CFD Modelling of the Microreactor for the Ammonia Synthesis

By

Mohammad Khairulanam bin Azeman

Dissertation submitted in partial fulfilment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
Chemical Engineering Programme
UniversitiTeknologi PETRONAS
in partial fulfilment of the requirement for the
BACHELOR OF ENGINEERING (Hons)
(CHEMICAL ENGINEERING)

Approved by,

____

(Dr. Mohd Zamri bin Abdullah)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
September 2012

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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MOHAMMAD KHAIRULANAM BIN AZEMAN

ABSTRACT

This project is related to the microreaction technology under the microengineering field. The development of microreactors has been researched worldwide due to their better performance over conventional reactors. Mixing is one of the key components in chemical process especially in microreactors. With good mixing, a better control on the quality of the final product and its properties are ascertained to comply with the specification of the product. However, poor mixing will result in a non-homogenous distribution of the product that certainly lacks consistency with the specification desired. The study of mixing behaviour in microreactors is crucial due to the laminar behavioural of the flow in microchannels. Together with the advancement in technology, the study of mixing can be done through Computational Fluid Dynamics (CFD) simulations. With CFD simulations, the design for the optimum mixing in a microreactor can be made based on a trial-and-error method. Through simulation, the best location of the catalyst placement can be predicted according to the mixing behaviour in the microreactor. This project involves the investigation of the effect of the micromixer geometric design and the inflow configuration for the micromixer on the mixing performance using CFD.

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CHAPTER 1 : INTRODUCTION

1.1 Background of Study

Synthetic ammonia and carbon dioxide are used to produce synthetic urea in liquid or solid form. Ammonia was first commercially synthesized in 1870 through Haber-Bosch process at extremely high pressure and temperature. Today, the Haber-Bosch process is used to produce more than 500 million tons of artificial fertilizer per year; roughly 1% of the world's energy is used for it, and it sustains about 40% of our planetary population. OneBAJA program introduces a new method of synthesizing ammonia and urea so called green urea production, which is energy saving, economical and safe. This new method involved the design of a new reactor and a new product that could enhanced the process and performance, respectively.

Ammonia is produced by reacting two gases, nitrogen (N_2) and hydrogen (H_2) to produce NH_3. In OneBAJA program, ammonia will be formed at ambient operating condition by means of magnetic induction zone to produce even higher ammonia yield compared to the conservative Haber-Bosch method. In such a process, catalyst plays significant role to assist the process.

In a typical ammonia synthesis, two reactant gases i.e. nitrogen and hydrogen are reacted with the aid of a catalyst in a high temperature, high pressure reactor. Regardless of the lower conversion and yield, the technique which is also known as Haber–Bosch process imposes a costly method to produce ammonia, in addition to the higher safety and control regulation that have to be looked upon. In an effort to improve the production, the OneBAJA program has proposed a new way for the synthesis of ammonia through a magnetic induction system which is performed at an ambient temperature and pressure. Besides generating higher conversion and yield, the OneBAJA process have the advantage in reducing the operating cost and lowering the safety risk of the overall system.

In OneBAJA program, the production of ammonia is to be done in a microreactor consisting of supported catalyst in a nanoscale channels through which fluid passes and undergoes a chemical reaction. According to Akiti and Amanente (2004), in the order of tens to hundreds of nanometers in size, the very small cross-dimensions of these channels offer large surface area to volume ratios allowing for rapid heat and mass transfer. This small scale also creates a more efficient use of reactive sites, improving yield and selectivity. The addition of packing particles to these channels further improves their efficiency.

1.2 Problem Statement

Ineffective mixing in microreactors or micromixers is primarily due to the laminar flow behaviour of the fluid in the microfluid devices. This has become an important and significant key interest for researchers in the field of micro reaction engineering. Current researches done on mixing process includes experimental work, theoretical studies and numerical methods. The research is often done together with the simulation of Computational Fluid Dynamics. (Salim, 2011)

Falk (2010) stated that the design of micromixers is based upon trial-and-error process which usually results in inefficiencies and suboptimal design. The issues related to mixing are complicated, and at times counterintuitive. This is because the results are the outcome from complex process integration between fluid mechanics, mass transfers and reactions.

Nevertheless, it is costly for industry to apply the trial-and-error method for a new product within a commercial industry without accurate theoretical knowledge together with proper testing method and supported with modelling process. The occurrence of bad mixing, if any, may lead to cost increment and reduction of the end product. A handbook published recently on the topic of industrial mixing estimates the cost of poor mixing up to US$100 million per year. (Tekchandaney, 2009).Hence, modelling is important to predict the mixing behaviour prior to process designing. Through modelling and simulation, the mixing can be optimised using the trial-and-error of the parameters involved.

This project is the continuation on the previous design of the microreactor for ammonia synthesis. The work is to simulate various mixing inlet geometries in order to pre-mix nitrogen and hydrogen gases prior entering the microreactor. The Computational Fluid Dynamics (CFD) simulation will be utilised to predict the mixing behaviour and estimate the optimum localization of catalyst in the microreactor for the ammonia synthesis.

1.3 Objectives and Scope of Study

The objectives of this project are as the followings:

1. To simulate several microreactor inlet designs through CFD modelling.
2. To study and analyse the mixing behaviour of the developed microreactor.
3. To investigate the variability of several specified parameters on the mixing behaviour of microreactor.

Due to the wide and diverse area of study for micro reaction technology, this project will be restricted to phenomena related to hydrodynamics study for gas-gas phase medium only. The incoming stream used for this project will be the reactant for ammonia synthesis which is nitrogen gas (N_2) and hydrogen gas (H_2). The field of study will include the study of fluid mechanics and transport phenomena.

The scope of modelling development will be focused on the development of at least three (3) different inlet models for the microreactor. The model for the microreactor will be taken from the previous geometry developed in OneBAJA project and modified accordingly. ANSYS CFX 14.0 will be used to construct the geometries of the microreactor, grid designs, and simulate the mixing behaviour inside the microreactor.

CHAPTER 2 : LITERATURE REVIEW

2.1 Mixing

Global consumer nowadays demands products not only with better quality, but also innovative products from various industries (EmmanuelaGavi, 2010). All of these industries have one thing in common, which is the process that is involved. In products' manufacturing and synthesis industry, chemical reactions involve the flow of reactants or raw materials that are mixed in a channel or a chamber to produce the desired output.

In fluid mixing, the main objective is to obtain uniform distribution in the mixture solution, achieve homogenisation of components in the mixture and attain uniform properties. (Baldyga, 1990) Thus, the study on the scale of its variability is needed to distinguish the degree of homogenisation (Nunes, 2007). Several words are used for the term 'mixing'such as stirring, blending, agitation and kneading that differ from each other in terms of its definition. Nevertheless, the plausible definition defined by Aref (1984), which differentiate between mixing and stirring provides a suitable explanation that relates to the real mixing process.

The term 'mixing' is defined as the physical process where simultaneous action of stirring and diffusion occurs. The word stirring here means the transport of fluids due to bulk fluid movement during mixing without the diffusive action. This further emphasize that good mixing of low diffusivity materials happens at two levels; stirring in the first level and diffusion in the second level (Kang, 2011).

Nunes (2007) stated that there are three different scales of mixing; micromixing, mesomixing, and macromixing. Macromixing occurs at macroscopic scale involving large-scale flows which affects the large-scale distribution such as residence time distribution (RTD). Therefore, macromixing influences meso- and micromixing. Mesomixing is the dispersion of the feed just after it enters the mixer or reactor. The scale is approximately at the size of the reagent feed pipe, which is smaller than macromixing but larger than micromixing. (Edward, 2004; Baldyga, 1990).Micromixing, on the other hand, is the final mixing stage that relates to the contacts of fluids in microscopic or molecular scale. The degree of the contact is governed by the fine texture of the fluid and the dynamic force induced or applied at molecular level. The inhomogeneity doesn't have a direct effect on the mesomixing and macromixing process but it does have a quite strong effect at micromixing scale (Nunes, 2007).

Fluid mixing phenomenon can lead towards reaction when the contact between the fluids or reactants is likely to synthesize new product/s with the aid of catalyst. When the reaction occurs in a microfluidic environment, the term 'microreactor' is used to describe the state of the vessel applied to the reaction process. Microreaction technology is concerned with microstructured reactors (microreactor), capillary and tube reactors of small inner dimensions, and, to a lesser extent, mini-fixed bed or small sized foam reactors. (Hessel et al., 2007).The technology has attracted much interest recently from the scientific and industrial fraternity due to the performance observed that is much better than the conventional batch reactors (Mason et. al., 2007; Tu et. a.l, 2010).

The efficiency and success of many industrial processes are dependent on the mixing condition of the material. The mixing process and the distribution of the products highly influence the progress of the reactions especially when involving complex reactions such as competing chemical reactions. (Salim, 2011).Thus, knowledge on the influence of mixing on the behaviour of a chemical process is very crucial in controlling and optimizing the distribution of the products. This allows the opportunity for the improvement of the yield with efficient usage of raw materials and reduction of byproduct formation. (Baldyga, 1990)

Baldyga and Bourne (1990) stated that the objective of the mixing process is to distribute the components evenly and obtain homogenization of components in one another. The homogenization of components enables uniform properties of the mixture to be attained. The process includes the processing and the preparation of the reactants involved, the composition mixture (weighing process), the actual mixing process (mixing time and intensity) and post-sequential treatment of the product through downstream processing (Weinkötter, 2011). Subsequently, fluid mixing in channels with a submillimeter dimension is a fundamental operation in microfluidic devices. The flow in such microfluidic devices is laminar, making it challenging to mix the fluids, especially in a smooth simple microchannel (Nguyen & Wu, 2005).

The mixing of two streams at laminar flow region has evoked considerable interest because of its usage in micromixers, whereby the operating conditions and dimensions of the mixing system that prevents turbulence effects (Cemal, 2010). Judat et al. (2004) and Fourcadea et al. (2001) agreed that molecular scale mixing (micromixing) can drastically affect the selectivity, yield and quality of products in chemical processes including polymerization, organic synthesis, and crystallization.

The unique applications related with microchemical industry including microreactor, micromixer and microheat-exchanger is what made microreaction technology one of the most rapid development and innovative fields with on-going research in chemical engineering and related disciplines (Adeosun, 2009). In this study, the synthesis of ammonia through the reaction of nitrogen and hydrogen gases in microfluidic environment will be investigated through the manipulation of geometry variables that will induce the mixing phenomenon. The geometry developed through Computational Fluid Dynamics simulation is hoped to predict the optimum hydrodynamics condition of the mixing process, which would further identify the suitable localization of catalyst in the microreactorleading to the synthesis of ammonia.

2.2 Mixing Index

Mixing index is one of the characteristic quantities for mixing. Maeng et al. (2006) studied on the model for fluid mixing in passive micromixers and proposed the definition of mixing index as follows.

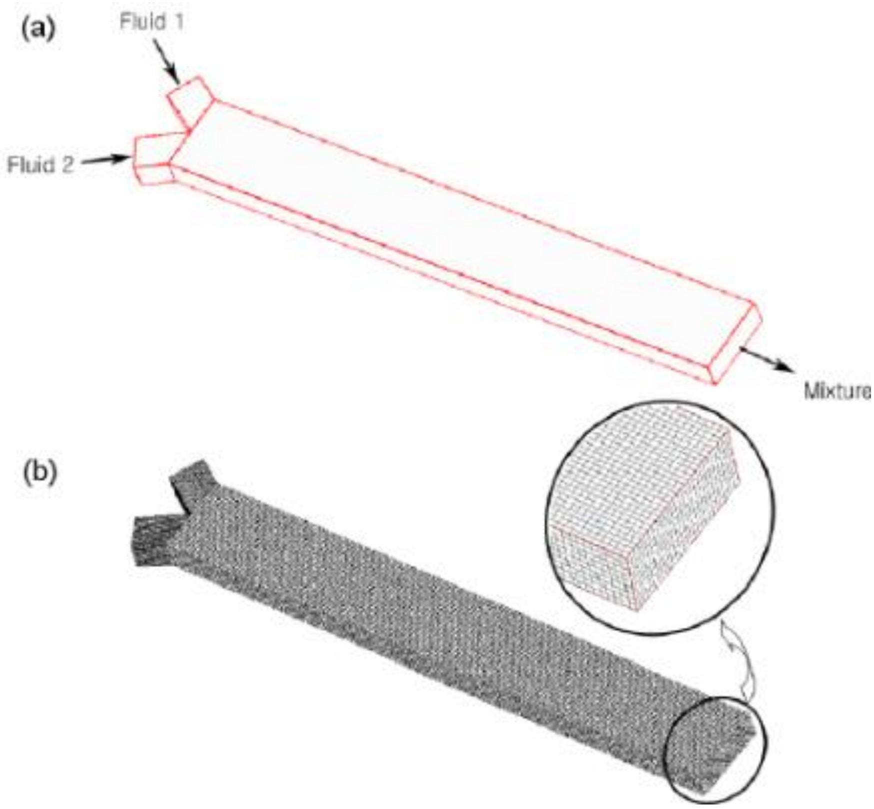


FIGURE 2-1: Y-shaped microchannel and generated grid (Maeng, Yoo, & Song, 2006)

Maeng et al. (2006) investigated the mixing of two fluids inserted into the Y-shaped microchannel as shown in Figure 1(a). The microchannel is divided into small volumes through grid generation as shown in Figure 1(b).

The mixing index (M) to quantify mixing in the microchannel is defined using the equation below:

$$M = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_i - C_{in})^2}$$

where C_i is the local, dimensionless concentration at a node of a given cross section channel, C_{in} is the dimensionless, average concentration at the inlet, at the junction of the Y-shape channel and N is the number of nodes at the cross section. The mixing index is equal to 0 at complete mixing of both fluids and 0.5 at the inlet.

2.3 Micromixer/Microreactor Introduction

Tu et al. (2010) reviewed on the development of micro reaction technologies and concluded that micro reaction technologies have attracted much interest and attention from the scientific and industrial community.

Micro reaction technology is concerned with microstructured reactors (microreactor), capillary and tube reactors of small inner dimensions, and, to a lesser extent, mini-fixed bed or small sized foam reactors. (Hessel et al., 2007)

The term “micromixer” and/or “microreactor” in the context of present invention are devices that comprise of microfluidic channels at micrometer dimensions. Thus, this term will be used interchangeably in this report.

According to Mason et al. (2007), micro reaction technology device specifically microreactors have been used in many reaction recently, and the performance of the microreactors are much better than conventional batch reactors.

The efficiency and success of many industrial processes is dependent on the mixing condition of the material. The mixing process and the distribution of the products highly influence the progress of the reactions especially when involving complex reactions such as competing chemical reactions. (Salim, 2011)

Thus, knowledge on the influence of mixing on the behaviour of a chemical process is very crucial in controlling and optimizing the distribution of the products. This allows the opportunity for the improvement of the yield with efficient usage of raw materials and reduction of byproduct formation. (Baldyga, 1990)

Baldyga and Bourne (1990) stated that the objective of the mixing process is to distribute the components evenly and obtain homogenization of components in one another. The homogenization of components enables uniform properties of the mixture to be attained. The mixing process includes the processing and the preparation of the reactants involving the composition mixture (weighing process), the actual mixing process (mixing time and intensity) and post sequential treatment of the product through downstream processing. (Dr. R Weinkötter, 2011)

Subsequently, fluid mixing in channels with a sub-millimeter dimension is a fundamental operation in microfluidic devices. The flow in such microfluidic devices is laminar, making it difficult to mix the fluids especially in a smooth simple microchannel. (Nguyen and Wu, 2005)

The mixing of two streams at laminar flow region has evoked considerable interest because of its usage in micromixers whereby the operating conditions and dimensions of the mixing system that prevents turbulence effects. (Cemal, 2010)

Judat et al. (2004) and Fourcadea et al. (2001) agreed that, molecular scale mixing (micromixing) can drastically affect the selectivity, yield and quality of products in chemical processes including polymerization, organic synthesis, and crystallization.

The unique applications related with microchemical industry including microreactor, micromixer, micro heat exchanger, and etc. is what made micro reaction technology one of the most rapid development and innovative fields with on-going research in chemical engineering and related disciplines. (John T. Adeosun, 2009)

2.4 Computational Fluid Dynamics (CFD) Introduction

CFD is termed as the art of predicting flow in fluid, mass and heat transfer, chemical reactions, and etc. through solving the mathematical equations involved in the process. A numerical method is used to solve the equations. Bakker (2008) highlighted the usage of result from CFD analysis as relevant engineering data in detailed product development, conceptual studies of new design, redesign and also troubleshooting.

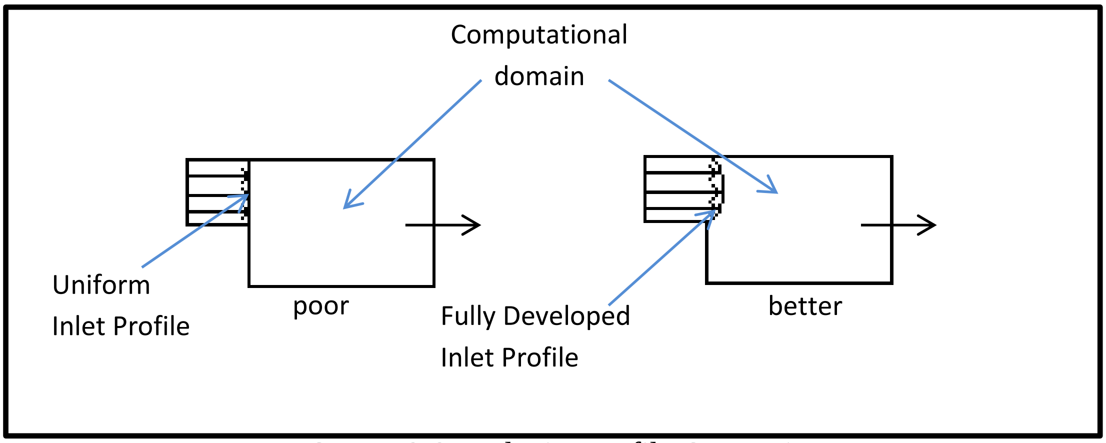


FIGURE 2-2: Velocity Profile Comparison

CFD provides additional valuable insight in developing and demonstrating technologies required to realize efficient and compact reactors. The basic CFD problems or simulation usually uses the Navier-Stokes equations, which defines single-phase fluid flow. Besides that, the Euler equations are also used which is the simplified equation from the Navier-Stokes equations by removing viscosity describing terms. The important consideration in CFD is using the correct way of treating a continuous fluid in a discretized manner on a computer.

2.5 State of the Art Micromixers

Micromixers are classified into two categories which are active and passive micromixers. (Shakhawat Hossain, 2009), (Ling-Sheng Jang, 2009)

An active micromixer uses mechanism or external source to induce mixing where else passive micromixer do not require external energy for mixing. The mixing process depends on diffusion and chaotic advection.

TABLE 2.1: Classifications of Micromixing (Ling-Sheng Jang, 2009)

Active Mixers	Passive Mixers
• Pressure field disturbance • Electro-hydrodynamic disturbance • Dielectrophoretic disturbance • Electro-kinetic disturbance • Magneto-hydrodynamic disturbance • Droplet shaking by electrowetting	• Injection • Droplet • Multi-lamination micromixers • Chaotic micromixers

According to John T. Adeosun (2009), active micromixers are more complex and difficult to operate, fabricate and integrate into the microfluidic environment. Due to this, passive mixers are the most used in microfluidic applications because of its simplicity.

Since the yield and selectivity of chemical processes highly depends on mixing, the selection of mixing devices often influences the profitability of the process.(Salim, 2011)

In this research, the mixing performances are investigated. Different geometric regime and configuration are studied to facilitate mixing.

2.6 Related Works

Throughout the simulation of the project, the operating conditions needs to be constant to achieve good and accurate results based on the real process. Baldyga (1990) reported many factors that can affect the mixing behaviour and these factors vary depending on the type of industries process. However, the typical factors that affect mixing are usually pressure, temperature, surface area and velocity. For this project, the scope of study includes the following factors:

a) Geometry design
b) Inflow configuration

a. Geometric design

Improvement of the geometric design can further improve the mixing behaviour of fluids. According to J. M. Miranda (2010) and Elmabruk A. Mansur (2008), additional parts in geometries such as obstacles, sharp bends, slanted walls or junctions can cause discontinuity of fluid flow and increase the mixing performance. The molecules interact with each other when the fluid flows through sharp bends due to the change in flow direction. An improvement in mixing performance can be obtained by utilising this lateral flow field.

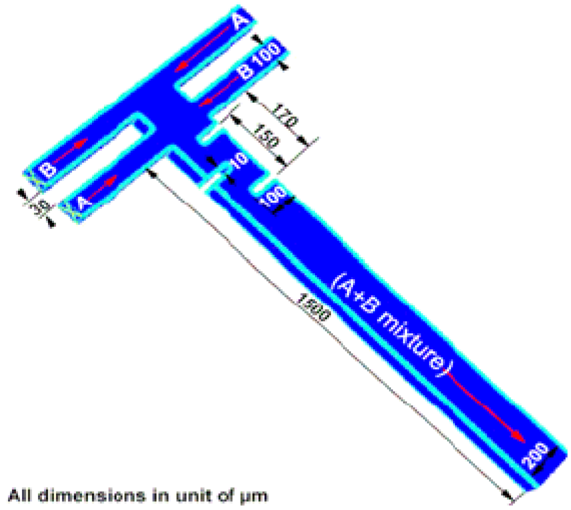


FIGURE 2-3: Passive DT-micromixer(Elmabruk A. Mansur, 2008)

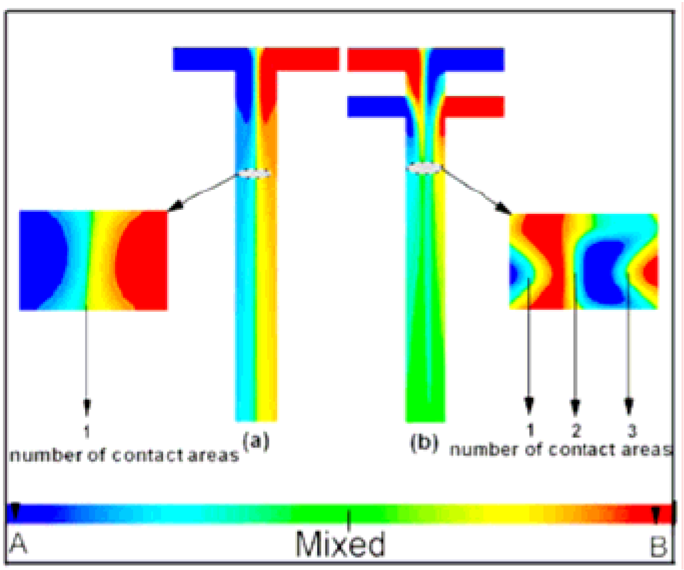


FIGURE 2-4: Mass fraction contour in T- and DT-micromixer

Elmabruk A. Mansur (2008) analysed the flow behaviour in T- and DT-micromixers under laminar conditions. From the simulations, DT-micromixer gives a better mixing performance than T-micromixer. The number of contact area in DT-micromixer is more than the number of contact area in T-micromixer, reducing the molecular diffusion distance to achieve mixing.

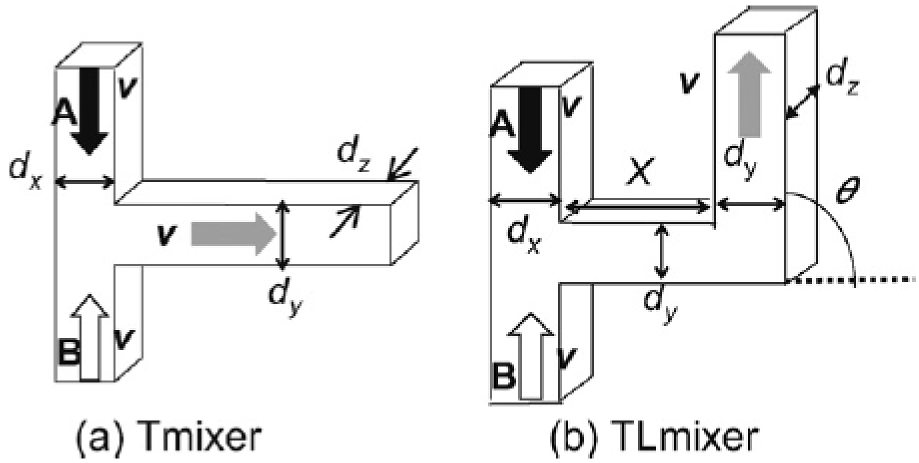


FIGURE 2-5: Schematic of T-mixer and TL-mixer (N. Aoki, 2010)

N. Aoki (2010) studied the effects of channel confluence and bends on mixing performance and found out that the combination of channel confluence and bend (TL-mixer) gives a better mixing performance.

b. Inflow configuration

The inflow configuration in this project is defined as how the reactant gas N_2 and H_2 come into contact at mixing. The N_2 stream may be the main stream with the H_2 stream joining as the minor stream or vice versa.

Up to now, there is no direct investigation on the how the inflow come in contact will affect the mixing efficiency. However, Wang et al. (2005) and Le (2006) stated that the density effect and the difference in molecular weight will have an effect on the mixing performance.

Wang & Li (2005) simulated the gas mixing in microchannel with the two gas species are at equal molecular masses to avoid the density effect on the investigation of the flow mixing behaviour.

Le (2006) investigated the effect of gas species on the mixing performance by using helium gas flow and argon gas flow and reported that the speed of the helium gas flow is greater than that of the argon flow with the velocity difference increasing with an increasing pressure ratio between the inlet and the outlet flow in the microchannel. The lighter gas which is helium is more sensitive to pressure drop and gains acceleration as the pressure drop increase, giving a higher difference in velocity.

CHAPTER 3 : METHODOLOGY

3.1 Introduction

The project utilizes ANSYS CFX 14.0 to investigate the hydrodynamics during the mixing of N_2 and H_2 gases in the microfluidic environment. There are three major processes in CFD modelling which includes problem identification and pre-processing, solver execution, and post processing. Figure 3.1 below illustrates the works that are carried out during the course of this project.

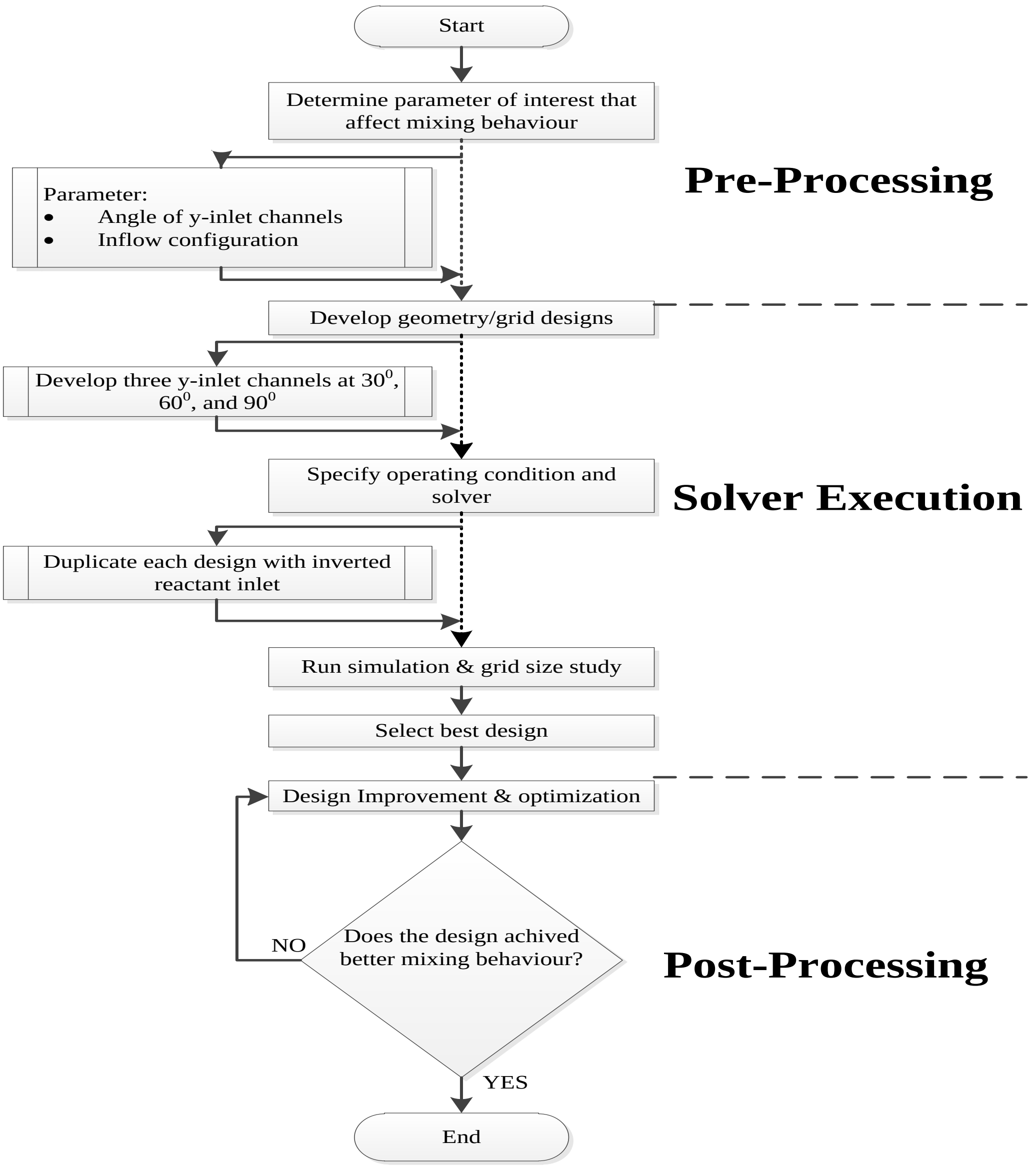


FIGURE 3-1: Block Diagram for Simulation Flow

3.2 Pre-processing

The pre-processing phase is the preparation of the model that is needed for the simulation to be done. This includes the creation or modification of the geometry, meshing of the geometries and setup of the physical properties for the simulation.

3.2.1 Geometry

The geometry is produced in the computer-aided design (CAD) system. ANSYS Design Modeler software is the user interface for geometry handling and analysis. ANSYS Design Modeler has connection to all major CAD systems, allowing easy transfer of existing data including the parameters from other CAD software. The parameters can then be adjusted and the design can also be updated with the addition of feature removal or simplification.

For this project, three different inlet geometries are used. The geometries are modified from the previously proposed geometry for the microreactor done by Rosli (2012). These geometries can have different parameters in order to study the effect of it towards fluids mixing pattern and its characteristics. The table below shows the configuration for the geometries.

TABLE 3.1: Inlet Geometry Configuration

Case Studies	Parameter To Be Test	Variables
Case Study 1	Angle of y-inlet	• 30^o • 60^o • 90^o
Case Study 2	Inflow configuration	• Hydrogen in main flow with nitrogen entering from the side • Nitrogen in main flow with hydrogen entering from the side

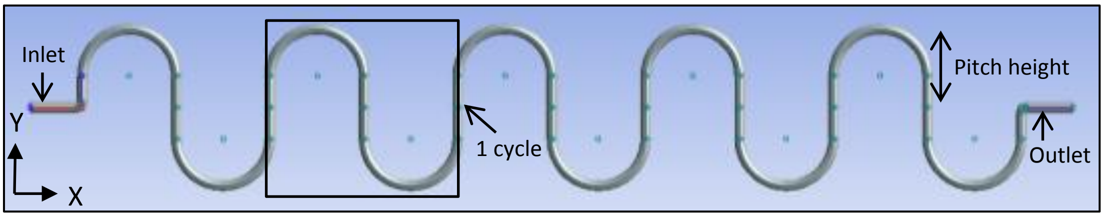


FIGURE 3-2: General microreactor geometry (Rosli, 2012)

The figures for the inlet geometries are shown in Figure 3.3 (a) to (f):

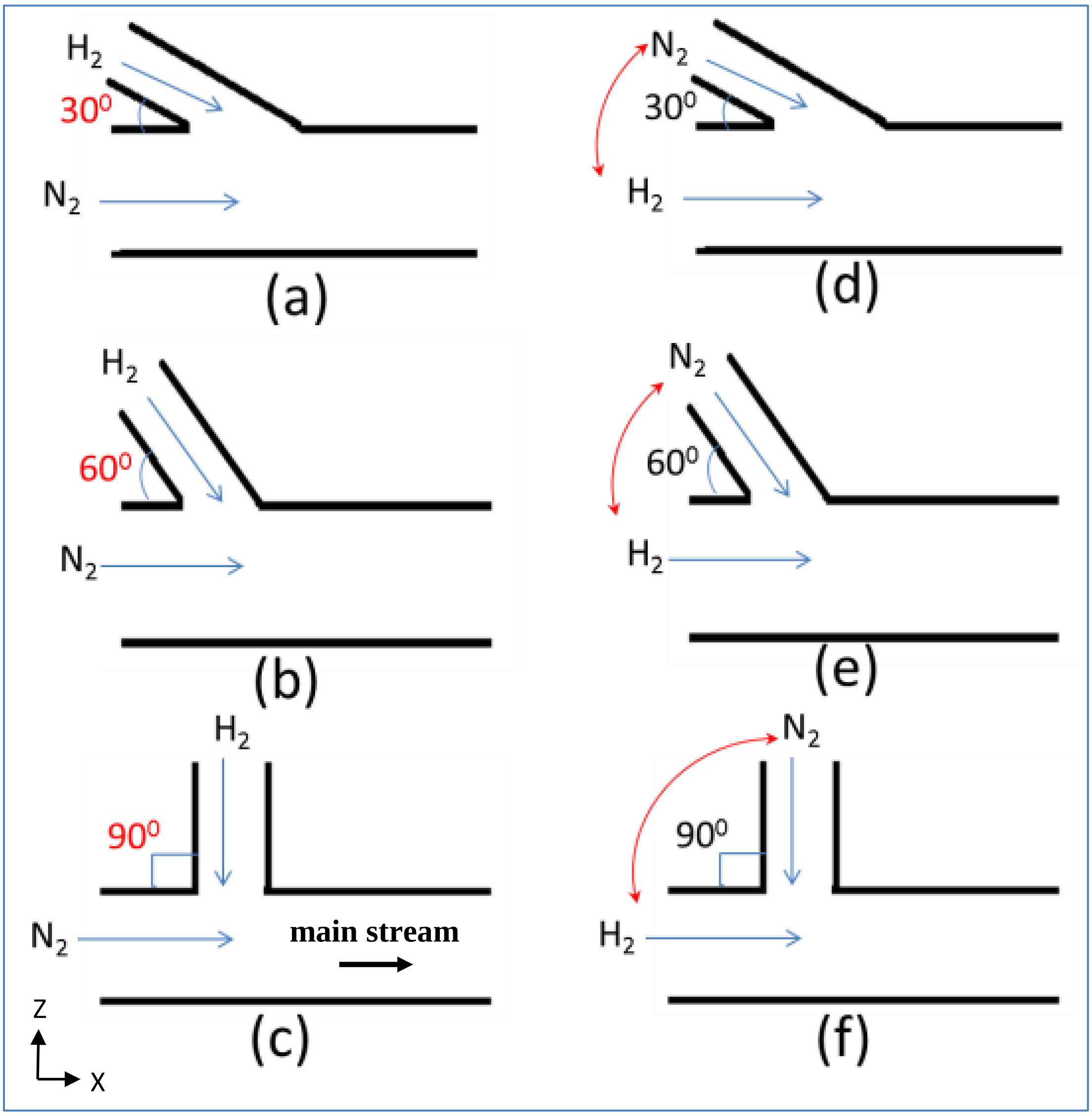


FIGURE 3-3: (a) Inlet geometry of 30^0 and nitrogen in the main stream, (b) Inlet geometry of 30^0 and hydrogen in the main stream, (c) Inlet geometry of 60^0 and nitrogen in the main stream, (d) Inlet geometry of 60^0 and hydrogen in the main stream, (e) Inlet geometry of 90^0 and nitrogen in the main stream, (f) Inlet geometry of 90^0 and hydrogen in the main stream.

The proposed geometry by Rosli (2012) has a cycle number of 5 and a pitch height of 0.15 cm. Figure 3.2 shows the microreactor on the XY-axis.The inlet geometries as in Figure 3.3 are construced in the XZ-axis. In Figure 3.3 (c), the main stream refers to the flow in the direction of X-axis.

3.2.2 Mesh

The meshing of the geometry will determine the accuracy of the simulation done. A generated mesh with too many cells may take a long time to solve, while a generated mesh with too few cells may give inaccurate result.

However, the meshing properties can be optimized to obtain the most appropriate mesh quality for an accurate result. A grid sensitivity study is done to analyse different meshing properties to find the appropriate meshing. Many meshing properties that need to be considered but in this project only the number of nodes and elements together with the orthogonal quality are considered. The orthogonal quality is considered as to see the grid quality in terms of the angle at the point of intersection between cells. The angle nearing to 90^0 between the cells give a better distribution among the cells in the grid. The orthogonal quality calculated is between 0 and 1 where the best cells will have an orthogonal quality of 1.

For the grid sensitivity analysis, meshed geometries with 4 different total numbers of nodes ranging from 200,000 nodes to 510,000 nodes (maximum number of nodes due to licensing limitation) are created for analysis.

The selected meshing properties are used for the other simulations for constant and accurate result. Figure below shows the detail of meshing parameters that have been used for this project.

Details of "Mesh"

Defaults	
Physics Preference	CFD
Solver Preference	CFX
Relevance	0
Sizing	
Use Advanced Size Function	On: Curvature
Relevance Center	Fine
Initial Size Seed	Active Assembly
Smoothing	Medium
Transition	Slow
Span Angle Center	Fine
Curvature Normal Angle	46.50 °
Min Size	1.e-006 m
Max Face Size	1.e-004 m
Max Size	4.e-004 m
Growth Rate	1.0
Minimum Edge Length	1.9101e-005 m
Inflation	
Patch Conforming Options	
Triangle Surface Mesher	Program Controlled
Advanced	
Defeaturing	
Statistics	
Nodes	509988
Elements	2354534
Mesh Metric	Orthogonal Quality
Min	0.219441781280483
Max	0.997844017837099
Average	0.853885022276322
Standard Deviation	8.86822094636258E-02

FIGURE 3-4: Mesh Properties

The mesh properties are inputted before meshing is done. The curvature normal angle is adjusted to acquire the desired number of nodes.

3.2.3 Setup

The setup defines the material and other parameters in the simulation. Several parameters are determined which includes the boundary condition, meshing domain physics and the boundary physics. The settings for all of these are as the figures below.

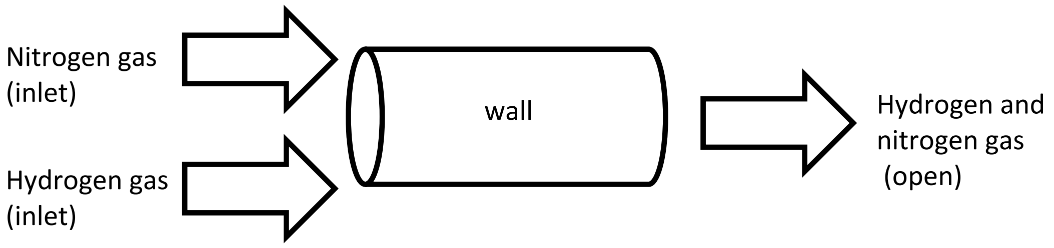


FIGURE 3-5: Boundary Condition

Domain - Default Domain	
Type	Fluid
Location	B39
Materials	
H2 at STP	
Fluid Definition	Material Library
Morphology	Continuous Fluid
N2 at STP	
Fluid Definition	Material Library
Morphology	Continuous Fluid
Settings	
Buoyancy Model	Non Buoyant
Domain Motion	Stationary
Reference Pressure	1.0000e+00 [atm]
Heat Transfer Model	Isothermal
Fluid Temperature	2.5000e+01 [C]
Homogeneous Model	On
Turbulence Model	k epsilon
Turbulent Wall Functions	Scalable

FIGURE 3-6: Domain Physics for CFX

Domain	Boundaries	
Default Domain	**Boundary - hydrogen inlet**	
	Type	INLET
	Location	F84.39
	Settings	
	Flow Regime	Subsonic
	Mass And Momentum	Normal Speed
	Normal Speed	3.3300e+00 [m s^-1]
	Turbulence	Medium Intensity and Eddy Viscosity Ratio
	Fluid	hydrogen
	Volume Fraction	Value
	Volume Fraction	1.0000e+00
	Fluid	nitrogen
	Volume Fraction	Value
	Volume Fraction	0.0000e+00
	Boundary - nitrogen inlet	
	Type	INLET
	Location	F74.39
	Settings	
	Flow Regime	Subsonic
	Mass And Momentum	Normal Speed
	Normal Speed	3.3300e+00 [m s^-1]
	Turbulence	Medium Intensity and Eddy Viscosity Ratio
	Fluid	hydrogen
	Volume Fraction	Value
	Volume Fraction	0.0000e+00
	Fluid	nitrogen
	Volume Fraction	Value
	Volume Fraction	1.0000e+00
	Boundary - out	
	Type	OPENING

	Location	F75.39
	Settings	
	Flow Direction	Normal to Boundary Condition
	Flow Regime	Subsonic
	Mass And Momentum	Opening Pressure and Direction
	Relative Pressure	0.0000e+00 [Pa]
	Turbulence	Medium Intensity and Eddy Viscosity Ratio
	Fluid	hydrogen
	Volume Fraction	Zero Gradient
	Fluid	nitrogen
	Volume Fraction	Zero Gradient
	Boundary - wall	
	Type	WALL
	Location	F40.39, F41.39, F42.39, F43.39, F44.39, F45.39, F46.39, F47.39, F48.39, F49.39, F50.39, F51.39, F52.39, F53.39, F54.39, F55.39, F56.39, F57.39, F58.39, F59.39, F60.39, F61.39, F62.39, F63.39, F64.39, F65.39, F66.39, F67.39, F68.39, F69.39, F70.39, F71.39, F72.39, F73.39, F85.39
	Settings	
	Mass And Momentum	No Slip Wall
	Wall Roughness	Smooth Wall

FIGURE 3-7: Physics Boundary

The inlet configurations are changed depending on the requirement for the study case for the inflow of nitrogen and hydrogen gas.

3.3 Solver Execution

The phase where the software computes the solution is named the Solver Execution in ANSYS CFX. The software solves the discretized conservation equation in an iterative manner until it converges to one value. The accuracy of a converged solution depends on the accuracy of the developed geometry, the meshing quality, the assumptions made and additional numerical errors.

3.4 Post Processing

The post-processing involves the analysis of the results. ANSYS offers a complete set of post-processing tools for displaying the results on the models as contours or vector plots. The tools allow the user to get more detailed results over given parts of the geometries.

3.5 Governing Equations

In this project, the fluid is assumed to be incompressible. The Mach number (the ratio of the flow velocity to the local speed of sound) at the inlet and throughout the microchannel of the microreactor is 0.01 and 0.02 respectively. Since the Mach number is less than 0.3, the gas flow in the system is considered to be incompressible. The constant flow of an incompressible Newtonian fluid in micro channels can be described by the Navier-Stokes equation and continuity equation. In addition, the species distribution follows the diffusion convective equation with the adoption of no-slip boundary.

For incompressible fluid, the continuity equation is

$$\frac{\partial u_k}{\partial x_k} = 0 \tag{1}$$

and the momentum equation is

$$\frac{\partial(\rho u_j u_i)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(-P\delta_{ij} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) + \rho g_i \tag{2}$$

where

P = pressure;

u = velocity;

i,j,k = cartesian axis;

x = cartesian coordinate direction;

δ_{ij} = 1 if i = j and 0 if otherwise;

μ = dynamic viscosity;

ρ = density.

The convective diffusion equation is

$$\frac{\partial c}{\partial t} + \frac{\partial u_k(c)}{\partial x_k} = D\frac{\partial^2}{\partial x}c \tag{3}$$

where

c = concentration;

t = time;

D = diffusivity

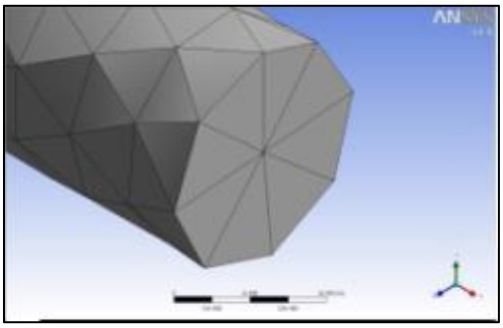
3.6 Tools

The software used for the CFD simulation is ANSYS CFX 14.0

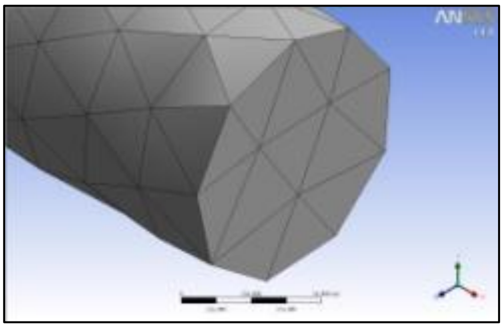
CHAPTER 4 : RESULTS AND DISCUSSION

4.1 Grid Sensitivity Study

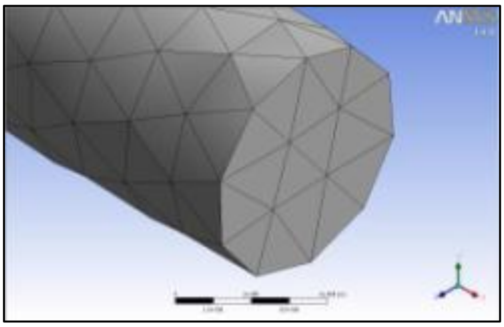
For evaluation of the optimum mesh size, a grid sensitivity study was conducted. This study helps to produce accurate results and findings with less computation errors as compared to other mesh sizing. The velocity parameter was chosen as the reference for evaluating the mesh sizes. The location selected is at the outlet of the geometry. The mesh size evaluated is at 250,000 nodes, 330,000 nodes, 410,000 nodes and 510,000 nodes. The results of the meshing and the velocity profile for each meshing are shown in Figure 4.1:



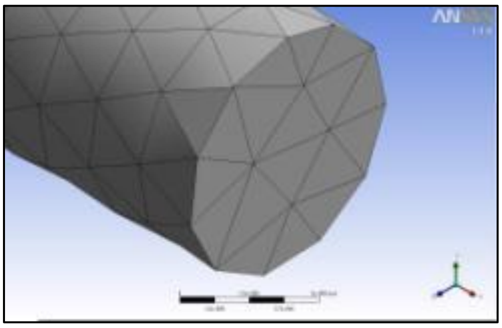
(a)



(b)



(c)



(d)

FIGURE 4-1: Meshing (a) 250,000 nodes (b) 330,000 nodes (c) 410,000 nodes (d) 510,000 nodes

The nitrogen velocity profiles at the outlet are shown in Figure 4.2:

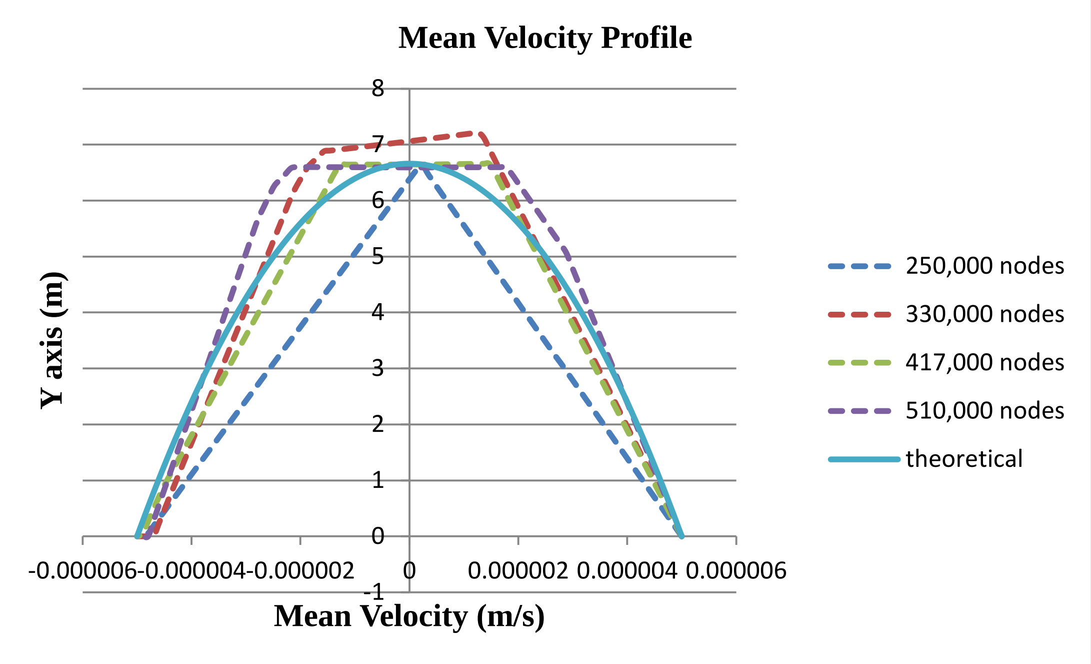


FIGURE 4-2: Nitrogen Velocity Profile

The actual number of nodes and elements together with the orthogonal factor and the time to complete simulation is as Table 4.1:

TABLE 4.1: Meshed properties

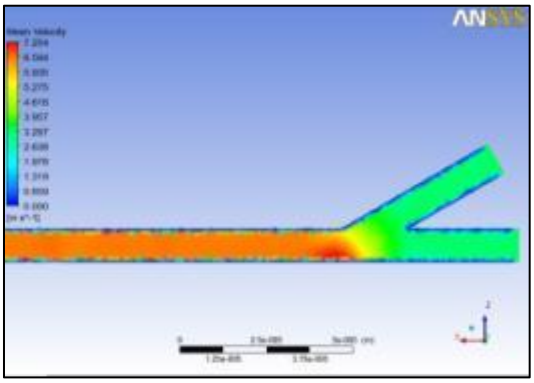
Nodes	Actual no. nodes	Elements	Orthogonal Factor				Simulation time (min.)
			Min.	Max.	Average	Standard deviation	
250k	248,347	1,024,355	0.212	0.997	0.86	9.02	10
330k	330,034	1,444,149	0.213	0.996	0.85	9.10	47
417k	417,800	1,880,572	0.173	0.997	0.85	8.87	19
510k	509,988	2,354,534	0.220	0.998	0.85	8.87	28

For geometry at a microscale, the nitrogen velocity profile for all the mesh quality does not reflect the real velocity profile; the profile should show for laminar flow behaviour. The addition of two inlets for the geometry disrupts the balance of the meshing distribution as compared from the meshing before adding the inlets. As a result, more nodes are needed to provide accurate results. Unfortunately, the limit for the licensed software is only at 512,000 nodes.

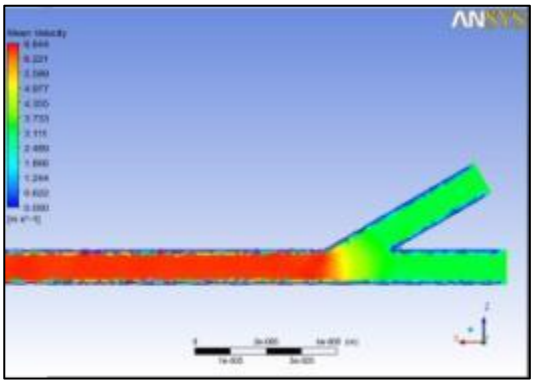
With reference to the simulation time and the orthogonal factor, the higher the orthogonal factor represents a better mesh quality and a larger number of nodes usually requires a longer time for the solver to run. The meshing at 330,000 nodes took the longest time. This may be due to the unevenly distributed element quality and node quality given by the highest orthogonal factor standard deviation. The meshing at 417,000 nodes and 510,000 nodes shows similar orthogonal factor although there is a difference in the simulation time. However, the nitrogen velocity profiles for the mesh at 510,000 nodes (Figure 4.8) shows a better distribution of velocity across the tabulated line, hence gives a better representation of the actual/theoretical fluid flow in the microchannel.

Based on the study, the mesh quality of 510,000 nodes is chosen solely due to the licensing limitation of the software. The meshing at 510,000 nodes gives a better representation of the flow although it is not accurate. Nevertheless, modifications can be made to evenly distribute the element quality throughout the geometry especially at the center to provide better accuracy.

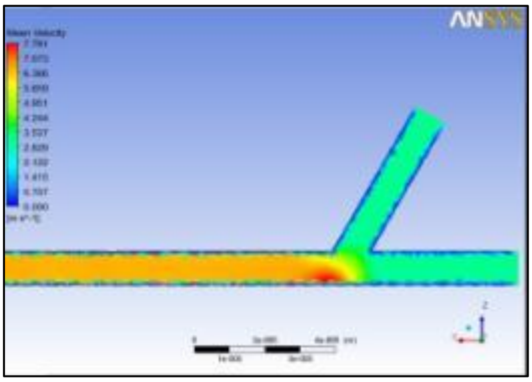
4.2 Contour



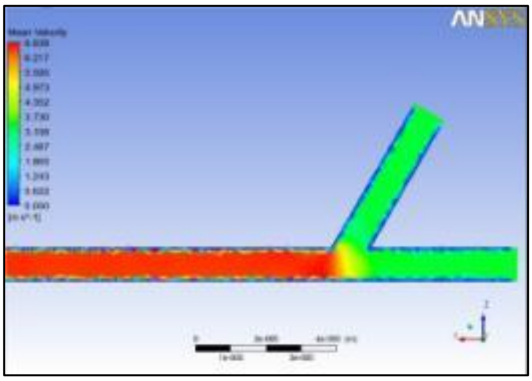
(a)



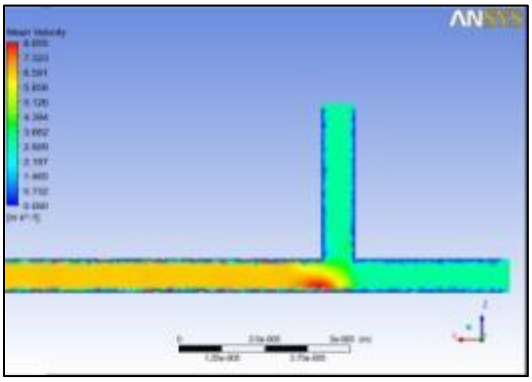
(b)



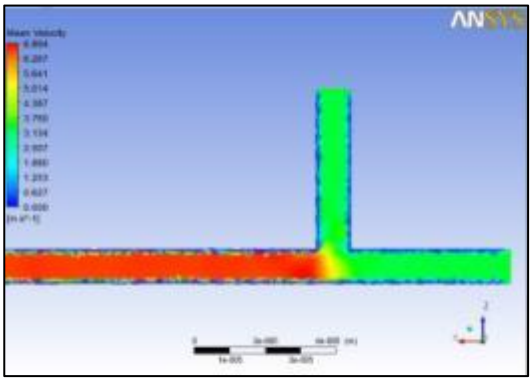
(c)



(d)

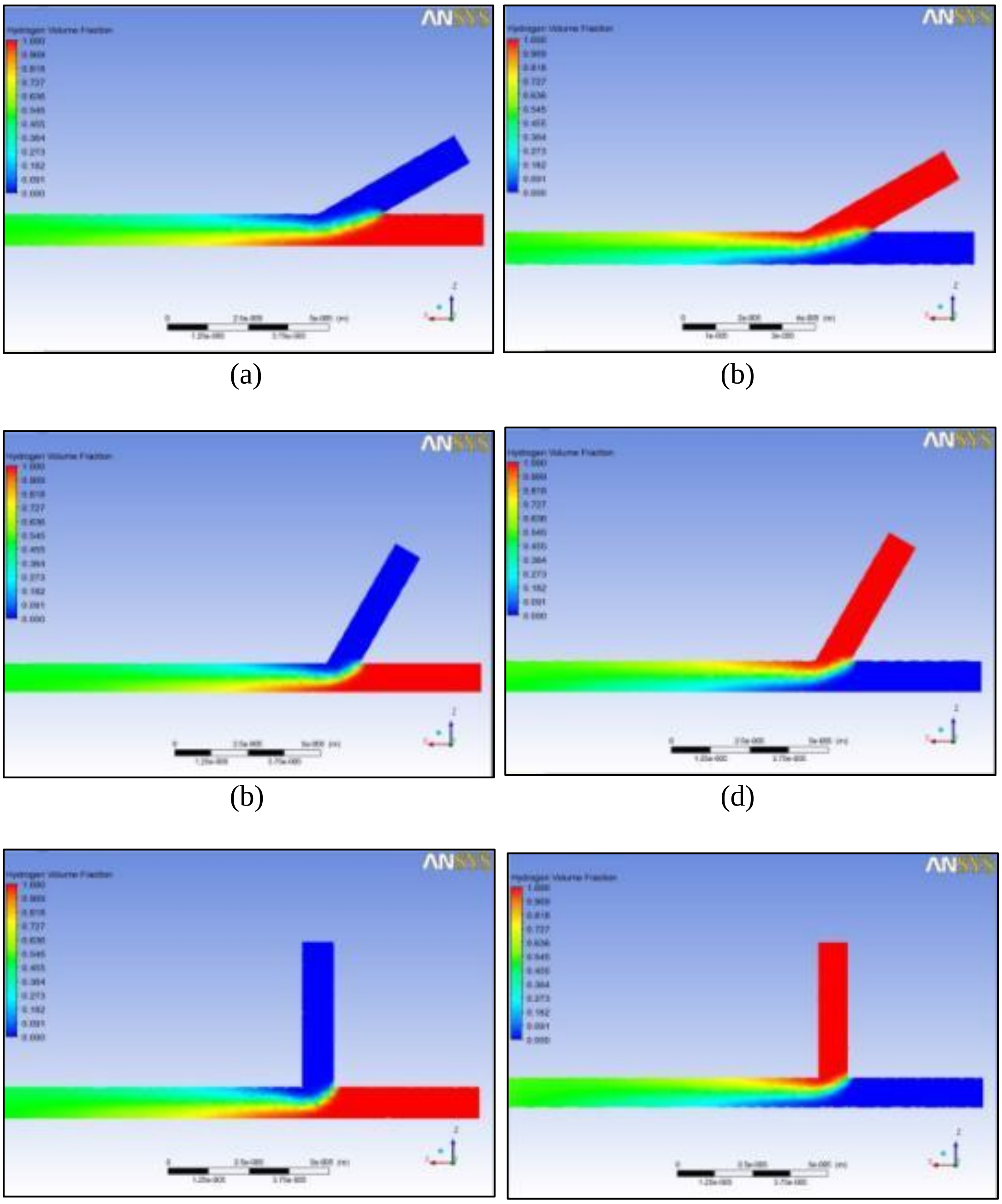


(e)



(f)

FIGURE 4-3: Velocity contour plot: (a) Inlet geometry of 30^0 and hydrogen in the main stream, (b) Inlet geometry of 30^0 and nitrogen in the main stream, (c) Inlet geometry of 60^0 and hydrogen in the main stream, (d) Inlet geometry of 60^0 and nitrogen in the main stream, (e) Inlet geometry of 90^0 and hydrogen in the main stream, (f) Inlet geometry of 90^0 and nitrogen in the main stream



(a) (b)

(b) (d)

(c) (f)

FIGURE 4-4: Hydrogen fraction contour (a) Inlet geometry of 30^0 and hydrogen in the main stream, (b) Inlet geometry of 30^0 and nitrogen in the main stream, (c) Inlet geometry of 60^0 and hydrogen in the main stream, (d) Inlet geometry of 60^0 and nitrogen in the main stream, (e) Inlet geometry of 90^0 and hydrogen in the main stream, (f) Inlet geometry of 90^0 and nitrogen in the main stream

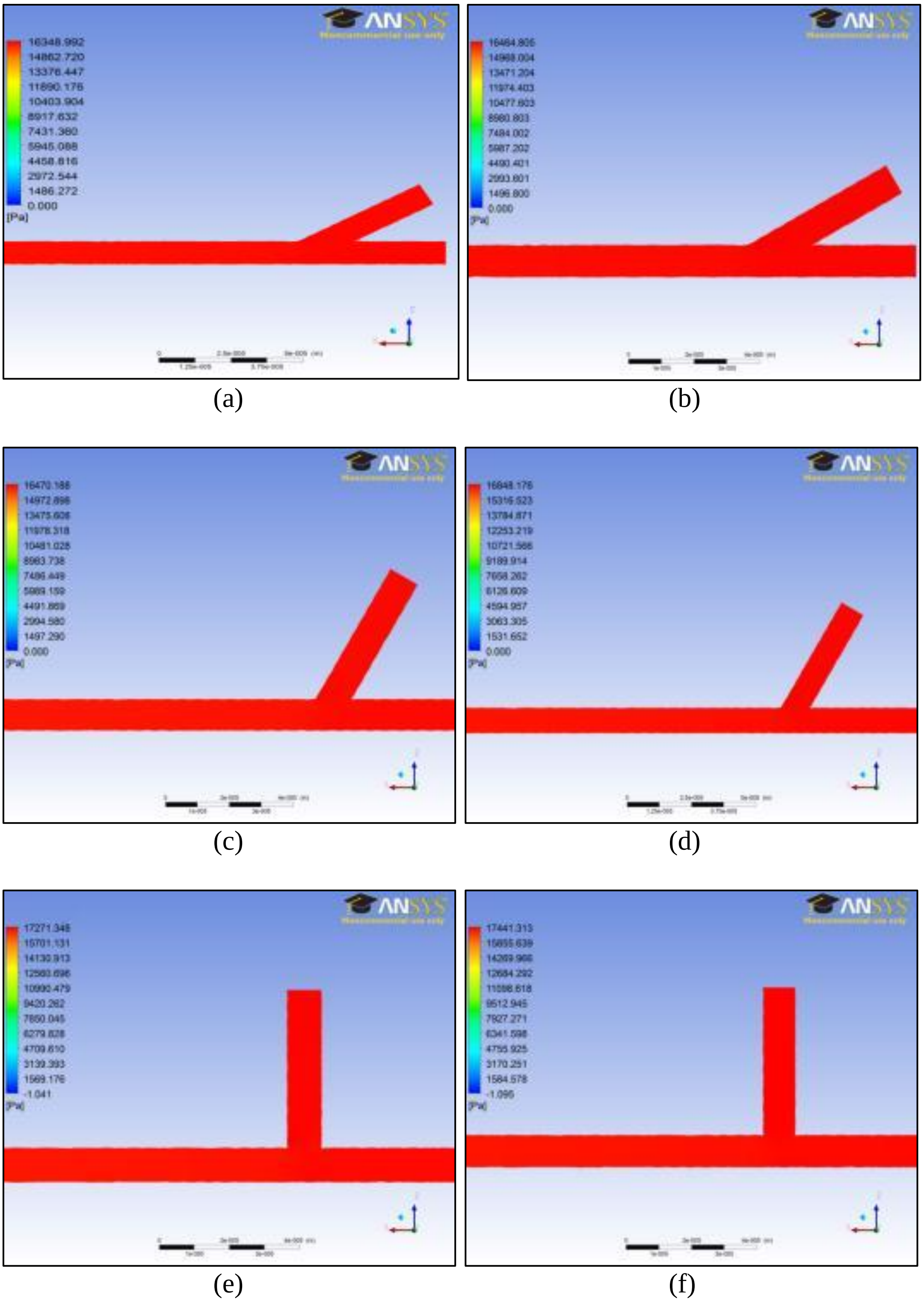


FIGURE 4-5: Pressure contour plot for (a) Inlet geometry of 30^0 and hydrogen in the main stream, (b) Inlet geometry of 30^0 and nitrogen in the main stream, (c) Inlet geometry of 60^0 and hydrogen in the main stream, (d) Inlet geometry of 60^0 and nitrogen in the main stream, (e) Inlet geometry of 90^0 and hydrogen in the main stream, (f) Inlet geometry of 90^0 and nitrogen in the main stream

Salim (2011) highlighted the inter-relation of velocity and velocity pressure as below:

$$Q = 0.5\rho V^2$$

where,

Q = velocity pressure (pascal);

ρ = density (kg/m^3);

V = velocity (m/s).

According to the equation, a higher velocity gives a higher velocity pressure at constant density. At constant inlet velocity of 3.33m/s for each species, the components interact and have contact with each other throughout the microchannel especially at the point of first contact (Y or T junction) in the microreactor. Higher interaction of the components will have a higher probability for better mixing.

The velocity profile in Figure 4.3 shows several apparent differences in the velocity profile. Figures 4.3 (b), (d) and (f) show a higher overall mean velocity. Meanwhile, Figures 4.3 (a), (c) and (e) shows a visibly higher velocity at the junction. The significant difference is due to the momentum effect of the components with respect to the component setup (hydrogen or nitrogen in the main stream). For Figures 4.3 (a), (c) and (e), the higher molecular weight of nitrogen gas compared to the molecular weight of hydrogen caused a sudden disrupt in flow at the junction when nitrogen gas enters the main stream and decreases the overall velocity. The situation is vice versa for Figures 4.3 (a), (c) and (e) where the nitrogen gas in the main stream can maintain its momentum despite the entrance of hydrogen gas in the main stream.

According to Banaszek (2010) and Salim (2011), mixing process occurs mainly in the red colour area of the velocity contour with slow mixing in the blue colour area. Thus, the areas with high velocities show high interaction and mixing rate. It is expected that the velocity pressure is also high at high velocities. However, the pressure contour near the inlet as per Figure 4.5 doesn't show any significant increase due to only small difference in velocity near the inlet. Nevertheless, when viewing the overall microreactor contours, the pressure contour in Appendix C shows a visible decrease of pressure together with a decrease of velocity in the velocity contour (Appendix B).

Salim (2011) also stated that the process of mixing two or more components will continue until the mixture is uniform in composition. From the hydrogen volume fraction contour in Figure 4.4, blue and red hues correspond to the hydrogen volume fraction of 0 and 1, respectively, whereas the green tone corresponding to a volume fraction of 0.5. It is observed that the mixture will reach a near uniform composition (green-yellow colour) after flowing in a certain length in the microchannel. The volume fraction will not reach a uniform and constant composition due to changes in the mean velocity throughout the microchannel. The microchannel length for the fluid to reach homogeneous condition is discussed in the entrance effect part of this discussion.

As a whole, from the contour study of velocity, pressure and volume fraction, it is observed that the setup of having hydrogen in the main stream gives a better mixing at the junction due to the disruption or discontinuity of fluid flow from the momentum of the entering nitrogen. This coincides with Salim (2011) which mentioned that having geometry with sudden bends, junctions or obstacles can lead to discontinuity in the flow of fluid and enhance the mixing performance. The disruption at the junction gives rise to interaction between hydrogen and nitrogen molecules which increases mixing performance. Yet, the optimum angle of inlet for mixing cannot be determined with the velocity contour only. The selection is made based on the discussion in the entrance effect part of the discussion.

Meanwhile, according to the microreactor contour plot in Appendix B and C, there is no distinct or specific location with a higher mixing rate throughout the microchannel in the microreactor. This may be due to the meshing quality of the geometry which is limited at 510,000 nodes due to license limitation. Thus, the results from the simulation could produce less accuracy. In addition, the design of the microreactor may also contribute to the mixing behaviour. The radius of the curves in the cycle may be too large that the fluid flow is not disrupted to induce mixing.

Nevertheless, as there is no specific site along the microchannel in the microreactor with a higher mixing rate, the catalyst for the H_2 and N_2 reaction (ammonia synthesis) is proposed to be placed uniformly throughout the microreactor.

4.3 Entrance effect on hydrogen volume fraction

The entrance effect of different angle of inlet is studied on the hydrogen fraction. Six locations on x-axis were selected depending on the degree of homogeneity based on the hydrogen volume fraction. The location selected for the analysis are at X = 50µm, 234µm, 418µm, 602µm, 786µm and 970µm, respectively.

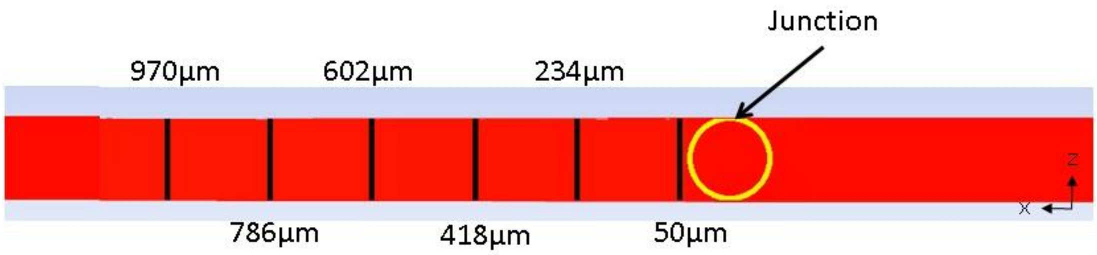
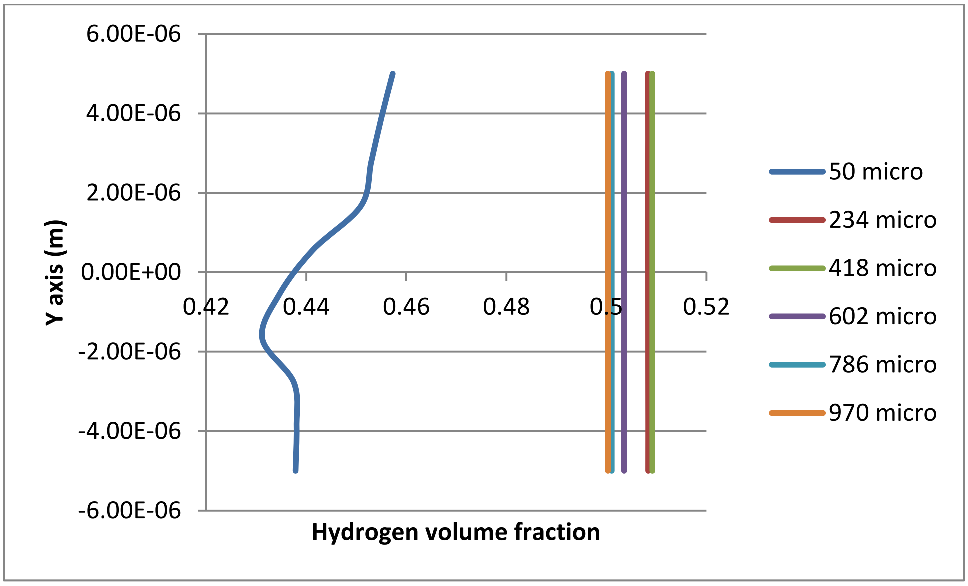
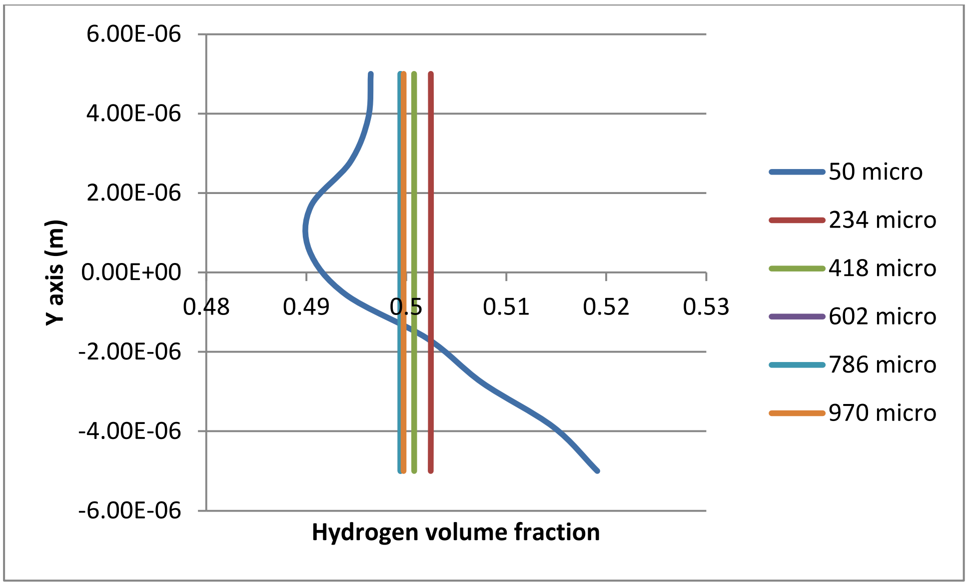


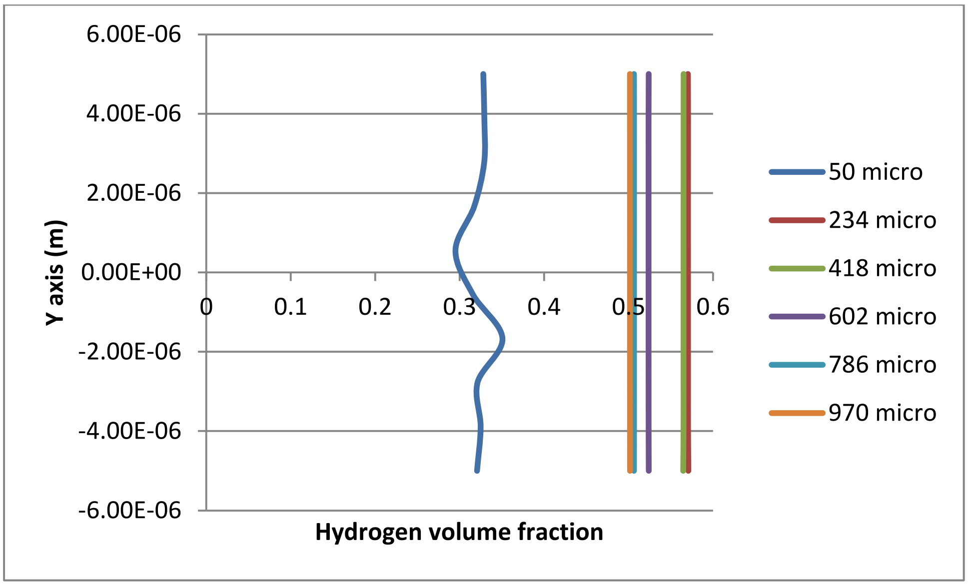
FIGURE 4-6: Position of hydrogen volume fraction profile taken along X-axis



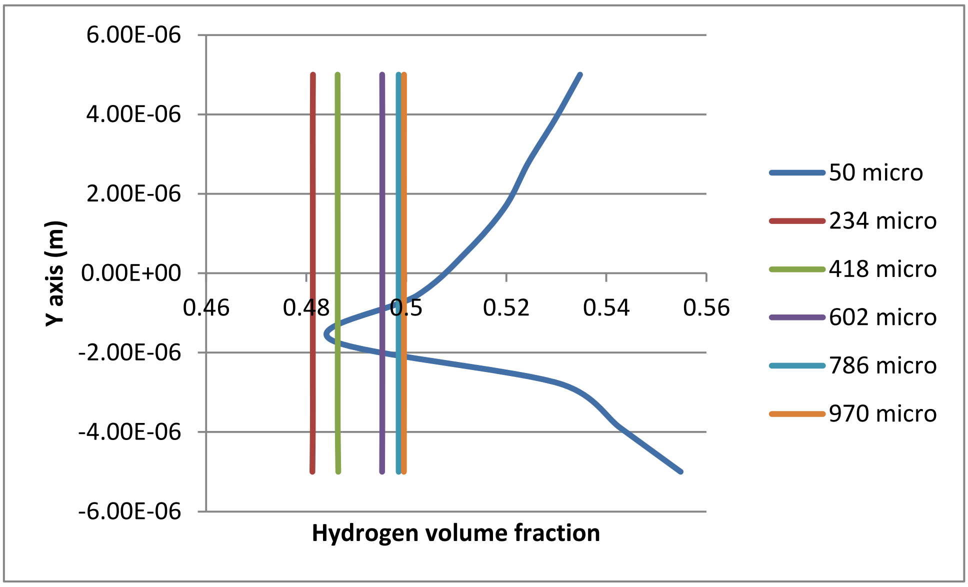
(a)


6.00E-06
4.00E-06
2.00E-06
0.00E+00
-2.00E-06
-4.00E-06
-6.00E-06
0.48
0.49
0.5
0.51
0.52
0.53
Y axis (m)
Hydrogen volume fraction
50 micro
234 micro
418 micro
602 micro
786 micro
970 micro

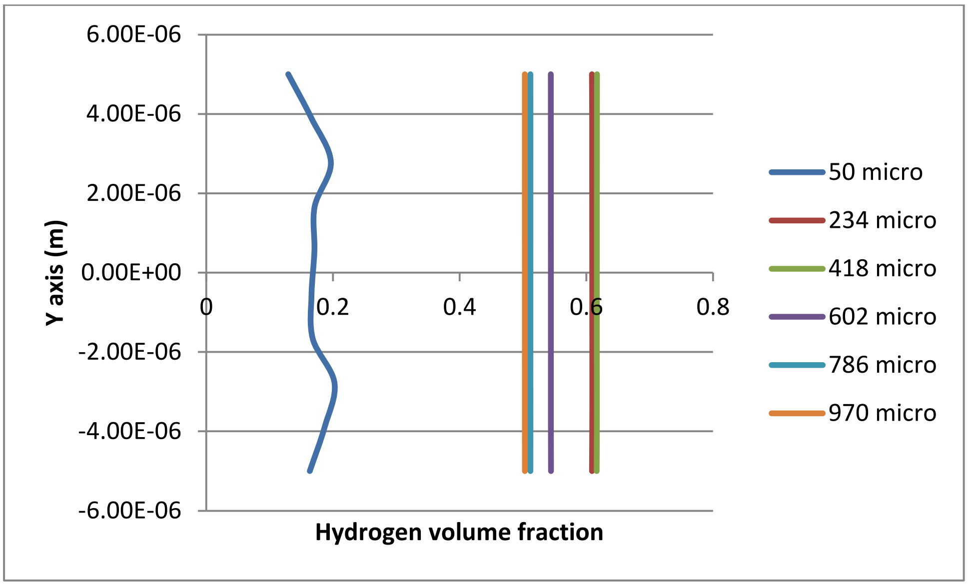
(b)


6.00E-06
4.00E-06
2.00E-06
0.00E+00
-2.00E-06
-4.00E-06
-6.00E-06
0
0.1
0.2
0.3
0.4
0.5
0.6
Y axis (m)
Hydrogen volume fraction
50 micro
234 micro
418 micro
602 micro
786 micro
970 micro

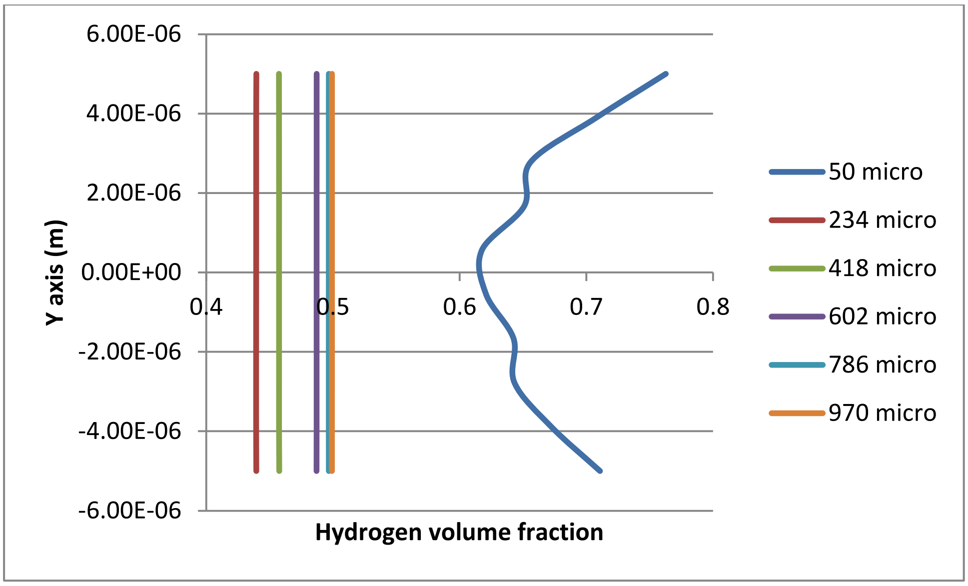
(c)


6.00E-06
4.00E-06
2.00E-06
0.00E+00
-2.00E-06
-4.00E-06
-6.00E-06
0.46
0.48
0.5
0.52
0.54
0.56
Y axis (m)
Hydrogen volume fraction
50 micro
234 micro
418 micro
602 micro
786 micro
970 micro

(d)


6.00E-06
4.00E-06
2.00E-06
0.00E+00
-2.00E-06
-4.00E-06
-6.00E-06
0
0.2
0.4
0.6
0.8
Y axis (m)
Hydrogen volume fraction
50 micro
234 micro
418 micro
602 micro
786 micro
970 micro

(e)



(f)

FIGURE 4-7: Hydrogen volume fraction at different x-axis (a) Inlet geometry of 30^0 and nitrogen in the main stream, (b) Inlet geometry of 30^0 and hydrogen in the main stream, (c) Inlet geometry of 60^0 and nitrogen in the main stream, (d) Inlet geometry of 60^0 and hydrogen in the main stream, (e)Inlet geometry of 90^0 and nitrogen in the main stream, (f) Inlet geometry of 90^0 and hydrogen in the main stream

Figure 4.6 shows the hydrogen volume fraction taken at several locations along X-axis. Comparison between Figures 4.6 (a), (c) and (e) and Figures 4.6 (b), (d) and (f) shows that the mixture having hydrogen in the main stream reaches near uniform composition within a shorter length along X-axis as compared to having nitrogen in the main stream.

Figure 4.6 (b), (d) and (f) shows hydrogen volume fraction along X-axis for nitrogen in the main stream at different angle of the inlet; 30^0, 60^0, and 90^0. The mixture of the 30^0 inlet angle gives the shortest distance (234µm) for the mixture to attain near uniform composition, followed by the 60^0 angle (602µm) and the 90^0 angle (786µm). It is observed that the 30^0 inlet angle gives a shorter length for the fluid flow to reach near uniform composition.

The length for the flow to fully develop the velocity profile, l_e in the laminar region is

$$l_e = 0.06(D)Re \qquad (4)$$

where, D = the diameter and Re = Reynolds number (Entrance Length and Developed Flow)

The distant for the flow to reach uniform composition indirectly represent the length for the flow to be fully developed, l_e. From (4), the Reynolds number must be low to have a shorter l_e. Through the computational study, in the laminar region, the Reynolds number needs to be at minimum in the junction to obtain a shorter l_e. This means that minimum turbulence intensity is needed for flow in the laminar region to achieve uniform composition.

The study shows that the 30^0 angle at the junction induces less turbulence in the flow compared to the 90^0 angle and as a result a shorter distance in needed for the flow to be fully developed and achieve uniform composition. With respect to the inlet configuration, the 30^0 angle at the junction shows a better mixing performance than the other angle designs.

CHAPTER 5 : CONCLUSION AND RECOMMENDATION

The objective of this work is to investigate the mixing dynamics of nitrogen and hydrogen gases during the synthesis of ammonia in a microreactor at ambient temperature and atmospheric pressure. The significant of the study is to determine the localization of catalyst in the microreactor for the enhancement of the ammonia synthesis reaction through the mixing capability between the gases. Several inlet configurations for the microreactor are selected prior the gases participated in the flow to enhance the mixing dynamics. This include 30^o, 60^o and 90^o joining angle at the inlet. In addition, either N_2 or H_2 gases is also chosen to flow in the main stream to investigate the effect of molar mass of the gases in the creation of turbulence in the microreactor.

Through CFD simulation, it is found out that the inlet design of the 30^o angle with hydrogen in the main stream is having the best mixing performance among the other designs and component setups. The selection is made based on the fluid flow discontinuity at the junction, together with a shorter length to reach near uniform condition due to the momentum effect of nitrogen entering the main stream and the entrance effect.

In addition, the overall mixing performance of the microreactor is uniform with no specific site having higher mixing rate despite the different inlet configuration and angle. Thus, it is proposed that the catalyst placement is to be localized throughout the microreactor.

Nevertheless, the suggested work for future is as below:

1. To obtain a better mesh quality by using a licensed ANSYS CFX software with a higher/no limiting number of nodes. Another alternative for better meshing quality is to do the face extrusion meshing or blocked meshing to obtain a better distribution of the nodes.

2. To modify the microreactor design based on the current general microreactor design proposed by Rosli (2012). The study may include the number of cycles, the radius of the cycle and the pitch height.

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APPENDIX

APPENDIXES A: TIME LINE FOR FINAL YEAR PROJECT 2

TABLE A-1: Time line for Final Year Project 2

No.	Detail / Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	3D geometry development and simulation														
2	3D simulation analysis and study														
3	Geometry improvement and optimization														
4	Finalize optimum design														
5	Submission of progress report														
6	Pre-SEDEX														
7	Submission of draft report														
8	Submission of Dissertation (soft bound)														
9	Submission of technical paper														
10	Oral presentation														
11	Submission of Dissertation (hard bound)														

APPENDIXES B: OVERALL MICROREACTOR VELOCITY CONTOUR

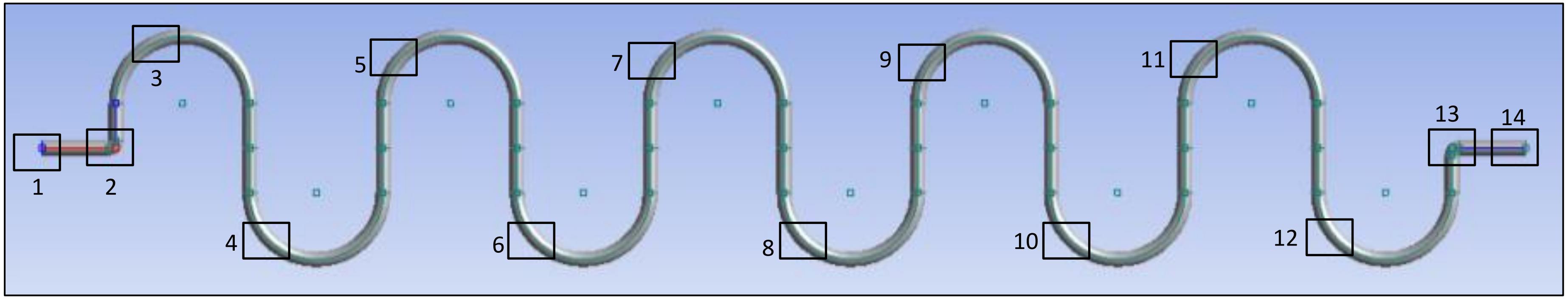
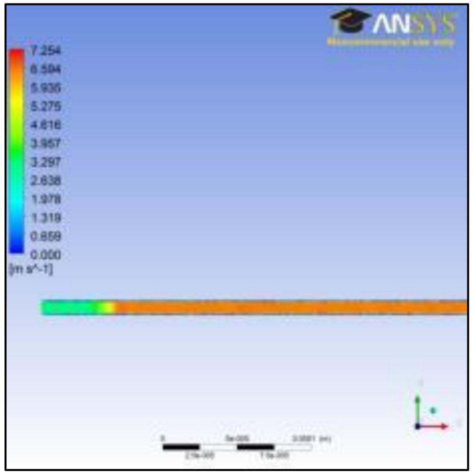
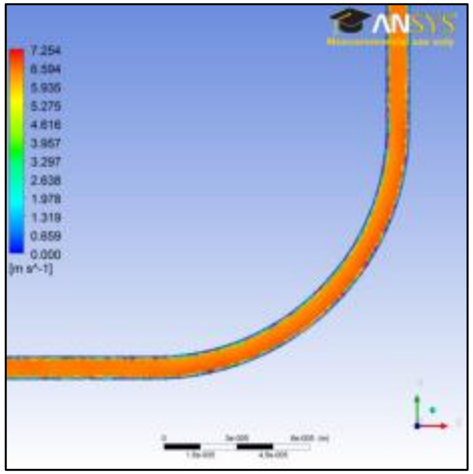


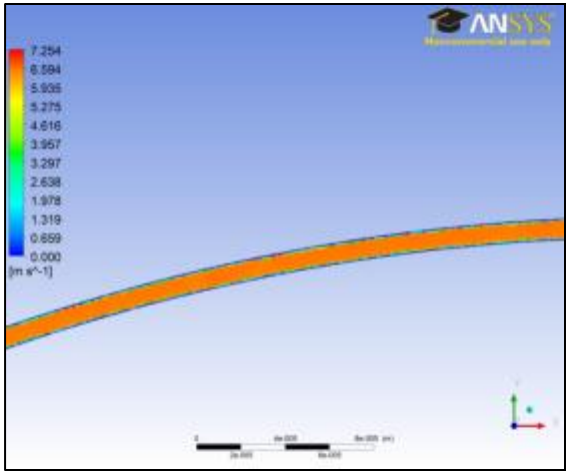
FIGURE B-1: Clipped contour segments from the microreactor geometry


7.254
6.594
5.935
5.275
4.616
3.957
3.297
2.638
1.978
1.319
0.659
0.000
[m s^-1]

(1)


7.254
6.594
5.935
5.275
4.616
3.957
3.297
2.638
1.978
1.319
0.659
0.000
[m s^-1]

(2)


7.254
6.594
5.935
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3.957
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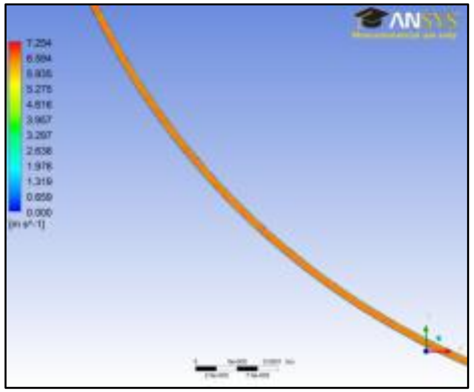
2.638
1.978
1.319
0.659
0.000
[m s^-1]

(3)



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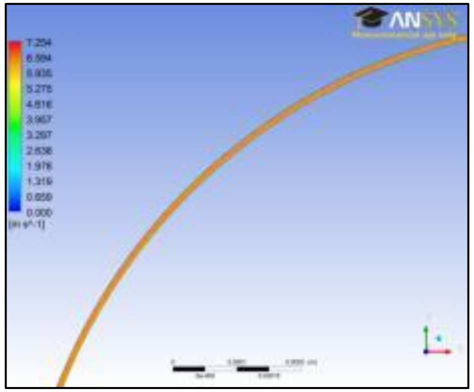

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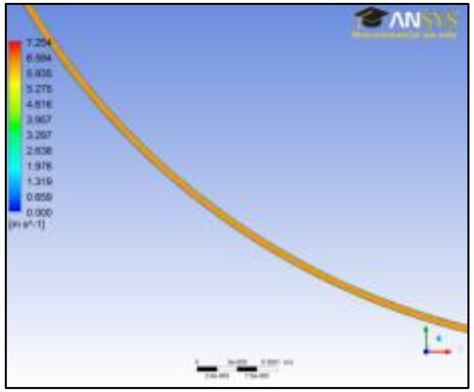

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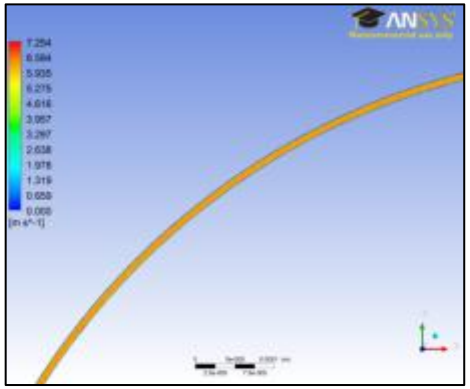

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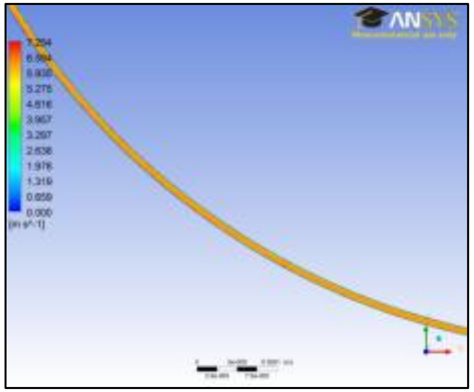

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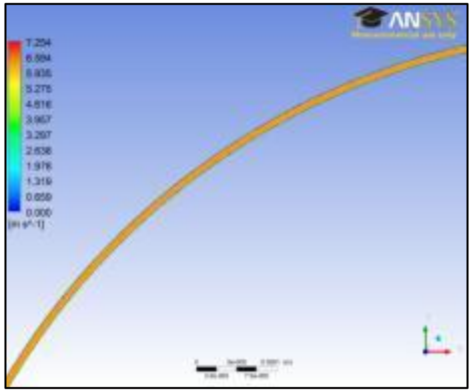

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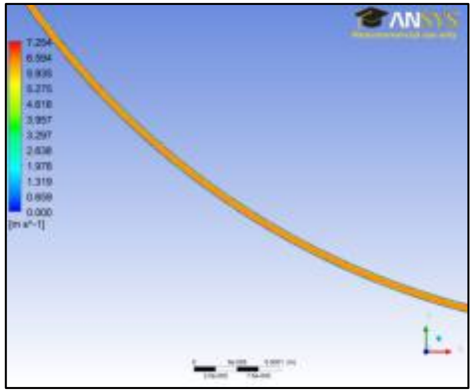

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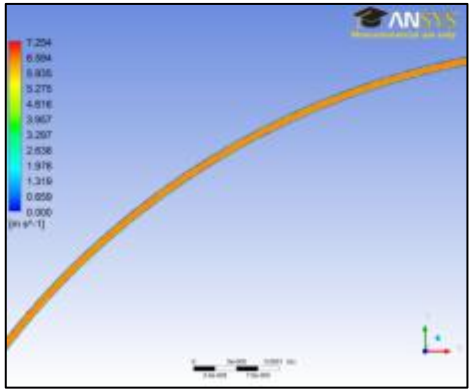

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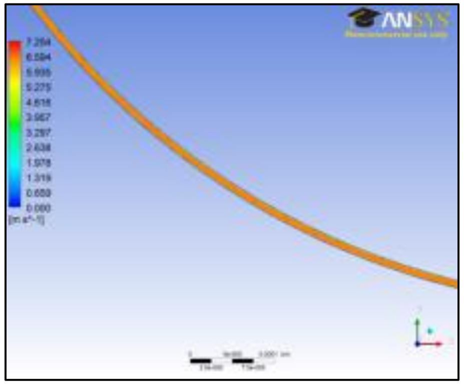

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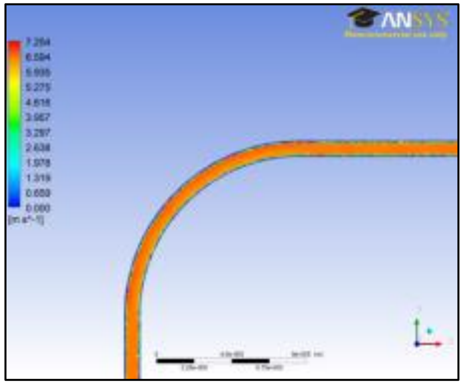

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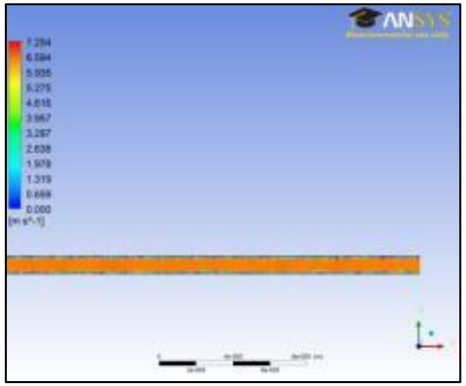
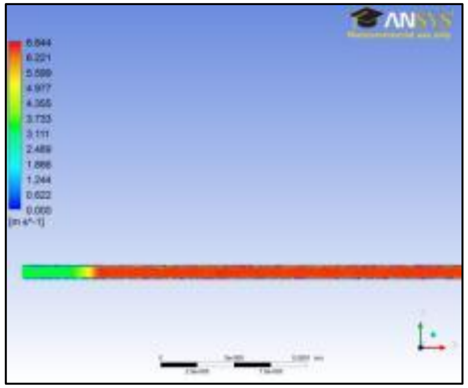


(14)

FIGURE B-2: Velocity contour for 30^0 angle and hydrogen in main stream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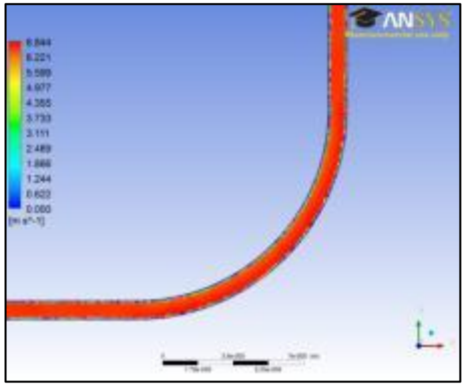
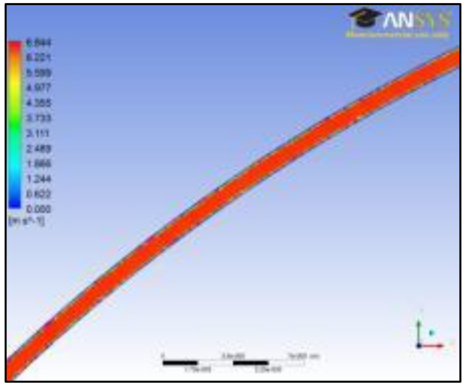
6.844
6.221
5.599
4.977
4.355
3.733
3.111
2.489
1.866
1.244
0.622
0.000
[m s^-1]

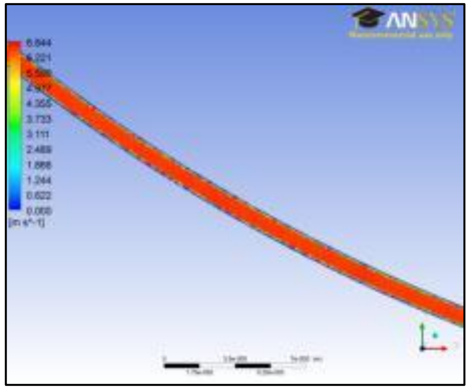
(1)


ANSYS
6.844
6.221
5.599
4.977
4.355
3.733
3.111
2.489
1.866
1.244
0.622
0.000
[m s^-1]

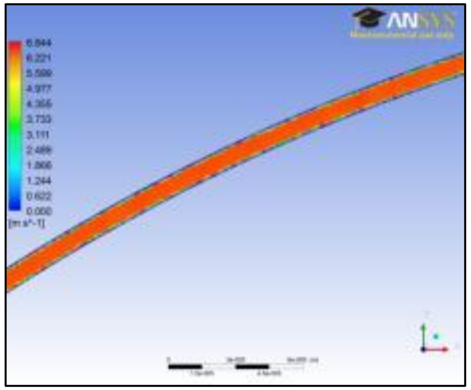
(2)


ANSYS
6.844
6.221
5.599
4.977
4.355
3.733
3.111
2.489
1.866
1.244
0.622
0.000
[m s^-1]

(3)


ANSYS
6.844
6.221
4.355
3.733
3.111
2.489
1.866
1.244
0.622
0.000
[m s^-1]

(4)


ANSYS
6.844
6.221
5.599
4.977
4.355
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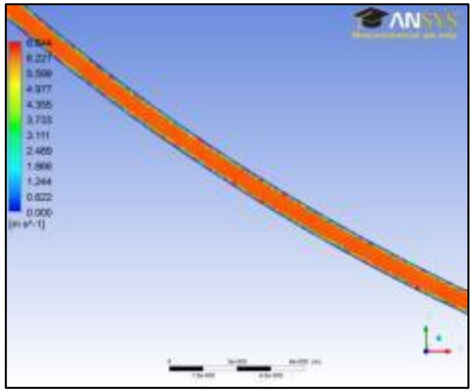
3.111
2.489
1.866
1.244
0.622
0.000
[m s^-1]

(5)


ANSYS
6.221
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3.733
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2.489
1.866
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0.622
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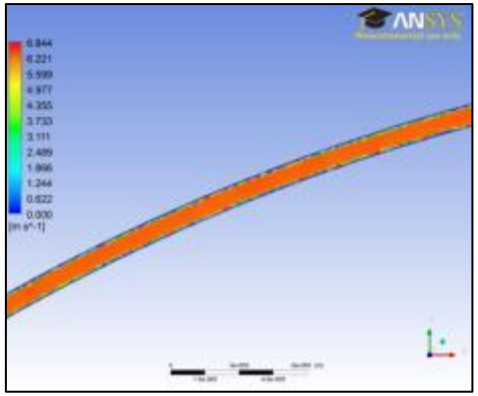
[m s^-1]

(6)


ANSYS
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5.599
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3.733
3.111
2.489
1.866
1.244
0.622
0.000
[m s^-1]

(7)

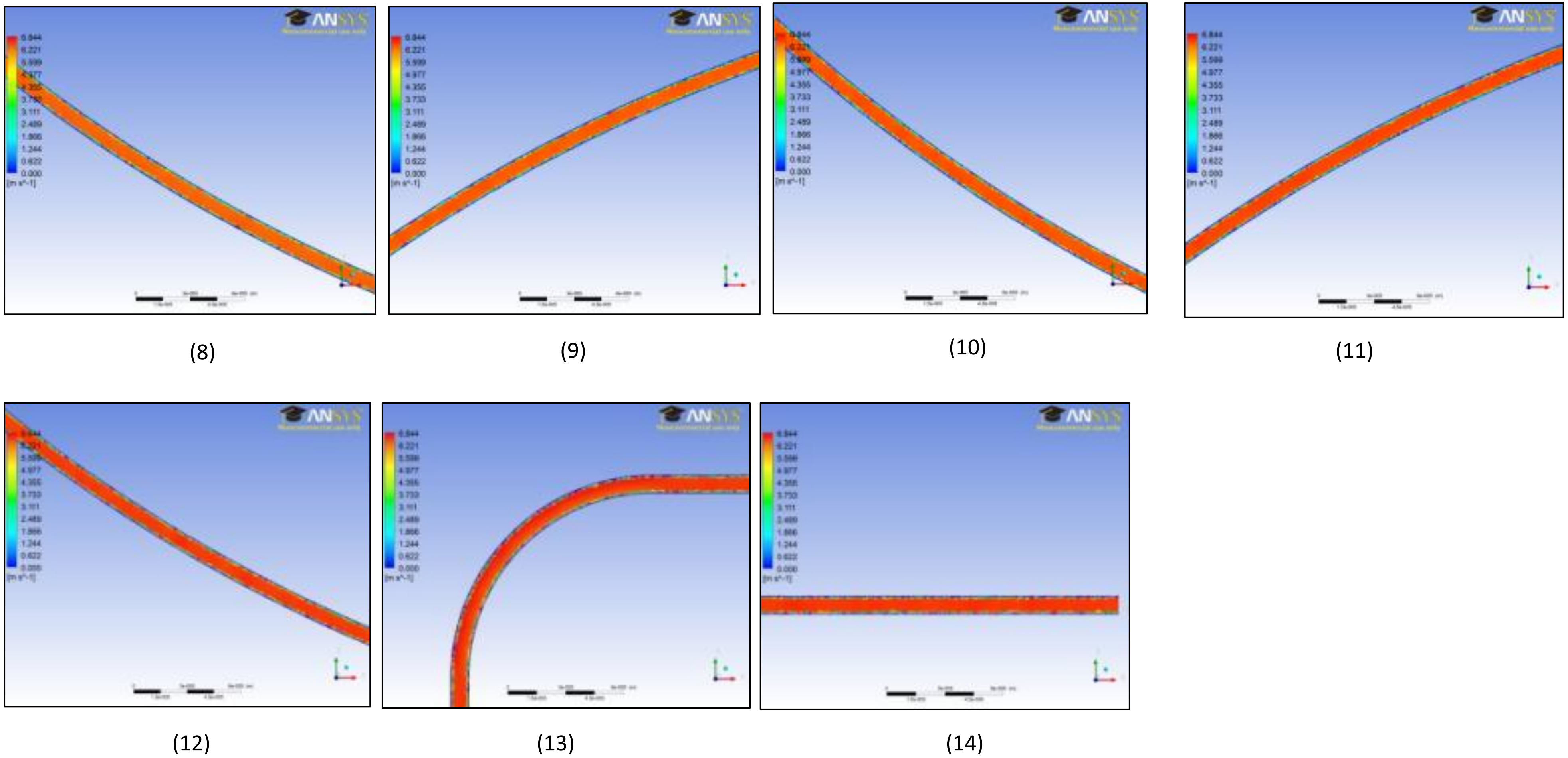
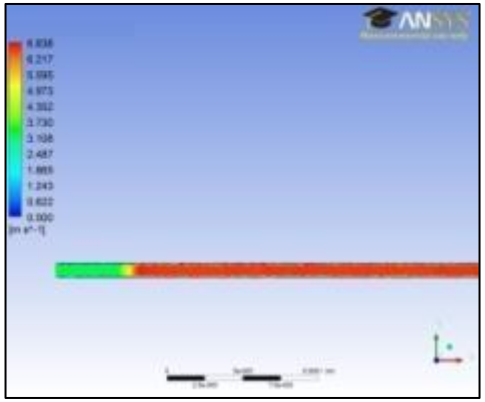
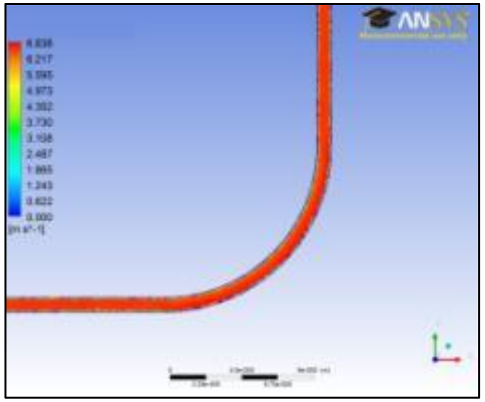


FIGURE B-3: Velocity contour for 30^0 angle and nitrogen in main stream


ANSYS
6.836
6.217
5.595
4.973
4.352
3.730
3.108
2.487
1.865
1.243
0.622
0.000
[m s^-1]

(1)


ANSYS
6.836
6.217
5.595
4.973
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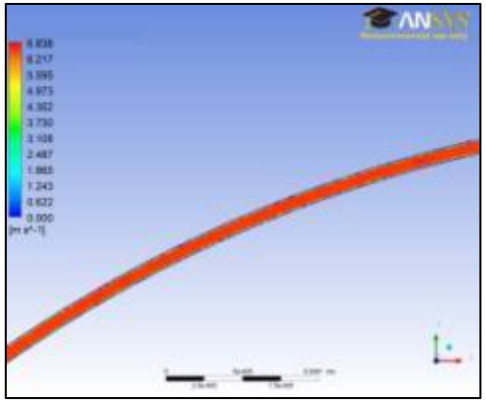
3.730
3.108
2.487
1.865
1.243
0.622
0.000
[m s^-1]

(2)


ANSYS
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6.217
5.595
4.973
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3.730
3.108
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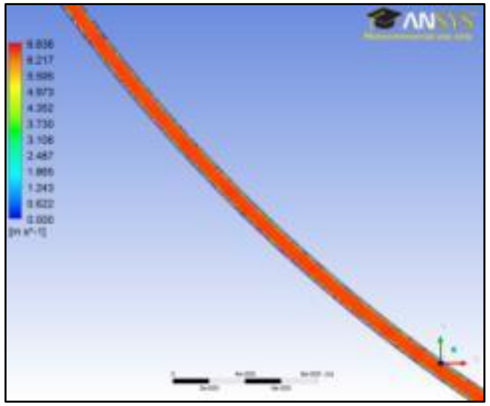
1.865
1.243
0.622
0.000
[m s^-1]

(3)


ANSYS
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6.217
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4.973
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3.730
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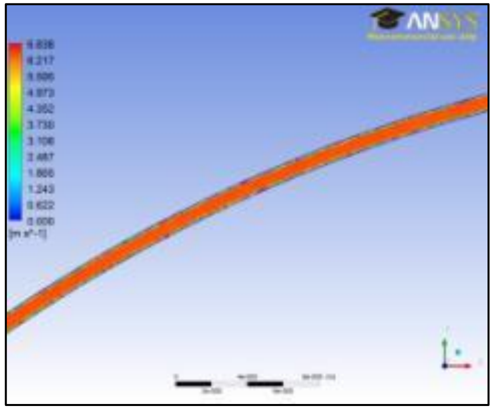
1.865
1.243
0.622
0.000
[m s^-1]

(4)


ANSYS
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1.243
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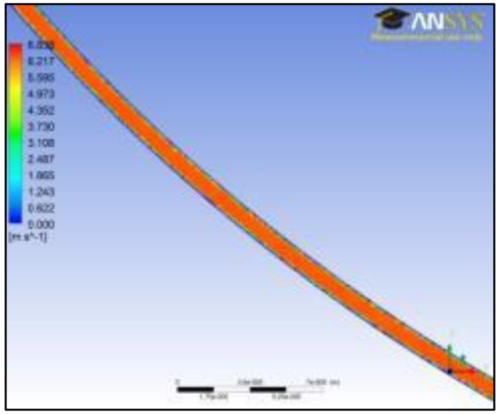
0.000
[m s^-1]

(5)


ANSYS
6.217
5.595
4.973
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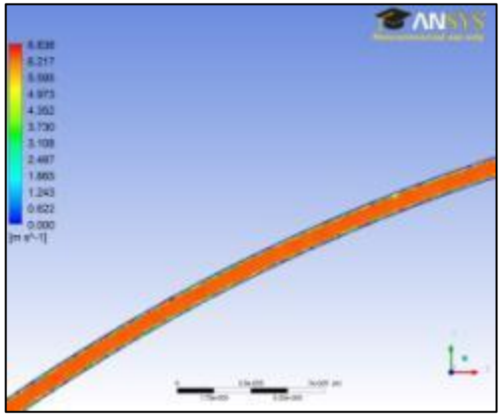
0.622
0.000
[m s^-1]

(6)


ANSYS
6.836
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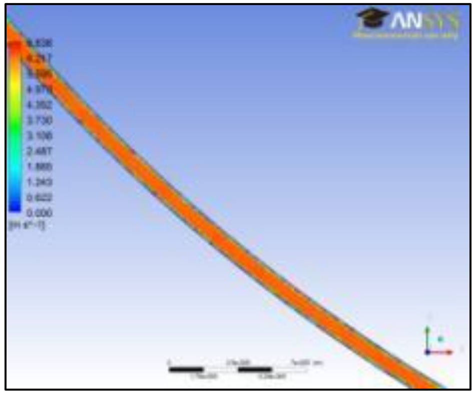
[m s^-1]

(7)



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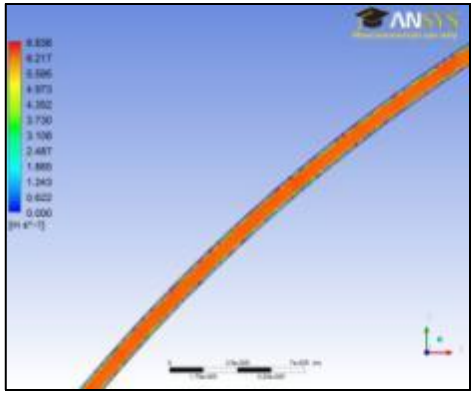

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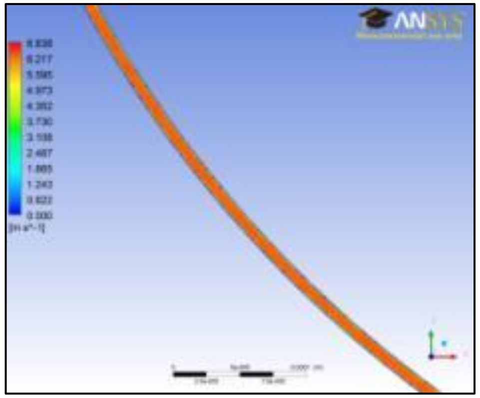

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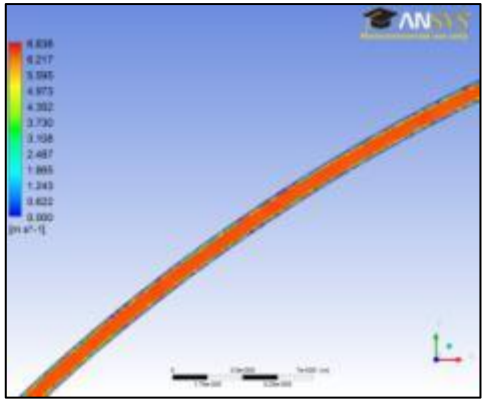

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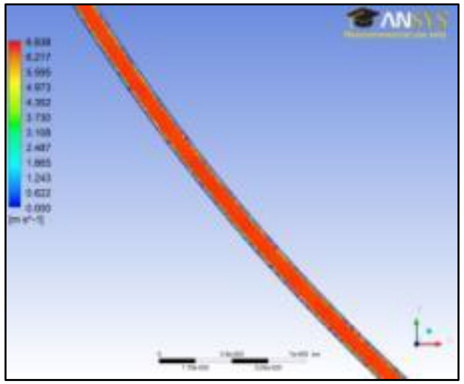

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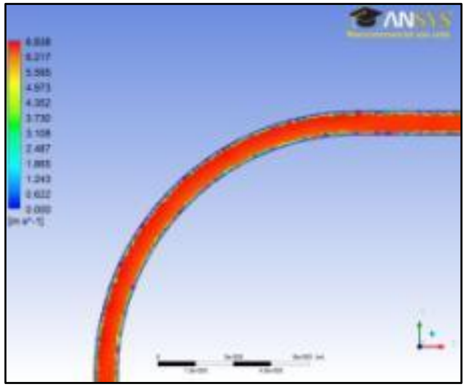

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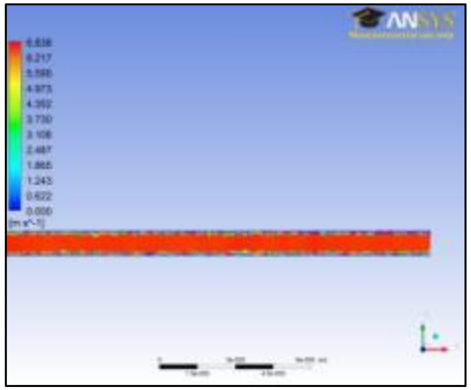

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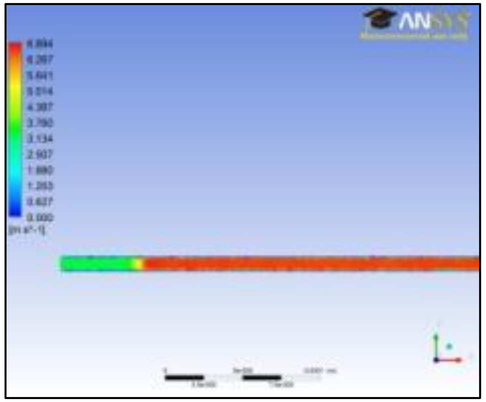
FIGURE B-3: Velocity contour for 60^0 angle and nitrogen in main stream



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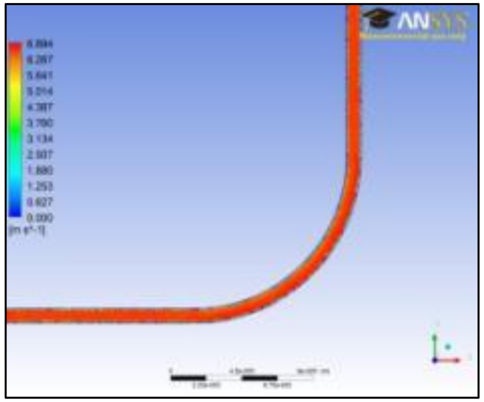

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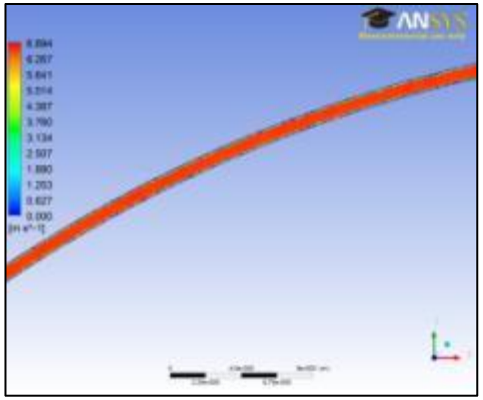

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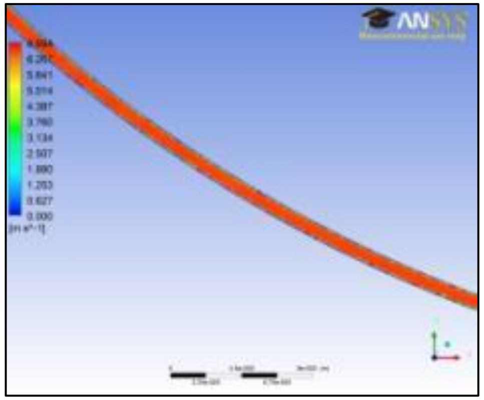

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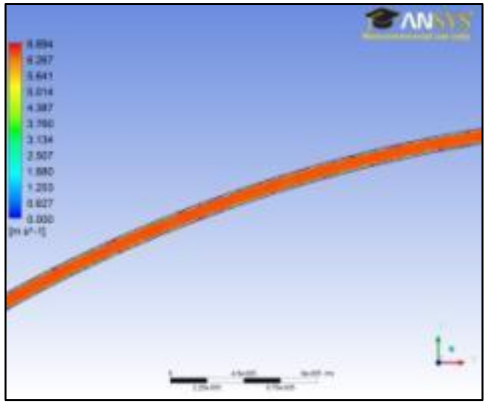

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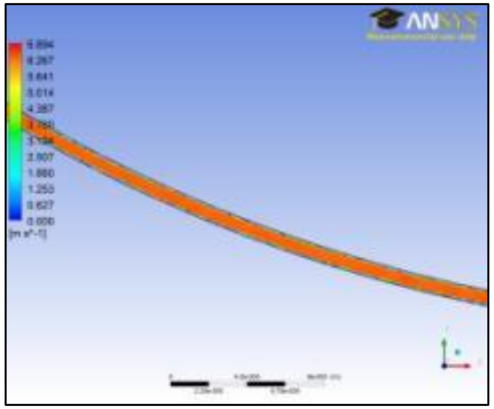

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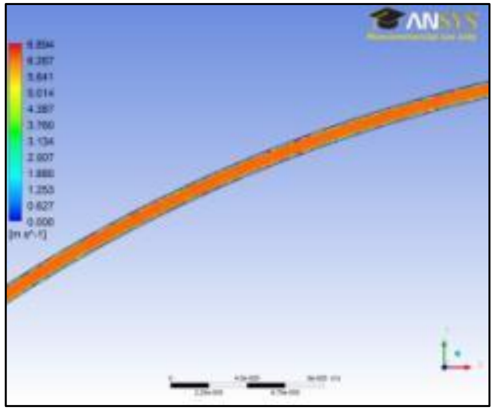

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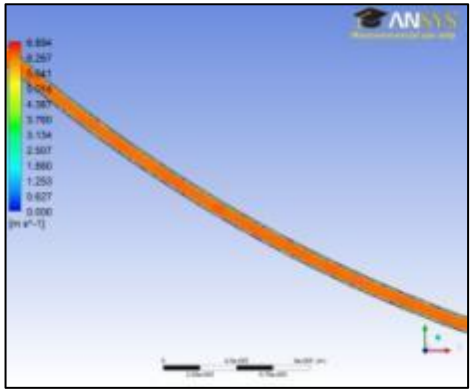

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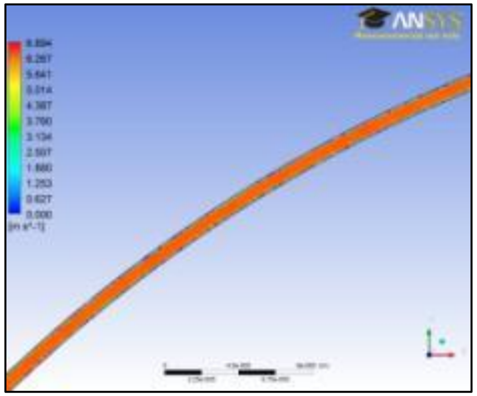

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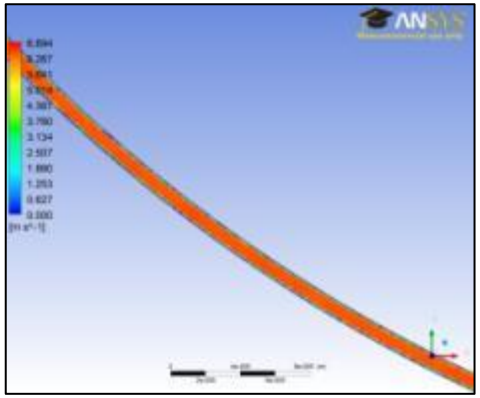
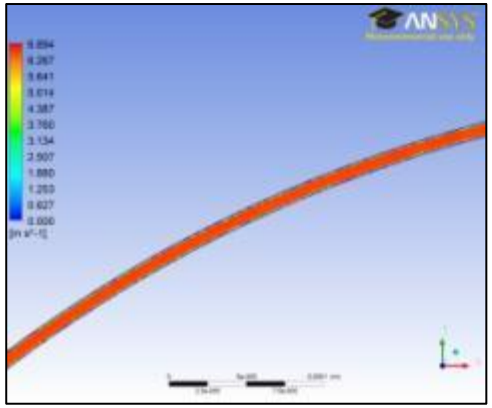
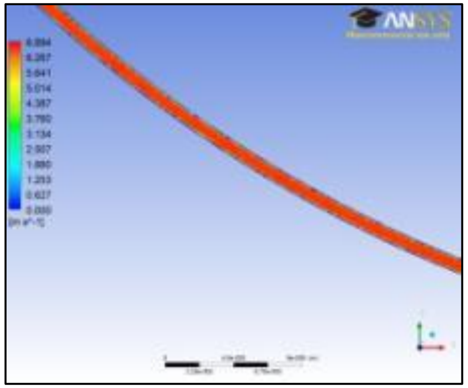


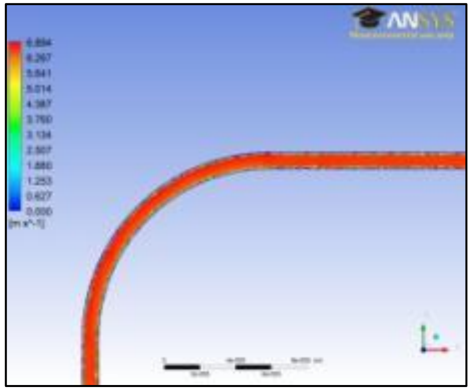
(10)



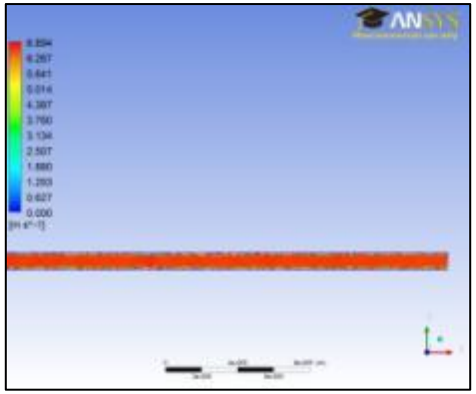
(11)



(12)



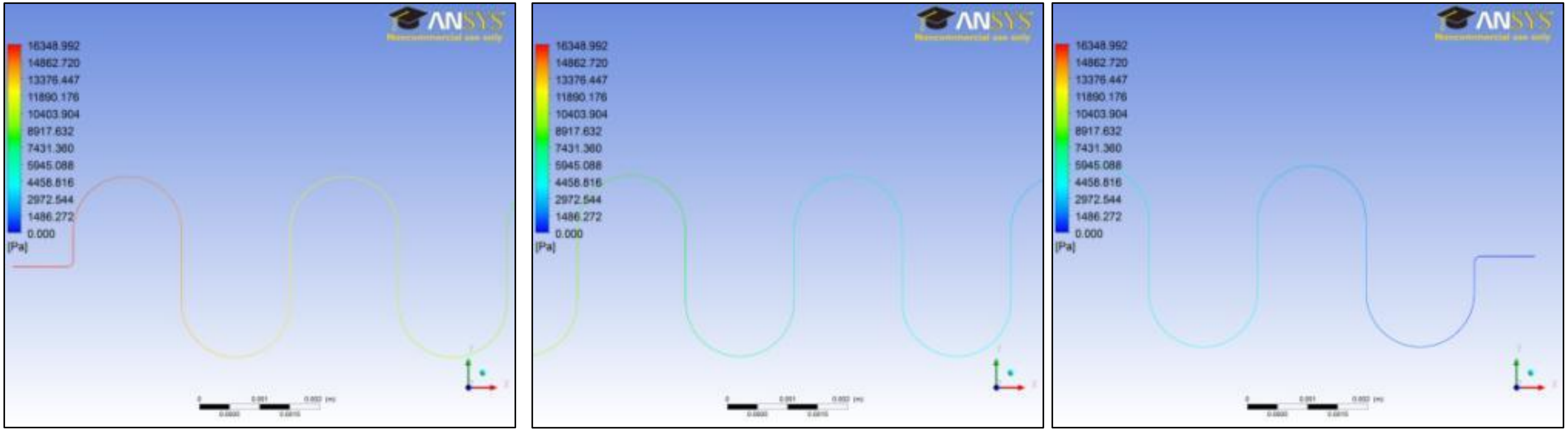
(13)



(14)

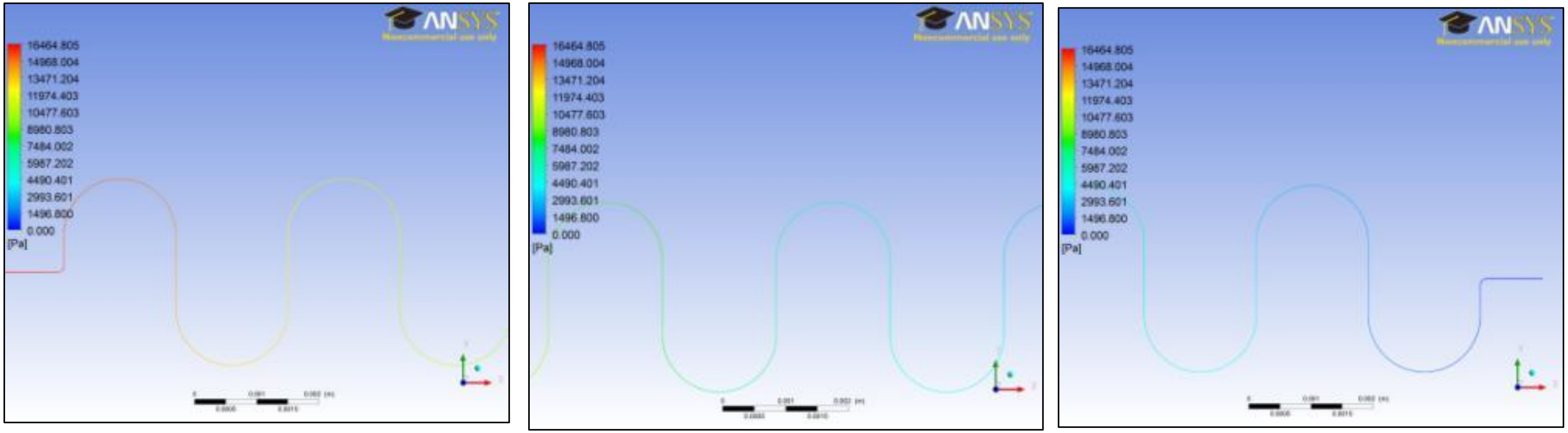
FIGURE B-4: Velocity contour for 90^0 angle and nitrogen in main stream

APPENDIXES C: OVERALL MICROREACTOR PRESSURE CONTOUR



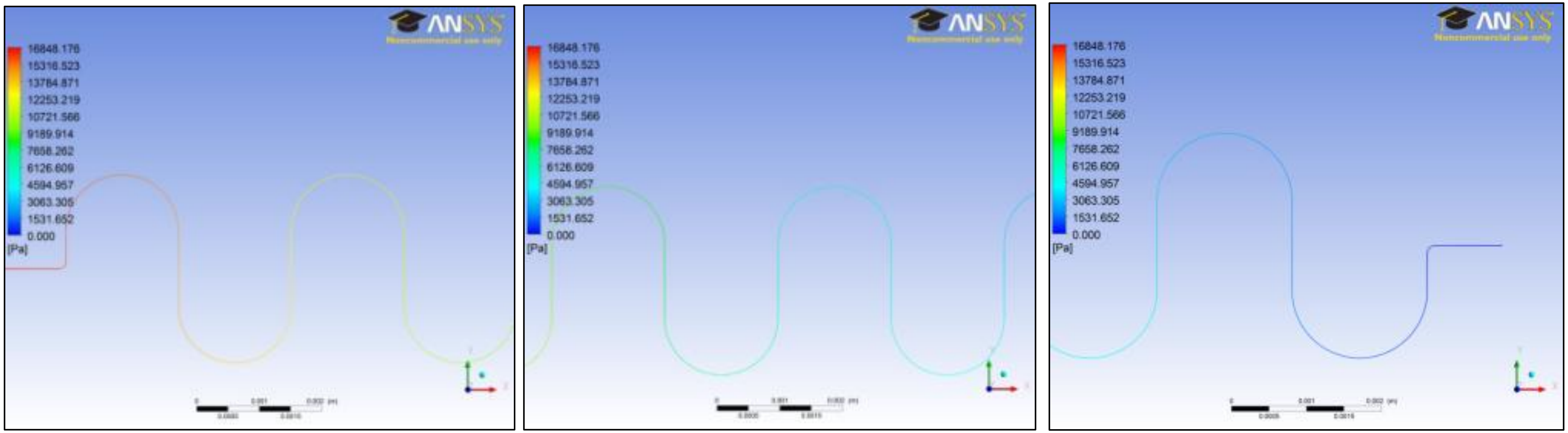
(1) (2) (3)

FIGURE C-1: Pressure contour for 30^0 angle and hydrogen in main stream



(1) (2) (3)

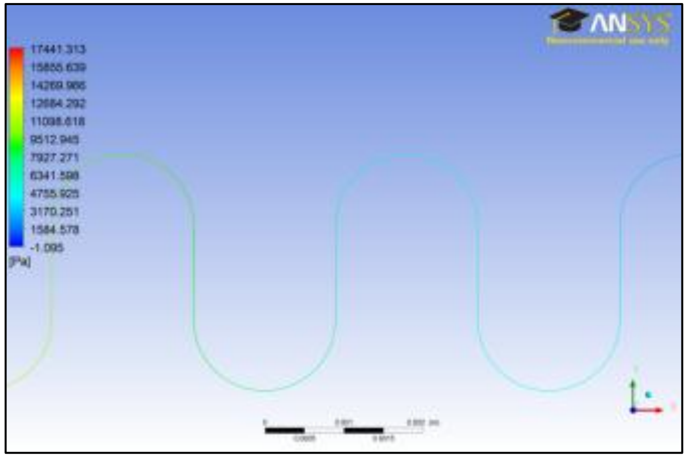
FIGURE C-2: Pressure contour for 30^0 angle and nitrogen in main stream



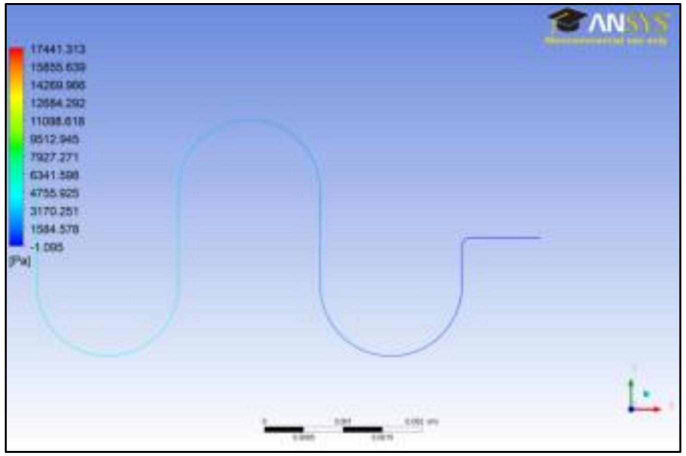
(1) (2) (3)

FIGURE C-3: Pressure contour for 60^0 angle and nitrogen in main stream

(1)



(2)



(3)

FIGURE C-4: Pressure contour for 90^0 angle and nitrogen in main stream