Dissertation Report

Study of the Flow Dynamics of Nitrogen and Hydrogen Gases in a Monolithic Microchannel.

by

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14923

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

May 2014

Universiti Teknologi PETRONAS
32610 Bandar Seri Iskandar
Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

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A project dissertation submitted to the

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(CHEMICAL)

Approved by,

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(Dr. Mohd Zamri Abdullah)

UNIVERSITI TEKNOLOGI PETRONAS

32610 BANDAR SERI ISKANDAR, PERAK

MAY 2015

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.

TAN LOO SEN, 14923

CHEMICAL ENGINEERING,

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ABSTRACT

A technological breakthrough allowed the production of Ammonia to be synthesize in ambient conditions. This method is called Magnetic Induction Method (MIM) where induced magnetic fields polarizes the hydrogen and nitrogen gases to the wires covered with catalysts to allow the synthesis of ammonia. This synthesis method however is done in microfluidic environments where micro mixing may not be favorable due to micro dimensions. In order to enhance the yield of Ammonia via this method, a better design of microreactor needs to be developed. Micromixing efficiency needs to be enhanced to improve the rate of reaction. Hence, this research is conducted to develop a microreactor that utilizes the wires arrangement in the microreactor to create chaotic advection that will induce greater mixing efficiency. These wires will be placed in the monolithic Microchannel acting as longitudinal vortex generators (LVG) that creates chaotic advection to the flow of the gases. This fluidic chaotic advection will then cause the mixing of gases to be increased. This theory was proven at the end of this project where three designs that incorporated wires as LVGs successfully created disruption in gases' velocities and change in Reynolds number as the fluid progresses through the whole channel. It was then deemed that Geometry Design 2 and 3 are more suitable for micromixing as the velocity variation are equally distributed along the channel. The development and design of the microreactor is done via a computational fluid dynamics (CFD) approach using the software ANSYS coupled with CFX module.

ACKNOWLEDGEMENT

I would to express my deepest gratitude to Universiti Teknologi PETRONAS (UTP) for providing me the platform and facilities for my education and for this project. Without that support this project would not have been successful and brought me invaluable experience.

I would like to express my appreciation to OneBAJA as this project was supported by it. OneBAJA is a long term grant scheme by Ministry of Education led by UTP's very own professors and researchers. OneBAJA has allowed me to gain experiences from various instances like the 4^{th} OneBAJA Colloquium where I was one of the presenters. That experience has been wonderful and an eye-opening one.

Besides that, I would like to thank Dr. Zamri Abdullah who is my supervisor since Structured Internship Training (SIT) and Structured Internship Project (SIP). From there he offered me to continue to be his student for the Final Year Project (FYP) where he asked me to conduct more Computational Fluid Dynamics projects which I have a deep interest in it. Without the opportunity given by Dr. Zamri, I would have not embarked on this project that is involved in the OneBAJA project.

I would like to thank my family and friends for the support and the fun times while conducting this project. Their emotional and knowledge support have proven to be a driving factor in the development of this project. I treasure the knowledge and motivation dearly to my heart.

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CHAPTER 1
INTRODUCTION

1.1 Background

Synthetic fertilizers are produced commonly from ammonia through a process named Haber - Bosch. The process uses hydrogen and nitrogen gases as raw materials to produce ammonia which will subsequently use to develop ammonia (Murzin, D. Y., 2013). This process is usually accompanied by an iron catalyst (can be accompanied by other oxides) and usually operates under a high operating condition where such conditions poses safety risks to the operators and the plant facilities. An example of such incidents is the Texas Fertilizer Plant explosion where 5 to 15 casualties were reported (Than, 2013). The high operating temperature and pressure also consumes a lot of energy. The Haber-Bosch process uses up to 1% of the world's energy per year. In order to reduce the hazard and the energy consumption of ammonia production, researches have been made to discover new ways of producing ammonia. An example of such research is using MIM (Yahya & et al., 2010). This synthesis using MIM allows the production of ammonia in ambient conditions therefore reducing the risk and improved energy saving. Microfluidics were considered in this research to improve the efficiency of the production by exposing the raw materials to a higher surface area and micromixing efficiency. Combining MIM and microfluidics, the research discovered that the conversion and yield of the process was much higher than to the conventional Haber-Bosch process (Yahya et al., 2010). This research will employ microfluidics to design a microreactor which enhances the micromixing of the raw materials. This project will study the effects of various geometries on the flowpath and mixing of the gases.

1.2 Problem Statement

The presence of catalyst inside a microchannel will assist the synthesis of ammonia through the reaction of N_2 and H_2 gases. As the flow inside a micro channel is typically in laminar regime due to the microchannel size, the reaction rate could be increased by inducing mixing in a microfluidic environment that will enhance collision between the two gases (Nguyen & Wu, 2005). One method to generate micromixing is by altering the geometry of the microchannel so that pseudo-turbulent region could be produced, by which catalyst would be placed in the location. In the previous projects, various micro channel geometries such as serpentine, cyclic and zigzag-type channels, have been designed to achieve greater micromixing dynamics. However, due to the current microreactor system has a space limitation, only cylindrical microchannel with a shorter configuration could be applied, where catalysts grown on wires will be placed inside to assist reaction. This project will investigate on the possible tweak of the inner cylindrical part that could be developed to enhance micro mixing dynamics in lieu of the small length-scale challenge. As the placement of wires in the internal section of the microchannel resembles a monolith reactor, hence, the term monolithic microchannel will be used throughout this project.

1.3 Objectives

This project aims to design a microreactor that uses wires as chaotic advection inducers to create changes in flowpath of hydrogen and nitrogen gases that will lead to an increase in mixing efficiency. The project will also identify locations along the microreactor design for catalyst to grow in order to increase the efficiency of ammonia production. Results will be processed in forms of contour plots and profiles.

1.4 Scope of Study

This project will focus on the study of the flow regime and its characteristics of hydrogen and nitrogen gases through 3 different types of nanowire arrangement. It is desirable to generate a micro geometry that will create a turbulent flow for mixing. This project will be employing ANSYS CFX to simulate the flow dynamics of the Microchannel. The expected results are in forms of contour plots of temperature, pressure, flow regimes and composition distribution throughout the flow path or the geometry. MIM will not be considered as a milestone in this project.

CHAPTER 2
LITERATURE REVIEW

2.1 Literature Review

Haber Bosh process is a conventional method to produce ammonia in the industry where this technique have dated since more than 100 years ago (Murzin, 2013). Ammonia produced will be used to make fertilizers for farming where the required raw materials used in this process are nitrogen gas and hydrogen gas. Equation 1.1 explains the conversion process from Nitrogen and Hydrogen gases to Ammonia.

$$N_2(g) + 3H_2(g) \leftrightarrow 2NH_3(g)$$

Equation 2.1: Haber - Bosch process

This method requires the process to be in high temperature and pressure range. The range for temperature is approximately from 300^0C to 550^0C whereas the range for pressure is around 15 to 25 MPa. The yield of this Haber-Bosch process is approximately 15% if done in a single pass manner. In order for the process to increase the overall yield of ammonia production the raw materials are separated from the product and recycled into the reactor. Using this recycling process, the synthesis can achieve an overall 95% yield. The high operating conditions is necessary as it helps the reaction to achieve higher conversion and selectivity as supported by the Le Chatelier's Principle, a higher pressure will highly favor the production of the product based on Equation 2.1: Haber - Bosch process

. Not only that, the pressure helps the gases to meet together at the catalyst by compressing it to the walls of the catalysts. Besides that, the high temperature at the reactor is caused due to the highly exothermic energy release from the reaction. Due to this reason, the reactor is usually an isothermal reactor to ensure that the temperature do not exceed dangerous levels.

There are various alterations that have been made to the Haber-Bosh process to accommodate certain requirements in the industry. Table 1 shows a comparison of the various processes used to produce ammonia (Yahya, 2010). Each companies may have modified the processes according to their own technology, the operating conditions of the ammonia synthesis are still considerably very high. Again, this high operating conditions will still prove to be hazardous to the components of the industry like employees and equipment of the plant.

Table 2.1: Various production method of ammonia

Process	**Pressure, atm**	**Temp, C**	**Conversion%**
Stami Carbon	310	500	10-30
Fauster-Montecatini	220-230	500	10-30
Casale	500-700	500	15-25
Clued	330-630	540-590	15-25
Haber-Bosch	330	500-550	10-30
Nitrogen Eng. Corp	200-300	500-550	10-30
Lummus	270-330	500-510	10-25
Kellogg	300-350	---	10-30
Du Pont	900-1000	500-600	40-80

This ammonia industry uses up to 1% of the world's energy and sustains about 40% of our planetary population and this industry is important as it provides raw materials to fertilizer industries (Murzin, 2013). As technology advances, new methods of ammonia productions are researched and developed. In one particular research, the use of Magnetic Induction Method (MIM) was introduced (Puspitasari et al., 2012). Helmholtz coils were used to generate the electromagnetic waves and this research successfully increased the yield to approximately 76%. Besides that, using MIM the operating conditions of the process was brought down to a room temperature of 28C and ambient pressure of 1.01 bar (Puspitasari et al., 2012). This method also uses micro reactors to enhance the efficiency of the production.

As technology advances, reactor sizes have known to be reduced to micron scales. The microreactors have proven to be more than or as effective as its macro siblings. The usage of microtechnology does not only limits to the development of microchips in electronics industry but also to the chemical process industry where it is used in fluid dynamics. Microchannels are defined when the dimensions of the flow path are less than 1 mm and greater than 1 micron (Sharp, et al, 2005). Any flow path with dimensions greater than 1mm will exhibit a behavior like in macroscopic flow. A smaller reactor will provide better yield compared to a bigger reactor (David et al, 2008). In the book, it was stated that a catalytic plate reactor in micron scale provides a higher yield compare to the Sasol and Exxon reactor as the ratio of surface area of catalyst to the volume of reactor is much higher hence the effective contact area for synthesis of product is higher and more efficient. The results of that study is as shown in Table.

Table 2.2: Reactor Size and Yield Comparison

Reactor	**Reactor Volume m^3**	**Yield of C5, $kg/m^3/hr$**
Sasol	432.1	29.98
Exxon	23.8	43.84
Catalytic Plate Reactor	1.0	163.12

Microreactors can be designed to increase the mixing efficiency. Mixing is an important factor in a reactor as an increment in mixing efficiency will allow materials to interact among each other more effectively hence improving reaction rate. Primarily, mixing can be enhanced by various means usually separate by two categories namely passive mixing and active Mixing. Passive mixing does not use external energy or input to create mixing and it is achievable by altering the flow path of the fluid. On the other hand, active mixing uses external forces to induce interaction of molecules and agitate the flow of materials entering the micro reactor by either kinetically or thermally (Hsieh & Huang, 2008). As mentioned by Aubin, Fletcher and Xureb (2005), there are no rule of thumb to design a micro reactor. The mixing coefficient is shown as below (Hsieh and Huang, 2008).

$$m_{eff} = \left(1 - \frac{\int_0^w |V - V_\infty| dx}{\int_0^w |V_0 - V_\infty| dx}\right) \times 100\%$$

Equation 2.2: Mixing efficiency equation

Where,

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

V_∞=volume fraction of complete mixing

V_0 = Initial distribution of the volume fraction before mixing

W = width of micro mixer

Due to the micro size of microreactors, passive mixing is more suitable instead of active mixing. A more vigorous mixing can be attained if the fluid’s movement falls into a turbulent region that creates a pseudo-mixing or external forces can be applied into the mixing process. Such turbulent flow can be generated using bends or uneven geometries (Cherlo & Puspavanam, 2009). A study conducted by Afzal and Kwang-Yong (2014), where a T-Shape and Serpentine geometries were studied. This paper shows that with a change in the flow of the fluid (caused by the geometry) will cause the different fluids to mix due to eddy current or turbulence and this geometry proved to have a better mixing efficiency at different mass flowrates. In a separate research where it focuses on the effect of cyclic curve bends on the mixing of Hydrogen and Nitrogen gases (Liaw I. & Abdullah Z., 2013). As the number of cyclic bends were manipulated, it was discovered that the velocity have the highest variation at all cyclic bends regardless of the number of cyclic bends. However, this study also shows that the velocity of the flow stabilizes almost immediately after exiting the bends which indicates that the overall design may not fully favor mixing throughout the chamber. Another research shows that when the cyclic bends are changed into sharp bends, a better mixing efficiency can be achieved. The study was conducted by Amadin (2013) where two geometries were designed and studied. The ZA geometry have a mixture of “Z” and “A” letters design pathway whereas the Sharp Bends which flat out at the edge of the design. The ZA geometry has more sharp bends that causes higher pressure drop compared to the other geometry. This pressure drop indirectly causes the fluid to mix due to the chaotic eddy currents after the bends. However, these designs are similar to the research conducted by Liaw and Abdullah where the flow develops fully almost immediately after the bends. It is more favorable if the flow is not allowed to be stabilize at any point along the flowpath to increase the efficiency of reaction. Another method can be applied to induce artificial mixing in cylindrical microchannels which probably is more favorable in increasing the effectiveness of reaction.

Microchannels can be fitted with Longitudinal Vortex Generators (LVG) to induce mixing along the fluid pathway. LVG acts as an obstacle that the fluid will require to improvise a new pathway along the flow. Studies shown that LVG designs in microreactors will be able to provide good mixing efficiency (Ebrahimi, Roohi & Kheradmand, 2014). Higher velocity of a fluid will create longer recirculation regions or eddy currents behind the LVG which proves to have good mixing efficiency in these regions. This research also proves that LVGs increases heat transfer due to the recirculation of the fluids. This recirculation or eddy currents is usually called Chaotic Advection.

The design of LVGs are very similar to the design of a tube and shell heat exchanger where the wires are like the tube arrangements in the heat exchanger. The parameters and their effect on heat exchangers are listed in table 3.

Table 2.3: Parameters that affect heat exchanger's performance

Parameter	**Description**	**Effect**
Tube diameter	Diameter of tubes will define the total number of tubes in the heat exchanger	A higher number of tubes increases the heat transfer area but creates a higher pressure drop
Pitch height	Distance between tubes	A higher pitch height will increase the hydraulic area hence reducing pressure drop
Tube layout	Triangular pitch (30^{O})	Highest heat transfer due to high turbulent flow path
	Rotated Triangular Pitch (60^{O})	Highest heat transfer due to high turbulent flow path
	Square Pitch (90^{O})	Usually applied when there is a high chance of fouling. Design of square pitch disallows fouling materials to be swept by the fluid flow
	Rotated Square Pitch (45^{O})	Usually applied when there is a high chance of fouling. Design of square pitch disallows fouling materials to be swept by the fluid flow

In relation with the shell and tube heat exchanger design principles, the research hopes to relate the arrangement of wires will affect the flow characteristics of the gases. If an increase of number of tubes due to reduction of tube diameters can cause a high pressure drop, the flow will undergo various changes in aspect of flow patter. The increment of tube surface area will have a higher friction factor that affects the flow of the fluid. Besides that, triangular pitch will create a high turbulent flow path due to the chaotic advection caused from the triangular arrangement. This form of LVG will cause the fluid to alter its path successfully into a turbulent region in a macroscopic geometry. From the understanding of heat exchangers, this research suggests that with a design of LVG created by wire arrangement in a monolithic microchannel, a passive mixing chaotic advection is attained hence increasing homogeneity of gases. Being able to create such scenario will allow researchers to identify locations where catalysts will be cultivated on the nanowire to achieve optimum synthesis of ammonia.

CHAPTER 3
METHODOLOGY

3.1 Geometry Development

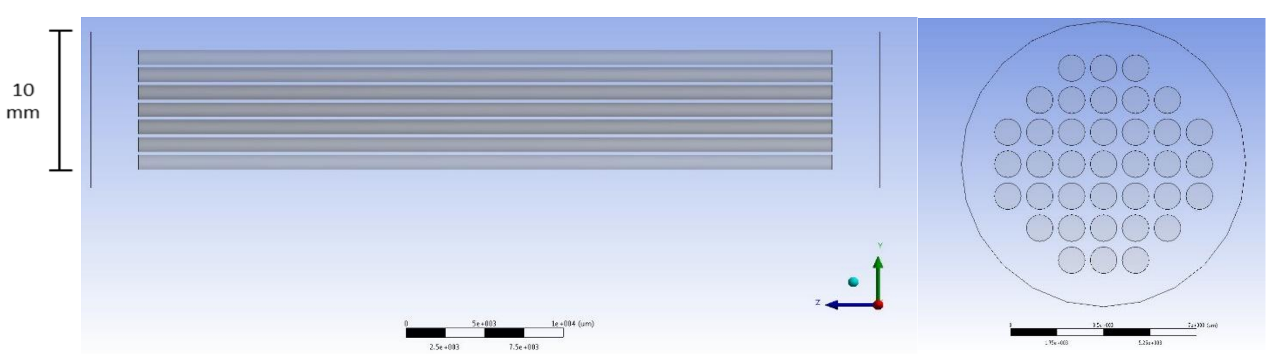
In this project, three designs will be suggested to be studied for each of its mixing efficiency. Generally, the microreactor will be designed in a cylindrical manner, where the wires will be arranged in the axial configuration. As the axial arrangement resembles a monolith reactor, hence the term “monolith microreactor” is used in this project. The main microreactor has a dimension of 10mm in diameter and 50 mm in length, while the wires are of 0.5 mm diameter. The wires will have a dimension of a 0.5 mm in diameter. The length varies depending on the design of the nanowire arrangement aimed to create chaotic advection.

3.1.1 Design 1

Design 1 has 21 straight nanowires placed along the cylindrical tube. There is no intersections of wires and no change in nanowire path. The wires are arranged in a square manner and has a distance of 300 microns from one and another as shown in the figure 3.1. Further details are listed below:

Wire length = 4.4cm

Figure 3.1: Geometry 1

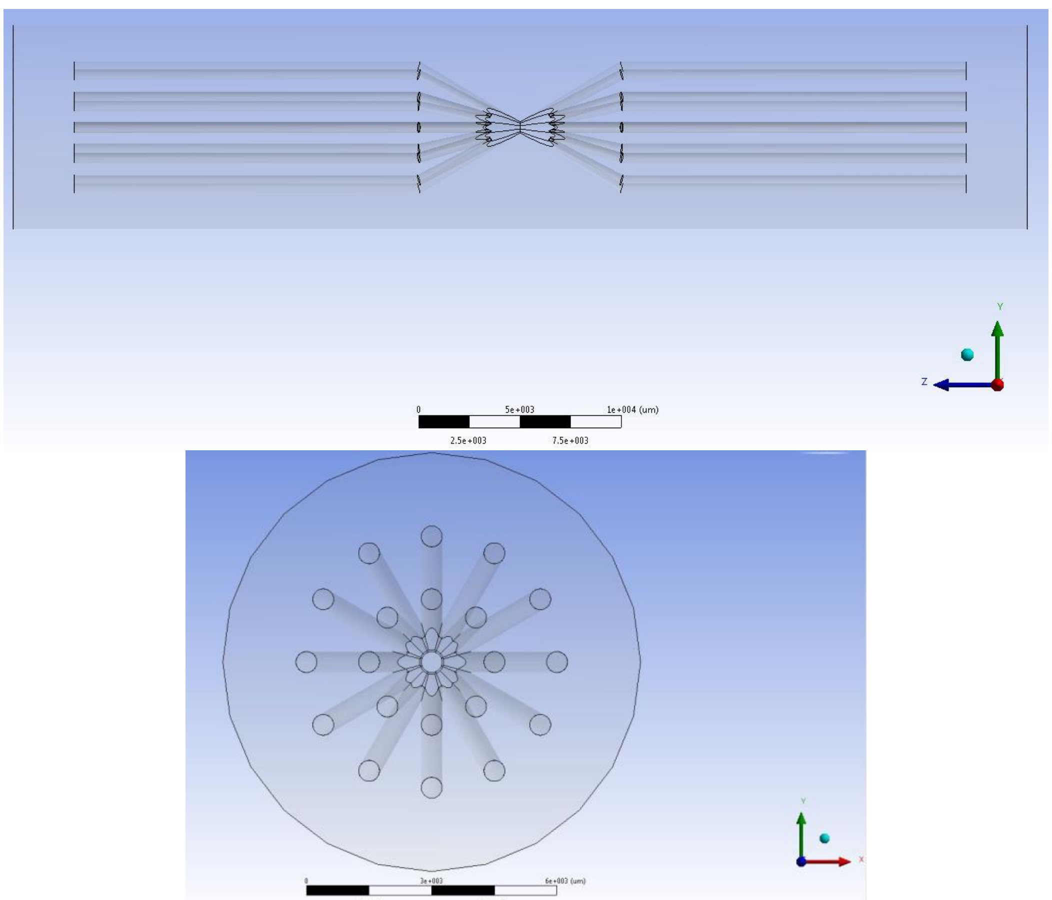


3.1.2 Design 2

Design 2 consist of 21 wires that will meet at the middle of the tube and then spread out again after the middle. This converging-diverging configuration is expected to create disruptions to the flow of the gases. This disruption will create turbulence which will increase the mixing of the gases in the middle region.

Point	Dimensions
Distance of ring 1 from center	0.15cm
Distance of ring 2 from center	0.30cm
Wire length	4.4cm
Converging/Diverging angle- Ring 1	17^o
Converging/Diverging angle- Ring 2	31^o

Figure 3.2: Geometry 2

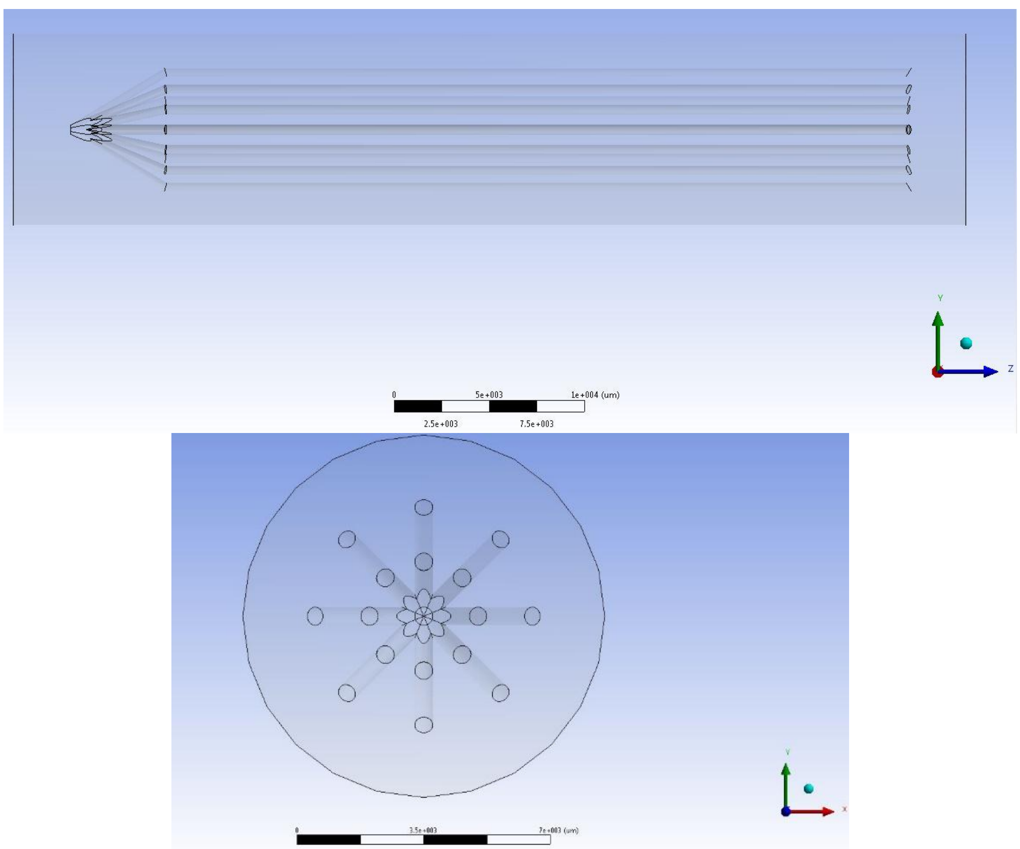


3.1.3 Design 3

Design 3 starts from a single point to fan out into 20 wires. This initial fanning will create disturbance to the flow at the start of the tube. This geometry is developed based on an assumption that the gases will be able to react quickly upon disturbance. This assumption will be studied in this project.

Point	Dimensions
Distance of ring 1 from center	0.15cm
Distance of ring 2 from center	0.30cm
Wire length	4.4cm
Converging/Diverging angle- Ring 1	17^{o}
Converging/Diverging angle- Ring 2	31^{o}

Figure 3.3: Geometry 3



3.2 Simulation Methodology

3.2.1 Physics Pre-Setup

After completion of the geometry design and the meshing of the model, ANSYS will require several pre-setup inputs before simulating the design. The meshing parameters were selected as moderate due to license limitations. The model will be fed with Hydrogen and Nitrogen gases at a volume fraction of 0.75 of Hydrogen Gas to 0.25 of Nitrogen Gas. The gases are fed at 3.33m/s as proposed by the OneBAJA team. The mode of the simulation will be steady state with isothermal ambient conditions (Temperature: 25^{o}C & Pressure: 1atm). This project will not consider magnetic induction in the simulation. The physics are summarized in the table below.

Table 3.1: Flow parameters setup

Parameter	Selection
Simulation mode	Steady State
Fluids	Nitrogen & hydrogen gases (at STP)
Fluid Inlet Ratio	0.25 Nitrogen: 0.75 Hydrogen (Volume Fraction)
Fluid Morphology	Continuous Fluids
Buoyancy Model	Non-buoyant
Reference Pressure	1 atm
Heat transfer Model	Isothermal (25^{O}C)
Turbulence Model	K-Epsilon
Fluid Inlet Velocity	3.33m/s

3.2.2 Governing Equations

The governing equations are summarized in the following table.

Table 3.2: Governing equations in ANSYS

Equation	Mathematical Form
Navier Stokes	$\rho\left(\frac{dv}{dt}+V.\nabla V\right)=-\nabla p+\nabla.T+f$
Continuity Equation	$\frac{dv_k}{dx_k}=0$
Momentum equation	$\frac{\partial\left(pv_j v_k\right)}{\partial v_j}=\frac{\partial}{\partial x_j}\left(-p\delta_{ij}+\mu\left(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\right)\right)$ $=\rho g_i$
Diffusion convective equation	$\frac{\partial c}{\partial t}+\frac{\partial v_k(c)}{\partial x_k}=D\frac{\partial^2}{\partial x}c$

3.2.3 Results Analysis

The results will be extracted in forms of contour plots at several different locations depending on the geometry. The distances between the contour plots (YZ axis plots) will also have to be based on the geometry as there are several places of interest to be studied (example, the concaving and diverging sections of geometry 2 and geometry 3). Besides that, the Reynolds number will also be identified using the following equation.

Equation 3.1: Reynolds equation (Original)

$$Re=\frac{\rho VD}{\mu}$$

Where,

ρ= density (kg/m3)

V = velocity m/s

D = diameter of cylinder (m)

μ = fluid viscosity (m^2/s)

This equation uses the overall diameter of the cylinder when calculating the Reynolds number and may not be representative to this research as the project aims to inserts wires as obstacles in the channel. Hence the equation is needed to be modified to represent the design. First the mixture density can be calculated via the following equation.

Equation 3.2: Mixture density equation

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

Where,

ρ_{mix} = mole fraction of component i of viscosity u_i

$\rho_{1\ldots}\rho_2$= density of each of the components (kg/m^3)

$V_1 + V_2 + \cdots + V_n$= volume share of each of the components (m^3)

After that the mixture viscosity is calculated using the equation:

Equation 3.3: Mixture viscosity equation

$$\mu_{mix} = \frac{\sum X_i u_i \,(M_i)^{1/2}}{\sum X_i \,(M_i)^{1/2}}$$

Where

X_i = mole fraction of component i of viscosity u_i

M_i= molecular weight of component i

The diameter in the Reynolds equation will be represented by the hydraulic diameter where the hydraulic diameter can be calculated via:

Equation 3.4: Hydraulic diameter

$$D_H = {}^{4A}/_{P}$$

Where

A = Subtraction of Cross Sectional Area & total area of void area (m^2)

P= Wetted perimeter area (m)

The Reynolds equation after modification which will be used in this project is

Equation 3.5: Modified Reynolds equation

$$Re = \frac{\rho_{mix} V D_H}{\mu_{mix}}$$

Where,

ρ= density (kg/m3)

V = velocity m/s

D = diameter of cylinder (m)

μ = fluid viscosity (m^2/s)

CHAPTER 4
RESULTS AND DISCUSSION

4. 1RESULTS

The required results to be extracted from the simulation are the velocity and volume fraction contour plots in both radial and axial manner. Both results will be used to analyze the behavior of the gases and to estimate the area of mixing and catalyst growth. The results are extracted in the Post-CFX module of the ANSYS 15.0 CFD software.

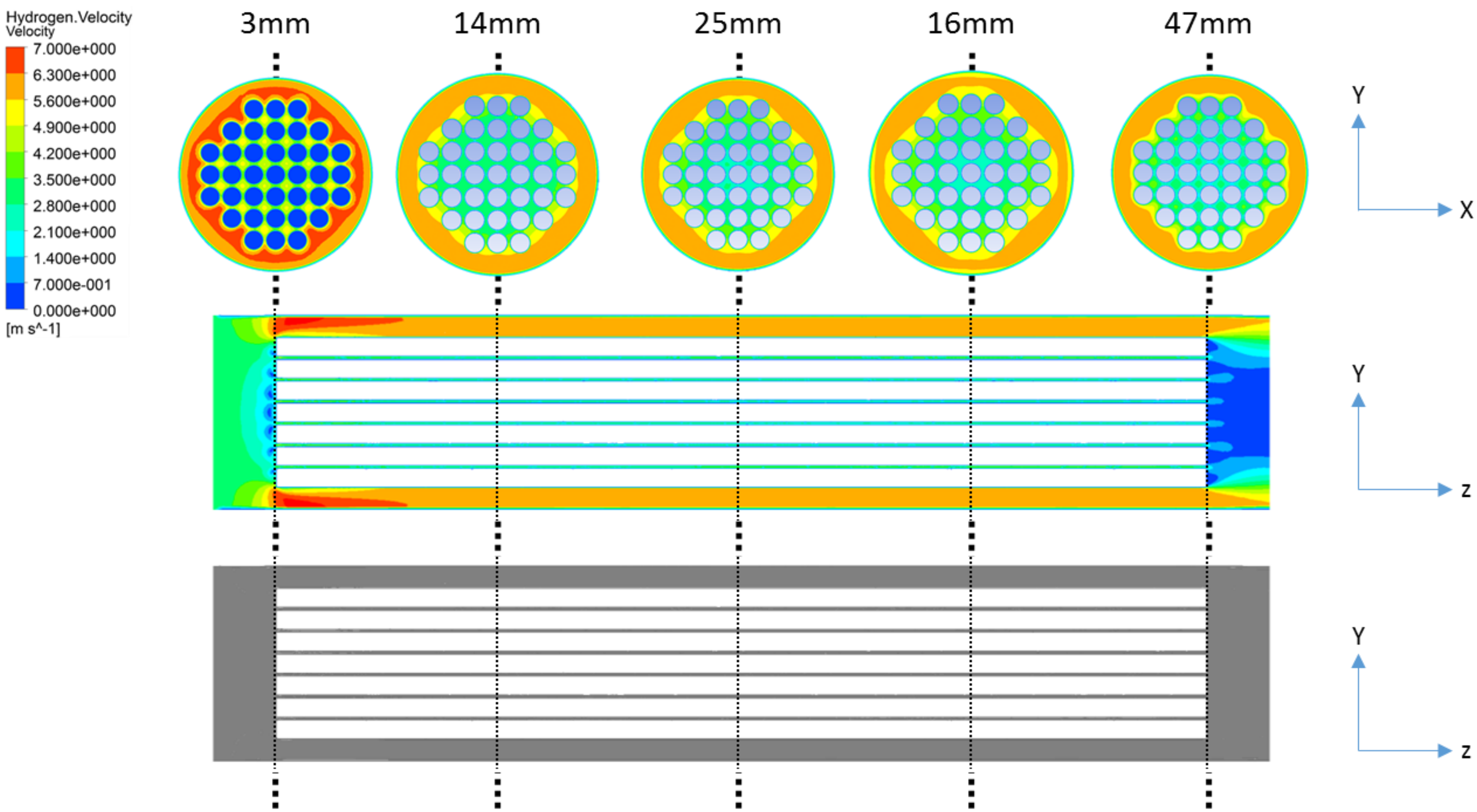
The results are extracted are separated into several sections. The results extracted are:-

(1) Geometry 1
  (a) Velocity Contour (Radial)
  (b) Velocity Contour (Axial)
  (c) Volume Fraction
(2) Geometry 2
  (a) Velocity Contour (Radial)
  (b) Velocity Contour (Axial)
  (c) Volume Fraction
(3) Geometry 3
  (a) Velocity Contour (Radial)
  (b) Velocity Contour (Axial)
  (c) Volume Fraction

4.1.1Geometry 1

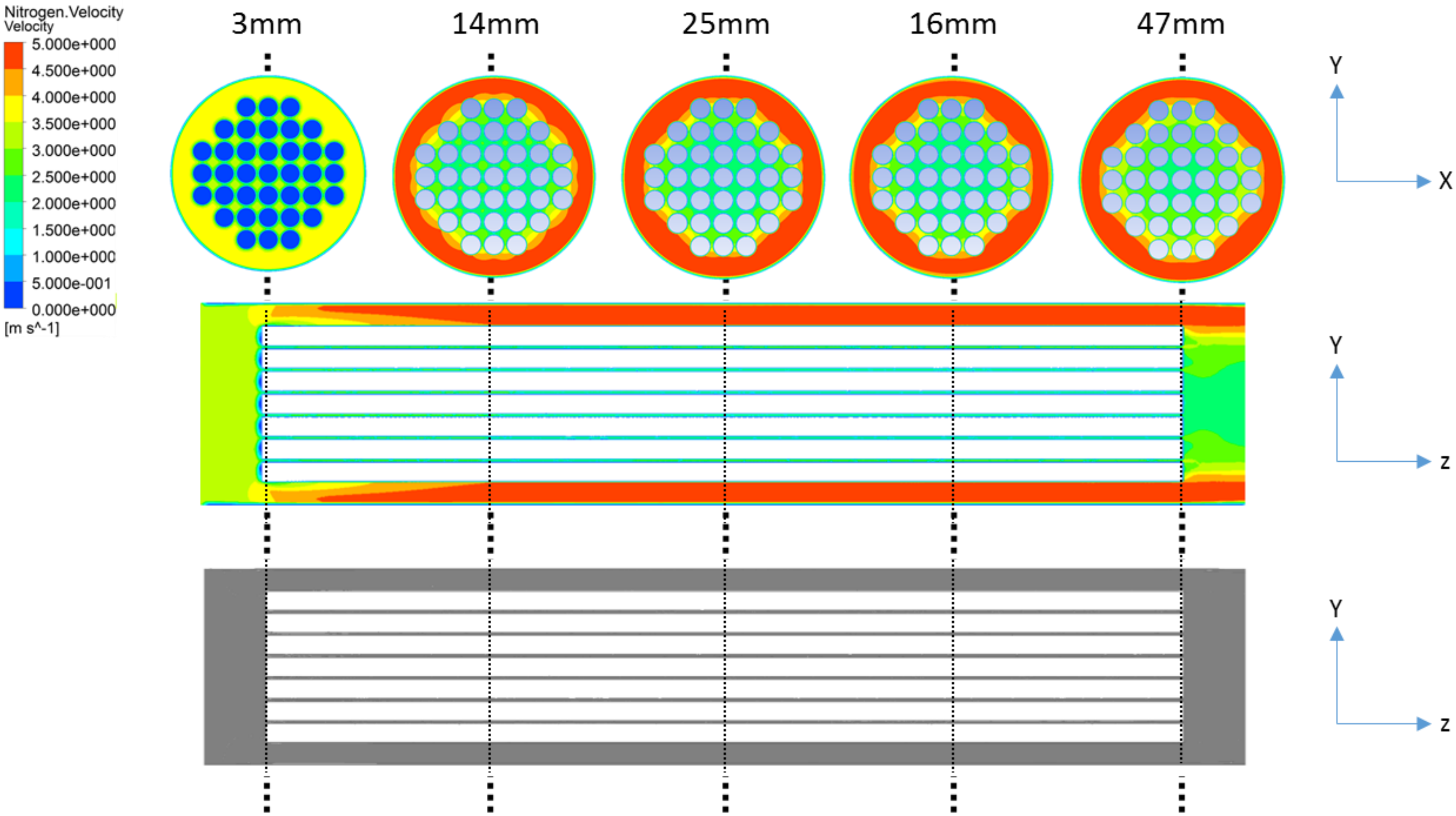
Hydrogen Velocity Plot (Radial)

Figure 1: Hydrogen contour plot for Geometry 1

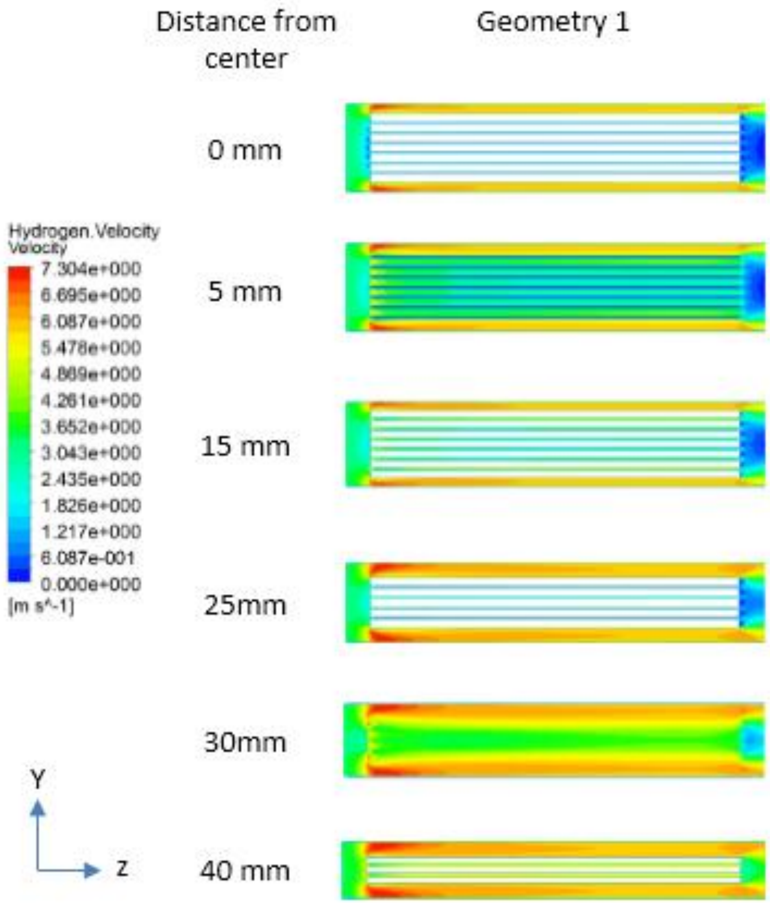


Nitrogen Velocity Plot (Radial)

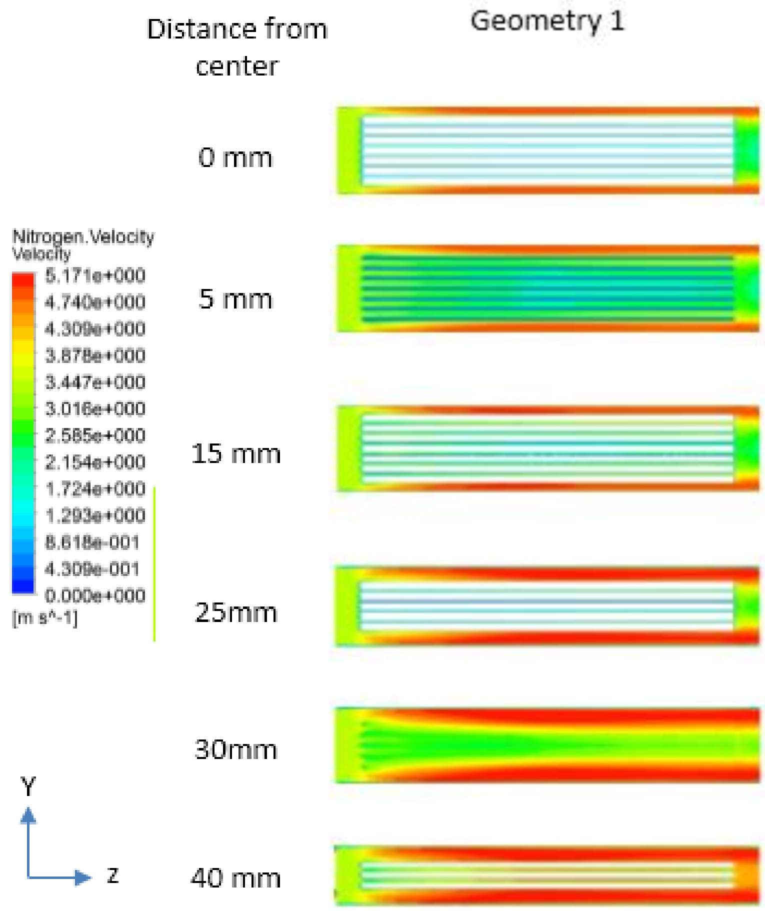
Figure 2: Nitrogen contour plot for Geometry 1



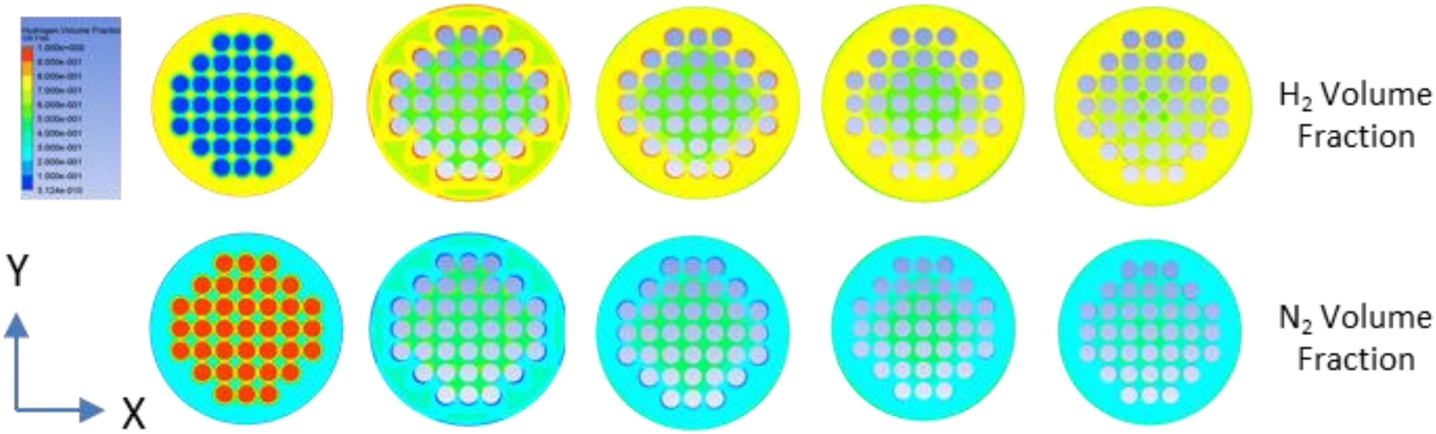
Hydrogen Velocity Plot (Axial)



Nitrogen Velocity Plot (Radial)



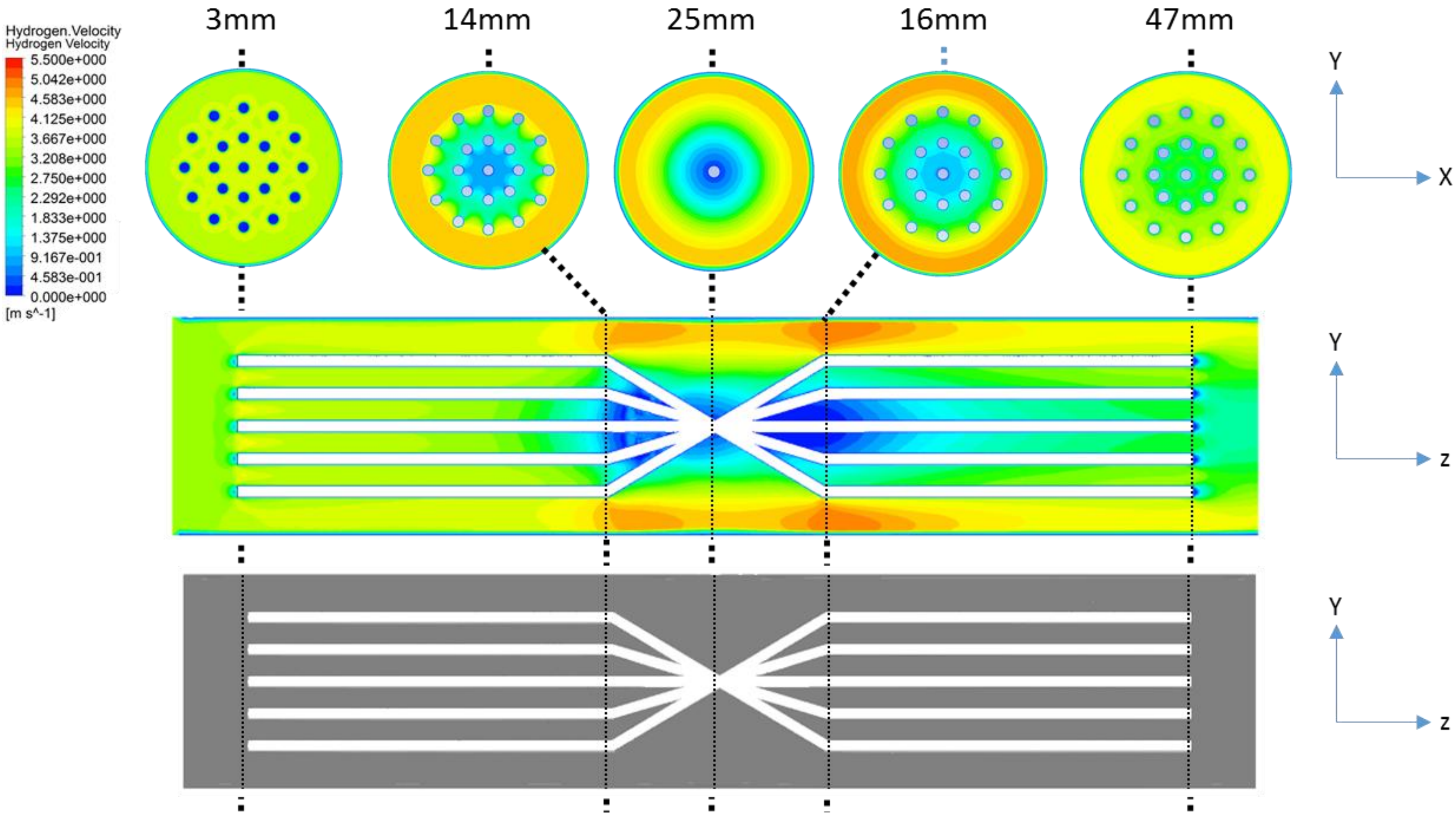
Hydrogen and Nitrogen Volume Fraction



4.1.2 Geometry 2

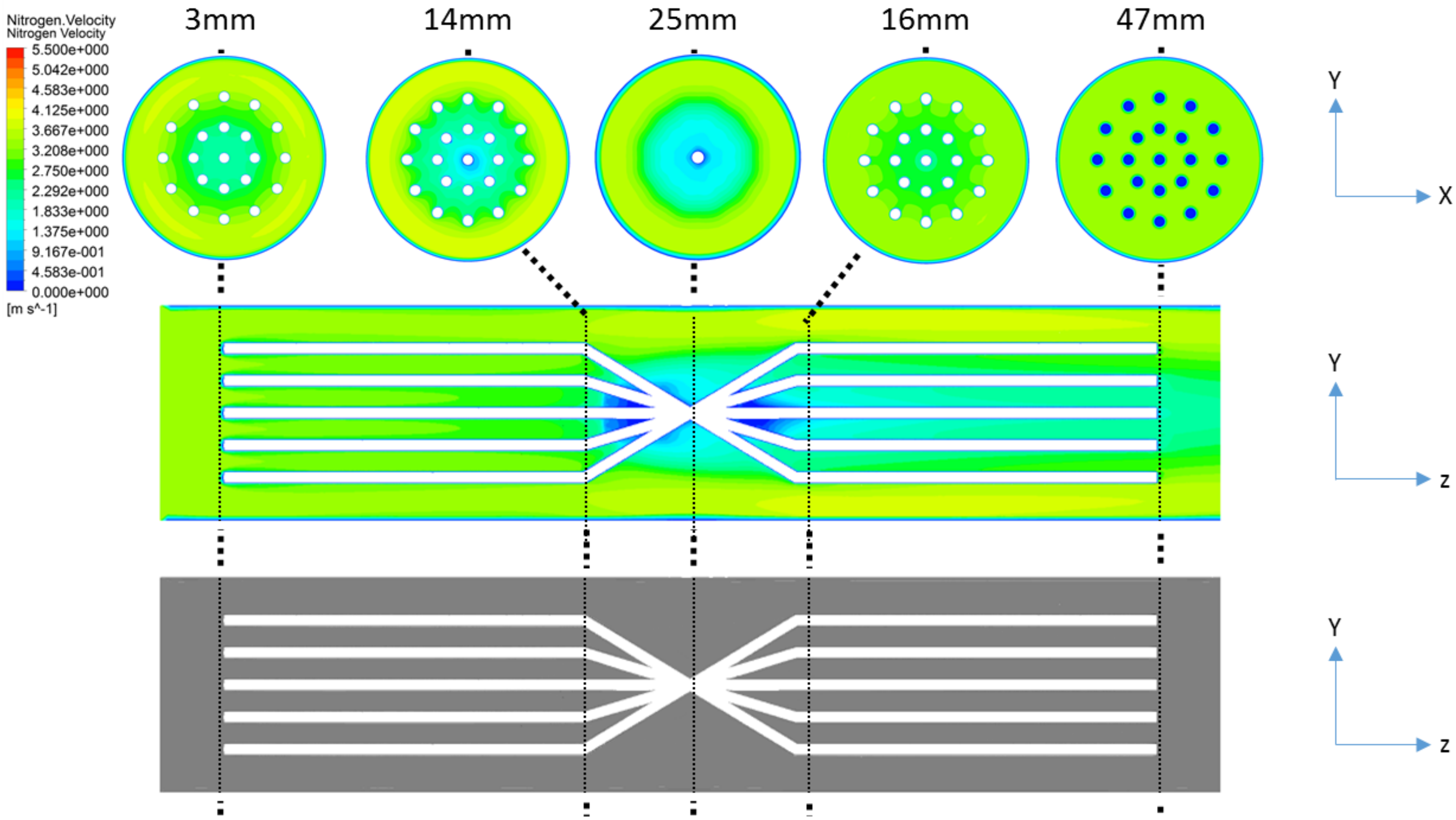
Hydrogen Velocity Plot

Figure 3: Hydrogen contour plot for Geometry 2

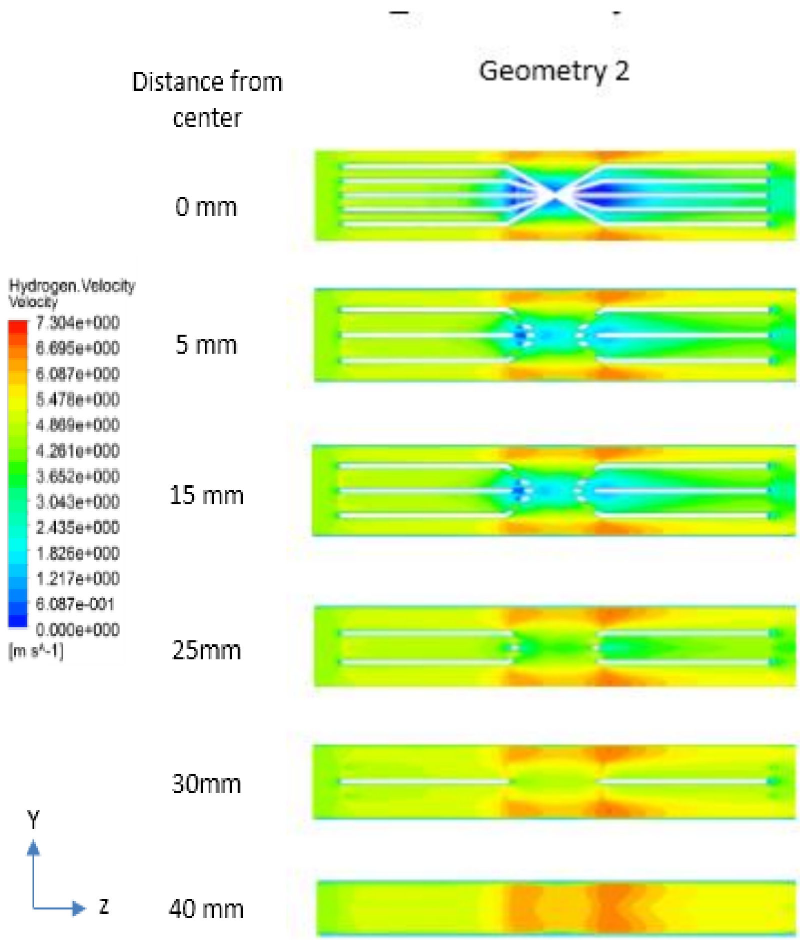


Nitrogen Velocity Plot

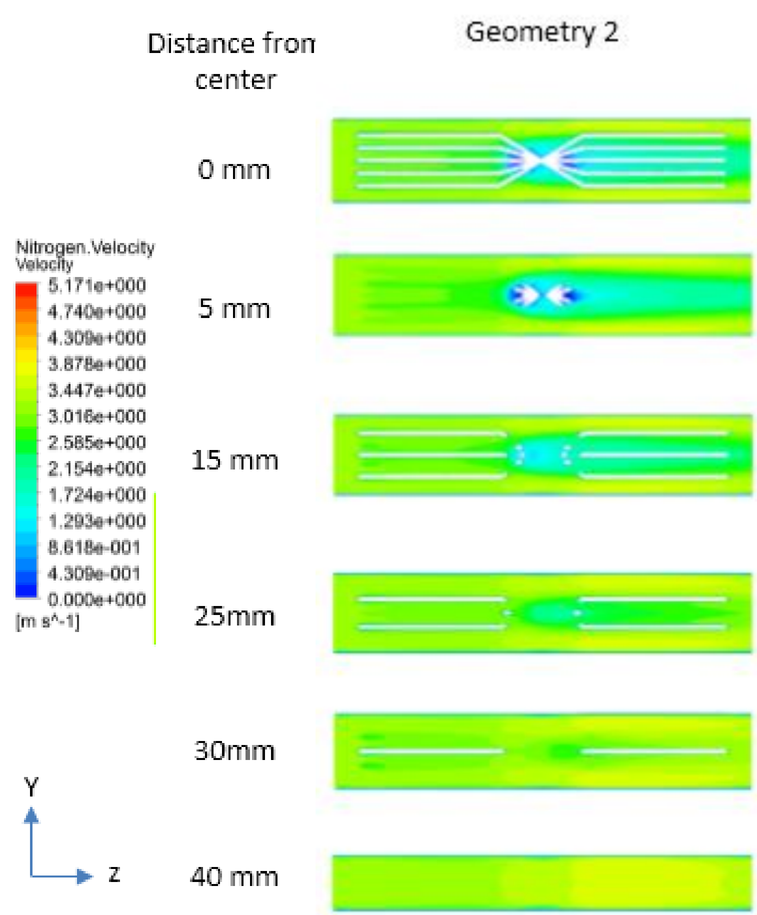
Figure 4: Nitrogen contour plot for Geometry 2



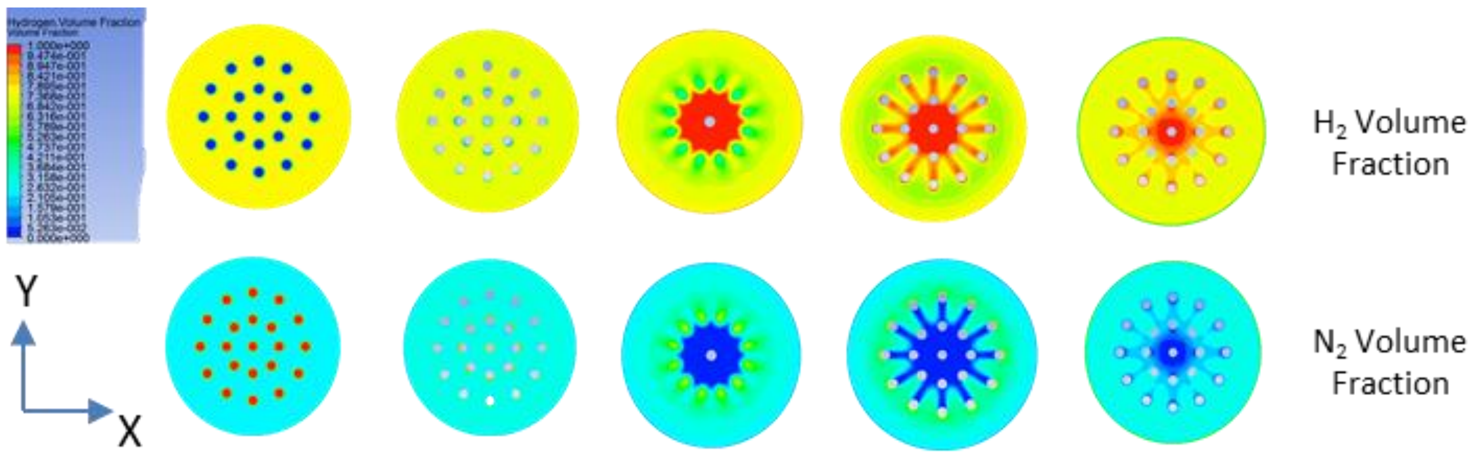
Hydrogen Velocity Plot (Axial)



Nitrogen Velocity Plot (Radial)



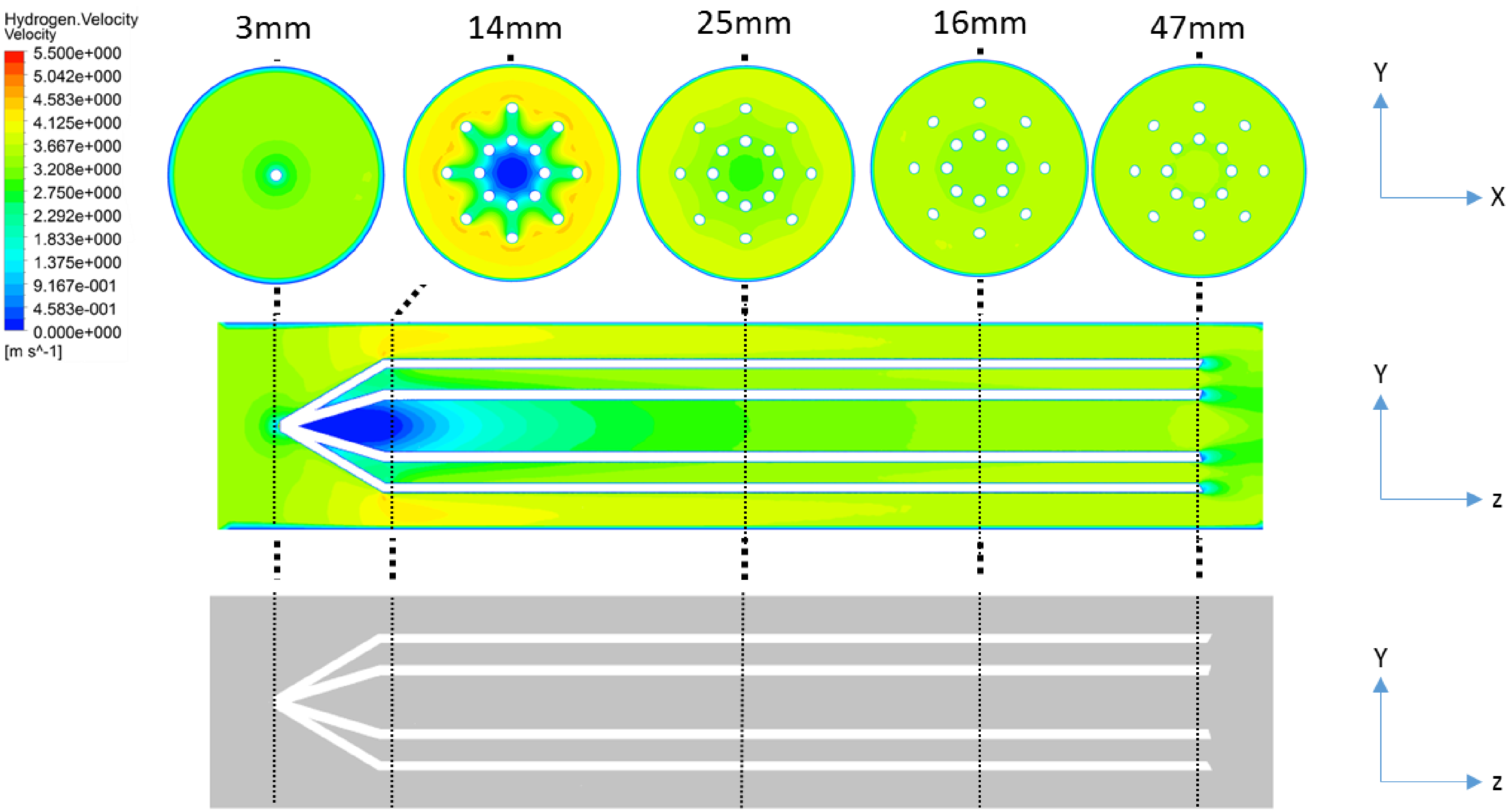
Hydrogen and Nitrogen Volume Fraction



4.1.3 Geometry 3

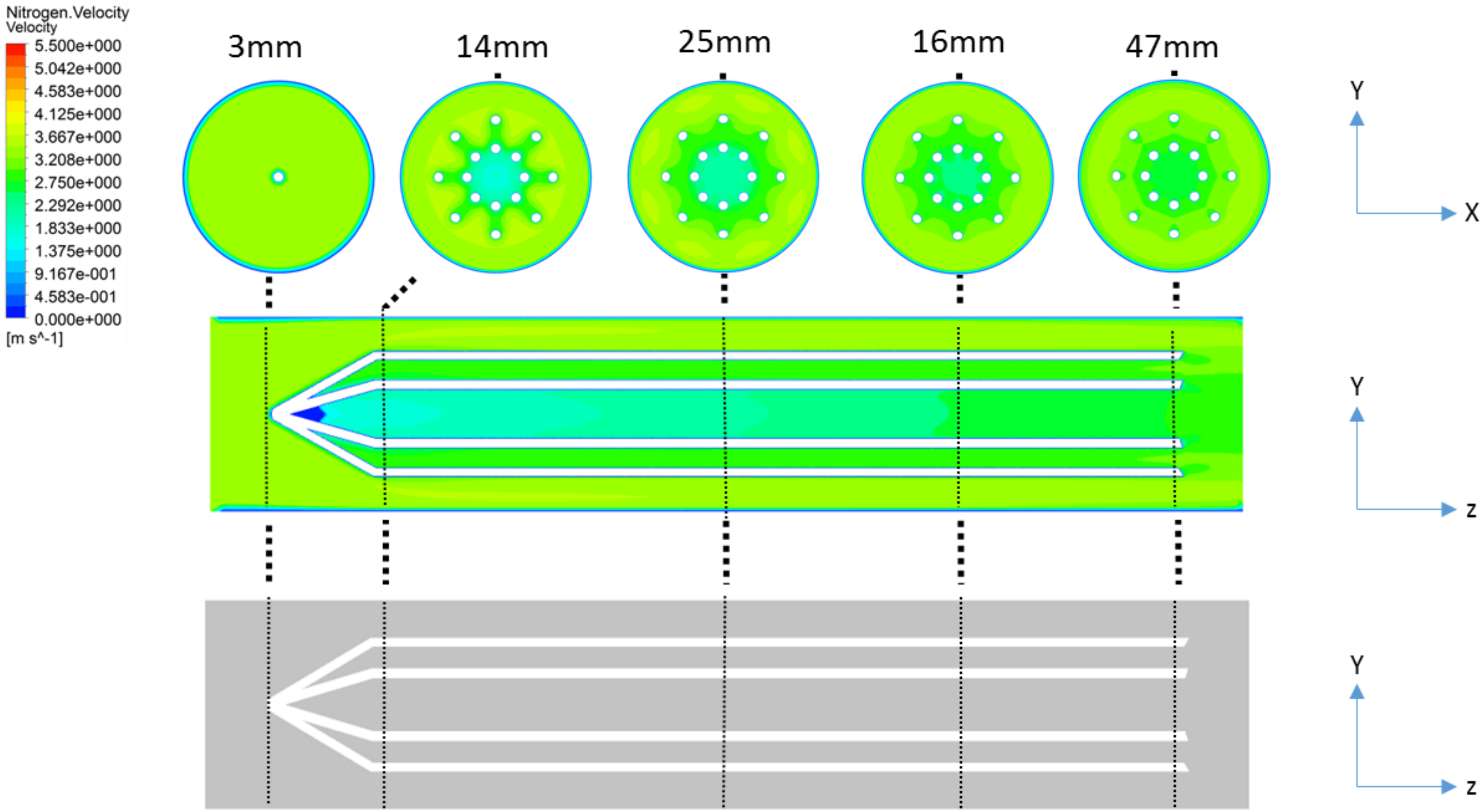
Hydrogen Velocity Plot

Figure 5: Hydrogen contour plot for Geometry 3

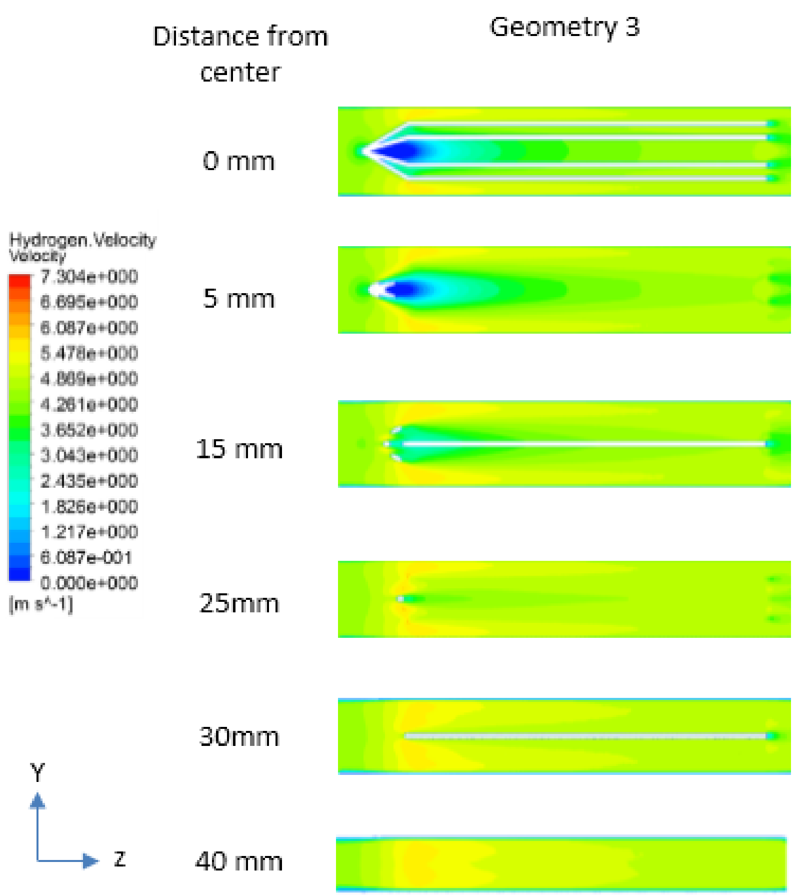


Nitrogen Velocity Plot

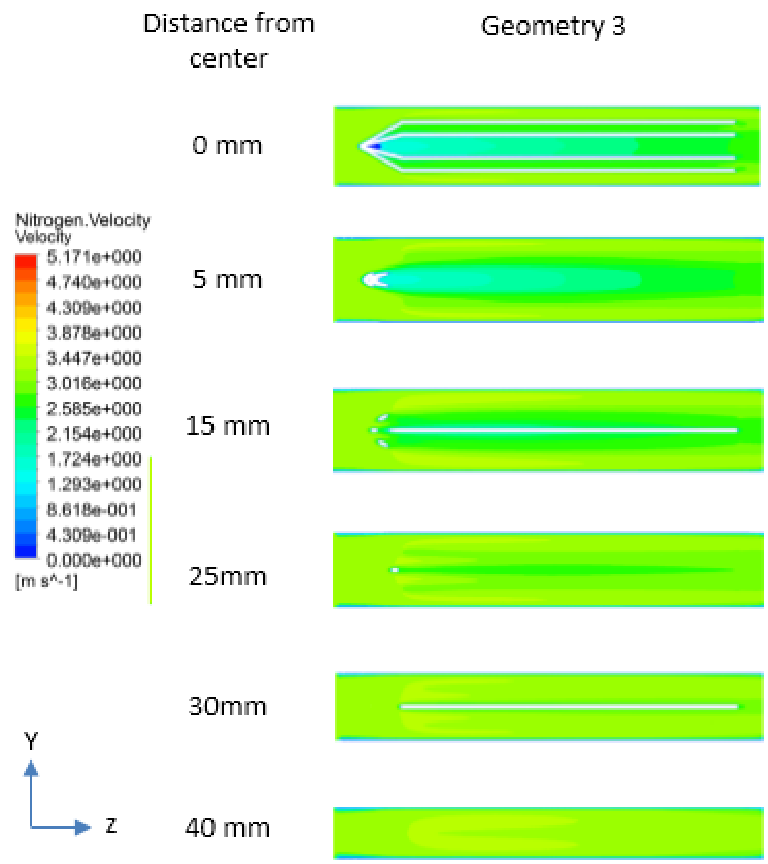
Figure 6: Nitrogen contour plot for Geometry 3



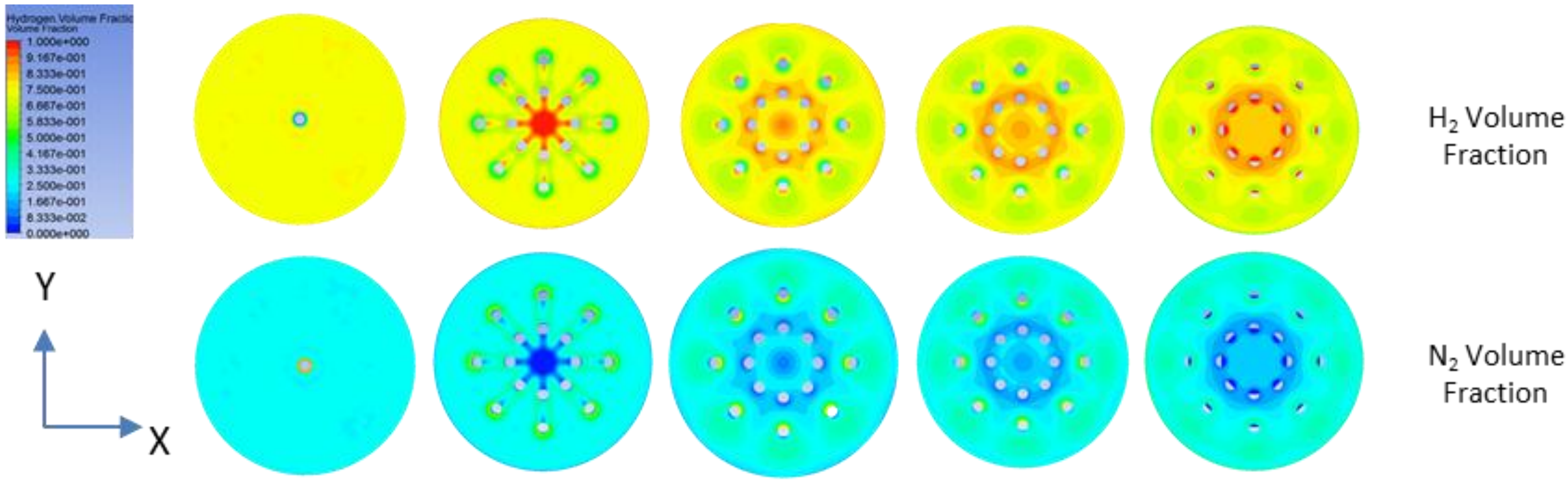
Hydrogen Velocity Plot (Axial)



Nitrogen Velocity Plot (Radial)



Hydrogen and Nitrogen Volume Fraction



4.2 Discussion

4.2.1 Geometry 1

Based on the velocity contour plots, it was shown that the velocities of the gases changes immediately after meeting with the wires. The wires created chaotic advection that causes the fluid to seek a different pathway to exit the microreactor. However the velocity of the gases however becomes develops after an approximate10mm (in relative to the length of the microreactor) where there is no change in velocity anymore. The development of the flow was possibly caused because of the dense nature of the wires and there is no apparent change of flowpath. It was also found that after meeting with the wires, the hydrogen and nitrogen gases disperse well in the middle of the microreactor. The gases however disperse after 10 mm in accordance with the length of the microreactor. Hydrogen gas tends to flock around the outer area of the wires as shown in Contour 6 to Contour 12. The nitrogen gas however remains in the middle of the microreactor. This could possibly due to the size of nitrogen particles. Nitrogen gases have a bigger atomic number and size compared to Hydrogen gas hence there is a difficulty to disperse in a confined space generated by the dense wires. Escaped nitrogen can be seen around the inner wall of the microreactor. The highest velocity of the gases noted in the simulation results are up to 7.3m/s. the velocity of the gases ranges from 3.0m/s to 7.3m/s. The Reynolds number calculated for geometry 1 are summarized in the below table:

Table 4.1: Reynolds number calculation for geometry 1

Parameter	**Value**	**Unit**
Cross section area of channel	7.85E-03	m2
Total area covered by wires	7.26E-04	m2
Wetted perimeter	8.95E-01	m
Hydraulic Diameter	3.18E-02	m
Mixture Viscosity	3.62E-05	m2/s
Mixture density	3.80E-01	kg.m3
Velocity	3.30E+00	m/s
Reynolds Number @ Inlet	3.50E+03	-
Reynolds Number (37 wires)	1.11E+03	-

The Reynolds number reduces as the fluid meets the wire arrangement. It can be said that the characteristic flow of the fluid changes to try to reach laminar along the flowpath. The value of the Reynolds number are comparable as the velocity of the gases stabilizes almost immediately after 10mm from the inlet of the channel.

It can be said chaotic advection was achieved in this geometry but the rate of gases leaving the channel may not be favorable as the gases should remain in the channel for a while in order for the gases to mix and meet at the tip of the catalysts for reaction to occur.

4.2.2Geometry 2

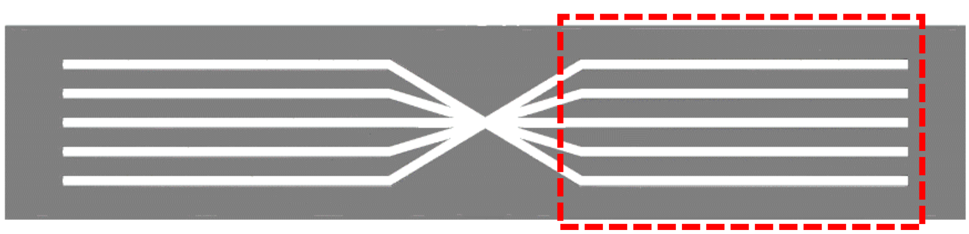
There is a slight disturbance to the velocity of the gases when the gases meet the wires at z=3000 micron. The gases stabilizes almost immediately. As we move along axially, the gases start to have significant velocity changes when the wires start to concave at the middle. The gases showed almost synchronized velocity changes especially the Hydrogen gases. Layers of different velocity is noticeable compared to the Nitrogen Gas. When the nanowire arrangement starts to diverge back, the gases are mixed and dispersed evenly in the microreactor. There is however a void area in the center immediately when the wires diverge outwards. Nitrogen gas does not exist in the middle of the microreactor after the wires diverge till the end. It was found that the Nitrogen gas are highly concentrated at the middle of the channel when the wires start to converge to the center. This design somehow created a trap for the Nitrogen gas. It was hypothesized that due to the size of the Nitrogen gas molecules, it is difficult for the gas to disperse well as the wires created some sort of filter or trap due to the density of nitrogen gas. Hydrogen gas is highly concentrated in the middle. The highest velocity of the gases noted in the simulation results are up to 5.0 m/s. the velocity of the gases ranges from 1.3m/s to 5.0m/s.

The Reynolds numbers for the Geometry 2 are summarized in the table below.

Table 4.2: Reynolds number calculation for geometry 1

Parameter	**Value**	**Unit**
Cross section area of channel	7.85E-03	m2
Total area covered by wires (21 wires)	7.26E-04	m2
Total area covered by wires (1 wires)	1.96E-05	m2
Wetted perimeter (21 wires)	6.44E-01	m
Wetted perimeter (1 wires)	3.30E-01	m
Hydraulic Diameter (21 wires)	4.62E-02	m
Hydraulic Diameter (1 wires)	9.50E-02	m
Mixture viscosity	3.62E-05	m2/s
Mixture density	3.80E-01	kg.m3
Velocity	3.3	m/s
Reynolds Number (Inlet, no wires)	3.50E+03	
Reynolds Number (21 wires)	1.62E+03	
Reynolds Number (1 wires)	3.33E+03	

As the fluid passes through the wire network, there is a change in Reynolds number too. It is calculated that the Reynolds number will reduce and then increase at the middle of the channel before reducing again due to an increment in the area of the wires. This change of Reynolds number can also be seen related to the change of velocities. Chaotic advection occurs as the flow changes its direction and velocity varies and the change of Reynolds number supports that. And as the Reynolds number change, it can be inferred that mixing of gases are achieved in this geometry.With this design, chaotic advection is successful and the results can be inferred to have good mixing of gases as the fluid progresses through the microchannel. The area of catalyst placement is described in the diagram below.



4.2.3 Geometry 3

Immediately after the gases meet with the nanowire the gases starts to disperse slightly along the diverging section of the nanowire. The gases flow along the wires and once the wires diverge sufficiently, the gases starts to flow into the middle section of the microreactor. Similar to Geometry 1 and 2, Hydrogen gas seems to favor the middle section of the wires due to its smaller atomic size. Besides that, Hydrogen gas seems to be stagnant or moving very slowly in the middle section. Perhaps the wires have created a sieve that disallows particles to interrupt the Hydrogen gases. Both gases however, disperse fairly quickly after an approximate 10mm from the start of the nanowire arrangement. In this geometry however, the gases seems to linger around the wires instead of dispersing equally along the microreactor. The velocity of the gases however stabilizes after 15mm in relative to the microreactor's length. The highest velocity of the gases noted in the simulation results are up to 4.5m/s. the velocity of the gases ranges from 0.3m/s to 4.5m/s.

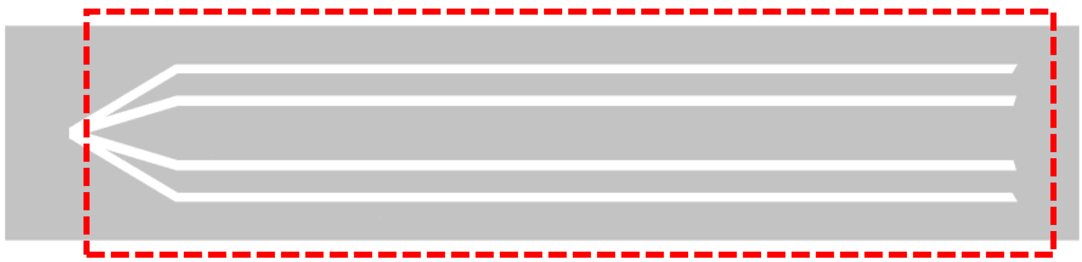
The Reynolds number calculated is described in the following table.

Table 4.3: Reynolds number calculation for geometry 3

Parameter	**Value**	**Unit**
Cross section area of channel	7.85E-03	m2
Total area covered by wires (20 wires)	3.93E-04	m2
Total area covered by wires (1 wires)	1.96E-05	m2
Wetted perimeter (20 wires)	6.28E-01	m
Wetted perimeter (1 wires)	3.30E-01	m
Hydraulic Diameter (20 wires)	4.75E-02	m
Hydraulic Diameter (1 wires)	9.50E-02	m
Mixture viscosity	3.62E-05	m2/s
Mixture density	3.80E-01	kg.m3
Velocity	3.3	m/s
Reynolds Number (Inlet, no wires)	3.50E+03	
Reynolds Number (20 wires)	1.66E+03	
Reynolds Number (1 wires)	3.33E+03	

The Reynolds number calculation results are the same with Geometry 2 as the hydraulic diameter is actually the same. The diverging angle for ring 1 and ring 2 are the same and the total number of wires after diverging are similar. Hence the Reynolds number calculations show the same results. The only difference here is that the 21 wires region is much longer compared to geometry 2 hence creating a distance for good flow development to reach stability.

Geometry 3 also successfully created chaotic advection flow where mixing was achieved form the interpretation of velocity contours and Reynolds number calculations. This geometry however have a longer length compared to geometry 2 for flow development after the diverging of the wires (8000microns from inlet). This allows the gases to mix slowly along that flowpath and may bring good mixing efficiency also. The area suggested for catalysts growth is described in the following figure.



CHAPTER 5
CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Chaotic advection was successfully induced when wires are arranged axially in a different manner. This chaotic advection altered the flowpath of the gases and caused velocity changes. The project have proven that the wires can be arranged in the microreactor to create disturbance to the flow that will enhance mixing of two separate gases namely Hydrogen and Nitrogen gas. It is also believed that using the wires as a chaotic advection inducer may provide better results to an alternating geometry as previous studies have done. Besides that, from the three suggested geometry, it was discovered that all three geometries' provide different velocity changes. A very dense Geometry 1 have the biggest velocity variation ranging from 3.33 m/s to a staggering 7.0m/s. The other two however has a lesser velocity increment compared to Geometry 1. It was also discovered that the distribution of gases in in Geometry 2 and Geometry 3 are more favorable for a reaction mixing. Geometry 3 has the most evenly distributed velocity variation and sufficient concentration of both gases in the system. The Hydrogen and Nitrogen Gases are fairly distributed surrounding each wires. The change in Reynolds number proved that the characteristics of the fluid changes when the wires arrangement are present in the Microchannel.

5.2 Recommendation

A more thorough study can be done by selecting Geometry 1 and testing the design parameters like the number of wires in the microreactor, the general geometry design (circular or rectangular) or the diameter of wires. As this project does not include the reaction and magnetic module, it is suggested that future works can revolve around adding the reaction and magnetic module as MIM uses induced magnetic forces by the wires to attract the gases to the catalyst. ANSYS have the ability to couple these modules in the system and will represent the technology better. Besides that, the design parameters can be studied to further the understanding on the effects of design parameters on the flow of the Hydrogen and Nitrogen gases with Ammonia gas.

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