Study on the Effect of Catalyst Loading to the Flow Dynamics of Ammonia Reactant Gases in a Microchannel via Computational Fluid Dynamics (CFD) Approach

by

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13675

Dissertation submitted in partial fulfilment of

the requirement for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

MAY 2014

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CERTIFICATION OF APPROVAL

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(CHEMICAL ENGINEERING)

Approved by,

_____

(Mohd Zamri bin Abdullah)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

May 2014

CERTIFICATION OF ORIGINALITY

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

_____

(MUHAMMAD ASYRAFF BIN AZMI)

ABSTRACT

There are many advantages of using microreactor compared to the conventional mixing process in industry nowadays. In order to replace the conventional mixing process, researches need to be done to get the best design that gives good mixing and able to maximize the quality of the final product. This work investigates the effect of catalyst loading to the mixing dynamics of ammonia reactant gases in the microchannel using computational fluid dynamics (CFD) simulation. ANSYS CFX 14.5 is used to simulate the flow of gases in the microreactor. The geometry used for this study is a ZA channel. Mesh sensitivity study was conducted using three different mesh quality; coarse, medium and fine mesh. It is found that a finer mesh quality with higher number of nodes and elements will produce a better quality of contour and more accurate data but for this study, medium mesh is selected due to software limitation. Further analysis shows that the hydrogen and nitrogen gas that flow in a porous media are able to achieve its developed-flow state and increase its mixing rate between the gases at a shorter mixing length. As for radial view, it can be observed that both gas components flow uniformly across the diameter of the microchannel. In term of pressure drop, a lower porosity gives a higher pressure drop in the microchannel. Therefore, it is proposed that the catalyst with an optimum porosity ($\varepsilon = 0.45$) should be used throughout the microchannel.

ACKNOWLEDGEMENT

In completion of this final year project, I would like to thank Universiti Teknologi PETRONAS for providing me with the opportunity to conduct this study. I would also like to express my gratitude to my supervisor, Mr Zamri Abdullah for his unconditional guide and support throughout the project. Not forgetting, special thanks to Graduated Assistant (GA) in the simulation lab for their co-operation that helps me to conduct my simulation smoothly. Finally, I would like to thank my parents for their continuous support and encouragement which driven me to complete this project.

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

The project is related to ammonia synthesis from two reactant gases i.e. nitrogen and hydrogen gas. Ammonia was first commercially synthesized in 1870 by using Haber-Bosch process, by which it operates with the aid of catalyst in an extremely high temperature and high pressure reactor. Despite the lower conversion and yield, the process imposes a costly method and high safety risk to produce ammonia. Therefore, the OneBaja program has proposed a new method to replace the Haber-Bosch method by using a magnetic induction system which is performed at an ambient temperature and pressure. The purpose of this project is to study on the effect of catalyst loading to the flow dynamics of ammonia reactant gases in a microchannel via computational fluid dynamics (CFD) approach. CFD is the science of predicting fluid flow, heat transfer, chemical reaction and other related phenomena by solving numerical set of Navier-Stokes equations. CFD modelling is a cost saving, timely, safe and easy to scale-up, and can reduce the total effort required in the experiment design and data acquisition. In this project, ANSYS CFX 14.5 will be used to predict the process and product design in a green urea production.

1.2 Problem Statement

Ammonia is produced by reacting two gases, nitrogen (N_2) and hydrogen (H_2) to produce NH_3. In OneBaja program, NH_3 will be produced at ambient operating condition by the mean of magnetic induction zone in a microchannel system to produce higher NH_3 yield compared to the conventional Haber-Bosch method. In such technique, catalyst plays important role to facilitate the process. When the gases flow inside the microchannel the reactant gases will mix, in which their degree of mixing will create turbulent that enhances their chances to collide and react in producing NH_3. At various sites in the microchannel, flow mixing behaviour will vary. By determining the mixing dynamics between the reactant gases, optimum localization of the catalyst could be predicted in order to be placed on the said site for the reaction to take place. This prediction could be performed through the use of computational fluid dynamics (CFD) simulation, and 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.

1.3 Objective

The aim of the project is to investigate the effect of catalyst loading to the mixing dynamics of ammonia reactant gases in the ZA-type microchannel by using computational fluid dynamics (CFD) approach.

1.4 Scope of Study

The simulation will be done using ANSYS CFX software. The geometry of the microchannel and gas flow rates will be selected from the previous FYP 2013 (May 2013 and September 2013). The simulation will be conducted based on this operating parameter:

- Catalyst loading based on thickness

CHAPTER 2

LITERATURE REVIEW

2.1 Micromixing

The rapid development of microreaction technology in recent years has led to a considerable variety of microfluidic devices. The prefix "micro-" generally designates chemical systems fabricated with techniques originally developed for electronic circuits (Jensen, 2001). In particular, microreactors and micromixers are nowadays commercially available in numerous design and materials in order to increase the mixing performance and maximize the production. Mixing will affect various process parameters including heat and mass transfer rates, process operating time, cost and safety, as well as product quality.

Mixing can be defined as a transport process for species, temperature, and phases to reduce inhomogeneity (Nguyen, 2008). There are three established concepts of mixing which are macro-, meso- and micro- mixing (Fournier et al, 1996). Macromixing is the mixing process using the largest scale of fluid motion, while micro mixing is the smallest scale of fluid motion and molecular motion. On the other hand, mesomixing is the scale range between the both.

Micromixers can be categorized into two groups which are active and passive micromixers (Nguyen et al., 2005). Passive micromixers do not require any external energy due to the absence of moving parts. Generally, the mixing process depends on molecular diffusion or chaotic advection. The robust property of the passive structure is more stable in operation and easily integrated in a more complex system. On the other hand, active micromixers involve moving parts and utilizes disturbance provided by external fields for mixing process. Due to insulation of external disturbance, the structure of the active micromixers is more complicated and require high cost to fabricate. Thus, passive mixers are more favourable to be applied in microfluidic systems.

Table 1 below shows the classification of micromixers.

***TABLE 1**: Classification of Micromixers (Nguyen, 2008)*

Active	**Passive**
Pressure Disturbance	Lamination
Electrohydrodynamic	Injection
Dielectrophoretic	Chaotic advection
Electrokinetic	Droplet
Magnetohydrodynamic	
Acoustic	
Thermal	

General requirements for micromixers are:

- Fast mixing time
- Small device
- Integration ability in a more complex system

There are several factors that need to be considered in designing the micromixers in order to increase the mixing performance, either by manipulating the flow using channel geometry or external disturbances. Common channel widths are on the order of 100 to 500μm, while the length could be a few millimeters or more (Nguyen, 2008). The reduction of the internal diameter of the capillary tube will significantly increases reaction performance implying that narrower capillary diameters should provide even better performance (Berns et al., 1999).

Ultimately, practical problems such as blockages and pressure drops will provide a lower limit to the size of channels that may be exploited in microreactor design. An effective microfabricated channel could be designed by establishing the physical laws governing gas flow in small conduits (Harley et at., 1995). Among other things, such flow may differ from its macroscopic counterpart in that relatively high, subsonic Mach (M) numbers may be maintained concurrently with low Reynolds (Re) numbers; the surface area to volume ratio is huge, the fabrication process may lead to a relatively large degree of surface roughness; and non-continuum effects may occur at pressure above 1 atm.

For microfluidic system, the Reynolds number, Re is usually smaller than 100 that the flow is considered laminar. For a better mixing, turbulent flow is generally preferred in a microchannel. However, it is impossible for turbulence and inertial effects to occur under low Reynolds number condition in microdevices (Brody et al., 1996). Mixing can be done by diffusion since the existence of forces due to surface tension at fluid interfaces are much stronger at this scale. Diffusion can be defined as the process of dispersion of molecules from a region of higher concentration to lower concentration until it reaches equilibrium. Besides, mixing in microfluidic devices is generally achieved by taking advantage of the relevant small length scale, which dramatically increases the effect of diffusion and advection (Capretto et al., 2011)

Microfluidic devices are not merely a miniature version of their macroscale counterpart because of many physical characteristics, such as surface area-to-volume ratio, surface tension and diffusion are not linearly proportional from large to small devices. Microfluidic mixer should be designed in such ways that leverage the physical characteristic of the mixing in a confined space (Capretto et al., 2011).

2.2 Porosity

In this study, the localization of catalyst in a microchannel that behave as an apparent microreactor for the NH_3 synthesis will be investigated. As catalyst will be located throughout or at certain optimized locale in the microchannel based upon the mixing dynamics observed, it is termed as a porous medium; which is highly dependent on the porosity studied. Porosity or void fraction is a measurement of empty spaces in a material where it represents a ratio of the volume of voids over the total volume in a form of percentage between 0 and 100%. An experimental comparison between microchannel heat exchanger with microchannel and porous media was performed by Jiang et al. (2001) to analyse the effect of the dimensions on heat transfer. It was concluded that the heat transfer performance of the microchannel heat exchanger using porous media is higher than a microchannel without porous media, despite the pressure drop in the microchannel is observed to be much larger.

2.3 Computational Fluid Dynamics

Analysis can be done either by experiment or simulation via numerical method of the flow (Zhendong et al., 2012). Analysis of micromixers characterization through experiment could be time consuming and costly. For microfluidics, there is still no generally accepted experimental method to measure its flow field (Wang et al., 2003). Thus, numerical simulation method such as computational fluid dynamics (CFD) of flow within micromixers is an attractive alternative, where it enables different geometries to be quickly designed and tested in a virtual manner. CFD is a branch of fluid mechanics that predicts the fluid flow, heat transfer, chemical reaction and other related phenomena by solving numerical set of Navier-Stokes equation. The results from CFD analysis are relevant for conceptual studies of new design, detail product development, troubleshooting and redesign.

Determining pressure field of micromixer using the Navier-Stokes equation through CFD simulation can give a better understanding of the flow patterns created in the micromixer because it shows the velocity profile of the flow within the micromixers in all three Cartesian coordinates (x, y, z-axis) throughout the entire volume of the device. The residence time distribution (RTD) of the micromixer can be found through the CFD simulation method by applying Langarian method (Aubin et al., 2005). Besides, the simulation not only serve as a design tool, but also as a means to interpret experimental data (Quiram et al., 2013).

A study on fluid dynamics in microchannel was conducted by Amadin (2013) via simulation by using ANSYS CFX® 14.5. The study was conducted to determine the hydrodynamics of the mixing hydrogen and nitrogen gases in various geometry configurations of a microchannel in order to embed the catalyst for ammonia synthesis at the uttermost optimum location. The proposed geometry was a 10 cycles of zigzag-type with two different configuration as shown in Figure 1 and Figure 2. The dimension used for both configurations were summarized in Table 2

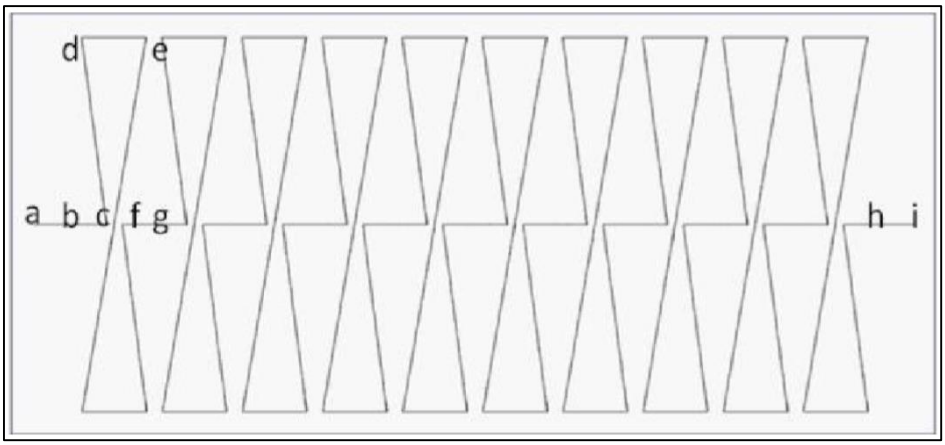


FIGURE 1: *Geometry Design A (Amadin, 2013)*

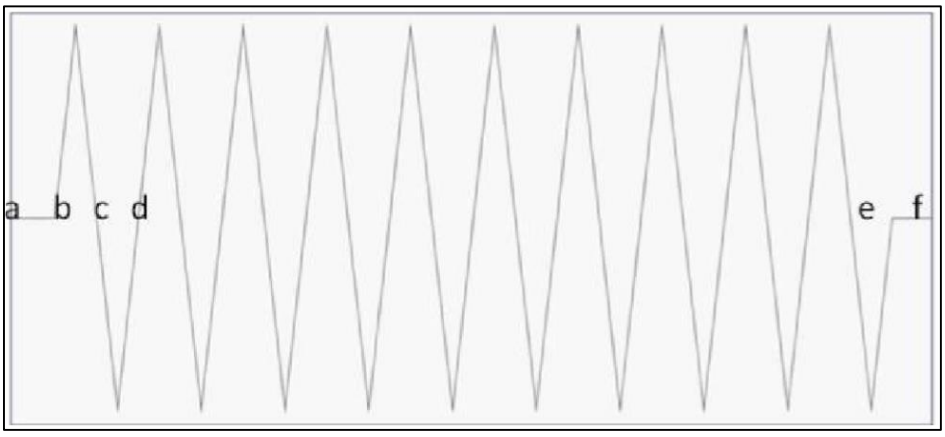


FIGURE 2: *Geometry Design B (Amadin, 2013)*

TABLE 2: *Dimension Used in Design A and B (Amadin, 2013)*

Dimension	Design A	Dimension	Design B
a – i	11 cm	a – f	11 cm
a – b	0.5 cm	a – b	0.5 cm
b – g (1 cycle)	1.0 cm	b – d (1 cycle)	1.0 cm
b – c	0.4 cm	b – c	0.5 cm
c – f	0.2 cm		
d – e	0.8 cm		

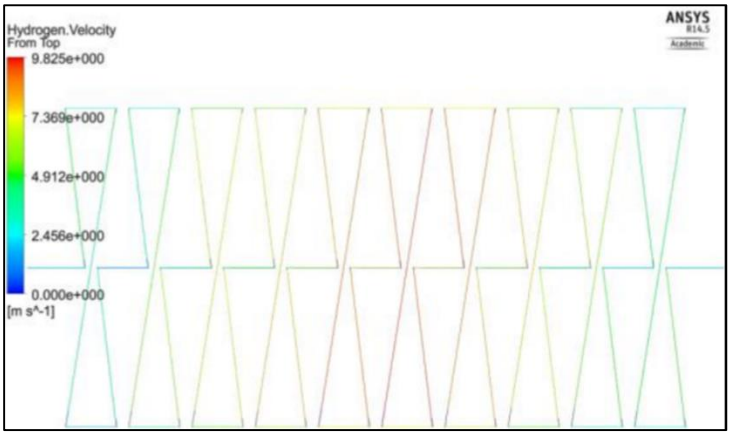


FIGURE 3: *Axial Hydrogen Velocity for Design A*

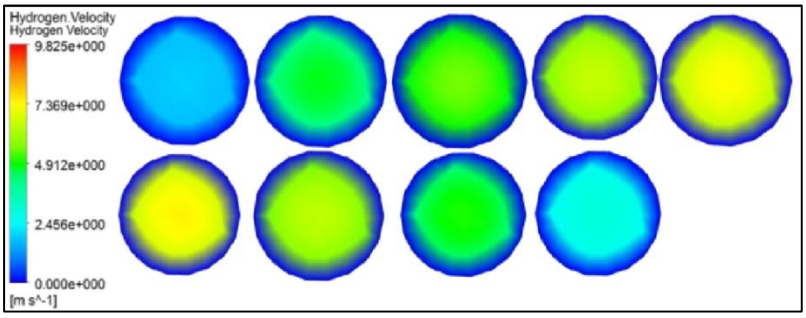


FIGURE 4: *Radial Hydrogen Velocity for Design A*

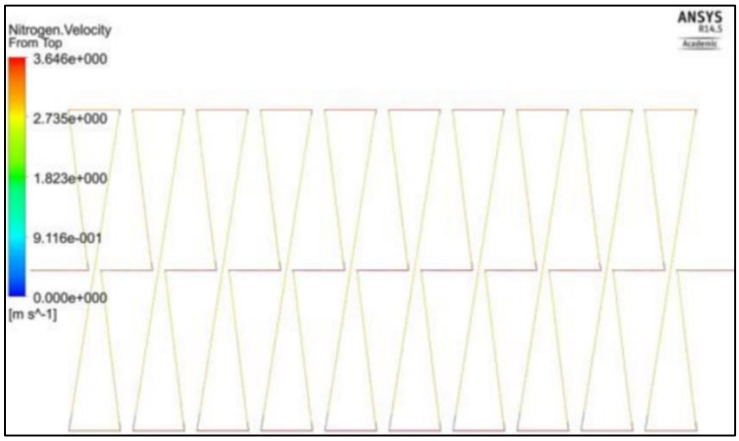


FIGURE 5: *Axial Nitrogen Velocity for Design A*

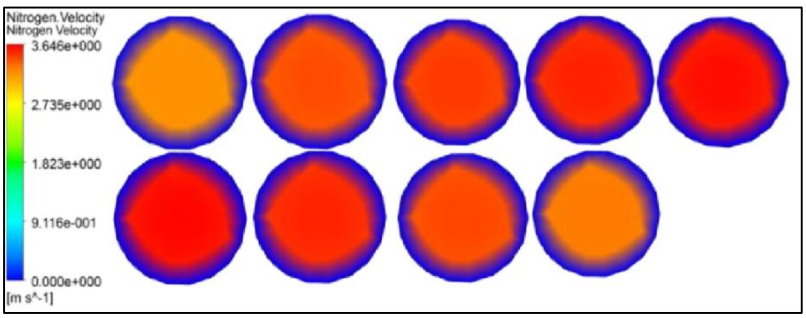


FIGURE 6: *Radial Nitrogen Velocity for Design A*

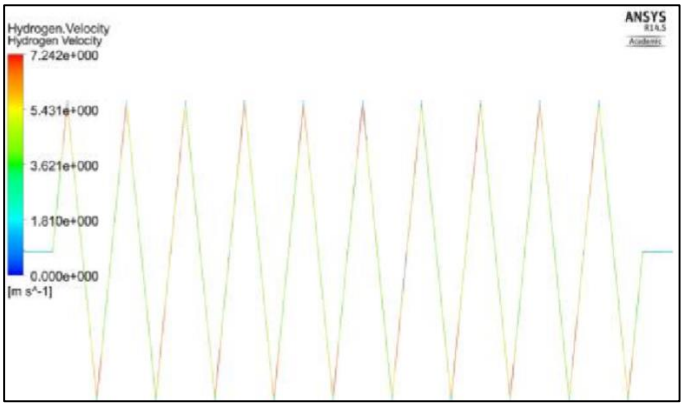


FIGURE 7: *Axial Hydrogen Velocity for Design B*

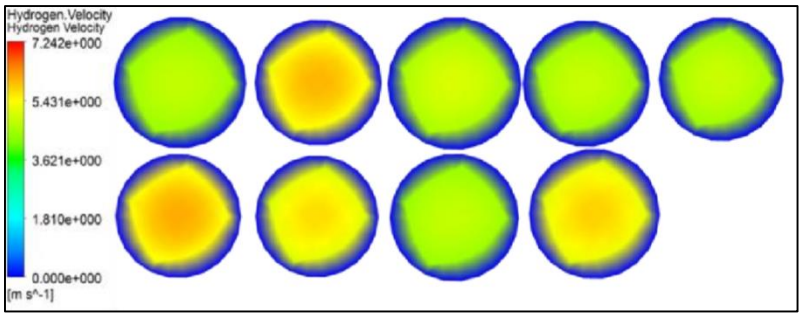


FIGURE 8: *Radial Hydrogen Velocity for Design B*

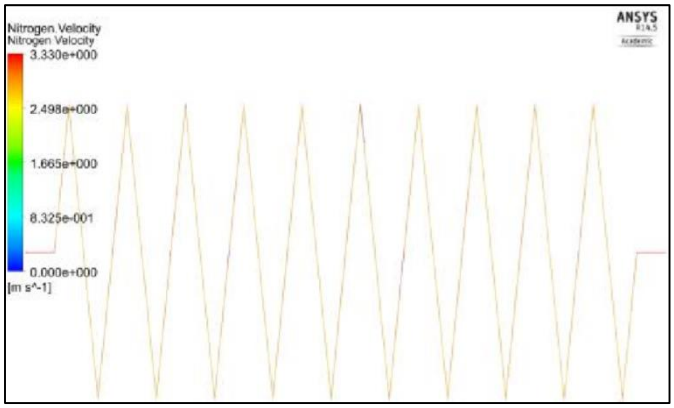


FIGURE 9: *Axial Nitrogen Velocity for Design B*

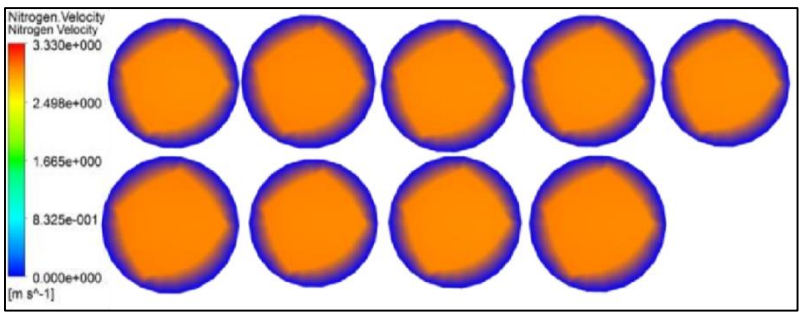


FIGURE 10: *Radial Nitrogen Velocity for Design B*

In this stage of the study, the reaction between hydrogen and nitrogen gas are ignored. The flow of nitrogen is at high velocity at short sections of mixing unit, and lower velocity at long sections for geometry A. Significant velocity changes are observed for hydrogen at every bends in the mixing unit of geometry B. As for nitrogen component, a more uniform flow with less significant change in velocity is observed.

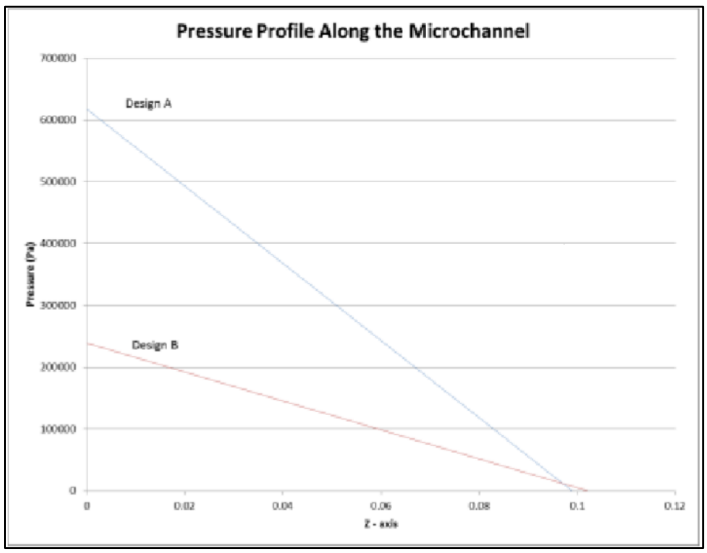


FIGURE 11: *Pressure Profile along the Microchannel*

Geometry A experiences much higher pressure drop compared to geometry B. This is due to the effective length of microchannel geometry A is longer than geometry B. Moreover, mixing unit in geometry A has double the number of bends compared to geometry B. This also contributes to higher pressure drop.

Based on the study, it was proposed for geometry A, the catalyst should be localized throughout the microchannel but concentrated more at the short sections of the mixing unit where both components are observed to be flowing at an almost equal velocity. It is expected that the reaction will occur more rapidly. As for radial view, the observation indicates both gas components flow almost uniformly throughout the microchannel. Hence, catalyst thickness should be localized evenly throughout the microreactor. As for geometry B, catalyst should be localized throughout the microchannel concentrating on the region with more stable flow of fluids which is between the two successive bends. As for catalyst thickness, it is similar to geometry A. In terms of pressure drop, geometry B is more preferable due to much lower pressure drop.

Another study on micromixing was done by Jiang et al (2000) where fluid flow and forced convection heat transfer in micro-heat-exchanger with either micro-channels or porous media have been investigated experimentally. The influence of the dimensions of the micro-channels on the heat transfer performance was first analysed numerically. Six different channel depths (0.1, 0.2, 0.4, 0.6, 0.8 and 1.6 mm) were used for the numerical calculations with the assumption of $W_c = W_w = 0.2$ mm and $h_w = 0.1$ mm.

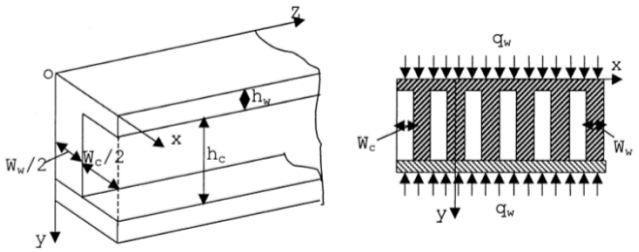


FIGURE 12: *Physical model and coordinate system for numerical simulation of micro-channel heat exchanger*

For these conditions, the pressure drop variation in the micro-channel with channel depth is presented in Figure 13(a) for Re = 224. The pressure drop variation with depth is significant, with deeper channels having less pressure drop. The relationship between the channel depth and the average convection heat transfer coefficient, Figure 13(b) is not monotonic, for $h_c < 0.4$ mm the average convection heat transfer coefficient decreases with increasing channel depth; whereas for $h_c > 0.4$ mm the average convection heat transfer coefficient increases with increasing channel depth. The ratio of the volumetric heat transfer coefficient and the pressure drop $K_v/\Delta P$ increases with increasing channel depth. Figure 13(c); therefore, deep channels have an advantage. The result in Figure 13 show that when $h_c > 0.6$ mm, the pressure drop decrease, the average convection heat transfer coefficient increase and the increase of the ratio $K_v/\Delta P$ are not significant. Therefore, since very deep channels will be difficult to manufacture and will increase the micro-heat exchanger size, the channel depth was selected as $h_c = 0.6$ mm.

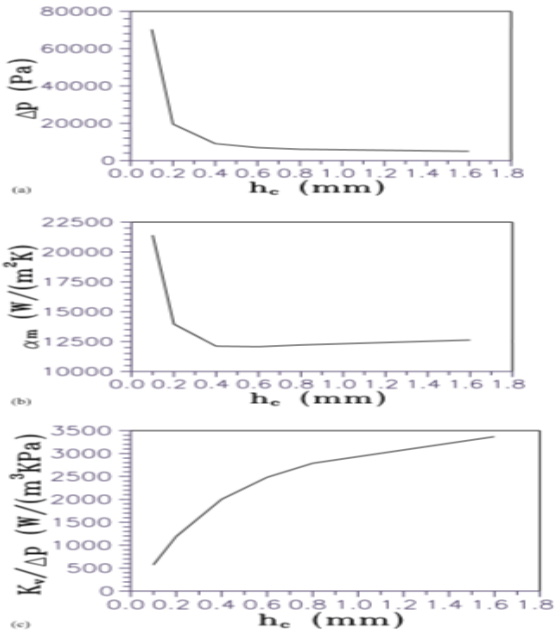


FIGURE 13: *Variation of pressure drop (a) and average convection heat transfer coefficient (b) in a micro-channel with channel depth and effect of channel depth on the ratio of the volumetric heat transfer coefficient and the pressure drop (c)*

Figure 14 presents the heat exchanger effectiveness of the micro-channel heat exchanger as a function of number of transfer units, NTU, for equal hot and cold side mass flow rates. For a single-pass, cross-flow heat exchanger with both fluids unmixed, the heat exchanger effectiveness is

$$\varepsilon = 1 - \exp\{NTU^{0.22}[\exp(-NTU^{0.78}) - 1.0]\} \qquad (1)$$

The experimental data for ε is a little higher than predicted by Equation (1) possibly because the hot and cold water mass flow rates in the experiments are not exactly the same. The differences between the experimental data for the heat exchanger effectiveness and the calculated results using Equation (1) are less than 5%. Therefore, from the heat transfer point of view, the micro-porous heat exchanger is better than the micro-channel heat exchanger.

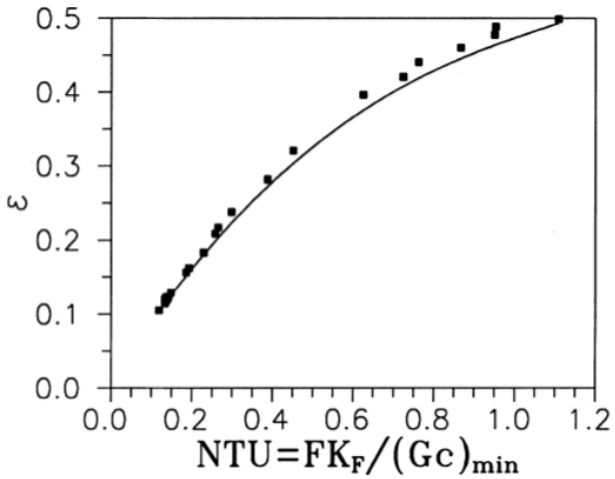


FIGURE 14: *Effectiveness of the cross-flow heat exchanger*

Based on the literature studies, for ammonia synthesis to occur, catalyst must be present and embedded in the microchannel. The effect of gases mixing can be enhanced with some geometric configuration. Therefore, more studies will be carried out to look into the impact of catalyst loading towards the overall flow dynamics of the microreactor.

CHAPTER 3

METHODOLOGY

3.1 Proposed Methodology

3.1.1 Development of Geometry

The geometry for the microchannel is designed by using the built-in Design Modeler computer-aided design (CAD). In this study, the geometry proposed is a ZA-type channel. The geometry parameters for the microchannel is based on the proposed geometry by Amadin (2013). Figure below shows the geometry in ZX-plane. The number of cycles of the proposed geometry is 10 cycles. Several parameters of the design are as stated below:

I. <u>ZA Channel</u>

Total Length of Geometry (a – i)	= 11.0 cm
Inlet/Outlet Length (a – b / h – i)	= 0.5 cm
Length of 1 Cycle (b – g)	= 1.0 cm
Length (b – c / f – g)	= 0.4 cm
Length (c – f)	= 0.2 cm
Length (d – e)	= 0.8 cm

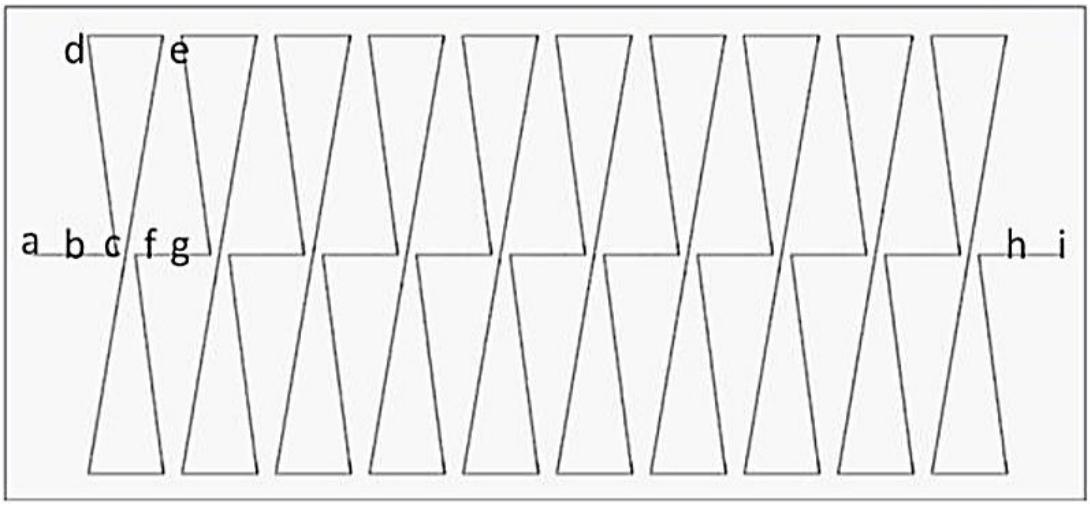


FIGURE 15: *Geometry configuration for the ZA-channel*

3.1.2 Mesh Generation

Mesh will be generated by using ANSYS Meshing right after the geometry creation. There are many meshing properties that need to be specified in order to create high quality of mesh and produce results with high accuracy. The quality of mesh can be identified from the number of nodes, element and orthogonal quality.

In this study, three different meshes are being generated for grid sensitivity analysis based on the geometry design of microchannel with 10 cyclic turns. The medium mesh is selected with the number of nodes of 3,285,264 and elements of 2,600,796 for further analysis of the flow behaviour of both gas components.

3.1.3 Flow Parameter Setup

After the mesh generation, the fluids properties and parameters for the flow is set up at the pre-CFX section. The fluid properties and parameters are as follows:

TABLE 3: *Fluid and Porous Medium Properties*

Fluid Properties	
Fluids	H_2 Ideal Gas N_2 Ideal Gas
Fluid Morphology	Continuous Fluids
Buoyancy Model	Non-Buoyant
Reference Pressure	1 atm
Turbulence Model	k-ε model
Fluid Inlet Velocity	3.33 m/s
Porous Medium Properties	
Type	Carbon Nanotube (CNT)
Thermodynamic state	Solid
Molar Mass	12.01 $gmol^{-1}$
Density	2.26 gcm^{-3}
Specific Heat Capacity	0.7214 $Jg^{-1}K^{-1}$
Thermal Conductivity	6600 $Wm^{-1}K^{-1}$
Porosity, ε	0.34, 0.45, 0.60, 1.00

Different porosities (ε = 0.34, 0.45, 0.60 and 1.00) are used in the microchannel to compare the fluid behaviour in term of velocity and pressure profile of the gas components. The type of porous medium used in the system is a Carbon Nanotube (CNT). Therefore, the value of molar mass, density and

specific heat capacity at 25 °C is based on the carbon-type of porous medium. Based on Berber et al (2000), they suggested an unusually high value of 6600 W/m-K for the thermal conductivity at room temperature.

In order to run the simulation, value of permeability, k and resistance loss coefficient, α has to be determined first based on the selected porosity. The equation involved for both calculation are as follow:

$$k = \frac{\varepsilon^3 \, x \, D^2}{150 \, x \, (1-\varepsilon)^2} \qquad (2)$$

$$\alpha = \frac{1.75 \, x \, (1-\varepsilon)}{\varepsilon^3 \, x \, D} \qquad (3)$$

Where ε = porosity, D = diameter (m)

3.1.4 Governing Equation

Next, the simulation will run in the Solver Manager section. The fluid is assumed to be incompressible and miscible. The constant flow of an incompressible Newtonian fluid in microchannel can be described by the Navier-Stokes equation and continuity equation.

For incompressible fluid, the continuity equation is

$$\frac{\delta u_k}{\delta x_k} = 0 \qquad (4)$$

And the momentum equation is

$$\frac{\partial(\rho v_j v_k)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(-P\partial_{ij} + \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\right) = \rho g_i \qquad (5)$$

Where,

P = pressure,

v = 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.

The species distribution follows the diffusion convective equation with assumption of non-slip boundaries as follows:

$$\frac{\partial c}{\partial t} + \frac{\partial v_k(c)}{\partial x_k} = D\frac{\partial^2}{\partial x}c \qquad (6)$$

Where c = concentration, t = time, and D = diffusivity.

In addition, for a high fluid velocity, the friction force is large enough to lift the particles. This represents the onset of fluidization. The frictional force can be expressed in terms of a friction factor. Thus, the Ergun equation is used to describe the flow through a packed bed.

$$\frac{\Delta P}{L} = \frac{150\mu(1-\varepsilon)^2 u_o}{\varepsilon^3 d_P^2} + \frac{1.75\,(1-\varepsilon)\rho u_o^2}{\varepsilon^3 d_P} \qquad (7)$$

Where ΔP = Pressure drop, L = Length/height of the bed, μ = fluid viscosity, ε = void space of the bed, u_o = fluid superficial velocity, d_P = particle diameter, ρ = density of the fluid.

3.1.5 Post-processing

In this stage, the results of the simulation will be finalized and displayed using a set of post-processing tools. Users can analysed the detailed results over selected parts of the geometry and export the data as a text files for further calculation. Based on the analysis of these data, the parameters can be manipulated in order to perform design optimization.

3.2 Gantt Chart and Key Milestone

GANTT CHART FOR FINAL YEAR PROJECT

No	Details	Week																										
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
1	Discussion of Project Title																												
2	Analyzing Research Articles																												
3	Collecting simulation information																												
4	Development of geometry													•															
5	Generating mesh																		•										
6	Run simulation																								•				
7	Flow Analysis																												
8	Reporting																												•

- Suggested Milestones

Process

CHAPTER 4

RESULT & DISCUSSION

The simulation was conducted by manipulating the porosity of porous medium at ambient condition. Three studies were carried out; mesh sensitivity study, flow of gas components in microchannel and pressure drop across the microchannel in order to determine the best porosity of porous medium to be used in the system

4.1 Mesh Sensitivity Study

The following summarized the mesh that was created for ZA channel geometry configuration.

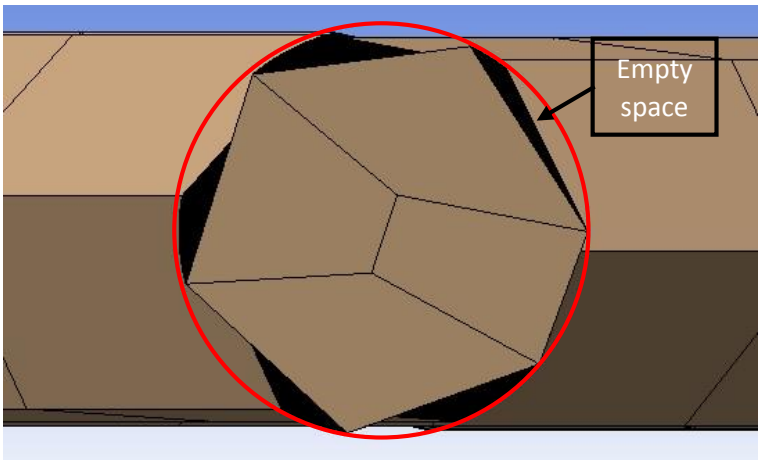


FIGURE 16: *Radial view of coarse mesh*

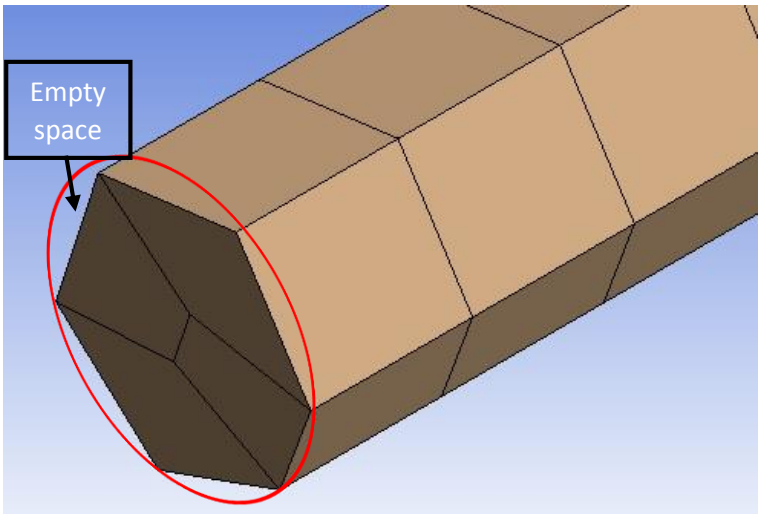


FIGURE 17: *Side view of coarse mesh*

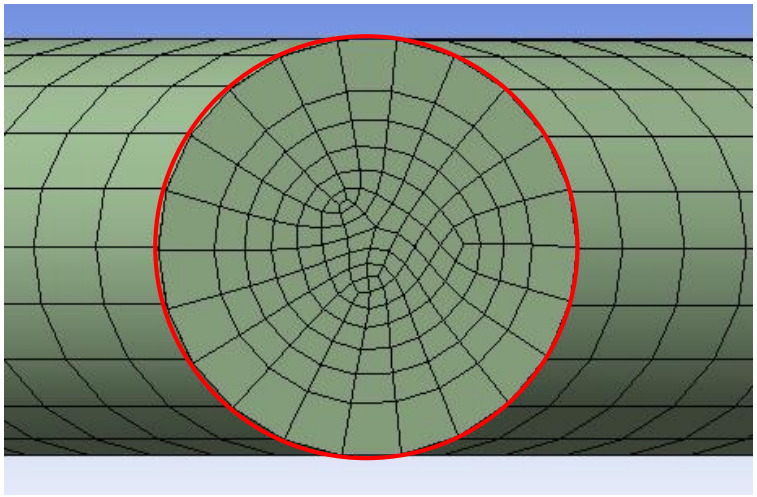


FIGURE 18: *Radial view of Fine mesh*

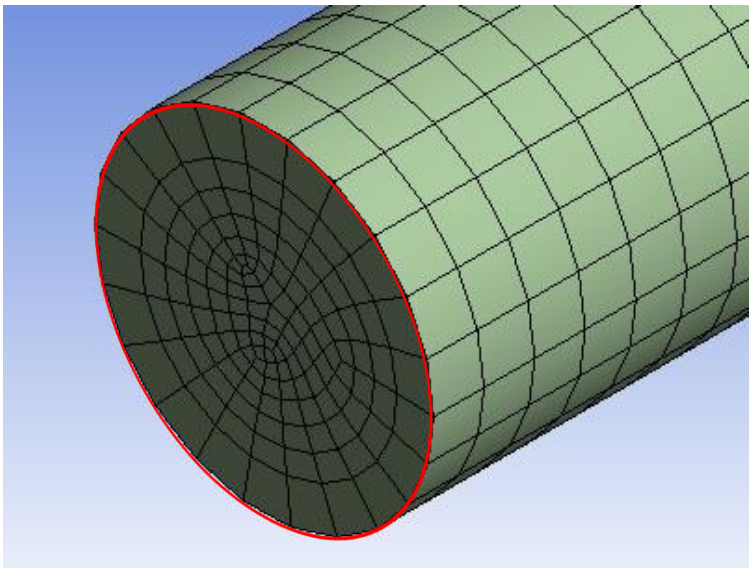


FIGURE 19: *Side view of Fine mesh*

TABLE 4: *Meshed Properties*

Geometry	Mesh Quality	No. of Nodes	No. of Elements	Orthogonal Quality	Simulation Duration
ZA	Coarse	161368	80680	59.3%	3 minutes
	Medium	3285264	2600796	67.8%	7 minutes
	Fine	13019314	12004680	69.2%	15 minutes

Good mesh is a very subjective matter. For a circular-based geometry, the rule of thumb is that the mesh shall fulfil the circumference of the actual circle. Also, mesh should be structured in order for good results to be obtained in the post-processing step such as in constructing contour plot. Mesh will determine the fluid domain behaviour during the flow. Based on Figure 16 & 17, the mesh result is in hexagonal shape rather than circle. It is not a good mesh and must be avoided. Furthermore, there are empty spaces around the shape which gives no data during the post-processing because no fluid domain exist there. Based on Figure 18 & 19, the mesh is better and acceptable as it forms a circle-like feature. The fluid domain is fully covered the circle shape and it will gives more accurate data compared to coarse mesh.

Based on Table 5, it shows that the higher the orthogonal factor, the better mesh quality produced. Besides, a finer mesh quality can be defined by the increment of number of nodes in the geometry. However, the simulation time required is longer for a finer mesh. The orthogonal quality shows that the finer mesh has higher percentage compared to coarse mesh and it indicates that finer mesh is a high quality mesh.

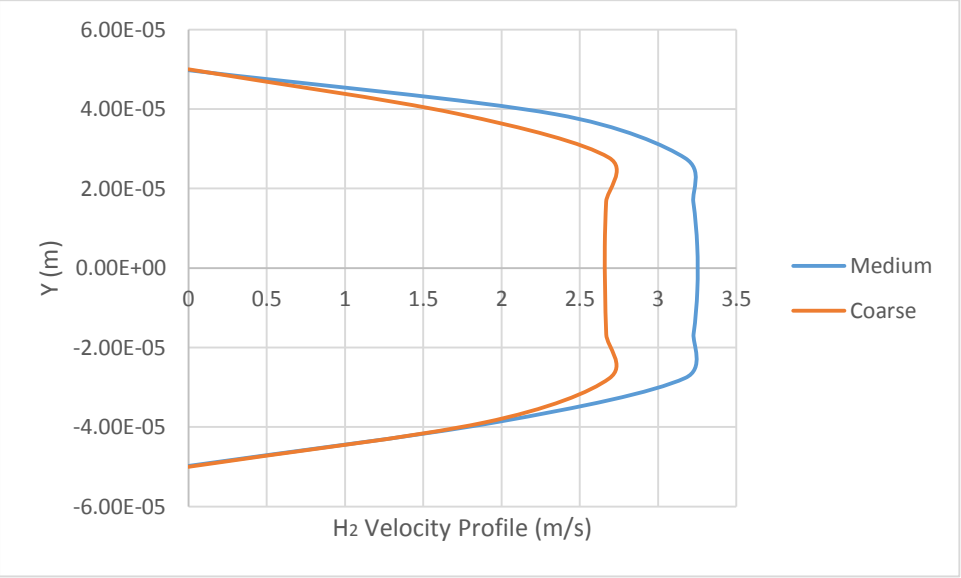


FIGURE 20: *Hydrogen Outlet Velocity Profile at Y-axis*

Figure 20 shows the comparison of hydrogen outlet velocity along y–axis for coarse and medium mesh quality. In this study, the hydrogen gas enter the microchannel at a speed of 3.33 m/s and expected to exit the channel at similar speed. From the figure, it is observed that for coarse mesh quality, the hydrogen gas exits at a speed of 2.7 m/s and for medium mesh quality, the hydrogen gas exits at the range

of 3.33 m/s. However, it is noted that the speed is lower at the side wall. This may due to the shear stress experienced by hydrogen gas component against the wall of the microchannel causing the decrease in the fluid flow.

Therefore, the sensitivity study shows that quality of meshes is indeed crucial in producing reliable and accurate results. A refined mesh is absolutely necessary so that the solver is able to compute the solution to a higher accuracy.

4.2 Flow of Gas Components in Microchannel

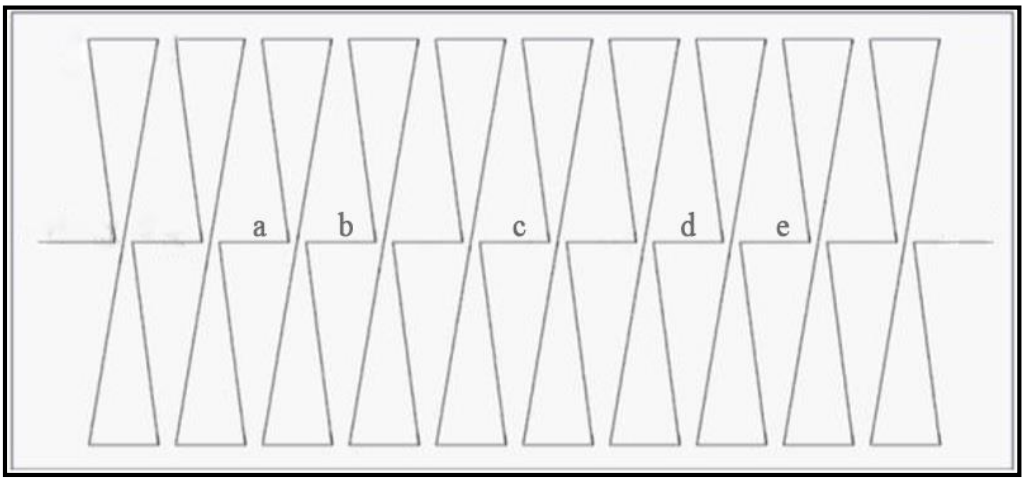


FIGURE 21: *Location of Velocity Contour Comparison*

TABLE 5*: Location of Velocity Contour Comparison of Hydrogen Gas for ε = 0.34, 0.45, 0.60 and 1.00*

Position	ε = 0.34	ε = 0.45	ε = 0.60	ε = 1.00
Default Legend	H2 at STP.Velocity Radial H2 Velocity 3.558e+000 3.349e+000 3.139e+000 2.930e+000 2.721e+000 2.511e+000 2.302e+000 2.093e+000 1.884e+000 1.674e+000 1.465e+000 1.256e+000 1.046e+000 8.372e-001 6.279e-001 4.186e-001 2.093e-001 0.000e+000 [m s^-1]	H2 at STP.Velocity Radial H2 Velocity 3.592e+000 3.380e+000 3.169e+000 2.958e+000 2.747e+000 2.535e+000 2.324e+000 2.113e+000 1.901e+000 1.690e+000 1.479e+000 1.268e+000 1.056e+000 8.451e-001 6.338e-001 4.226e-001 2.113e-001 0.000e+000 [m s^-1]	H2 at STP.Velocity Radial H2 Velocity 3.988e+000 3.754e+000 3.519e+000 3.284e+000 3.050e+000 2.815e+000 2.581e+000 2.346e+000 2.111e+000 1.877e+000 1.642e+000 1.408e+000 1.173e+000 9.384e-001 7.038e-001 4.692e-001 2.346e-001 0.000e+000 [m s^-1]	Hydrogen.Velocity Radial H2 Velocity 9.825e+000 9.247e+000 8.669e+000 8.091e+000 7.513e+000 6.935e+000 6.357e+000 5.779e+000 5.201e+000 4.623e+000 4.046e+000 3.468e+000 2.890e+000 2.312e+000 1.734e+000 1.156e+000 5.779e-001 0.000e+000 [m s^-1]

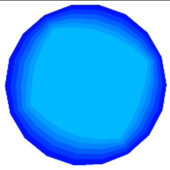
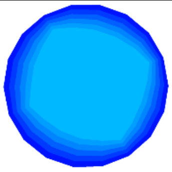
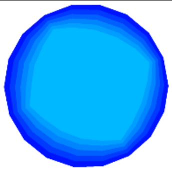
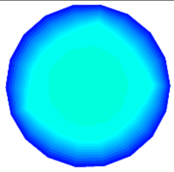
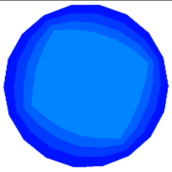
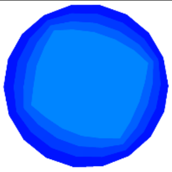
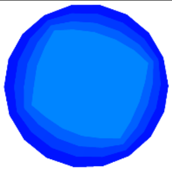
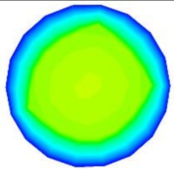
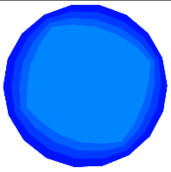
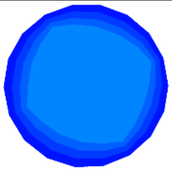
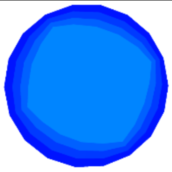
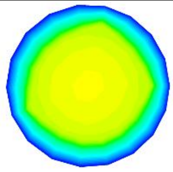
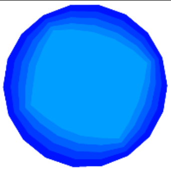
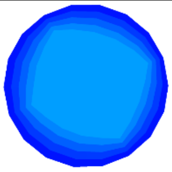
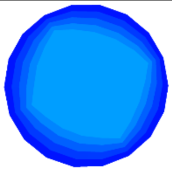
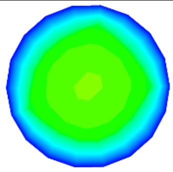
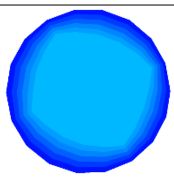
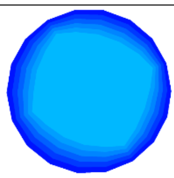
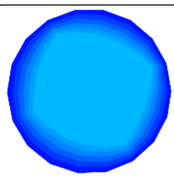
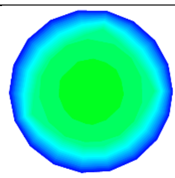
Location ‘a’				
Location ‘b’				
Location ‘c’				
Location ‘d’				
Location ‘e’				

TABLE 6: *Location of Velocity Contour Comparison of Nitrogen Gas for ε = 0.34, 0.45, 0.60 and 1.00*

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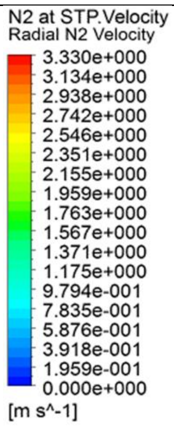
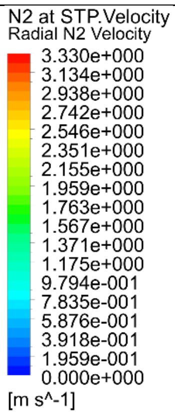
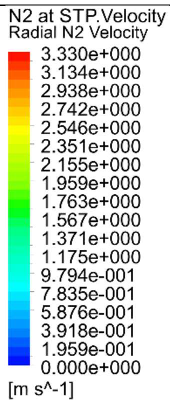
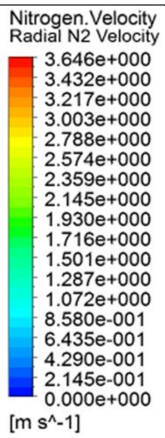
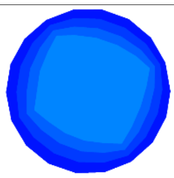
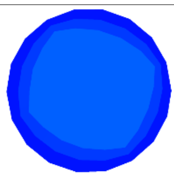
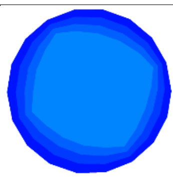
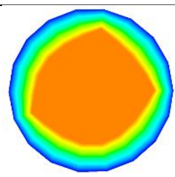
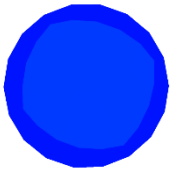
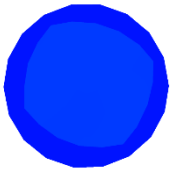
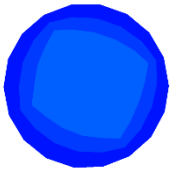
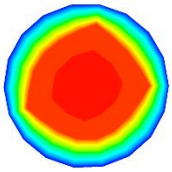
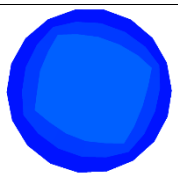
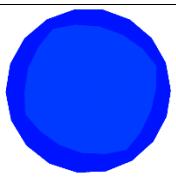
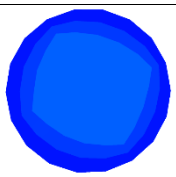
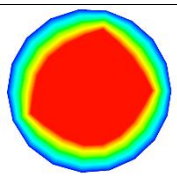
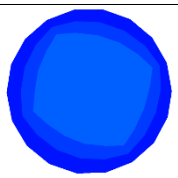
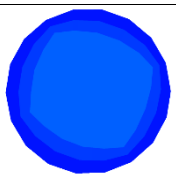
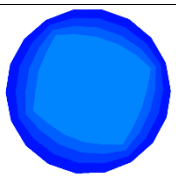
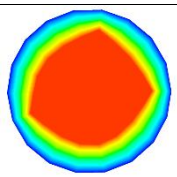
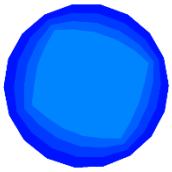
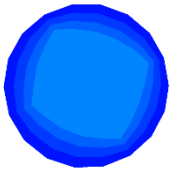
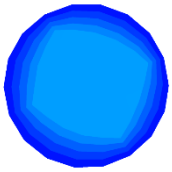
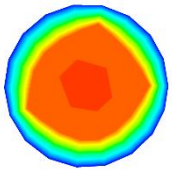
Default Legend				
Location ‘a’				

Location ‘b’				
Location ‘c’				
Location ‘d’				
Location ‘e’				

From Table 6 and Table 7, they clearly shows that the velocity from a radial view of the hydrogen and nitrogen gas flow is slower at $\varepsilon = 0.34$, 0.45 and 0.60 compared to $\varepsilon = 1.00$ (no porosity). This is happening because there are friction of fluid between the gases and the surface of the porous medium in the microchannel which causes the flow of the gases to decrease. Besides that, the contour plot also shows that the velocity profile in low porosity are more organized into localized, channel-like patterns while the velocity profile in high porosity media are more chaotic and uneven across the diameter of the microchannel. This proves that the hydrogen and nitrogen gases flow more stable in a microchannel that contain porous media. Other than that, from this point of view, there are sharp edges near the wall of microchannel. This situation might happen due to the usage of medium mesh quality which causes the formation of edges and data gathered is less accurate.

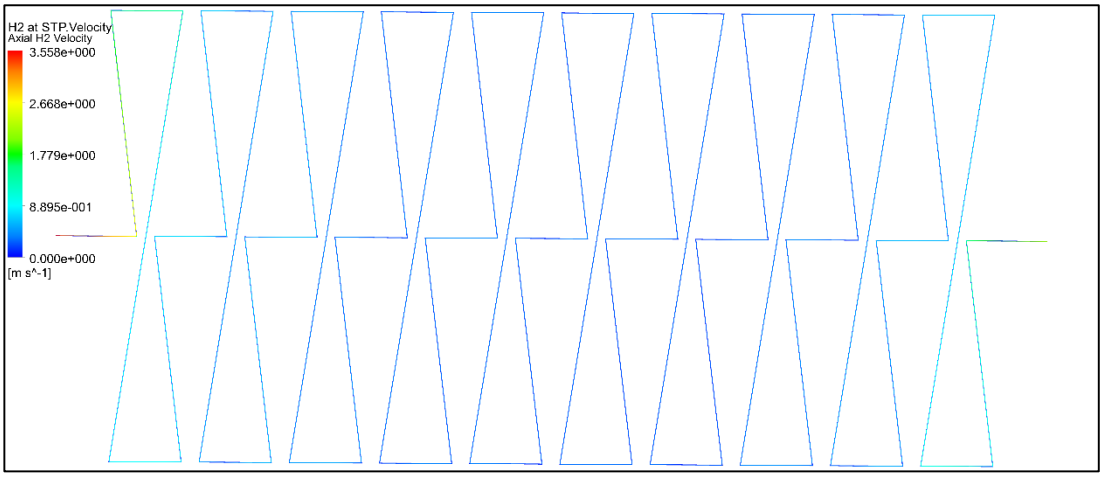


FIGURE 22: *Axial Hydrogen Velocity for ε = 0.34*

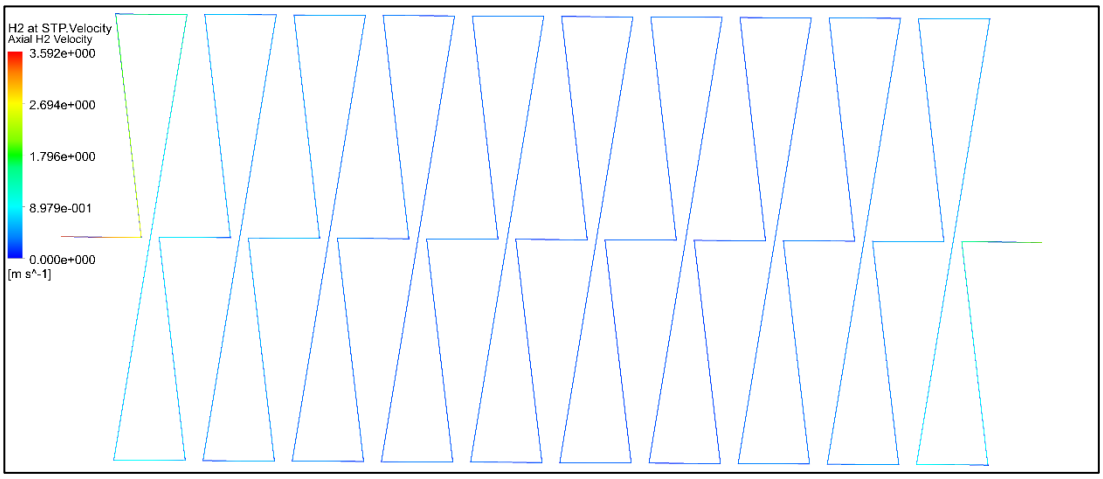


FIGURE 23: *Axial Hydrogen Velocity for ε = 0.45*

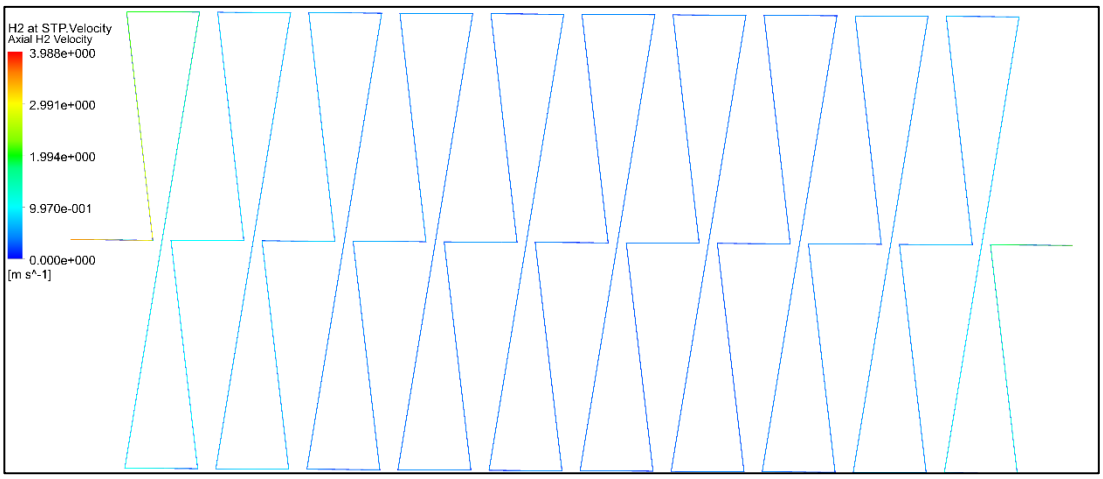


FIGURE 24: *Axial Hydrogen Velocity for ε = 0.60*

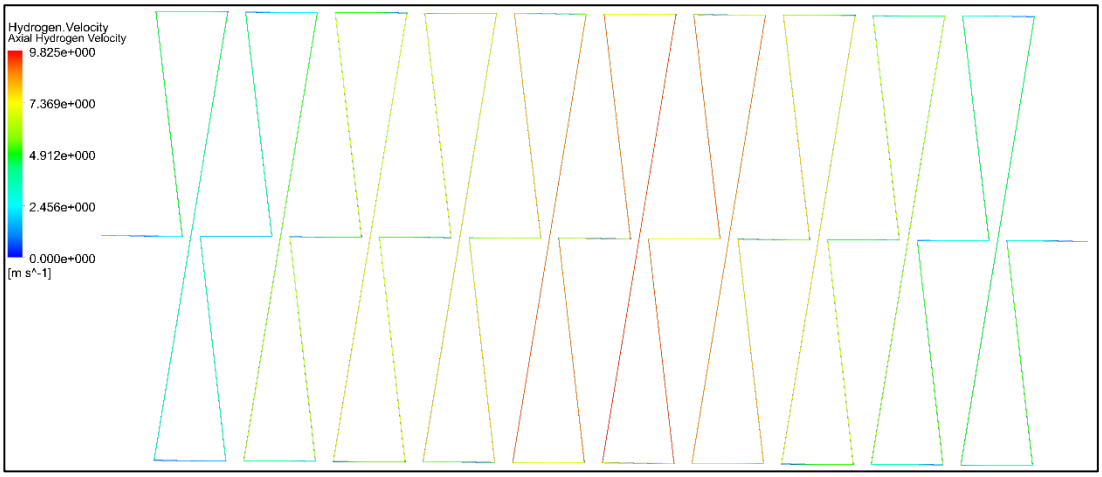


FIGURE 25: *Axial Hydrogen Velocity for ε = 1.00*

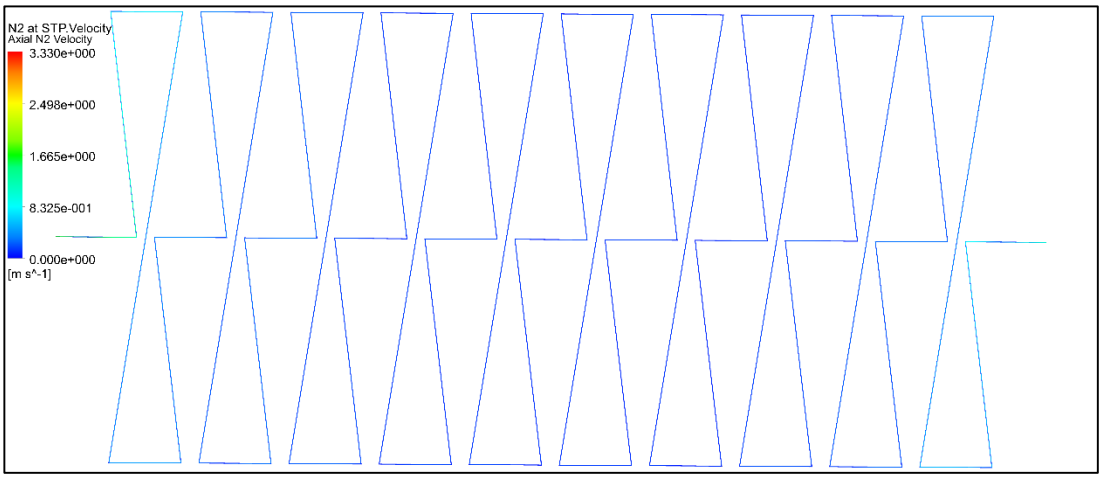


FIGURE 26: *Axial Nitrogen Velocity for ε = 0.34*

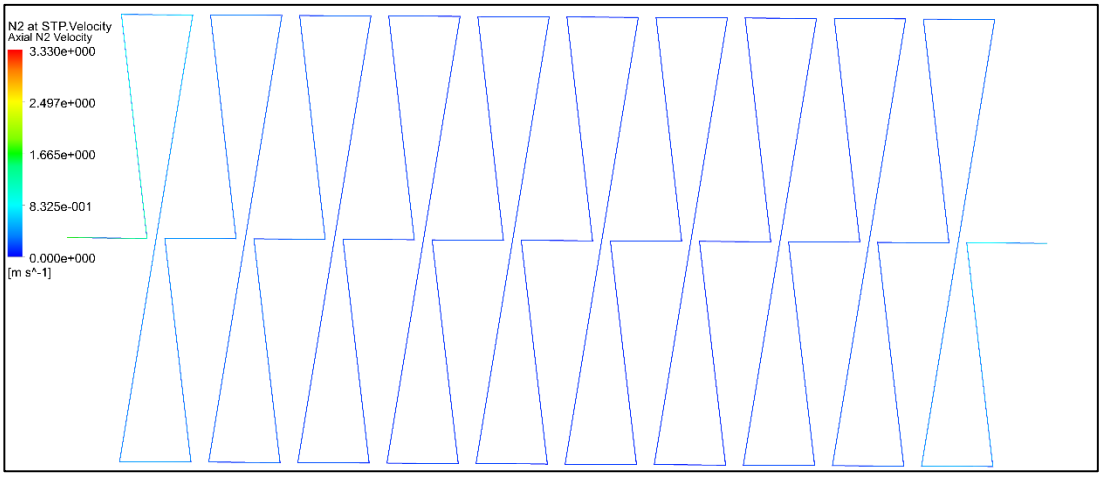


FIGURE 27: *Axial Nitrogen Velocity for ε = 0.45*

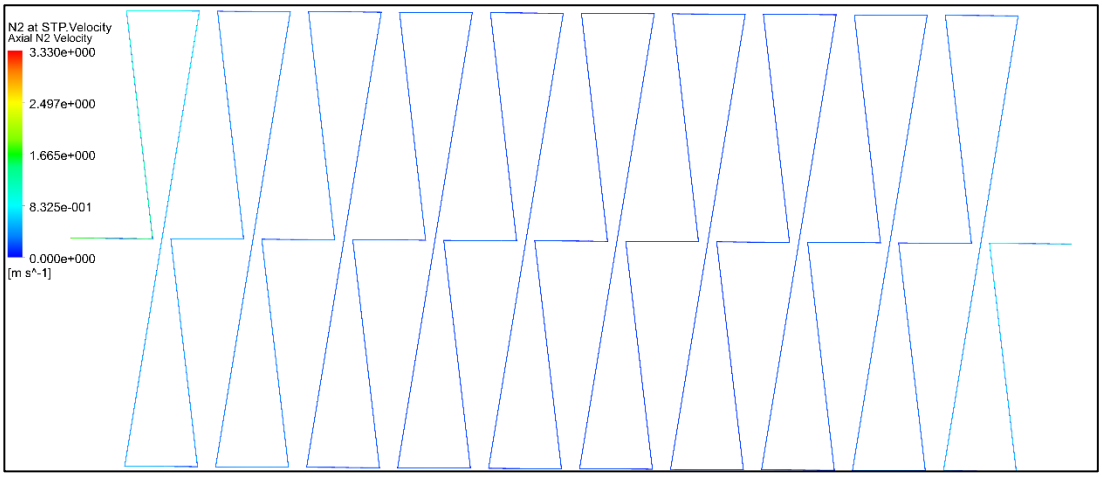


FIGURE 28: *Axial Nitrogen Velocity for ε = 0.60*

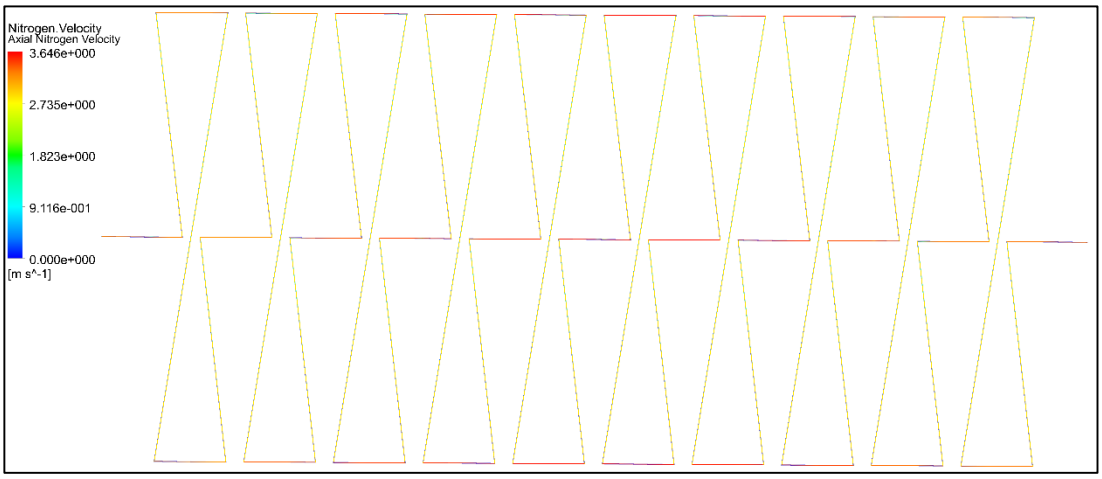


FIGURE 29: *Axial Nitrogen Velocity for ε = 1.00*

From axial point of view, Figure 22, Figure 23 and Figure 24 shows almost similar velocity contour plot. The hydrogen gas generally has higher velocity at the start point and slow down until it reaches a constant velocity at the middle section of the microchannel. These figures shows that the presence of porous medium inside the microchannel are able to change the flow of both gases become more stable (both gases show blue colour). The uniform colour in the middle section of the microchannel (mostly blue) shows that the gases has reached its developed-flow state compared to Figure 25 which shows uneven colour distribution throughout the microchannel. This might be due to two reasons:

1. The design of the microchannel itself allows better opportunity for developed-flow state to be achieved faster, as the zig-zag and all the turnings creates better turbulence.
2. The function of having porous media is to enhance the mixing between gases to occur faster. Hence, it creates shorter mixing length phenomenon.

Other than that, the contour plot from the axial view also shows the velocity profile at the outer-most wall of the microchannel. It indicates that the velocity at the wall is approaching zero for all porosity. This phenomenon may be due to the large shear stress of the microchannel wall on the hydrogen gas component, thus causing slowdown of the fluid flow. Similar observations are seen from Figure 26, Figure 27 and Figure 28 for nitrogen gas where it reaches the developed-flow state at the middle section of the microchannel as compared to Figure 29, where the developed-flow state is yet to be reached by the gas. Therefore, it shows that the presence of porous media are able to increase the mixing rate between hydrogen and nitrogen gas at a shorter mixing length.

4.3 Pressure Drop across Microchannel

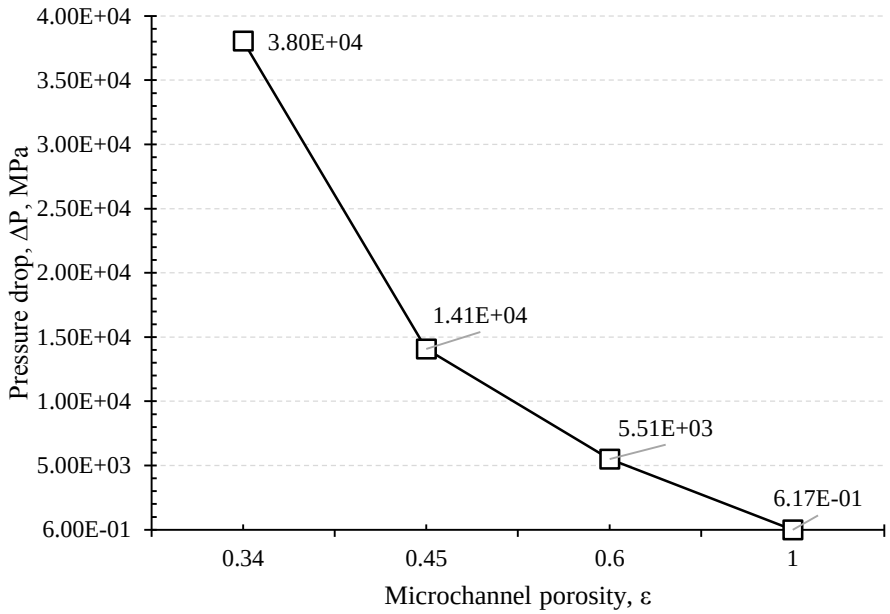


FIGURE 30: *Pressure Profile along the Microchannel*

The following Figure 30 illustrates the pressure profile along the microchannel at different porosity. Porosity at 0.34 experiences much higher pressure drop compared to porosity at 1.00. This is due to the increment of friction of fluid flowing over the surface of the porous media. Finer particles have a higher surface area per unit volume compared to coarser particles. Therefore, it will increases the flow resistance in the microchannel. Besides that, turbulences within the fluid inside the porous media, at higher flow rates, cause an additional flow resistance. Thus, it also contributes to the increment of pressure drop. Based on Jiang et al (2000), they found that, for the same flow rate with the presence of porous medium causes the pressure drop of the system is much larger. In term of manufacturing cost and safety purpose, low pressure drop is more preferable to be used in the microchannel because less material strength is needed to withstand the low pressure.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

In this project, computational fluid dynamics was applied to study the effect of catalyst loading to the hydrodynamics of hydrogen and nitrogen gas components in a microchannel at ambient temperature and atmospheric pressure. The significant of this study is to determine the optimum localization of catalyst in the microreactor for the enhancement of the ammonia synthesis reaction.

In this stage of study, the reaction between hydrogen and nitrogen gas are ignored. Four different porosity (ε = 0.34, 0.45, 0.60, 1.00) were chosen and tested. Mesh sensitive study was conducted using three different mesh qualities; coarse, medium and fine mesh. It is found that a finer mesh quality with higher number of nodes and elements will produce a better quality of contour and more accurate data solution. In this study, medium mesh with 3285264 nodes is selected as the contour plot of its gas components due to software limitation.

Further analysis shows that the hydrogen and nitrogen gas flow slower in porous media because of higher resistance in the microchannel. The velocity profile in a lower porosity are more organized into localized, channel-like patterns. Furthermore, gases flow in a porous media are able to achieve its developed-flow state and enhance the mixing rate between hydrogen and nitrogen gas at a shorter mixing length.

Based on this study, it is proposed that the catalyst with a lower porosity (ε = 0.60) should be used throughout the microchannel but concentrated more at the short sections of the mixing unit where both components are observed to be flowing at an almost equal velocity in an empty microchannel. It is expected that the reaction will occur more rapidly throughout the microchannel with a minimum catalyst loading. As for radial view, current observation shows both gas components flow uniformly across diameter of the microchannel. In term of pressure drop, the suggested porosity is more preferable because of its low pressure drop.

There are few recommendations that need to be apply for further improvement of the system:

- More refined mesh is used for the design in order to achieve more accurate data solution
- Modification of the catalyst thickness need to be more specific at certain area such as at the center of the microchannel or at the inner wall.
- Using different angle of bends
- Different diameter of the microchannel

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