CERTIFICATION OF APPROVAL

Study on the Flow Dynamics of Nitrogen and Hydrogen Gasses Subjected to Wires Element in Monolithic Microchannel

by

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15570

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Approved by,

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(Mohd Zamri Abdullah)

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CERTIFICATION OF ORIGINALITY

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

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NUR AMIRAH BINTI MOHAMED RASHIDI

ABSTRACT

The former method to produce ammonia (NH_3) was not sustainable and unenvironmentally friendly since the process required high energy consumption as well as high operating condition. The advanced of technology for the past few decades have enabled the production of NH_3 to occur in the ambient condition. The technique to achieve high yield of NH_3 is illustrated under nanotechnology and the Magnetic Induction Method (MIM) where induced magnetic fields polarizes the hydrogen (H_2) and nitrogen (N_2) gasses in the monolithic microchannel to allow the synthesis of NH_3. Previous study showed that chaotic advection was successfully induced when wires are arranged axially in different manners along the microreactor. Hence to further enhance the rate of reaction, design of the monolithic microchannel is improved. Therefore, wires elements with different configurations are introduced in this research where they are arranged in 30^0 and 90^0 pitch with different distance and number of wires in the monolithic microchannel to analyse the flow dynamic of H_2 and N_2. This simulation investigated the result of mixing index with effect of distance between centre of wires, effect of number of wires and effect of wire pitch with the production of ammonia. Based on the result obtained, the square pitch geometry with 13 wires is perceived to produce the most effective dynamic mixing. The development and design of the five monolithic microchannels are prepared via a computational fluid dynamics (CFD) approach using the software ANSYS 15.0 coupled with CFX module.

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LIST OF ABBREVIATIONS

t	diffusion time of molecules
L	square of the channel width
D	diffusion coefficient of a molecule
Re	Reynolds number
ρ	density (kg/m^3)
V	velocity (m/s)
D	diameter of cylinder (m)
μ	fluid viscosity (kg/ms)
n	number of chemical species
ρ_n	density of each of the component (kg/m^3)
V_n	volume of each component
n	number of chemical species
x_i, x_j	mole fractions of two species
μ_i, μ_j	viscosities of two species at specified temperature
M_i, M_j	molecular weight of two species in g/mol
A	subtraction of cross sectional area and total area of void area (m^2)
P	wetted perimeter area (m)
ρ_{mix}	density of mixture (kg/m^3)
D_H	hydraulic diameter (m)
μ_{mix}	viscosity of the mixture (kg/ms)
γ	variance
C_i	mass fraction at sampling point i
C_m	optimal mixing mass fraction
N	number of sampling points
M	mixing index
γ_{max}	maximum variance

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CHAPTER 1
INTRODUCTION

1.1 Background of Study

Ammonia (NH_3) is a chemical compound which consists of three atoms of hydrogen (H_2) and one atom of nitrogen (N_2). This gas substance is known universally in industrial for the various application as an additive such as explosives, detergent and fertilizer industry, chemicals, fibres and plastics, refrigeration, pharmaceutical, pulp and paper and mining and metallurgy [1]. A high percentage of 80% approximately, from the total production of this chemical substance has been applied in synthetic fertilizer, therefore causing a great market demand in the industry business. Consumption of fertilizer increased significantly in 2010 and is expected to grow in a stabilized way during the following years of the forecast period. World demand for total fertilizer is estimated to grow at 2.0 percent per annum from 2011 to 2015 [2].

Precisely, 48% of the NH_3 produced is deployed in the production of urea (the most commonly used nitrogen fertiliser and basic feedstock for industrial products like plastics, resins and adhesive) while 11% is employed in the production of ammonium nitrate. Production of other fertilisers like ammonium sulfate, ammonium phosphate, diammonium phosphate and monoammonium phosphate contribute about 20% of the ammonia consumption in the fertilizer industry and lastly 3% is directly used as fertiliser.

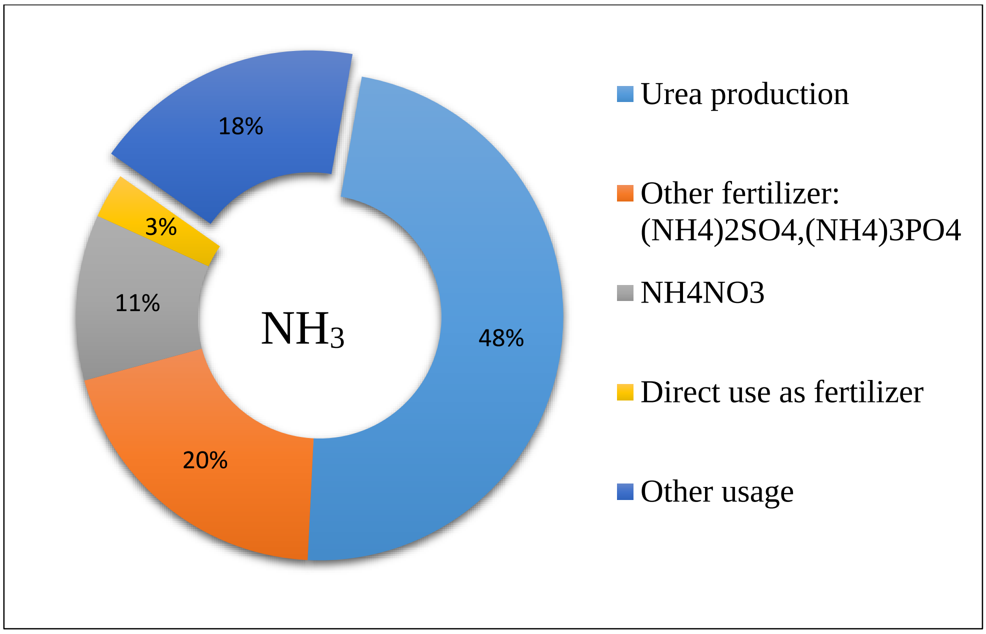


FIGURE 1.1 Ammonia Usage in Industry

Regrettably, the current production is only capable to generate 10-20% of NH_3 yields with capital and energy intensive [3]. This process of producing NH_3 which is known as Haber-Bosch process obliges to operate under a high operating condition temperature (400 – 500^0C) and pressure (130 – 300 atm) where such circumstances possess a very careful handling as well as increasing the hazards to the operators and the plant facilities which lead to the high energy consumption.

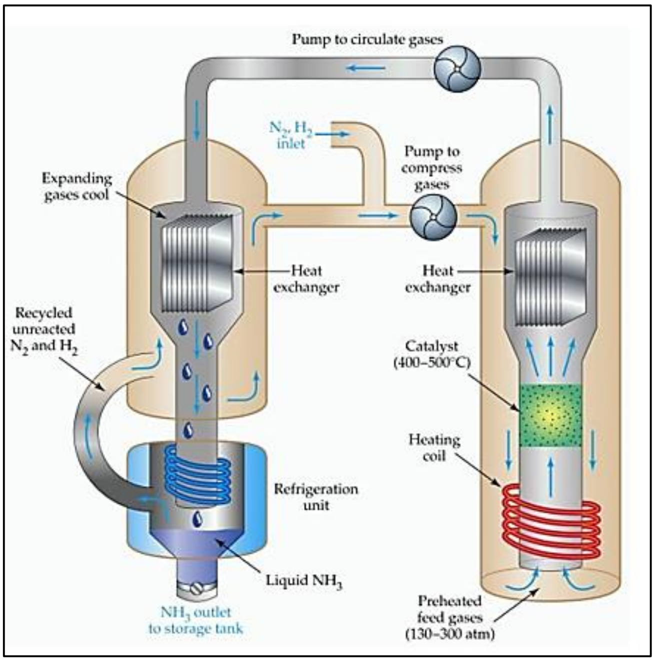


FIGURE 1.2 Haber - Bosch Process

In order to overcome these drawbacks, researches discovers new promising method to attain the high yield of NH_3 at ambient condition (at 25°C and 1atm), under the Magnetic Induction Method (MIM) in a microfluidic environment by applying six pairs of Helmholtz coils. The preliminary synthesis of NH_3 using this proposed method was previously proven at laboratory scale in which a microreactor containing Mn-based ferrite catalyst under the magnetic induction zone was able to yield 24.8% NH_3 [4].

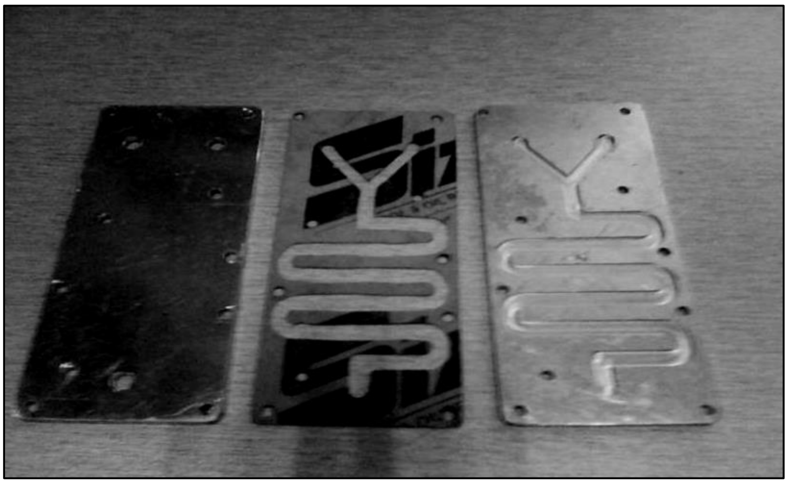


FIGURE 1.3 Microreactor with a Channel Diameter of 5-mm

This NH_3 synthesis works by charging the electron cloud of hydrogen and nitrogen atoms by magnetic induction as the first step. It is proven that the higher the applied magnetic field is, the more effective the catalytic activity will be as a better alignment of the electron spin of the catalyst (usually catalyst used is iron (III) oxide, Fe_2O_3) occurs and enhances the adsorption and desorption process. By this new route, synthesis of ammonia at low temperature is realized and offers NH_3 producers an economic advantage compared to the classical routes [5].

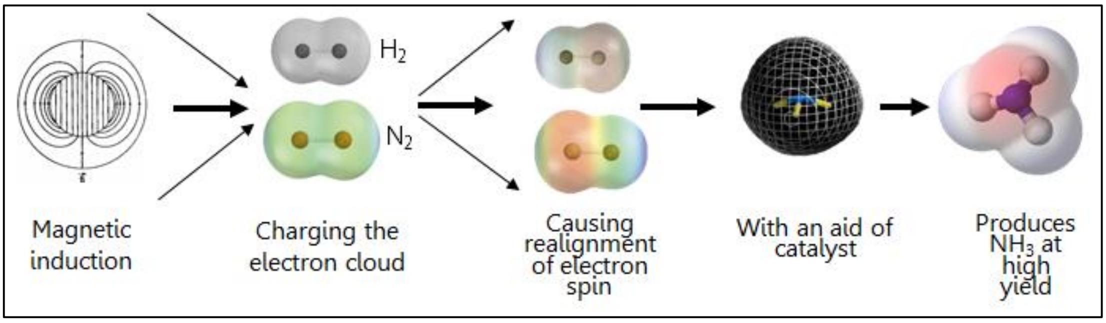


FIGURE 1.4 Magnetic Induction Method

NH_3 synthesis has been successfully achieved. The yield was 76% increasing by using the new version of magnetic induction method. The optimum condition in this system is using $Mn_{0.8}Zn_{0.2}Fe_2O_4$ and $Y_3Fe_5O_{12}$ as nanocatalysts while the room temperature is at 28^0C and ambient pressure is at 1.01 bar. The magnetic field strength used to attain the high production of NH_3 is 1 tesla [4].

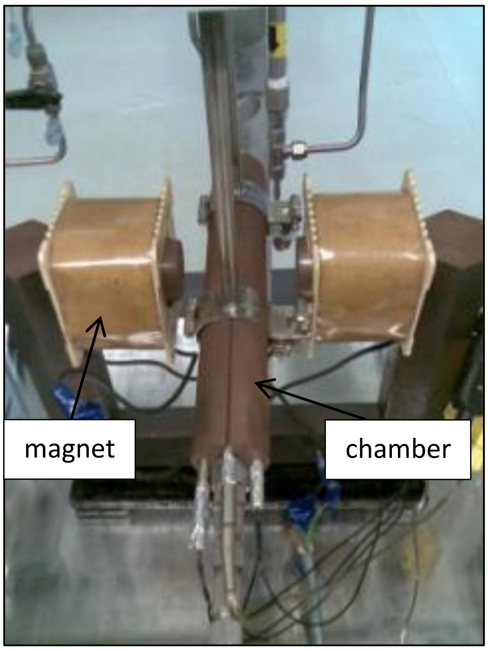


FIGURE 1.5 New Version of Magnetic Induction Method

This project also utilised the magnetic induction method with the addition of wires element into the monolithic microchannel to further enhance the rate of reaction of NH_3. Using wires element in monolithic microchannel is seen as an alternative to improvise the efficiency of NH_3 production by exposing the raw materials, hydrogen and nitrogen to high surface area to volume ratio. Due to their small volume, fast changes of operating conditions can be performed in minimal time demand to reach equilibrium state [6]. This project studied the effect of various geometries of wires in monolithic microchannel and possibility of prevalent gases mixing.

1.2 Problem Statement

In the former project report, the monolithic microchannel consist of varies design with different geometry, mesh and setup applied. The best applicable one is the design consisting of 13 monolithic microchannel that attain the most optimum mixing of H_2 and N_2 arranged as given in the illustration below. In the MIM, wire placement inside the microchannel that contains catalyst does not induce turbulence. Previous study shows that arrangement of wires in square pitch configuration would affect flow dynamics. However, with square pitch arrangement, less mixing occur because of low hydraulic diameter. The dynamic flows of both gases are observed to maintain its homogeneousness at almost the entire length of the monolithic microchannel. Parameters such as temperature and pressure of the gases are maintained throughout the design. Several arrangement and configuration is constructed in order to investigate the effect of using wires element for the ammonia synthesis. At the end of this project, we could determine whether the mixing has improved with the presence of wires in the monolithic microchannel.

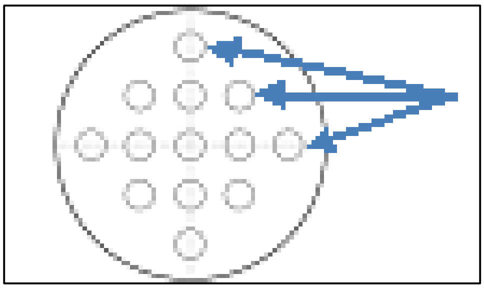


FIGURE 1.6 Radial View of Wires Arrangement in Monolithic Microchannel

1.3 Objectives

This project aims to design a monolithic microchannel that uses wires element as obstructions and support for catalyst that will create greater micromixing dynamics for N_2 and H_2 gases. This project will also identify arrangements along the monolithic microchannel for the wires in order to increase the efficiency of ammonia productions. Results will be processed in forms of chart, contour plots and profiles.

1.4 Scope of Study

This project will focus on the study of flow regime and the characteristics of H_2 and N_2 gases through 30° and 90° wires pitch with different distance of centre between the wires that is parallel to the flow. Number of wires element proposed in the monolithic microchannel are 19 wires for three design and 13 wires for two design respectively. Simulation will be done using ANSYS CFX 15.0 software. Typical methodology in CFD applies such as creation of geometry, development of mesh, and post-solver analysis. Despite the project emphasizes on the 'synthesis of ammonia', only flow dynamics without the reaction element will be simulated. It is desirable to create a micro geometry that will generate a great flow for the mixing.

CHAPTER 2
LITERATURE REVIEW

2.1 Literature Review and Theory

The problem of difficulties to synthesis ammonia on an industrial scale had been solved by German scientists Fritz Haber and Carl Bosch whom discovered new alternative way to convert nonreactive atmospheric nitrogen to ammonia at the early of ninetieth century. Currently, the Haber-Bosch process is used to produce about 100Tg of reactive nitrogen per year worldwide where most of the substances are used for nitrogen fertilizer manufacturing. Food grown with this fertilizer feeds approximately 2 billion people [7]. Haber-Bosch process shown in equation 1 describes the conversion process from nitrogen (N_2) and hydrogen (H_2) gases to ammonia (NH_3).

$$N_2(g) + 3H_2\ (g) \leftrightarrows 2NH_3\ (g) \qquad (1)$$

However, this process involves high pressure and temperature as well as the presence of an iron catalyst which is extensively an energy-consuming process. Iron catalyst such as Fe_3O_4 and Fe_2O_3 in Haber - Bosch process requires high temperatures between 400^{o}C to 500^{o}C for efficient catalyst usage. Ammonia production can be entropically enhanced with elevated gas pressure between 130 and 300 atm [5]. Despite the lower conversion and yield (10-20%), the Haber–Bosch process imposes a costly method to produce ammonia because the pressure of the system has significant economic costs as pressure is an expensive commodity. Besides that, the high temperature in the reactor is occurred due to the highly exothermic energy release from the reaction.

In fact, ammonia production is responsible for about 17% of the energy consumed in the chemical and petrochemical sector. In 2004, the ammonia manufacturing industry consumed 5.6 EJ of fossil fuels, of which 2.7 EJ was for energy and 2.9 EJ for feedstock use [8]. Due to this reason, the reactor is typically an isothermal reactor to ensure that the temperature does not go beyond dangerous level. Since it is operated in high operating conditions, greater safety measurement and control regulation have to be considered while performing this process.

After discovery of the Haber-Bosch process, various processing techniques including conventional and nonconventional have been developed to further improve the conditions which focuses to convert high temperature and pressure to ambient temperature and pressure and process to accommodate certain needs and simplicity of the industry nowadays. One of the alternatives is ammonia synthesis by electrochemical and biological approach. This research designed and tested a bio-electrochemical device that generates NH_3 through electrode induced enzyme catalysis. The ammonia creating device comprises of an electrode modified with a polymer that contains whole cell Anabaena variabilis, a photosynthetic cyanobacterium. A. variabilis contains nitrogenase and nitrate (NO_3^-)/nitrite (NO_2^-) reductase, catalysts for the production of ammonia. In this system, the electrode supplies driving force and generate a reductive microenvironment near cells to facilitate enzymatic production of NH_3 at ambient temperatures and pressures [9]. However, the efficiency of the bioelectrocatalytic device as compared to the efficiency of unaltered cyanobacteria in nature has not been calculated or estimated.

At the same time, more new processes have been developed recently for efficient production of ammonia as the demand of it increases throughout the years. In one particular research, the use of Magnetic Induction Method (MIM) and Helmholtz coils were used to generate the electromagnetic waves [4]. Besides that, MIM has an advantage because it is able to yield high production of Ammonia while operating under ambient conditions where the temperature and pressure is respectively at 25°C and 1atm. This method also uses micro reactors to improve the efficiency of the production.

As the technology in chemicals industries evolve, the usage of micro reactor proven to be more effective than normal size reactors. Micromachining technologies are being applied to the design of miniature devices for chemical synthetic applications such as microreactor. A microreactor is equipment that has microchannel, which in this project is known as monolithic microchannel on the order of micrometers and that enables chemical reactions to be performed in reaction space several orders of magnitude smaller than conventional batch reactor [10]. The downscaling of devices has brought attractive features to microreactors such as equipment installation time has been reduced as well as it higher yields achievement and product quality improvement.

Mixing is hardly achieved in microsystem without modification of geometry. Mixing plays a significant role to increase the conversion of N_2 and H_2 to form NH_3. Mainly the importance is to reduce inhomogeneity that leads to secondary effects such as reaction and change in properties [11, 12]. Furthermore, great flow dynamic is preferred in a channel if intimate mixing is desired between two streams [13].

Thus, one of the main purposes of using this device is the mixing efficiency varies accordingly to the different geometry of wires arrangement. This mixing performance can be explained in equation 2 known as mixing index relationship.

$$t \propto \frac{L^2}{D} \qquad (2)$$

where,

t = diffusion time of molecules

L = square of the channel width

D = diffusion coefficient of a molecule

Thus, following the equation above, t is to proportional to L. To elaborate more, when L is reduced to 1/10, the diffusion time is reduced to 1/100 and the fluids, in this case are hydrogen and nitrogen gasses can be mixed 100 times faster.

Other than that continuous flow in microreactors enables reaction processes to be monitored, controlled, analysed and intermediate storage to be reduced. Hence, the hazards and process safety risks may be reduced since the quantity of substances in the microreactor is much more less. Furthermore, the product profile improvement can be observed and using microreactor also creates constant product output quality [10].

As microreactor provides huge advantages to the output product, numerous researchers are interested to further investigate about microreactor and create variety of studies using different type of fluid flowing in the microchannel as well as using different design characteristic such as serpentine and grooved-based. The researchers explore new parameter that will produce their own findings and output with the different cross section of the microchannel.

TABLE 2.1 Previous Studies on Microchannel in Microreactor

Author	Fluid	Microchannel Design Characteristic	Cross Section Width/ Diameter	Parameter Tested	Findings / Output
Liaw S.Y. (2013), Rosli, M.F. (2012)	Gas	Serpentine	10µm (D)	Number of cycle and pitch height	Optimum mixing at lower pitch and more cyclic.
Fang et al. (2011)	Liquid	"T" inlet + staggered bars mixing unit	200µm (W_i), 300µm (W_o)	Period of mixing unit, 500µm (L) x 500µm (W).	Uniform mixing achieve at greater number of mixing unit.
Zhang et al. (2008)	Liquid	Grooved-based	50µm (W_i)	Different groove depths	Deeper grove depth, better mixing efficiency
Jiang et al. (2001)	Liquid	A deep micro-channel design	0.050 mm (D)	Porous & non-porous microchannel	Better heat transfer for porous channel than non-porous, but higher ΔP observed.

As the project is developed under micro environment, the Reynolds number obtained is low and contributes to laminar flows in the microchannel. Hence, the mixing of the two gasses is controlled by molecular diffusion which means longer time and length of the channel is necessary that leads to high cost and pressure drop [14]. To avoid this from happening, this project signifies the usage of MIM in the development of the monolithic microchannel to obtain efficient and active mixing even at low Reynolds numbers.

2.2 Physical Properties of Nitrogen and Hydrogen

The main components used in this project which are hydrogen gas (H_2) and nitrogen gas (N_2) comprises of different physical properties. By identifying several properties, the Reynolds number for the mixture is determined easily.

TABLE 2.2 Physical Properties of Nitrogen and Hydrogen

Properties	Hydrogen	Nitrogen
Molecular Weight (g/mol)	2.0159	28.02
Density at STP*, ρ (kg/m^3)	0.08988	1.2506
Viscosity at 0^{o}C, μ (cP*)	0.01064	0.016531187

*STP - Standard Temperature and Pressure - is defined as 0^{o}C and 1 atm

*1 cP (Centipoise) = 10^{-3} Pa s

CHAPTER 3
METHODOLOGY

3.1 Simulation Methodology

To proceed with the methodology, the flow of simulation methodology is determined. Fluid Flow (CFX) Design Modeller is used to develop five geometry designs in millimetre unit. Then, the simulation proceeded to mesh generation where the meshing were created with different relevance centre which are fine, medium and coarse via Meshing. In this stage, minimum and maximum size of the meshing is inputted accordingly and nodes, elements and orthogonal quality statistics were ensured not to exceed the limit. The flow properties is set up via CFX-PRE were the inlet, outlet and wall were defined as domain. The value of volume fraction of nitrogen and hydrogen gasses and pressure are constant for all geometry while the velocity of gas flow were differ for 13 wires and 19 wires design. CFX-SOLVER calculated volume fraction, momentum and mass for the geometry using the Navier-Stokes equation. Finally, flow dynamic analysis can be performed in the form of contour plots, profiles and mixing index with the help of CFX-POST.

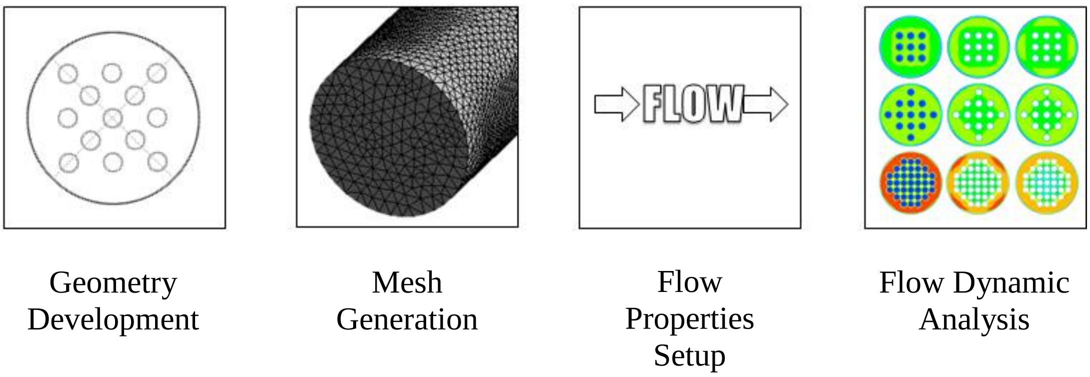


FIGURE 3.1 Flow of Simulation Methodology

3.2 Geometry and Meshing Development

Five designs were developed in this project and the flow dynamics of the nitrogen and hydrogen gasses will be observed and recorded. Basically, the monolithic microchannel will be designed in cylindrical manner where the wires will be arranged according to the wire layout of 30°. Even though it is called 30° triangular pitch, the inner angle for the triangle is 60°. It is also known as equilateral triangle. While one of the geometry design will be in 90° square pitch to compare the result with previous studies. As it is arranged in parallel order, there is no intersection of wires and no change in wires path. The microchannel has a dimension of 10 mm in diameter and the length of the channel has been determined which is 50 mm while the diameters of the wires are 1 mm. The wires assembly started at a distance on 3 mm from the inlet and ended 3 mm before the outlet as a mean to induce pre-mixing upon flowing inside.mm length located at the centre of microchannel which are constant for all five design. The wires are arranged parallel to the microchannel with different distance between the centres of the wires, different number of wires and different pitch aimed to create higher mixing efficiency.

An initial velocity before facing the obstacles is expected to result in better dynamic mixing. In order to calculate velocity of the flow stream with respect to 1s, these parameters is determined in advance:

1. Volume of empty microchannel
2. Volume of wires
3. Cross section area of flow stream
4. Number of wires

TABLE 3.1 Velocity Determination

Parameters	Equation
Volume of empty microchannel	$V_{microchannel} = \frac{\pi D^2}{4} \times h$ $V_{microchannel} = \frac{\pi(10mm)^2}{4} \times 50mm$ $\boldsymbol{V_{microchannel} = 3926.991mm^3}$
Volume of wires	$V_{wires} = \frac{\pi D^2}{4} \times h \times Number\ of\ Wires$ $V_{19\,wires} = \frac{\pi(1mm)^2}{4} \times 44mm \times 19$ $\boldsymbol{V_{19wires} = 656.593mm^3}$ $V_{13\,wires} = \frac{\pi(1mm)^2}{4} \times 44mm \times 13$ $\boldsymbol{V_{13wires} = 449.248mm^3}$
Cross section area of flow stream	$A = \frac{\pi D_{microchannel}^2}{4} - \left(\frac{\pi D_{wires}^2}{4} \times Number\ of\ Wires\right)$ $A_{19\,wires} = \frac{\pi(10mm)^2}{4} - \left(\frac{\pi(1mm)^2}{4} \times 19\right)$ $\boldsymbol{A_{19\,wires} = 63.617mm^2}$ $A_{13\,wires} = \frac{\pi(10mm)^2}{4} - \left(\frac{\pi(1mm)^2}{4} \times 13\right)$ $\boldsymbol{A_{13\,wires} = 68.330mm^2}$
Velocity w.r.t to 1s	$Velo = \frac{V_{microchannel} - V_{wires}}{A}$ $Velo_{19\,wires} = \frac{3926.991mm^3 - 656.593mm^3}{63.617mm^2}$ $\boldsymbol{Velo_{19\,wires} = 51.408\frac{mm}{s} = 0.05\frac{m}{s}}$ $Velo_{13\,wires} = \frac{3926.991mm^3 - 449.248mm^3}{68.330mm^2}$ $\boldsymbol{Velo_{13\,wires} = 50.896\frac{mm}{s} = 0.05\frac{m}{s}}$

Table 3.2 illustrated the dimensional characteristics of the monolithic microchannel with the embedded wires. The types of wires configured in the radial direction (XY-axis) for Design 1, 2, 3, 4 and 5.

TABLE 3.2 Geometry of Monolithic Microchannels

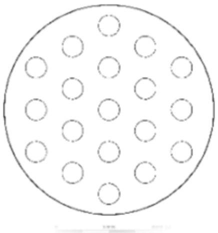
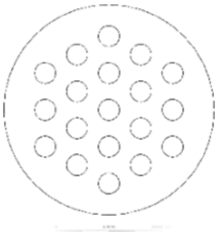
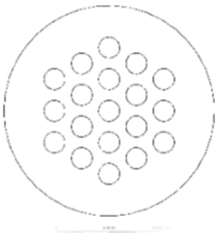
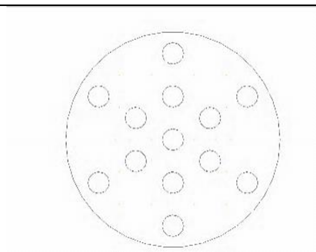
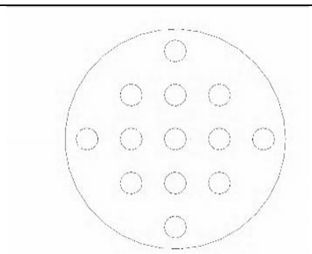
Design	Characteristics	XY-Axis View (Radial)
1	Number of wires: 19	
	Distance: 2 mm	
	Pitch: 30^0	
2	Number of wires: 19	
	Distance: 1.75 mm	
	Pitch: 30^0	
3	Number of wires: 19	
	Distance: 1.5 mm	
	Pitch: 30^0	
4	Number of wires: 13	
	Distance: 2 mm	
	Pitch: 30^0	
5	Number of wires: 13	
	Distance: 2 mm	
	Pitch: 90^0	

Figure 3.2 displayed the location of plane 1, 2, 3 and 4 along the monolithic microchannel which are similar for all five designs. Plane 1, 2, 3 and 4 are located at Z-axis where the position are 5.56 mm, 16.67 mm, 27.78 mm and 38.89 mm from the inlet respectively

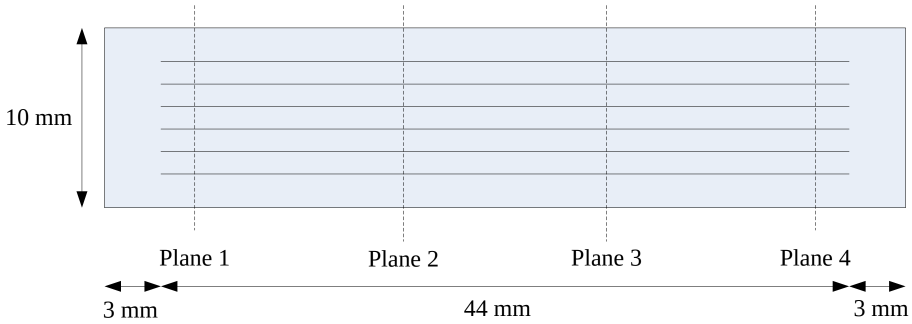


FIGURE 3.2 Location of Planes

The mesh properties for geometry 1 were set up to fine, coarse and medium. According to the orthogonal factor, mixing index and time taken to run the program, coarse mesh was selected to be the relevance centre for all design were the mixing is more dynamic and steady as shown in Figure 3.3.

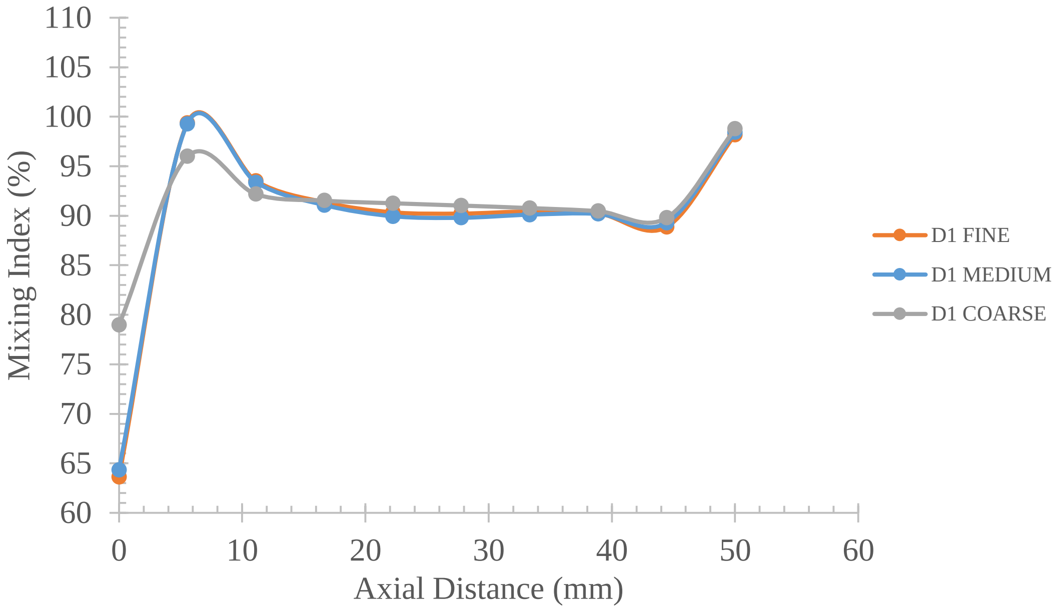


FIGURE 3.3 Mixing Index of Design 1 for Fine, Medium and Coarse Meshing

3.3 Physics Properties Setup

Once the geometry designs for the five configurations are accomplished, several pre-setup inputs are required by ANSYS before stimulating the design. The meshing parameters were selected so that the nodes are less than 512,000 due to license limitations. The simulation will have the inputs of hydrogen and nitrogen gases at a ratio of 3 atoms of hydrogen gas to 1 atom of hydrogen gas. The gas inlet velocity is the same for all type of design. . K-epsilon (k-ε) turbulence model is used in this simulation as it is the most common model used in Computational Fluid Dynamics (CFD) to simulate mean flow characteristics for turbulent flow conditions. This project will not consider any magnetic induction in the simulation. The physics are listed in the Table 3.3.

TABLE 3.3 Flow Parameters Setup

Parameter	Flow Properties
Gas Inlet Velocity	0.05 m/s
Gas Inlet Ratio	$H_2 : N_2 = 3 : 1$
Volume Fraction	$H_2 : N_2 = 0.75 : 0.25$
Temperature	25^0C
Pressure	1 atm
Heat Transfer Model	Isothermal
Buoyancy Model	Non-buoyant
Fluid Morphology	Continuous Fluids Model
Turbulence Model	K-Epsilon
Simulation Mode	Steady State
System Reactivity	Non-reactive System

3.4 Methodology Analysis

The analysis of the flow dynamics was based upon the volume fraction and velocity contour plots for each gasses selected at four plane at different axial location (YZ-axis). However the effect of magnetic induction field and reaction were not considered in this project. Other than that, to identify the mixing efficiency of each design, the Reynolds number need to be determined using equation 3.

$$Re = \frac{\rho V D}{\mu} \qquad (3)$$

where,

ρ = density (kg/m^3)

V = velocity (m/s)

D = diameter of cylinder (m)

μ = fluid viscosity (kg/ms)

Generally, this equation uses the overall diameter of the cylinder to obtain the Reynolds number. However, this may not be suitable to this research as the project intention is to insert wires as obstacles in the monolithic microchannel. Thus, modification of equation is necessary to obtain the accurate project result. The density of mixture can be calculated based on equation 4.

$$\rho_{mix} = \frac{\rho_1 V_1 + \rho_2 V_2 + \cdots + \rho_n V_n}{V_1 + V_2 + \cdots + V_n} \qquad (4)$$

where,

n = number of chemical species

ρ_n = density of each of the component (kg/m^3)

V_n = volume of each component

Next step is the modification of the viscosity of the mixture using equation 5 and 6.

$$\mu_{mix} = \sum_{i=1}^{n} \frac{x_i u_i}{\sum_{j=1}^{n} x_j \varphi_{ij}} \qquad (5)$$

$$\varphi_{ij} = \frac{1}{\sqrt{8}}\left(1 + \frac{M_i}{M_j}\right)^{-\frac{1}{2}}\left(1 + \left(\frac{\mu_i}{\mu_j}\right)^{\frac{1}{2}}\left(\frac{M_j}{M_i}\right)^{\frac{1}{4}}\right)^{2} \qquad (6)$$

where,

n = number of chemical species

x_i, x_j = mole fractions of two species

μ_i, μ_j = viscosities of two species at specified temperature

M_i, M_j = molecular weight of two species in g/mol

The diameter represented in the Reynolds number equation earlier is the hydraulic diameter which means diameter for a circular tube or wire. The diameter is calculated via equation 7.

$$D_H = \frac{4A}{P} \qquad (7)$$

where,

A = subtraction of cross sectional area and total area of void area (m^2)

P = wetted perimeter area (m)

After considering all equation that has been modified due to the project's aim, the new Reynolds number equation is formed as equation 8.

$$Re = \frac{\rho_{mix} V D_H}{\mu_{mix}} \qquad (8)$$

where,

ρ_{mix} = density of mixture (kg/m^3)

V = velocity (m/s)

D_H = hydraulic diameter (m)

μ_{mix} = viscosity of the mixture (kg/ms)

In order to quantify the mixing efficiency, data from CFD simulation is extracted from the location of each line that have been constructed in the monolithic microchannel. From the 40 lines, 10 samples are taken from each line that denoted as volume fraction of hydrogen are used to calculate the mixing index. Then, based on the points taken, mixing index graph will be created using equation 9 and 10.

$$\gamma = \sqrt{\frac{1}{N}\sum(C_i - \overline{C_m})^2} \qquad (9)$$

where,

γ = variance

C_i = volume fraction at points/nodes i

C_m = optimal mixing volume fraction

N = number of points/nodes

$$M = 1 - \sqrt{\frac{\gamma^2}{\gamma_{max}^2}} \qquad (10)$$

where,

M = mixing index

γ^2 = maximum variance

CHAPTER 4
RESULTS AND DISCUSSION

4.1 Results

The volume fraction and velocity of both nitrogen and hydrogen gases are extracted from the simulation in the form of contour plots in radial and axial manner. Each radial arrangement consists of four planes which are measured equally to observe the mixing of both gasses. Mixing index for each geometry are calculated and presented in line chart to show which geometry create greater mixing to produce ammonia. The range of velocity profile is standardized from 0 ms^{-1} until 0.09 ms^{-1} and the range for volume fraction from 0 to 1. The results are taken from Post-CFX.

The results obtained are:

1. Velocity Contours for Nitrogen Flow in XY-axis
2. Velocity Contours for Hydrogen Flow in XY-axis
3. Volume Fraction Contours for Nitrogen Flow
4. Volume Fraction Contours for Hydrogen Flow
5. Velocity Contours at Centreline in YZ-axis
6. Streamline Velocity of Nitrogen and Hydrogen
7. Mixing Index Line Chart

4.2 Discussion

Based on the results obtained from the simulation, effect of distance between centre of wires, effect of number of wires and effect of wire pitch are investigated. Design 1, 2 and 3 comprises the same geometry with different distance between centres of wires of 2 mm, 1.75 mm and 1.5 mm. Design 1 and 4 is studied with different number of wires, 19 wires and 13 wires respectively. For Design 4 and 5 different type of wire pitch is arranged for 30^{o} triangle pitch and 90^{o} square pitch.

Tables 4.1. 4.2, 4.7, 4.8, 4.13 and 4.14 indicating the velocity contours of nitrogen and hydrogen gases at four different planes created along the monolithic microchannel with different configuration of wires element accordingly. An active dynamic mixing was expected if the tone of the contour for both gases achieve similarities based on the set velocity which is shown at the legend on the right side of the tables.

On the other hand, volume fractions for nitrogen and hydrogen gases are presented in table 4.3, 4.4, 4.9, 4.10, 4.15 and 4.16 respectively. Since synthesizing ammonia requires 1 mole of nitrogen and 3 mole of hydrogen, the fraction of the gases should be in the ratio of 0.25:0.75. Therefore, lesser or higher fraction of the gases will result to lower the yield of ammonia when the actual reaction occurs in the microchannel [15].

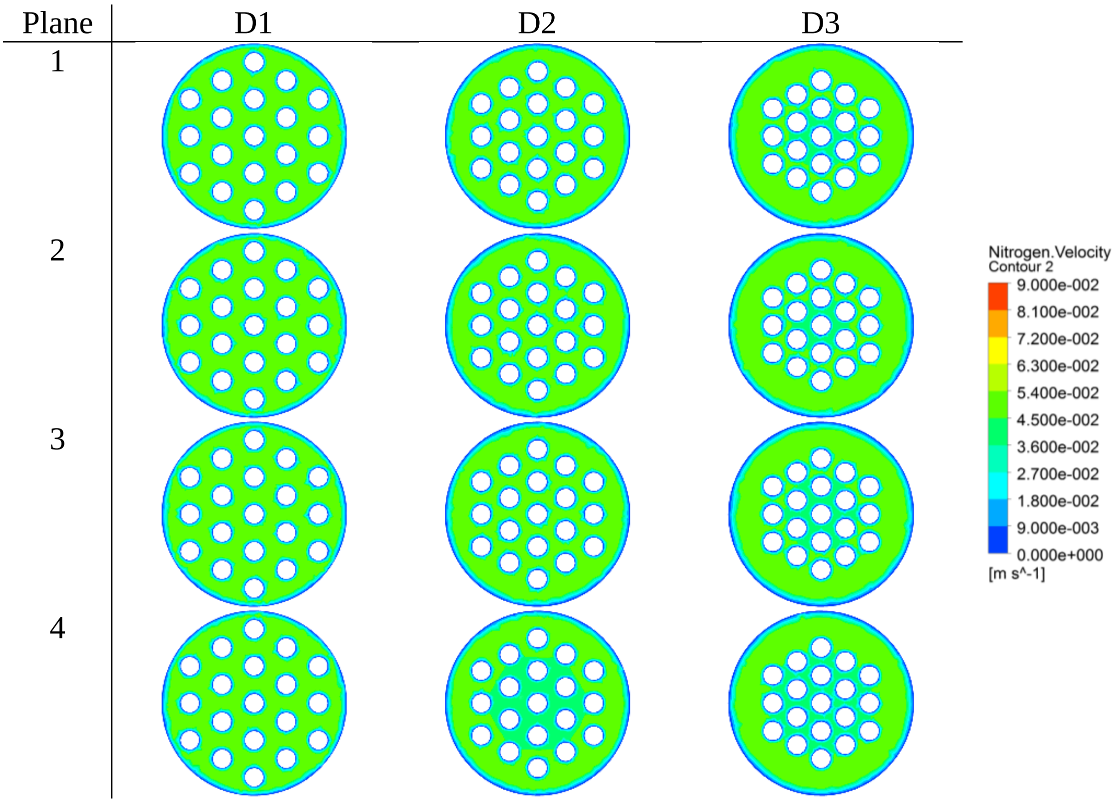
Velocity of nitrogen and hydrogen can be visualize in an altered angle in Tables 4.5, 4.11 and 4.17 where the contour is obtained at the point Z = 0 on YZ-axis, showing the radial centreline of the movement for both gases. Similar hue of contour for nitrogen and hydrogen contours along the microchannel indicating good mixing among the gases. When a good mixing occurred, the velocity streamline shown in Tables 4.6, 4.12, 4.18 provide better characterization of the gases flowing downstream.

Mixing Index plotted in Figure 4.1 will become the last reference to acknowledged which design provide better mixing based on the parameter of volume fraction and velocity contours at ten different axial distance distributed evenly throughout the monolithic microchannel.

4.2.1 Effect of Distance between Centres of Wires

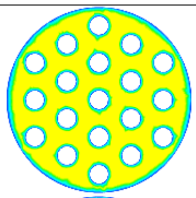
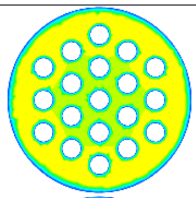
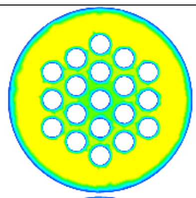
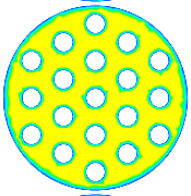
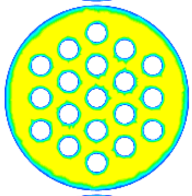
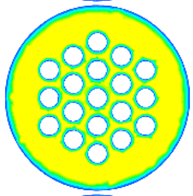
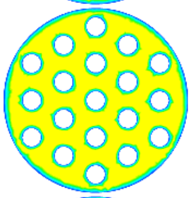
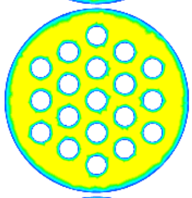
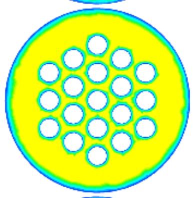
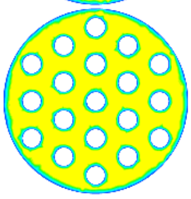
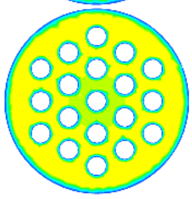
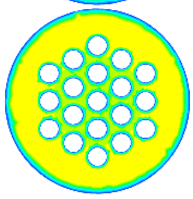
According to the XY-axis velocity contour for nitrogen gas, from Design 1, 2 and 3, Design 1 having the most stable velocity while Design 2 and 3 shows inconsistent velocity at the centre of the channel as the arrangement of the wires as closely packed at that position providing less space for mixing and the velocity become less than the set velocity.

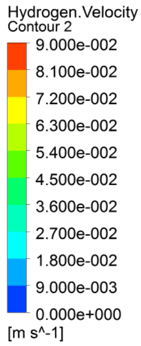
TABLE 4.1 Velocity Contour for Nitrogen Flow



For velocity contour of Design 1, the hydrogen gas moves at faster speed between 0.063 ms^{-1} and 0.072 ms^{-1} throughout the channel while Design 2 and 3 having lower velocity of hydrogen at the centre of microchannel than at the wall at Plane 1 and 4 around 0.06 ms^{-1} which lead to non-homogeneous mixing.

TABLE 4.2 Velocity Contour for Hydrogen Flow

Plane	D1	D2	D3
1			
2			
3			
4			



For the volume fraction results, Design 1, 2 and 3 are not able to produce consistent volume fraction of nitrogen and hydrogen ratio, 3:1 except at plane 1.

TABLE 4.3 Volume Fraction Contour for Nitrogen Flow

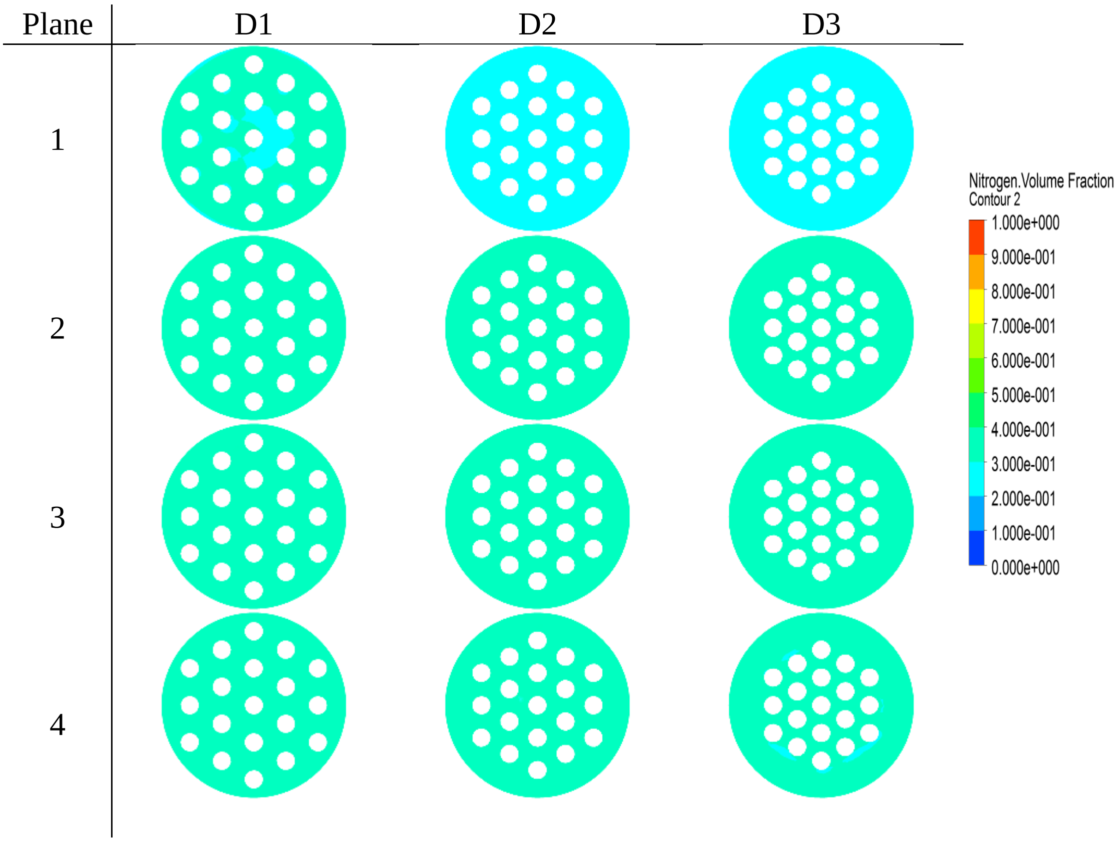
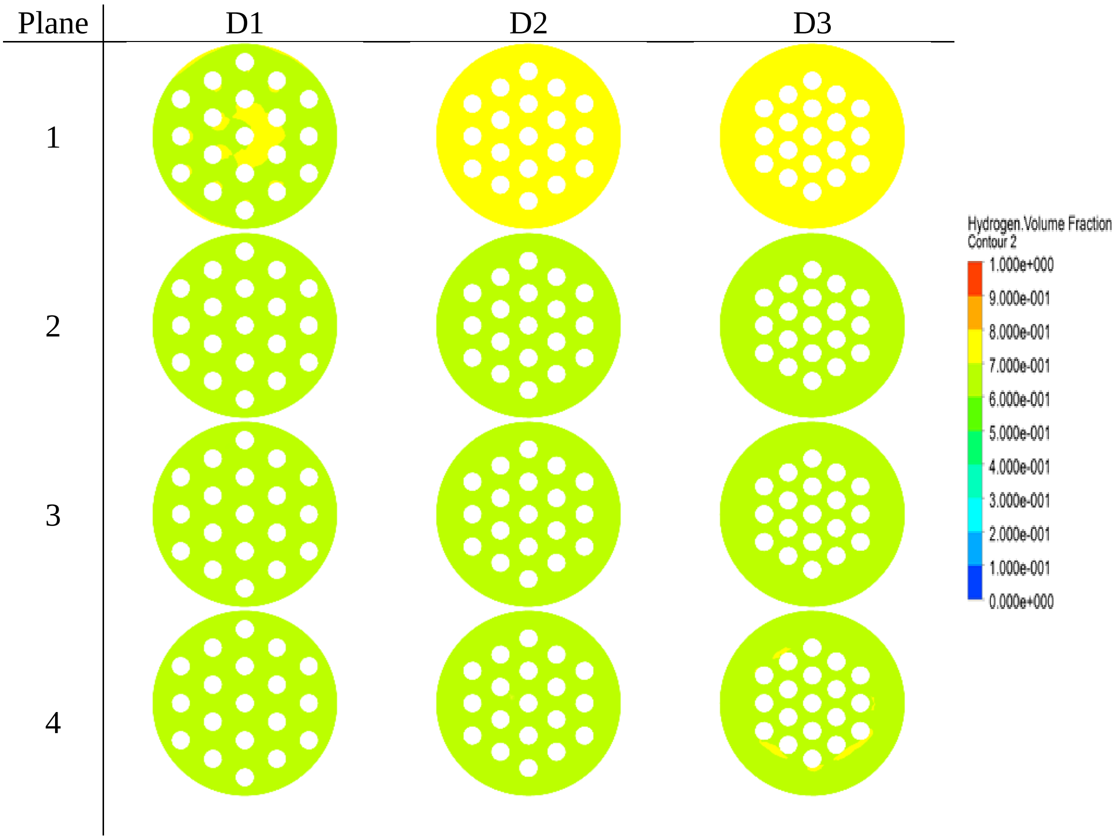
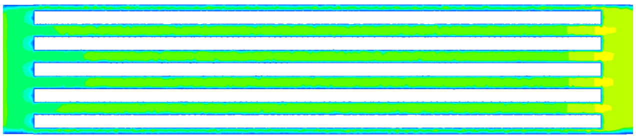
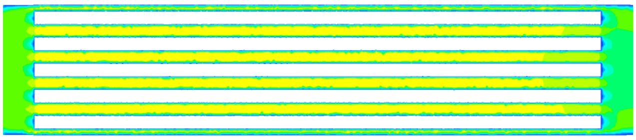
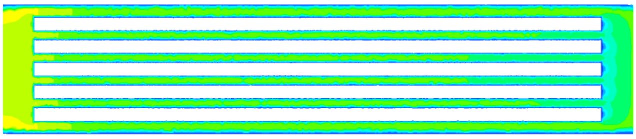
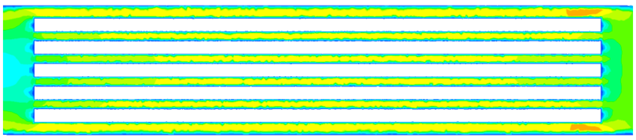
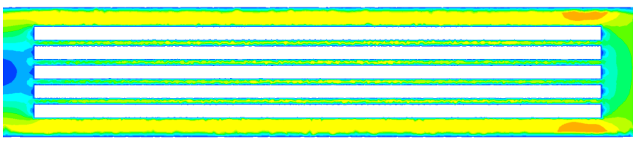


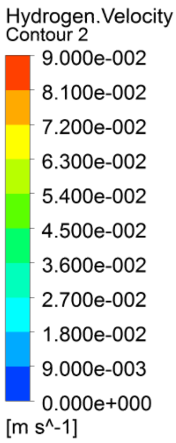
TABLE 4.4 Volume Fraction Contour for Hydrogen Flow



From the velocity contours at centreline in YZ-axis, Design 1 is seen to have constant velocity of nitrogen while the hydrogen possesses higher velocity than the set velocity. For Design 2 and 3, velocity of hydrogen gas is higher at the outlet of the channel.

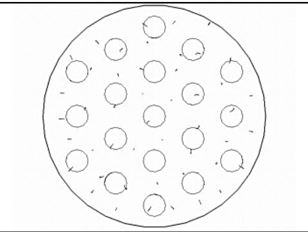
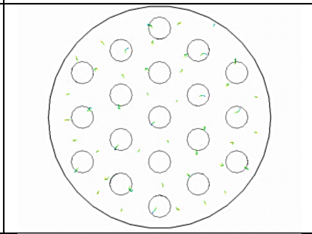
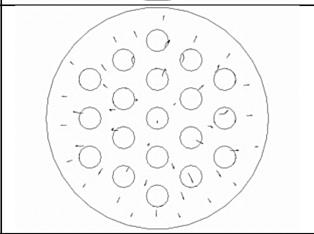
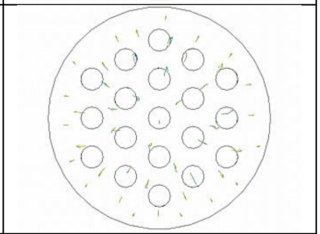
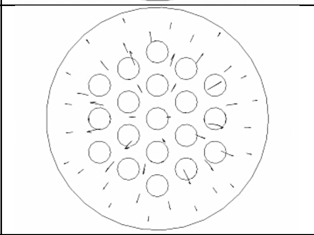
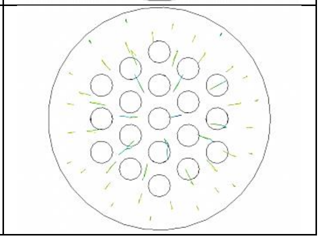
TABLE 4.5 Velocity Contours at Centerline

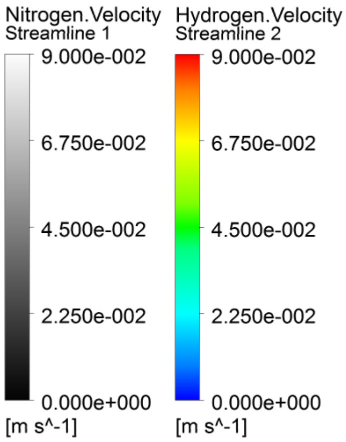
D1	N_2	
	H_2	
D2	N_2	
	H_2	
D3	N_2	
	H_2	



Observing the velocity streamline of both gasses, Design 3 presented higher literal shift of gasses which mean more chaotic advection occur in this design compare to Design 1 and 2. Unfortunately, the advection only occurs at the centre of the microchannel and not producing an even mixing.

TABLE 4.6 Streamline Velocity of Nitrogen and Hydrogen

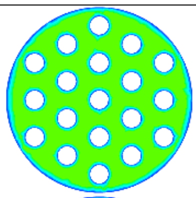
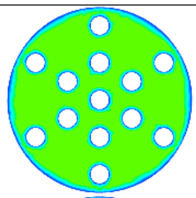
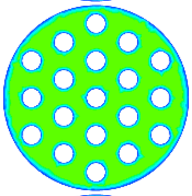
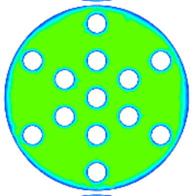
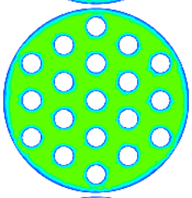
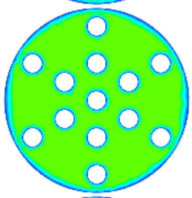
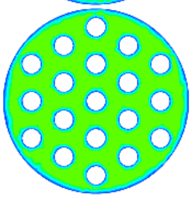
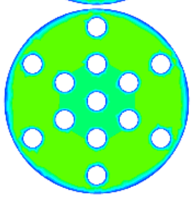
Design	N_2	H_2
1		
2		
3		



4.2.2 Effect of Number of Wires

From the results presented, Design 4 is having more uniform velocity of nitrogen and hydrogen at 0.05 ms^{-1} while Design 1 possess velocity of hydrogen flow approximately at 0.065 ms^{-1} which is higher than the set velocity. Since the velocity of nitrogen and hydrogen for Design 4 is nearly similar, it will lead to more uniform mixing.

TABLE 4.7 Velocity Contour for Nitrogen Flow

Plane	D1	D4
1		
2		
3		
4		

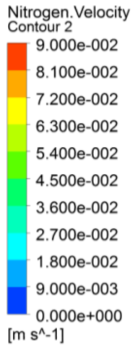
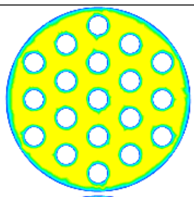
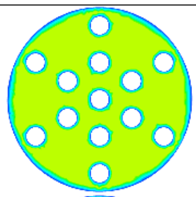
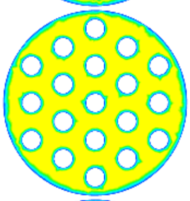
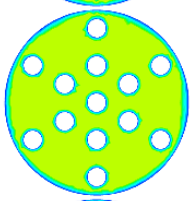
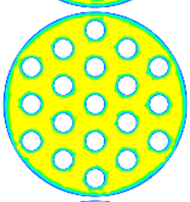
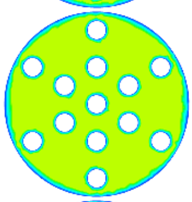
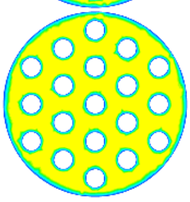
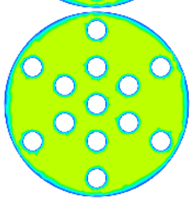
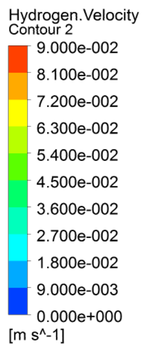


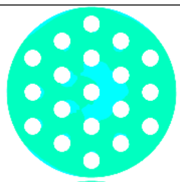
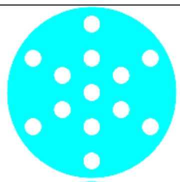
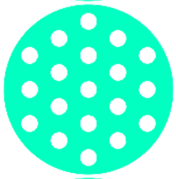
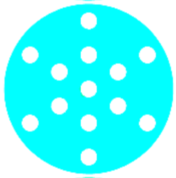
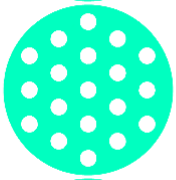
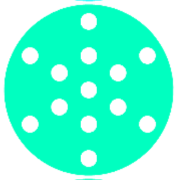
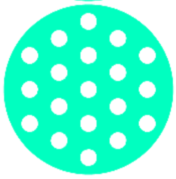
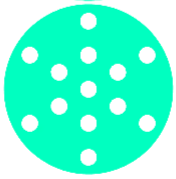
TABLE 4.8 Velocity Contour for Hydrogen Flow

Plane	D1	D4
1		
2		
3		
4		



Other than that, Plane 1 and 2 in Design 4 showed suitable volume fraction for nitrogen and hydrogen gasses which is 0.25:0.75 compare to Design 1 where only at Plane 1 it achieve the appropriate volume fraction.

TABLE 4.9 Volume Fraction Contour for Nitrogen Flow

Plane	D1	D4
1		
2		
3		
4		

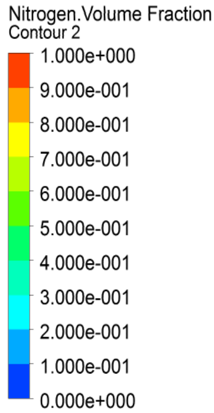
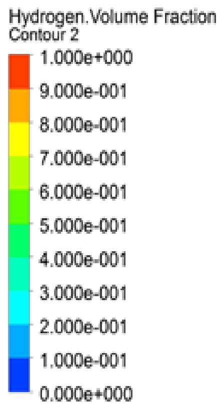


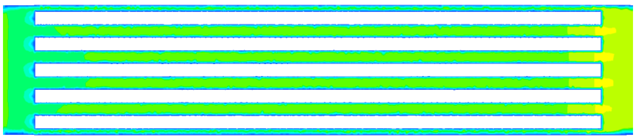
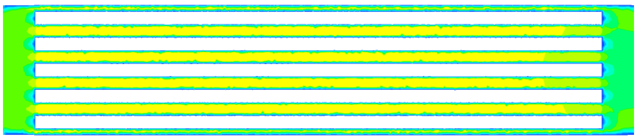
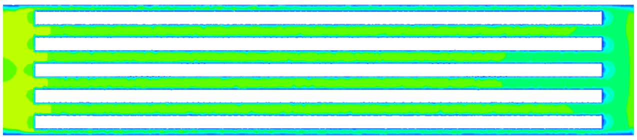
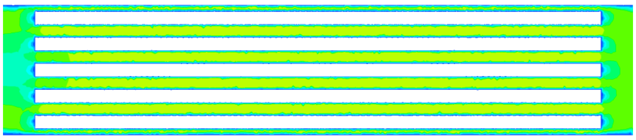
TABLE 4.10 Volume Fraction Contour for Hydrogen Flow

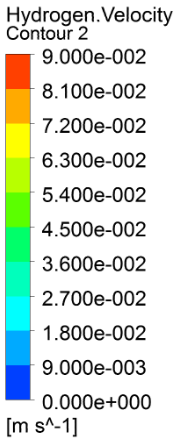
Plane	D1	D4
1		
2		
3		
4		



Based on the velocity contours at centreline in YZ-axis nitrogen and hydrogen gasses achieve similar velocity where an active mixing may occur along the channel.

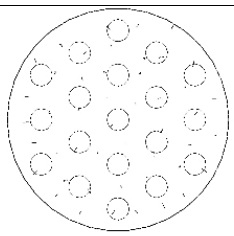
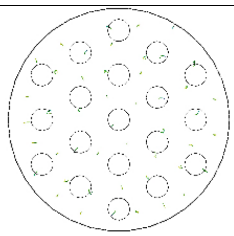
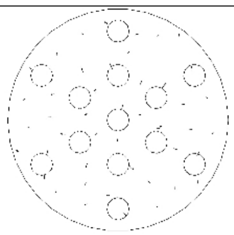
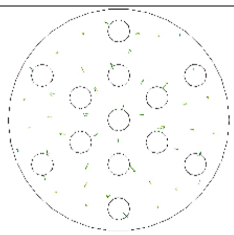
TABLE 4.11 Velocity Contours at Centerline

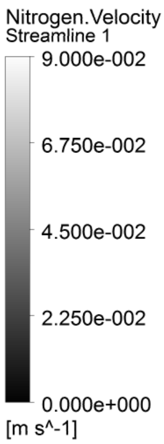
D1	N_2	
	H_2	
D4	N_2	
	H_2	

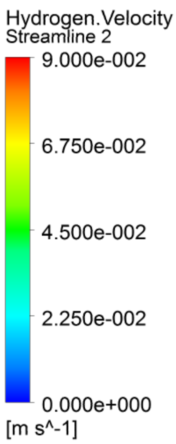


The velocity streamline for Design 1 and 4 illustrated similar shifting of gasses because the distance between centres of wires is the same for both geometries.

TABLE 4.12 Streamline Velocity of Nitrogen and Hydrogen

Design	N_2	H_2
1		
4		

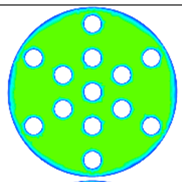
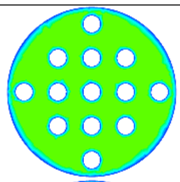
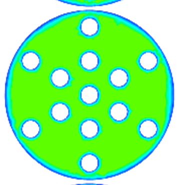
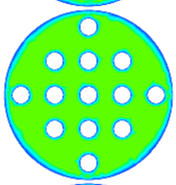
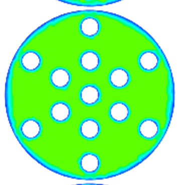
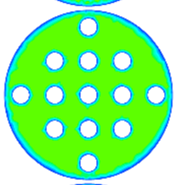
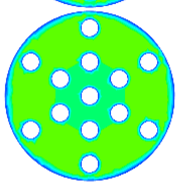
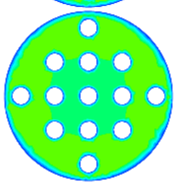




4.2.3 Effect of Wire Pitch

The velocity contour for Design 5 showed dissimilar velocity of nitrogen and hydrogen gasses at Plane 4 while Design 4 is having velocity that is constant throughout the monolithic microchannel.

TABLE 4.13 Velocity Contour for Nitrogen Flow

Plane	D4	D5
1		
2		
3		
4		

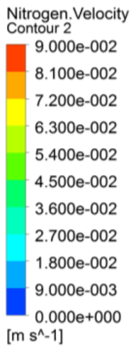
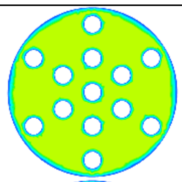
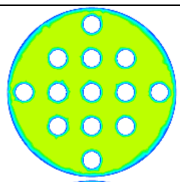
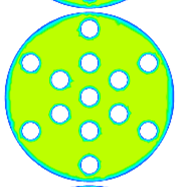
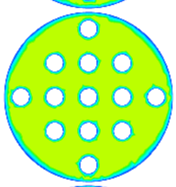
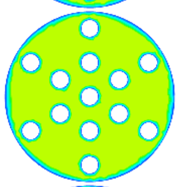
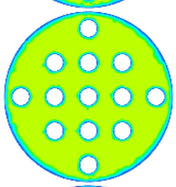
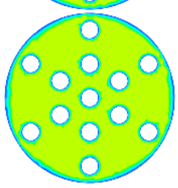
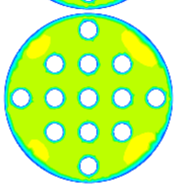
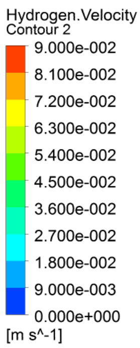


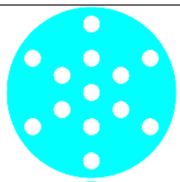
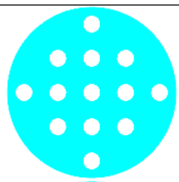
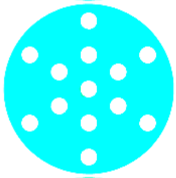
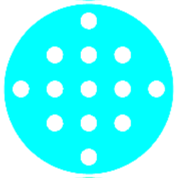
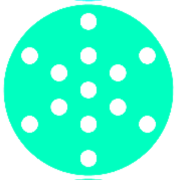
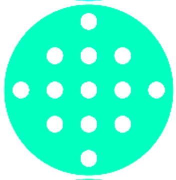
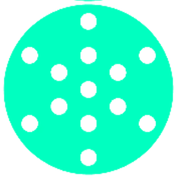
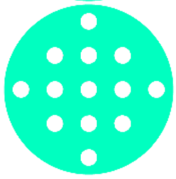
TABLE 4.14 Velocity Contour for Hydrogen Flow

Plane	D4	D5
1		
2		
3		
4		



However, this unlike wire pitch presented similar contours for volume fraction of hydrogen and nitrogen for Design 5 and Design 4.

TABLE 4.15 Volume Fraction Contour for Nitrogen Flow

Plane	D4	D5
1		
2		
3		
4		

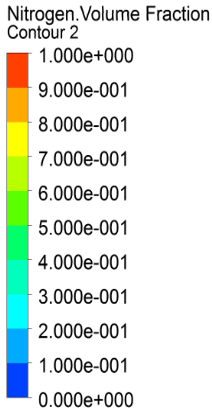
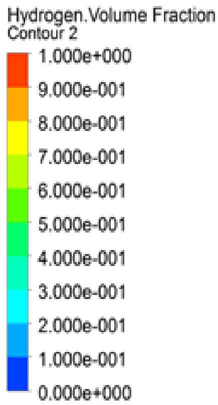


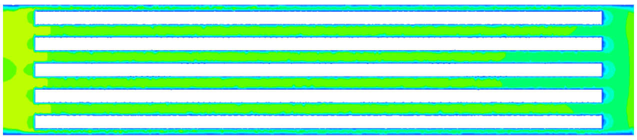
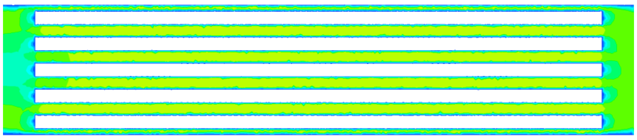
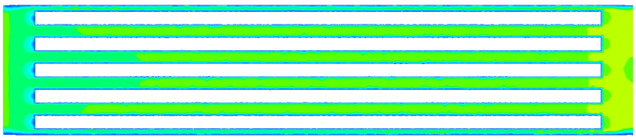
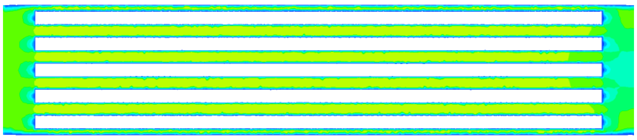
TABLE 4.16 Volume Fraction Contour for Hydrogen Flow

Plane	D4	D5
1		
2		
3		
4		



The velocity contours at centerline and streamline of hydrogen and nitrogen gasses producing alike readings for Design 4 and 5 where good mixing is achieved for both designs.

TABLE 4.17 Velocity Contours at Centerline

D4	N_2	
	H_2	
D5	N_2	
	H_2	

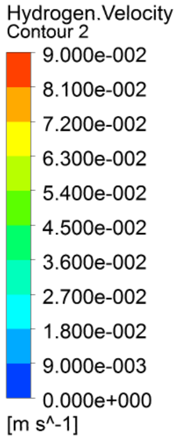
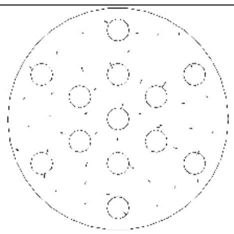
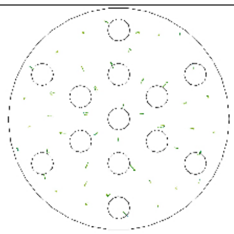
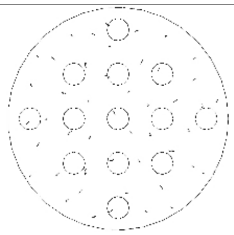
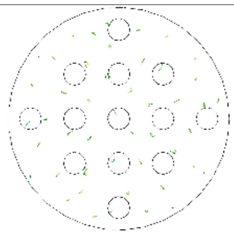
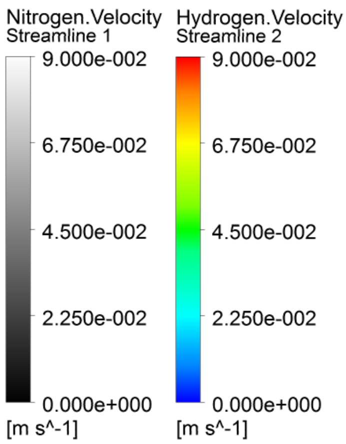


TABLE 4.18 Streamline Velocity of Nitrogen and Hydrogen

Design	N_2	H_2
4		
5		



According to Figure 4.1 mixing index of Design 1 is observed to be higher compare to Design 2 and 3. Therefore, Design 4 and 5 are created using 2 mm as the distance of centres between wires same as Design 1 as the results produce good convergence among the three designs.

The graph illustrated that Design 4 achieved greater dynamic mixing than Design 1. In this point of view, we can conclude that lower number of wires, 13 contributes to better mixing efficiency than 19 wires.

However, based on the mixing index calculation, it is indicated that Design 4 provided better mixing compare to Design 5 when the arrangement is in triangle pitch form.

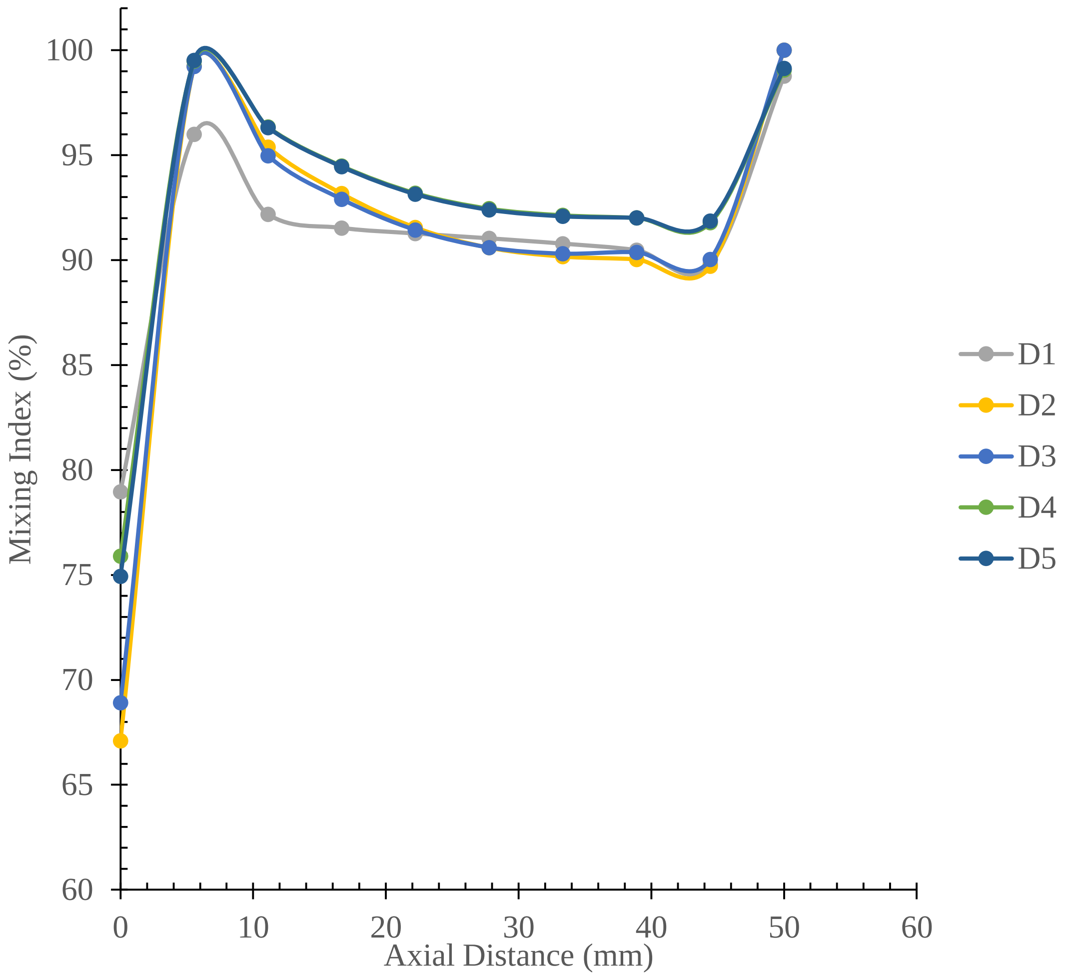


FIGURE 4.1 Mixing Index of Geometries

CHAPTER 5
CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

Among the five geometries, Design 4 showed the best mixing result with uniform speed and volume fraction and high mixing index throughout the monolithic microchannel. The hydrogen and nitrogen gasses are distributed uniformly along the monolithic microchannel.

Dynamic mixing was successfully induced when appropriate properties of parameters were used in this project. When the wires are configured in a different manner, the simulation presented different mixing index and contours accordingly. By placing obstructions to the flow, chaotic advection occurs and the flow direction of the gas stream altered laterally [16].

It is proven that creating suitable obstruction with larger obstruction space enhanced the mixing and rate of reaction between hydrogen and nitrogen gasses to synthesis ammonia [17]. Therefore the objectives of this project are achieved successfully with the appropriate methods that have been used.

5.2 Recommendation

1. More detail study need to be conduct to correct the minimum and maximum size of meshing to produce more accurate result.

2. The design parameters can be studied thoroughly to enable better understanding on the effect of design parameters on flow of hydrogen and nitrogen gasses to yield ammonia.

3. More design can be produced that can provide an active mixing and turbulent flow regime in the hydrogen and nitrogen stream.

4. The type of obstruction in the monolithic microchannel also can be improvised to provide suitable space and time for mixing of the two gasses to occur.

5. Mathematical model can be developed in order to obtain a better picture of mixing process for hydrogen and nitrogen gases.

6. Besides, MIM can be applied to the best design created in order to prove the simulation result.

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APPENDICES

Table 6.1 Data of Design 1 for Mixing Index

Axial Distance	Mixing Index
0.00000	78.9620060
5.5555552	95.9872818
11.11111	92.1833706
16.6666652	91.5314049
22.2222204	91.2658523
27.7777756	91.0343305
33.3333309	90.7812707
38.8888879	90.4684746
44.4444432	89.8007017
49.9999984	98.7723088

Table 6.2 Data of Design 2 for Mixing Index

Axial Distance	Mixing Index
0.00000	67.0952428
5.5555552	99.2441104
11.11111	95.3897065
16.6666652	93.1666549
22.2222204	91.5483739
27.7777756	90.5900886
33.3333309	90.1683140
38.8888879	90.0331906
44.4444432	89.7033729
49.9999984	99.9999930

Table 6.3 Data of Design 3 for Mixing Index

Axial Distance	Mixing Index
0.00000	68.9068508
5.5555552	99.2200559
11.11111	94.9773916
16.6666652	92.9035451
22.2222204	91.4346443
27.7777756	90.5977994
33.3333309	90.3054150
38.8888879	90.3734315
44.4444432	90.0264452
49.9999984	99.9999966

Table 6.4 Data of Design 4 for Mixing Index

Axial Distance	Mixing Index
0.00000	75.8977890
5.5555552	99.4816973
11.11111	96.3385958
16.6666652	94.4869045
22.2222204	93.1908758
27.7777756	92.4509036
33.3333309	92.1368027
38.8888879	92.0128499
44.4444432	91.7832820
49.9999984	99.0574372

Table 6.5 Data of Design 5 for Mixing Index

Axial Distance	Mixing Index
0.00000	74.9405229
5.5555552	99.5154150
11.11111	96.3094125
16.6666652	94.4473237
22.2222204	93.1400963
27.7777756	92.3942163
33.3333309	92.0826618
38.8888879	92.0101235
44.4444432	91.8532044
49.9999984	99.1283896

Table 6.6 Data of Design 1 with Fine Mesh for Mixing Index

Axial Distance	Mixing Index
0.00000	63.6098880
5.5555552	99.3567387
11.11111	93.5021581
16.6666652	91.3523257
22.2222204	90.3370678
27.7777756	90.2076187
33.3333309	90.4180149
38.8888879	90.2229702
44.4444432	88.8628677
49.9999984	98.1823015

Table 6.7 Data of Design 1 with Medium Mesh for Mixing Index

Axial Distance	Mixing Index
0.00000	64.3333161
5.5555552	99.2710670
11.11111	93.3655383
16.6666652	91.0669005
22.2222204	89.9402122
27.7777756	89.7814673
33.3333309	90.0970223
38.8888879	90.1730210
44.4444432	89.2843898
49.9999984	98.4279116