Convergence Criteria	
Residual Type	RMS
Residual Target	0.000001

3.2.2 Computation of Solution

Once the setup has been done, computation of the solution will be carrying out by using ANSYS CFX 14.5 software. The discretized conservation equations are solved iteratively until convergence is reached; where the overall property conservation is achieved in addition to the quantities of interest have reached steady values. Furthermore the changes in solution variables from one iteration to the next are also expected to be negligible.

The accuracy of the solver will be dependent on the developed geometry and meshing quality, as well as the assumptions made and the numerical errors. The results obtained from the computation will be analyzed and illustrated accordingly.

3.3 Post-Processing

In post-processing phase, the result obtained from the simulated computation will be examined by extraction of useful data. ANSYS 14.5 offers a complete set of post-processing tools for display of the results on models in the form such as contour plots and velocity plots. Furthermore, improvement and optimization can also be done at this phase by analyzing the result data, where parameters such as physical models, boundary conditions and mesh quality can be redefined and improved by observing the output of the simulated computation.

3.4 Governing Equations

The fluid component in this project is assumed incompressible as the Mach number at the inlet and throughout the microchannel is reported at 0.01 and 0.02 by the previous studies. As the Mach number is lesser than 0.3, the gas component flow in the system is therefore considered as incompressible. The constant flow of an incompressible Newtonian fluid in microchannel can be explained by the Navier-Stokes equation and Continuity Equation. Furthermore, the species distribution follows the diffusion convective equation with adoption of non-slid boundaries.

Continuity Equation for incompressible fluid is

$$\frac{\partial u_k}{\partial x_k} = 0$$

[Equation 3.1]

While Momentum Equation is expressed as

$$\frac{\partial(\rho u_j u_i)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[-P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho g_i$$

[Equation 3.2]

Where

P = Pressure

u = Velocity

i, j, k = Cartesian axis

x = Cartesian coordinate direction

δ_{ij} = 1 if i= j and 0 if otherwise

μ = Dynamic viscosity

ρ = Density

Whereas the Convective Diffusion Equation is expressed as

$$\frac{\partial c}{\partial t} + \frac{\partial u_k(c)}{\partial x_k} = D\frac{\partial^2}{\partial x}c$$

[Equation 3.3]

Where

c = Concentration

t = Time

D = Diffusivity

3.5 Tools

The software applied in this study for CFD simulation is ANSYS CFX 14.5.

3.6 Key Milestones

Progresses of this project study for Final Year Project I and Final Year Project II are shown in APPENDIX I and APPENDIX II.

CHAPTER 4

RESULTS AND DISCUSSIONS

4.1 Mesh Sensitivity Study

Three meshes have been conducted for the proposed microreactor with 10 cyclic turns. The results of the meshes are shown in FIGURE4.1, FIGURE 4.2 and FIGURE 4.3 below:

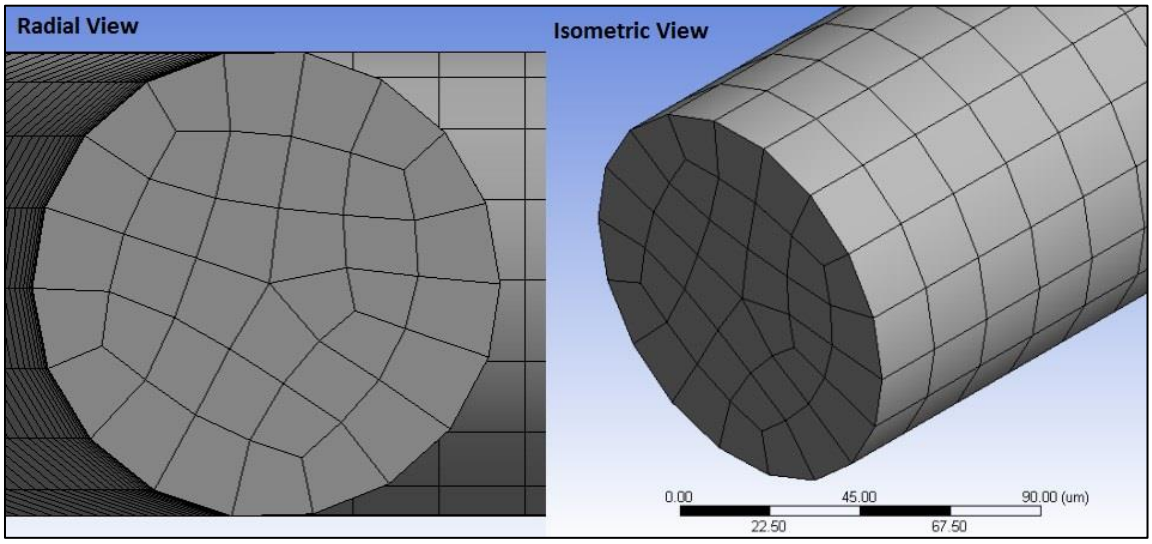


FIGURE 4.1: Coarse Meshing with 3,704,981 nodes

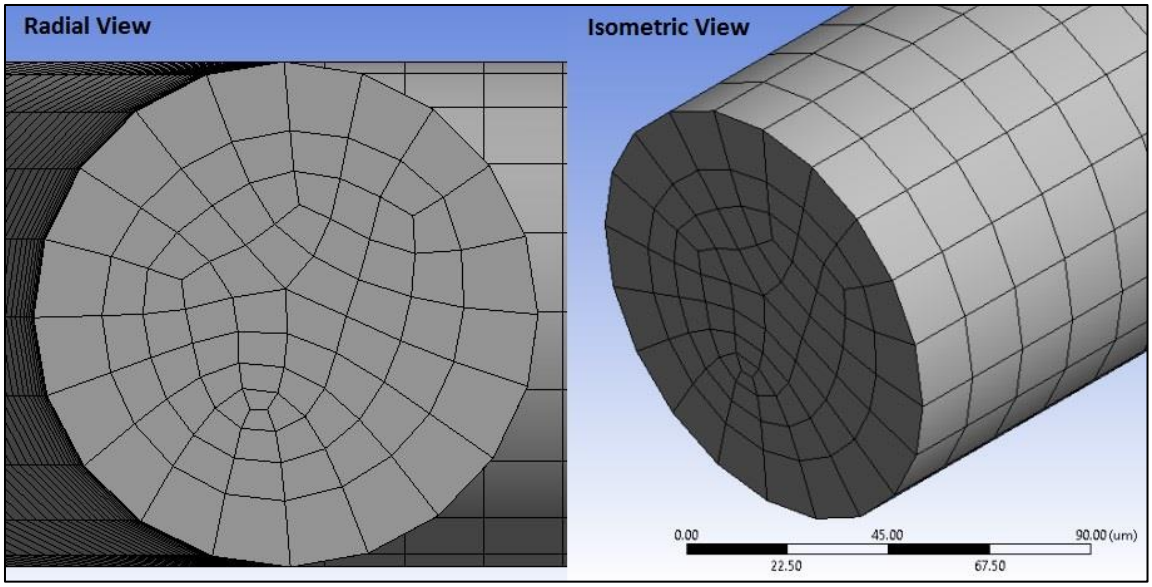


FIGURE 4.2: Medium Meshing with 3,829,868 nodes

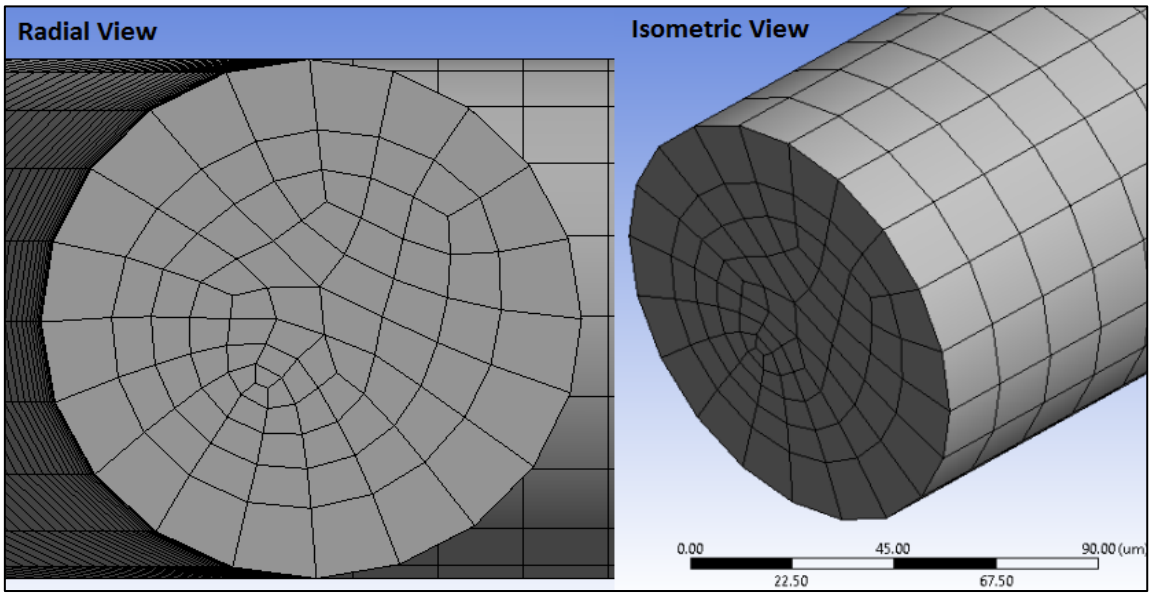


FIGURE 4.3: Fine Meshing with 4,162,900 nodes

The number of nodes and elements with its orthogonal factor is tabulated as in TABLE 4.1:

TABLE 4.1: Meshed Properties

Meshing Quality	No. of nodes	Elements	Orthogonal Factor				Simulation Duration
			Min	Max	Average	Standard Deviation	
Coarse	3,704,981	3,246,984	0.8725	0.9959	0.9718	0.0235	2 days 18 hours
Medium	3,829,868	3,371,868	0.8053	0.9949	0.9643	0.0324	2 days 19 hours
Fine	4,162,900	3,704,892	0.9028	0.9964	0.9745	0.1783	2 days 23 hours

Through the numerical data of orthogonal factor tabulate in TABLE 4.1, it is observed that the higher the orthogonal factor, the better the mesh quality and larger number of nodes will be produced. However the simulation time required (CPU Time) is also longer for a finer mesh. For a higher refined mesh, the number of cells per unit area is approaching maximum, therefore its required time to simulate is also relatively longer, and generates a solution of more inferior mesh quality.

A comparison of the contour plot qualities for each meshes are made in six locations of the microchannel as labeled in FIGURE 4.4.

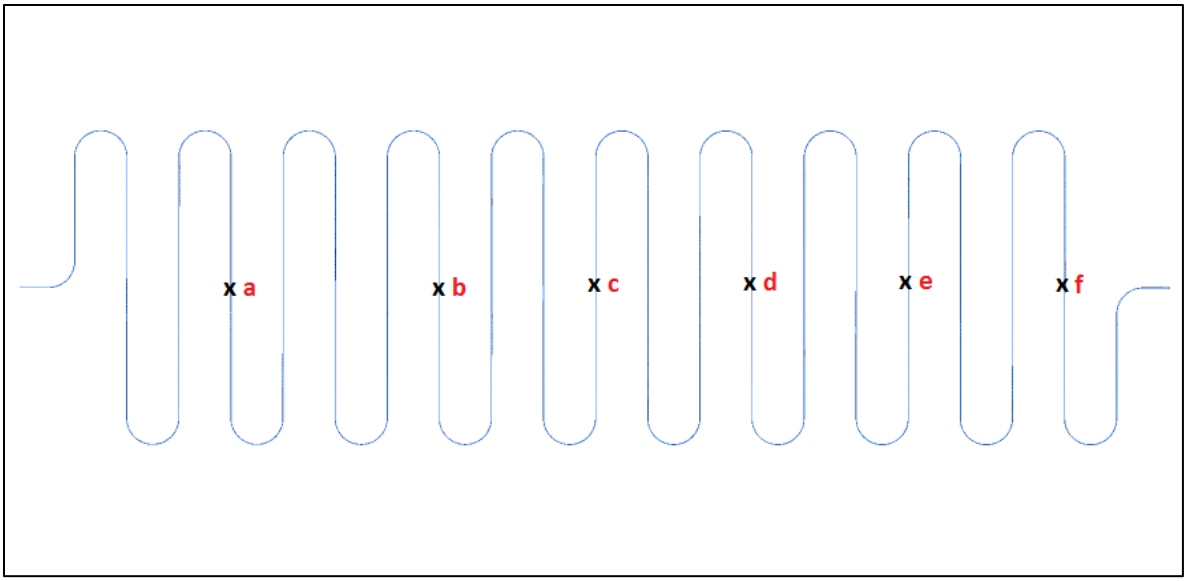
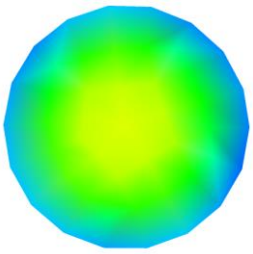
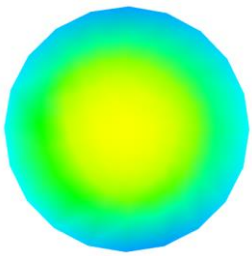
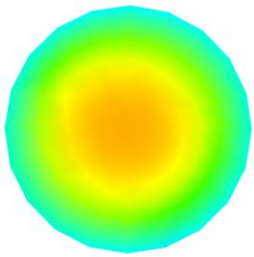
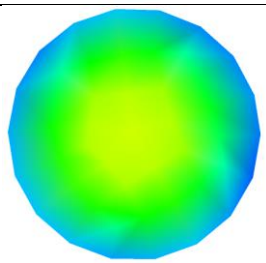
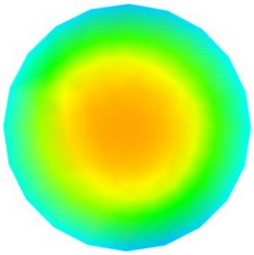
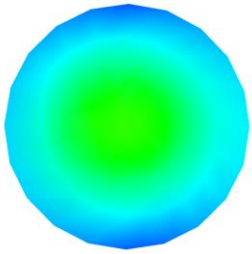
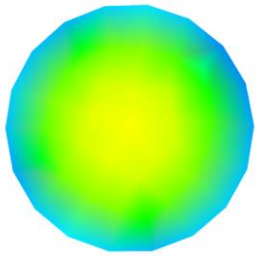
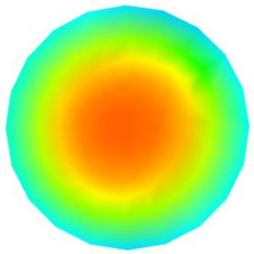
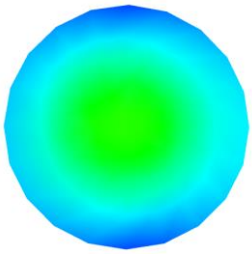
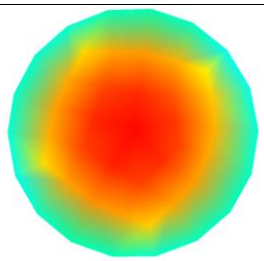
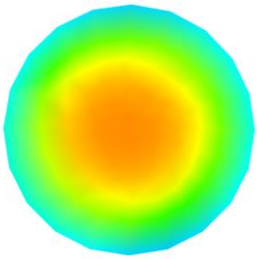
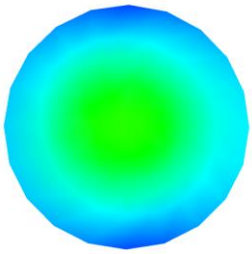
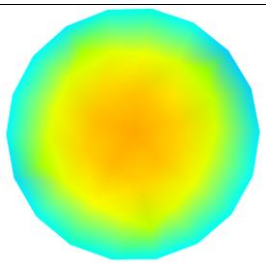
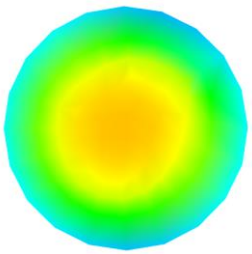
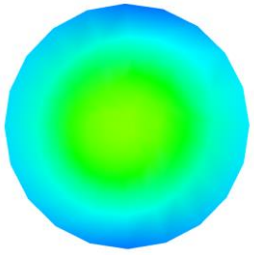
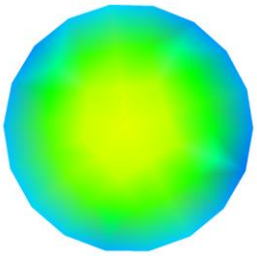
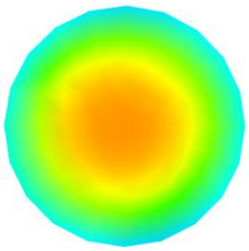
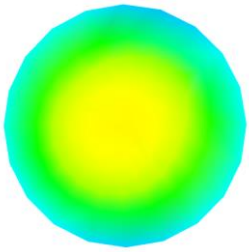


FIGURE 4.4: Location of Velocity Contour Comparison

TABLE 4.2 below shows the comparison of the velocity contour with their respective location coordinates. It is observed that the fluid flow in coarse mesh does not uniform radially throughout the circular tube as there are several visible sharp jagged contour near the edge of the microchannel tube. This is most visibly shown especially in location labeled ‘d’ for the coarse mesh, where the color contour shows the sharp lines for coarse mesh. Whereas the medium mesh produced a near uniform fluid flow, indicated by the color contour but part of the contour appeared to be in the unclear mixed regions, especially at location labeled ‘c’ in TABLE 4.2. Meanwhile for fine mesh, the contour is uniform radially throughout the microchannel tube, with no visible jagged or mixed contour.

TABLE 4.2: Comparison of Velocity Contour Plot Qualities

Coordinates (m)	Coarse	Medium	Fine
Location 'a' X = 0 Y = 0 Z = 0.09			
Location 'b' X = 0 Y = 0 Z = 0.07			
Location 'c' X = 0 Y = 0 Z = 0.055			
Location 'd' X = 0 Y = 0 Z = 0.04			
Location 'e' X = 0 Y = 0 Z = 0.025			

Location 'f' **X = 0** **Y = 0** **Z = 0.01**			

From the comparison made in TABLE 4.2, coarse and medium have shown less uniformity due to the meshing is not sufficiently refined; therefore its accuracy of the solution is also limited. Whereas a finer meshes quality with higher number of nodes and larger elements will produce a better quality of contour and produced a more accurate solution. Therefore this comparison has shown that mesh quality plays an important role to dictate the accuracy of the iteration solutions.

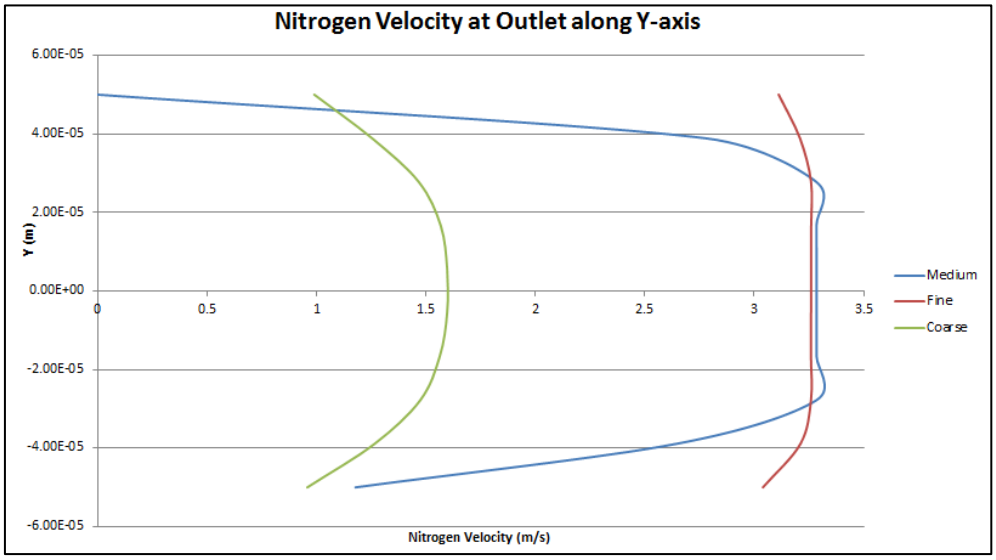


FIGURE 4.5: Nitrogen Velocity Profile

The velocity profiles of nitrogen gas component at the outlet in the direction of its microchannel height are tabulated in FIGURE 4.5. Velocity profile is often used to measure the flow condition of fluids within a pipe. In this study, nitrogen gas component enters the microchannel tube at a speed of 3.33 m/s, and it is also expected to exit the channel at similar speed. From FIGURE 4.5, it is observed that the nitrogen gas component of coarse mesh quality exits at a speed slower that the expectation even in the center of fluid stream (halved of expected velocity). Moreover, the speed throughout the tube is not uniform, with the speed decreases as it approaches the side wall. Other than that, for medium mesh the center of the fluid stream is approximately at the range of 3.33 m/s but the velocity variation is large when approaching the circular side wall of the microchannel. These phenomenons may be due to the large shear stress of the microchannel wall on nitrogen gas component, thus causing slowdown of the fluid flow and the large

Whereas for fine mesh, the fluid stream flows in the range of 3.10 m/s to 3.30 m/s throughout the microchannel in the direction of its height, with much better consistency as compared to the coarse and medium mesh quality results. The shear stress of the side wall on the fluid component is lesser, thus resulted in the uniformity of its fluid flow.

These result shows that the quality of meshes is crucial in designing of the microreactor. A refined mesh is highly recommended as it will not only iterate solutions with greater accuracy but also results a more uniform fluid flow with lesser shear stress effect on its side wall. Thus this will provides better stability for the flow of both the gas components when the study is further researched on its mixing behavior in the presence of catalytic components.

4.2 Velocity of Gas Components in Microchannel

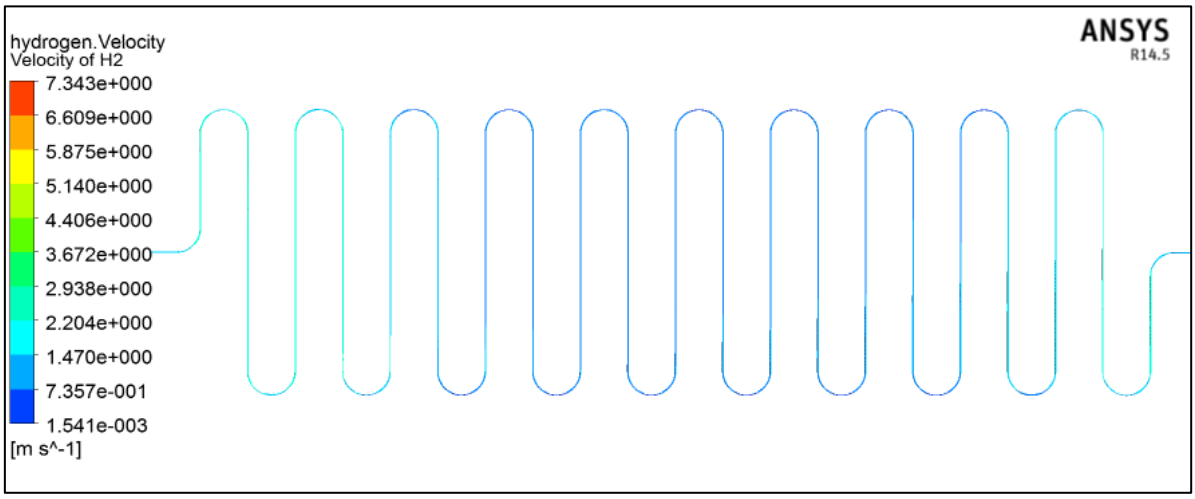


FIGURE 4.6: Axial Velocity Contour of Hydrogen Gas Component

Based on the results obtained in mesh sensitivity study, the study is further proceeding by applying fine mesh quality of microreactor design. FIGURE 4.6 shows the axial view of the velocity contour for hydrogen gas component. The radial view for the same gas component is shown in FIGURE 4.7 below. As observed from FIGURE 4.6, the contour shows that the velocity of hydrogen gas component decreases as it approaches inwards to the middle section of the microchannel. The decrement of the fluid flow may be due to the low molecular weight of hydrogen gas. Then as it approaching the exit of the microchannel tube, the differential pressure of the tube and its environment speeds up the fluid flow, thus the velocity tends to increase again before the exit.

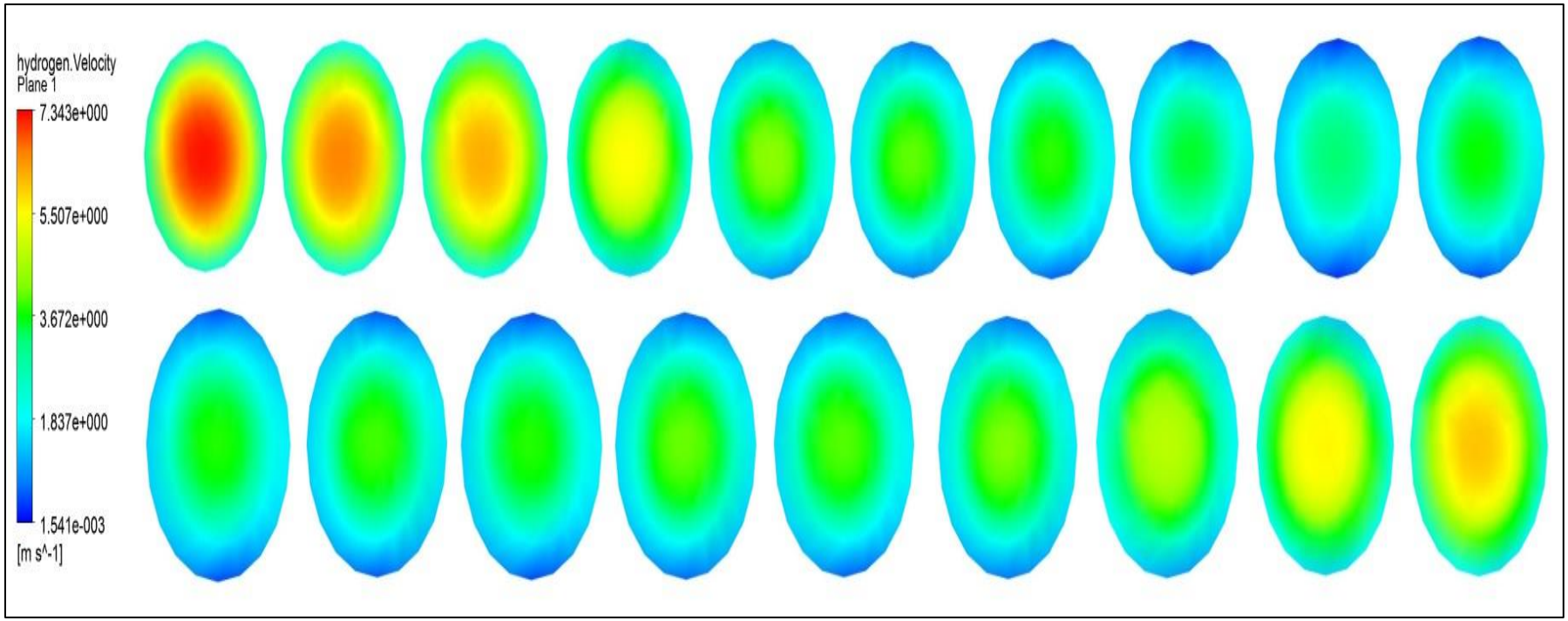


FIGURE 4.7: Radial Velocity of Hydrogen Gas Component

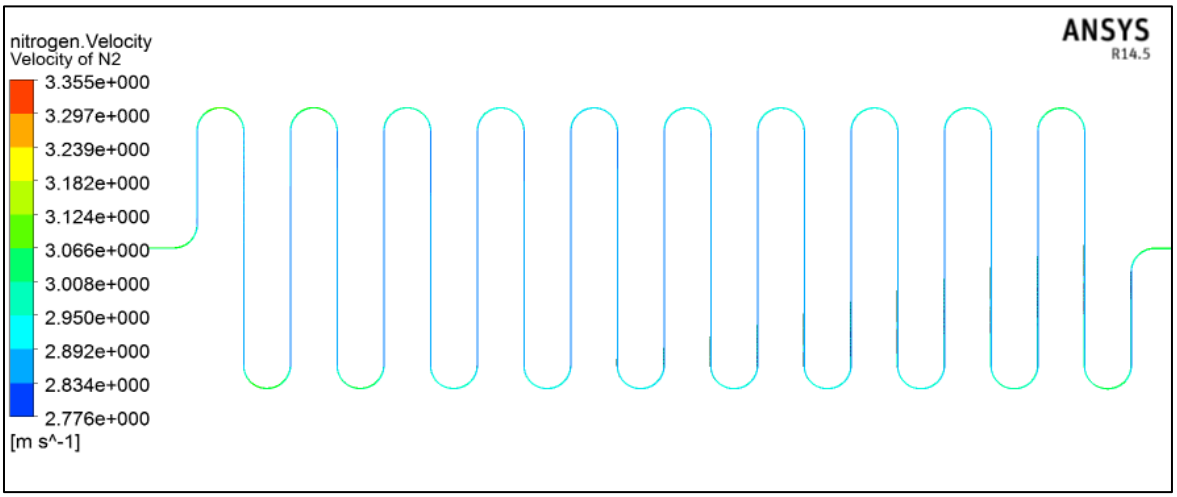


FIGURE 4.8: Axial Velocity Contour of Nitrogen Gas Component

Meanwhile, FIGURE 4.8 shows the axial velocity contour of nitrogen gas component. Its radial view is shown in FIGURE 4.9 below. From FIGURE 4.9, it can be seen that nitrogen gas component travels equally stable throughout each parallel section of the microchannel. However FIGURE 4.7 shows that the fluid flow tends to decrease at the junctions and bends. The decrement in nitrogen gas component velocity may be due to the momentum effect of the gas component itself, where the higher molecular weight of nitrogen component tends to have difficulties as accumulation occurs at the junctions caused sudden disruption and thus lowered the velocity of nitrogen component. In general, nitrogen gas component travels uniform axially and radially as observed in both FIGURE 4.8 and FIGURE 4.9.

In summary, from the study of velocity contour for both gas components it is observed that hydrogen component have a lower velocity as the fluid flows inward towards the middle of the circular microchannel; whereas nitrogen component will

decrease its fluid flow only each of the junctions and bend but at the parallel straight section it will flow steadily and in uniform.

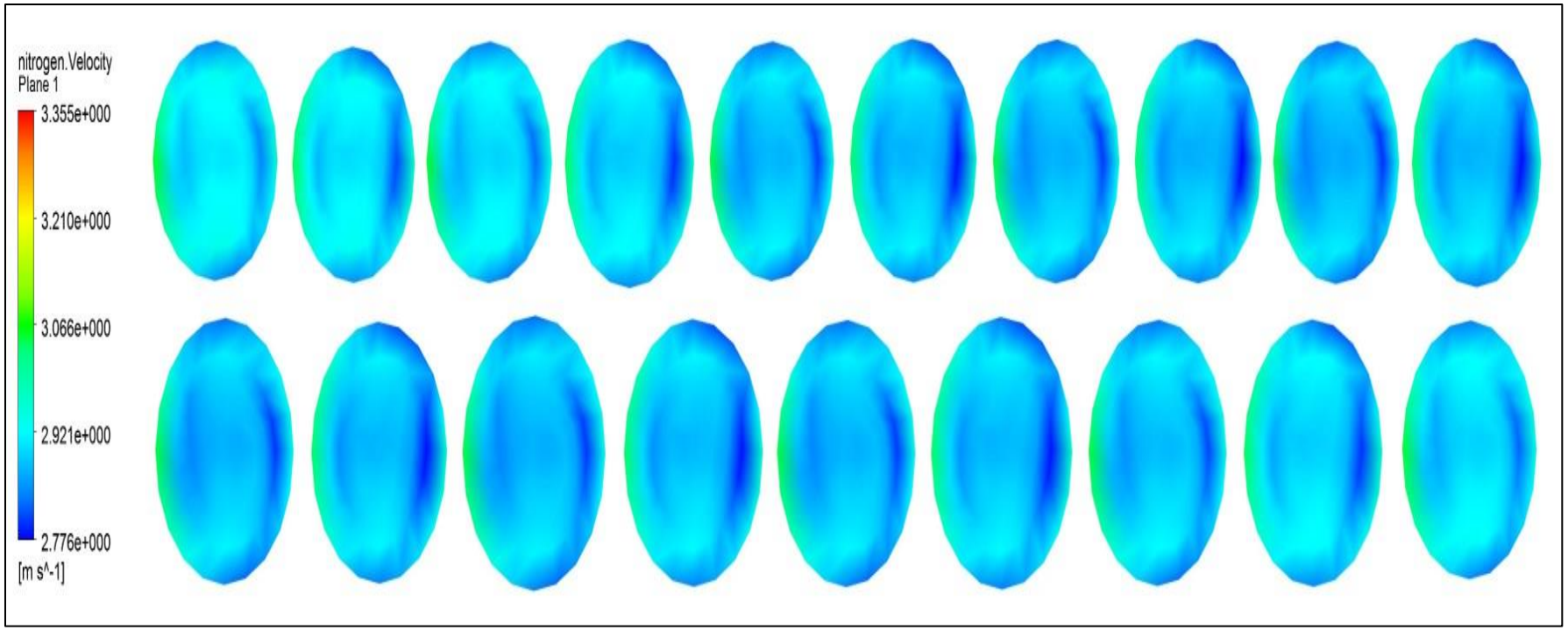


FIGURE 4.9: Radial Velocity of Nitrogen Component

4.3 Pressure Difference in Microchannel

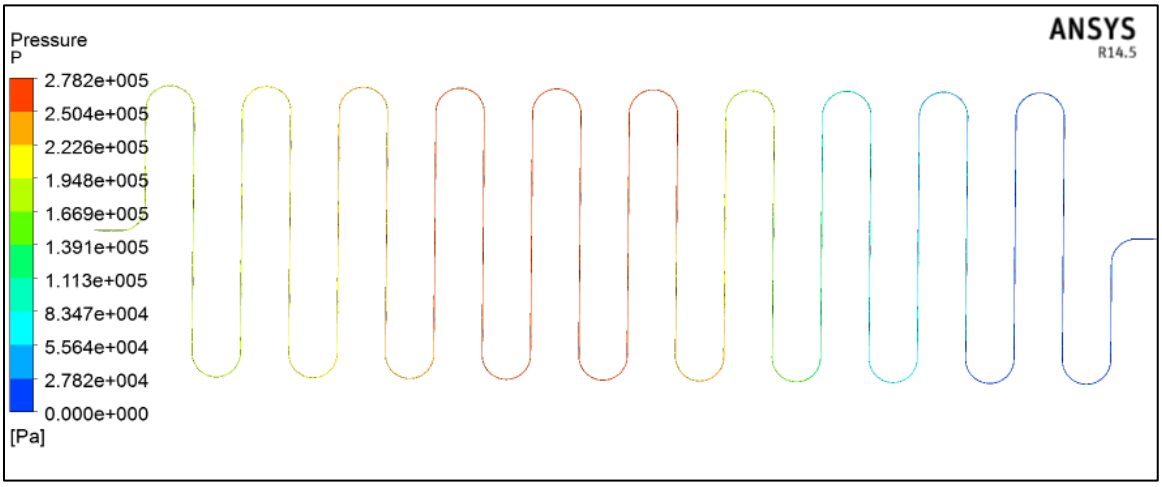


FIGURE 4.10: Axial View of Pressure Difference across Microchannel

FIGURE 4.10 shows the fluid pressure difference across the microchannel. From the color scheme, it is observed that the pressure of the fluid flow at the initial part of the microchannel tends to increases while the fluids flow towards the inner section of the reactor, before the pressure decreases and dropped when the fluid flows towards the exit of the channel.

As the fluid components are compacted into a small volume of the space in the microchannel, the moving fluid inside the microchannel tends to produce stresses and strains as it tries to stretch on the wall of the tube. This explains the increment of pressure as the fluid components are moving towards the middle section of the microchannel as shown in FIGURE 4.10 above. The collision between fluid component molecules and the microchannel wall due to the random movement of molecules while moving through the microchannel resulted in the decrease in the kinetic energy. The loss of kinetic energy is converted into other form of energy i.e. internal and pressure energy.

According to the law of continuity, that if a cross section of the microchannel is remained constant, the velocity of fluid flow is also assumed to keep constant throughout its flow. Thus as moving along the microchannel, pressure energy is to be converted to kinetic energy to keep the fluid moving at the constant velocity; therefore a drop of pressure is detected from the comparison of pressure at the inlet and the outlet of the microchannel.

The pressure drop across the microchannel can be calculated by:

1. Calculating the fluids' Reynolds number,

$$Re = \frac{1000 \times V \times D}{\gamma}$$

[Equation 4.1]

Where

V = Velocity of fluid, m/s

D = Diameter of channel, mm

γ = Kinematic viscosity of fluid, centistokes

Applying Equation 4.1, the Reynolds number of the fluid is calculated at 1443.43. This further proves that the moving fluid is a laminar flow (Re < 2100).

2. Friction factor for laminar flow,

$$f = \frac{64}{Re}$$

[Equation 4.2]

3. Pressure difference,

$$\Delta P = \frac{V^2 \times f \times L \times \rho}{2D}$$

[Equation 4.3]

Where

V = Velocity of fluid, m/s

f = Friction factor

L = length of microchannel, m

ρ = density of fluid, kg/m^3

D = Diameter of microchannel, m

FIGURE 4.11 below shows the radial view of the pressure difference across the microchannel.

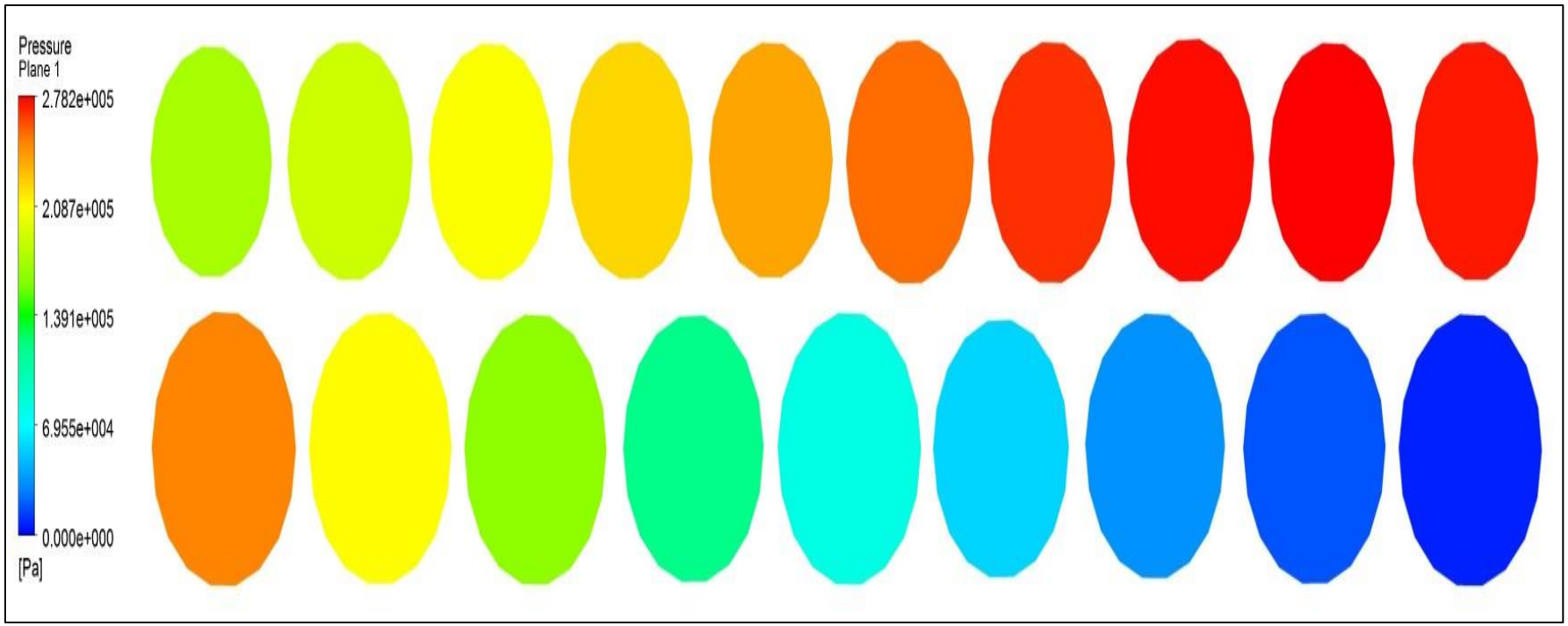


FIGURE 4.11: Radial View of Pressure Difference across Microchannel

CHAPTER 5

CONCLUSIONS AND RECOMMENDATIONS

The objective of this project study is to investigate the hydrodynamics of nitrogen and hydrogen gas components during the synthesis of ammonia in a microreactor at ambient operating condition. The significant of this study is to assist in optimizing the localization of the catalyst for the ammonia synthesis reaction to take place.

In this stage of the study, the reactions of the gas components are not being included. Three different meshing qualities are being studied, labeled as coarse, medium and fine meshes. Through mesh sensitivity study, the design with the best mesh quality will be further studied on the gas components flow behavior along the microchannel.

In mesh sensitivity study, it is found that a finer mesh quality with higher number of nodes and large elements will produce a better quality of contour and thus a more accurate solution. In this study, fine mesh with 4,162,900 nodes is selected as the contour plot of its gas components showed a better and uniform fluid radial flow.

Next, the microreactor with fine mesh quality is further simulated. Through CFD simulation, the velocity contour plots for both the gas components are obtained. It is observed that hydrogen component have a lower velocity as the fluid flows inward towards the middle of the circular microchannel; whereas nitrogen component will

decrease its fluid flow only each of the junctions and bend but at the parallel straight section it will flow steadily and in uniform.

Based on this study, it is proposed that the catalyst should be localized throughout the microchannel but concentrated more in the middle inner section of the microchannel, as the hydrogen component tends to slow down in the middle section of the microchannel it is expected that the reaction with nitrogen component will occurs more rapidly in the inner section of the microreactor. As from the radial view, since both components are showing equally steady fluid flow throughout the microchannel, it is proposed that the thickness of the catalyst should be localized evenly throughout the microreactor, so that the reaction can occur completely and equally while it channels down the microchannel.

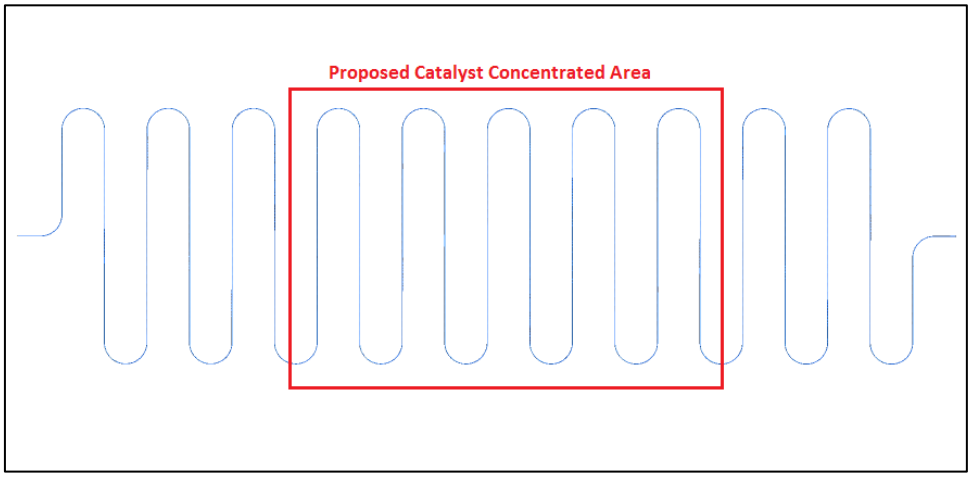


FIGURE 5.1: Proposal of Catalyst Concentrated Area

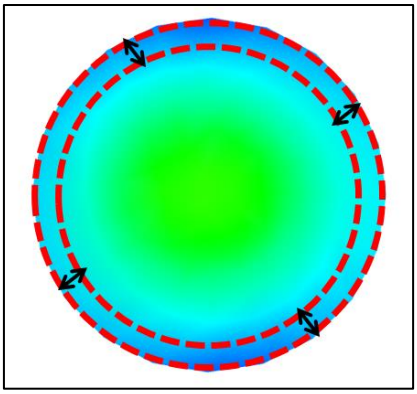


FIGURE 5.2: Proposal of Evenly-Distributed Catalyst Thickness

This project has a very bright prospect for future development. It is recommended that different parameters of the microchannel should be further look into in order to improve the mixing performance of ammonia gas components and the efficiency of the microchannel as the next step of the project. Among the suggestions proposed for future study should include the different overall design of the microreactor, number of inlets (hydrodynamic focusing), number of cyclic turns, diameter of the microchannel, different configuration of the junctions and also its pitch height.

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APPENDIX I: GANTT CHART FOR FINAL YEAR PROJECT I

NO	DETAIL / WEEK	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Selection of Project Title															
2	Preliminary Research Work															
3	Literature Review: introduction to microfluidics															
4	Literature Review: theory of microreactor system															
5	Literature Review: application of CFD software															
6	Literature Review: gas behaviour in microreactor															
7	Literature Review: affecting parameters on gas flow in microreactor															
8	Detail study on usage of CFD software															
9	Hands-on practice on CFD software															

APPENDIX II: GANTT CHART FOR FINAL YEAR PROJECT II

NO	DETAIL / WEEK	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Geometry development study															
2	Design of microreactor geometry															
3	Geometry development on CFD software															
4	Simulation of the designed geometry															
5	Simulation analysis study															
6	Geometry improvement and optimization															
7	Finalize optimum design															
8	Oral presentation															
9	Submission of reports and technical papers															