NUMERICAL SIMULATION OF FLUID HYDRODYNAMICS IN V-SHAPE MICRO-CHANNEL FOR AMMONIA PRODUCTION USING MICRO-REACTOR

By

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Dissertation submitted in partial fulfillment of

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CERTIFICATION OF APPROVAL

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Approved by,

(Dr. Anis Suhaila bt Shuib)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

May 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.

MUHAMAD FAIROL IZWAN BIN OSMAN

ABSTRACT

Micro-reactor and other micro-devices have received attention from the society nowadays. This field is unique and has its own advantages which are worth to be studied further. This project entitled 'Numerical Simulation of Fluid Hydrodynamics in V-Shape Micro-channel for Ammonia Production using Micro-reactor' has 3 objectives which are to develop a model for ammonia production in micro-reactor, to identify the optimal catalyst location and to study the effect of micro-channel diameter and inlet volumetric flow-rate toward the degree of mixing of the reactants.

Currently the production of ammonia widely is by using Haber-Bosh process. This Haber-Bosh process is proven in large-scale industrial process. However it uses high temperatures (e.g., at 748 K) and pressures (e.g., at 20 MPa), and has not been proven technically or economically effective below the ton per hour range (J.N. Sahu, 2010). The study will be focusing on replacing the bulk reactor in the Haber-Bosh process with micro-reactor.

The scope of study is focusing on hydrodynamics of fluid where the reaction to produce ammonia was not taken into consideration. The effect of micro-channel diameter and inlet volumetric flow-rate toward the ammonia production is assessed by using computational fluid dynamic (CFD) approach. ANSYS 14, CFD is the software for the simulation. Later the result from the simulation will be assessed in order to proceed to the next phase, manufacturing the micro-reactor under 'One Baja' project.

ACKNOWLEDGEMENT

Alhamdulillah praises to The Almighty Allah for blessing me with the strength and health towards completing this project. I would like to thank my supervisor, Dr Anis Suhaila bt Shuib for her countless guidance and supervision throughout the course of my Final Year Project. Her patience and insight in supervising me is greatly appreciated and will not be forgotten.

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Special thanks to my family, especially Osman bin Hassan and Fadziyah binti Mohd Saleh for their endless moral support and assistance. The love, support and precious time together has made this journey more meaningful.

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LIST OF ABBREVIATIONS

3D	3 Dimensional
abs	absolute
CFD	Computational Fluid Dynamic
CSTR	Continuous Stirred-Tank Reactor
DDPM	Dense Discrete Phase Model
EOF	Electroosmotic Flow
PBR	Pack Bed Reactor
PFR	Plug Flow Reactor

CHAPTER 1: INTRODUCTION

1.1 Background of Study

Ammonia is a bulk chemical that has numerous uses in a wide range of areas, especially in fertilizers production. Many industrial plants including industrial furnaces, incinerators and electric power generation industries require a supply of vast quantities of ammonia, which frequently must be transported through and stored in populated areas (H.B.H Cooper, 2004). Because of ammonia many uses, there are many large-scale production plants world wide, producing a total of 131,000,000 metric tons of ammonia in 2010. Ammonia is also used for the production of plastics, fibers, explosives and intermediates for dyes and pharmaceuticals.

These days, there are a numbers of chemical processes used in the production of ammonia. The three most common methods are the Haber-Bosh process, indirect electrochemical dissociation, and urea decomposition (T.A. Del Prato, 2005). The Haber-Bosh process is the formation of ammonia by nitrogen fixation reaction of nitrogen gas and hydrogen gas. The indirect electrochemical dissociation is an indirect synthesis via a molten alkali-metal halide electrolyte with nitrogen introduced at the cathode and hydrogen introduced at the anode whereas urea decomposition is conversion of urea into ammonia by hydrolysis process. Figure 1 shows the simplify process flow diagram of Haber-Bosh process.

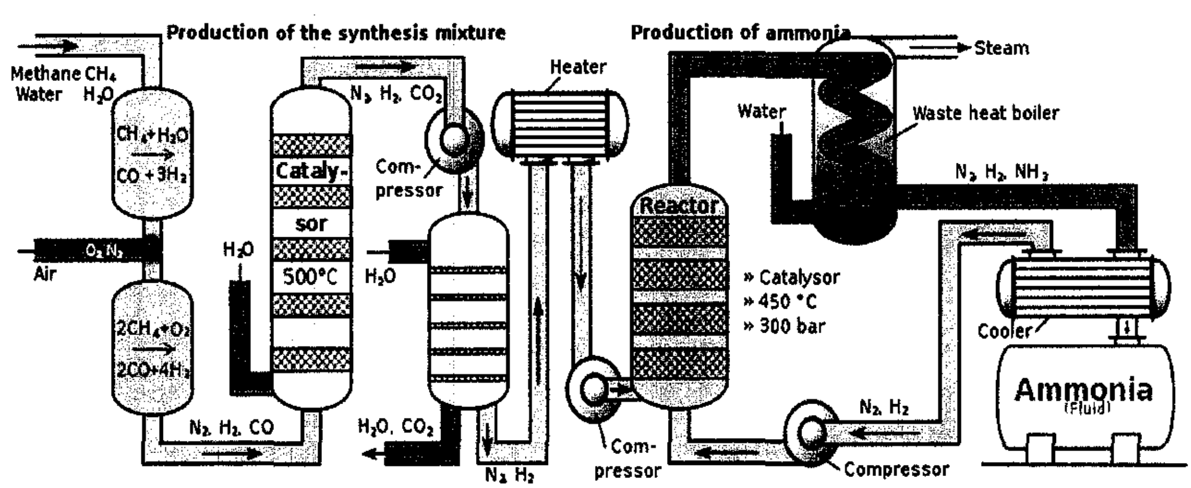


Figure 1: Process Flow Diagram for Haber-Bosh Process

1.2 Problem Statement

The Haber-Bosh process is proven in large-scale industrial process. However it has not been proven technically or economically effective below the ton per hour range (J.N. Sahu, 2010). Under 'One Baja' project, the study is focusing on replacing the bulk reactor in the Haber-Bosh process with micro-reactor. In 'One Baja' project, the iron-based catalyst is used for the ammonia reaction.

Due to the nature of the V-shape micro-channel which is curvature, the mixing of the reactants along the micro-channel varies. Therefore the best reaction sites need to be identified along the micro-channel. Other than that, the reactants degree of mixing and velocity is influenced by the micro-channel diameter and inlet volumetric flow-rate. So, the optimal micro-channel diameter and inlet volumetric flow-rate need to be studied in order to optimize the ammonia reaction inside the micro-reactor.

1.3 Objective

The objectives of the study are:

1. To develop a model for ammonia production in micro-reactor.
2. To investigate the optimal location for catalyst in V-shape micro-channel.
3. To study the effect of micro-channel diameter and inlet volumetric flow-rate in the degree of mixing of the reactants.

1.4 Scope of Study

The study is more thoroughly on the hydrodynamics of fluid where the reaction to produce ammonia was not taken into consideration. The study is by using computational fluid dynamic (CFD) approach. The volume fraction of reactants is compared in order to predict the best reaction sites inside the micro-channel. The parameters studied including the effect of micro-channel diameter and inlet volumetric flow-rate towards the degree of mixing of the reactants.

CHAPTER 2: LITERATURE REVIEW

2.1 Micro-reactor

Micro-reactor is one of the several chemical engineering unit process devices that are now being designed on the micrometer scale. Normally micrometer is used in the production of small scale chemicals such as perfume. There are two micro-reactor design, axial flow and cross flow. For the axial flow, the flow will be parallel with the long axis of the tube and the opposite for the cross flow.

There are some advantages of micro-reactor that make the subject interesting to be studied further. Usually, the heat exchange coefficients of a micrometer is very large, at least 1 MW m^{-3} K^{-1} up to 500 MW m^{-3} K^{-1}. This means that heat can be remove much more efficiently in micrometer thus critical reactions can be performed safely at high temperature (D. Roberge, 2005). The small scale in micro-reactor allows the subsequent processing of unstable intermediates and avoids typical batch workup delays. This rapid work up avoids decay of precious intermediates and allows better selectivity (T. Schwalbe, 2002). The concentration profile for micro-reactor is completely different from typical reactor. Two chemicals can be mixed nearly instantly in micrometer. Although micro-reactor can produce chemical in small quantities, scale-up to industrial volumes is simply increases the number of micro-channels.

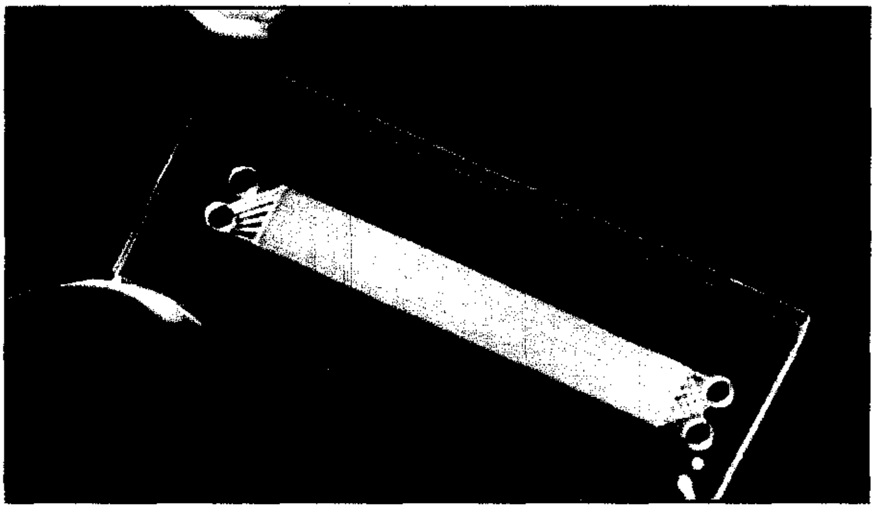


Figure 2: Micro-reactor

Common problem raise from micro-reactor application is the residence time of the reagents shortens from gas evolved by pushing out material much faster than anticipated. Other than that, mechanical pumping might generate a pulsating flow which can be disadvantageous. Nevertheless many researches are still on going to solve the issues. The shorten residence time can be solve by the application of backpressure. Meanwhile, a continuous flow solution can be created by using electroosmotic flow (EOF).

2.2 Ammonia Production (Bulk)

In chemical process, the three common type of reactor used are CSTR, PFR and PBR. Since ammonia synthesis process involved catalyst, PBR is commonly used in industry. The ammonia reaction equation is as follows:

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

Until today, there has been 3 generation of reactor technology development used to synthesis ammonia. The distinct between each generation is its process condition. For 1st generation, the pressure is ranging from 30-35 MPa (abs) and improves to 20-25 MPa (abs) for 2nd generation. The 3rd generation improved more as the operating pressure decrease to less than 5 MPa (abs). The details for each reactor generation are listed in Table 1.

Gen.	Reactor Type	Cooling type	Companies / Licensors	Process Conditions
1st	Vertical shell & tube heat exchanger	External (shell)	Ammonia Casale & TVA	Pressure : 30 -35 $\times 10^{6}$ Pa abs
	Vertical, multiple bed, intermediate cooling	Injection of quenching gas	BASF	
		Water tubes & steam production	Montecatini & OSW	Capacities : 600 t/day

2nd	Vertical, multiple catalyst beds (usually two), Axial flow.	Injection of quenching gas	Kellog* (Figure 3) Topsoe, ICI & Ammonia Casale	Pressure : 20 to 25 × 10^6 Pa abs Capacities: 1500 t/day
		Water tubes and steam production	Uhde & Montedison	
	2 shells, 1intermediate external heat exchanger	Water tubes and steam production	C.F. Braun	
3rd	Horizontal system, axial flow, catalyst bed	Quenching by gas injection	Kellogg * (Figure 4)	Low ΔP
	Vertical, radial flow catalyst bed	Built in gas/gas exchanger	Topsoe	-
	Vertical, axial and Radial flow, catalyst bed with high catalyst volumes	-	Ammonia Casale	Pressure : < 5×10^6 Pa abs

Table 1: Ammonia reactor technology development

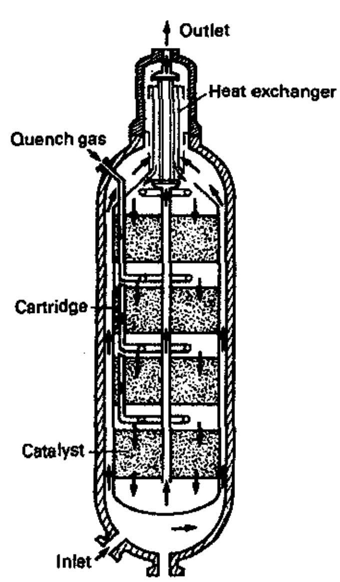


Figure 3: Kellogg reactor - 2nd generation

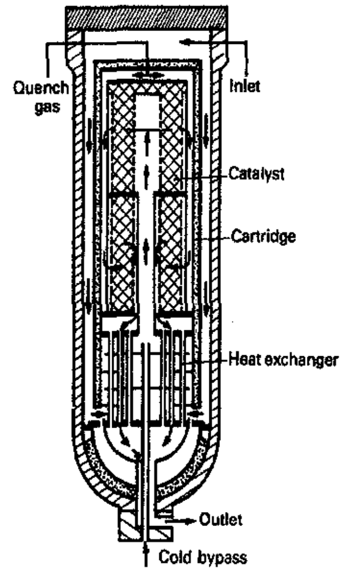


Figure 4: Topsoe's reactor - 3rd generation

According to J.N. Sahu (2010), the ammonia output from a reactor depends on four factors. There are feed input, temperature, pressure, and reactor volume

2.3 Catalysts

Catalyst is used to increase the rate of product formation without ideally changing the composition and quantity of catalyst used. Usually the use of a suitable catalyst can significantly reduce reaction temperatures and can improve conversion rate (Andrea Di Carlo, 2011). The common catalyst use in ammonia synthesis includes iron oxide, molybdenum, ruthenium, and nickel (Holladay JD, 2009). The performance of Ru catalysts is better than Fe catalysts, particularly at low temperature and close to thermodynamic equilibrium. However, Ru catalysts more expensive and have a shorter catalytic lifetime (Hellman A, 2008). Materials that employ Ni-alumina compound in the catalysts are more common and less expensive. It is claimed by many it has good conversion results in a wide temperature and pressure range (Gobina EN, 1995).

In micro-reactor, the catalysts particles are packed inside the whole reactor. In order to compute the kinetic expression of the catalyzed reaction, several resistances need to be considered. First is the gas film layer resistance, reagents and products diffuses respectively from the gas towards the external surface or from external surface towards the gas of the catalytic particle. Next is pores diffusion resistance. The inside of the particle contains most of the catalytic surface, therefore the reactions occur prevalently inside the particles. Lastly is superficial phenomena resistance. The reagents moving inside the catalyst are adsorbed by the solid surfaces, then they react following their kinetic mechanism and the products are desorbed to the gas phase (Andrea Di Carlo, 2011).

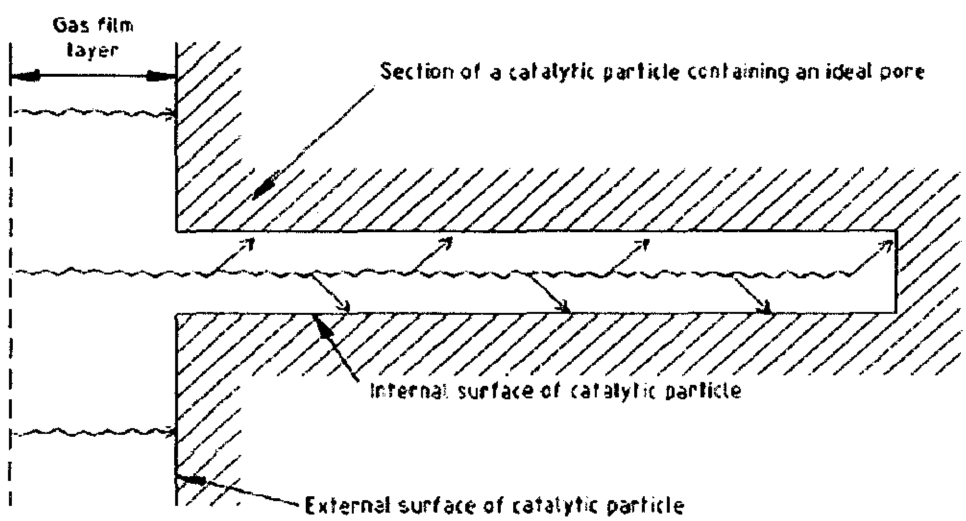


Figure 5: Catalyzed reaction resistances

2.4 The Navier-Stokes equations

The Navier-Stokes equations are the basic governing equations for a viscous, heat conducting fluid. It is a vector equation obtained by applying Newton's Law of Motion to a fluid element and is also called the momentum equation. It is supplemented by the mass conservation equation, also called continuity equation and the energy equation. In an inertial frame of reference, the general form of the equations of fluid motion:

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=-\nabla p+\nabla\cdot\mathbb{T}+\mathbf{f},$$

where v is the flow velocity, ρ is the fluid density, p is the pressure, T is the (deviatoric) stress tensor, and f represents body forces (per unit volume) acting on the fluid and ∇ is the del operator.

The conservation of mass equation:

$$\frac{\partial \rho}{\partial t}+\nabla\cdot(\rho\vec{V})=0$$

The conservation of momentum equation is

$$\rho\frac{\partial \vec{V}}{\partial t}+\rho(\vec{V}\cdot\nabla)\vec{V}=-\nabla p+\rho\vec{g}+\nabla\cdot\tau_{ij}$$

These equations are essential in the CFD modeling for the project.

CHAPTER 3: METHODOLOGY

3.1 Research Methodology

. Figure 6 shows the overview of the project methodology.

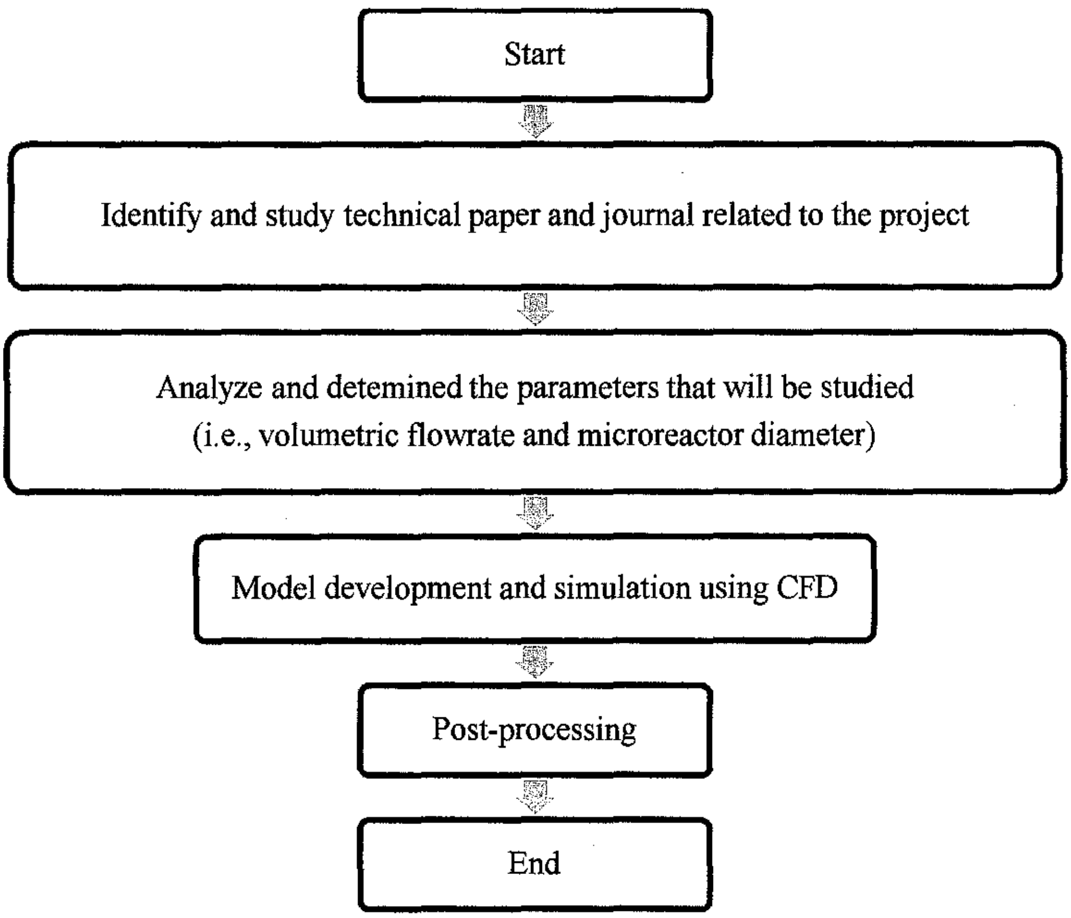
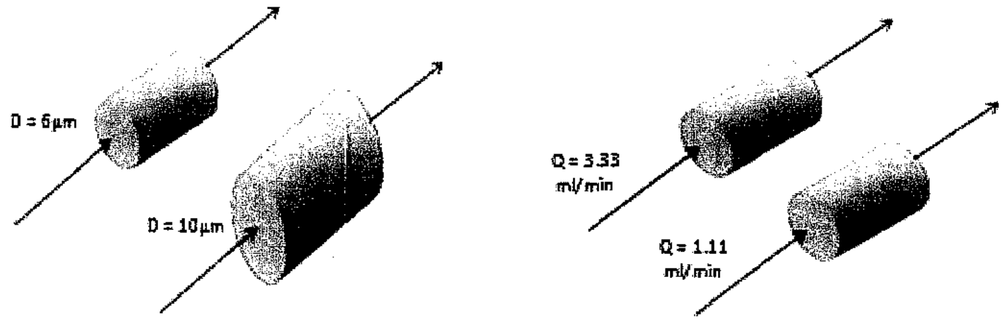


Figure 6: Research Methodology

The ammonia production will be studied by using CFD simulation software as the optimal location for catalyst is identified. Two parameters, which are micro-channel diameter and inlet volumetric flow-rate also is studied. Figure 7 and Table 2 summarized the information of the parameters:



(a) Micro-channel Diameter (b) Inlet Volumetric Flow-rate

Figure 7: Micro-channel Diameter and Inlet Volumetric Flow-rate

1. Effect of micro-channel diameter (Q = 1.11 ml/min)

Micro-channel Diameter (μm)	10	8	6

2. Effect of inlet volumetric flow-rate (D = 10 μm)

Inlet Volumetric Flow-rate (ml/min)	3.33	2.22	1.11

Table 2: Parameters information

3.2 Geometry Construction

The modeling of V-shape micro-channel inside the micro-reactor is the focus of this study. The 3D geometry construction is done using Design Modeler embedded in ANSYS 14 software. The dimension for micro-reactor geometry is suggested by 'One Baja' project team, and then modified according to the fitness and suitability for the study. The default dimension configuration is as follow:

Diameter	:	10 μm
Length	:	20, 000 μm
Wide	:	5,000 μm

Since the ratio between wide and length toward the diameter of the micro-channel is very large, it confirm the geometry is extremely long, regardless its unit. Figure 9 and Table 3 show the geometry dimension in details. The steps in geometry construction are as follows:

1. A circle is drawn with a diameter of 10 μm in XY plane.
2. A continuous line is drawn in YZ plane using polyline as shown in Figure 9.
3. Sweep command is performed for the solid creation. The circle in XY plane as the profile and polyline in YZ plane as the path.

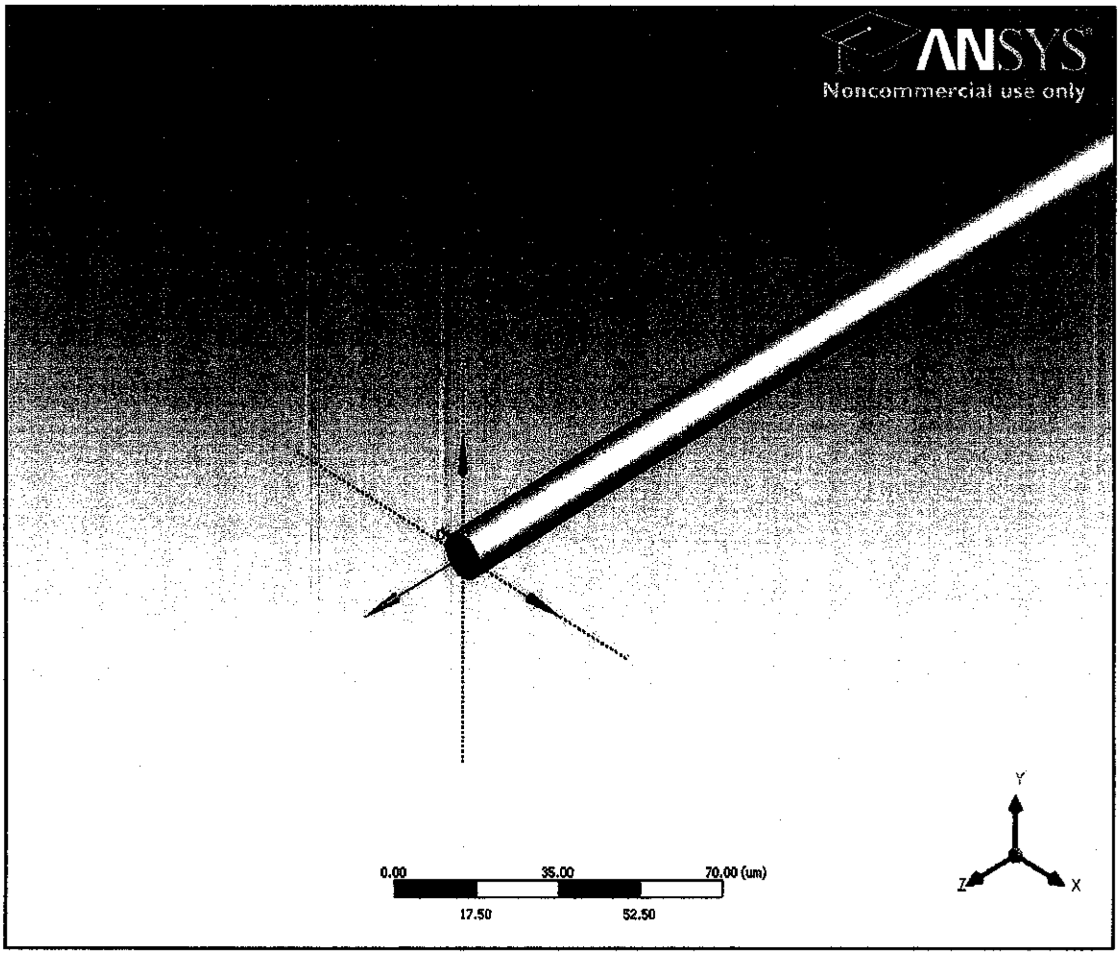


Figure 8: Geometry Isometric View

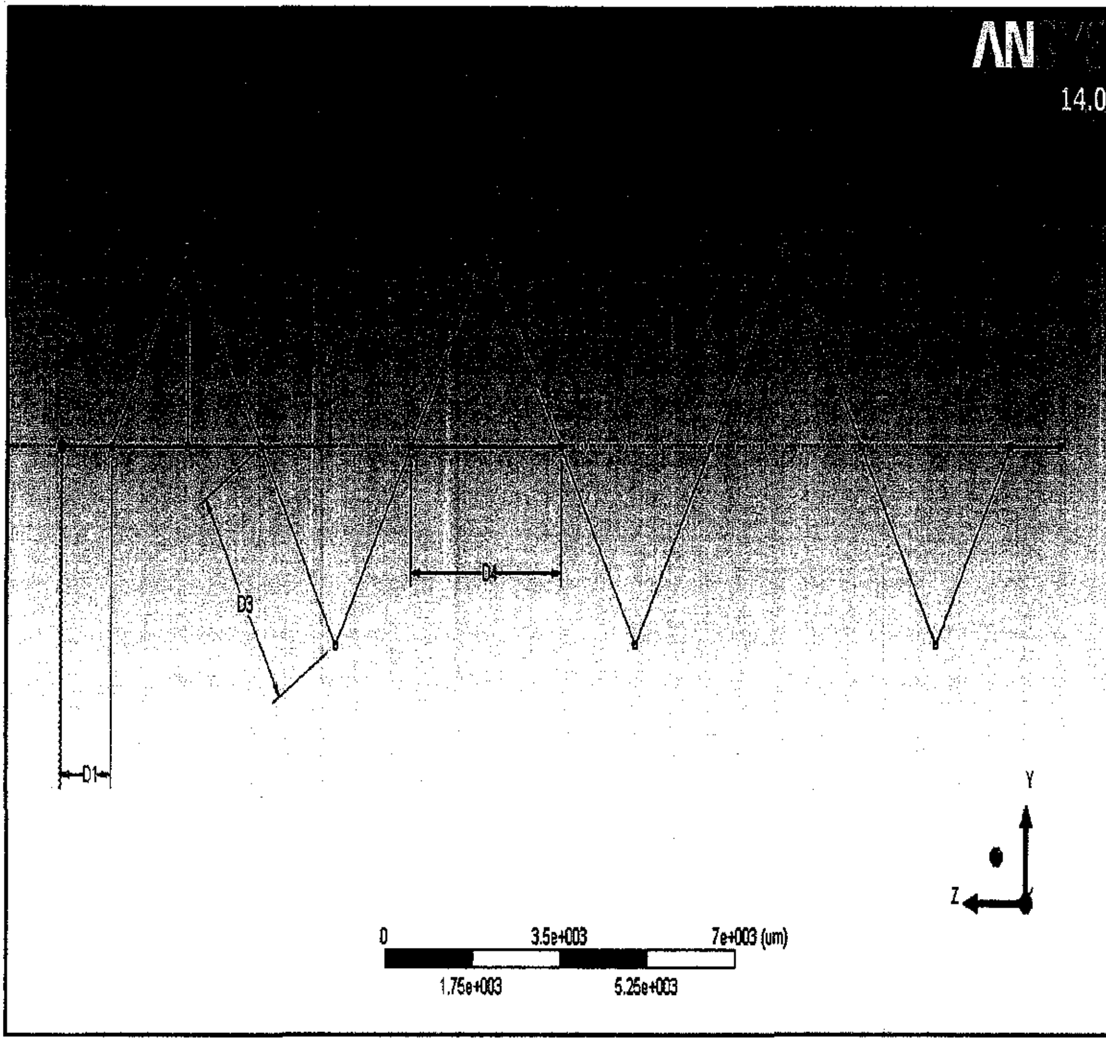


Figure 9: Geometry Top View

Dimension	Length/Degree
D1	1,000 μm
D2	2,500 μm
D3	2,915 μm
D4	3,000 μm
D5	61.98 °

Table 3: Dimension Details (based on Figure 9)

The total volume for the complete geometry created is **2.83 e-12 m^3**.

3.3 Mesh Generation

The next step was to generate mesh that suits the geometry well. The mesh quality is important in order to obtain an accurate simulation. A coarse mesh will cause large numerical errors, especially at the interested area of study from the geometry. The good quality mesh means that the mesh quality criteria are within correct range and can be measured by the orthogonal quality value. Meanwhile, bad quality mesh can induce convergence difficulties, bad physics description and diffuse solution. There are 8 mesh parameters in ANSYS 14 Meshing program: defaults, sizing, inflation, assembly meshing, patch conforming option, advanced and statistic.

The default parameter included physics preference, solver preference and relevance. CFD is chosen for physics preference and Fluent for solver preference. Relevance quality tangles with the fineness of the mesh, with a scale from -100 to 100. By default it is set at 0. The relevance is set to 25 to achieve a greater mesh quality. The second parameter will be sizing, which usually kept as the given default value. Some changes done are the advance sizing function is turn on into curvature. This is because of the nature of the geometry, which is a V-shape micro-channel configuration. Next is the relevance center adjusted from medium to fine. The function of relevance center is much alike the relevance in default parameter. Figure 10 explains the relevance and relevance center in ANSYS Meshing.

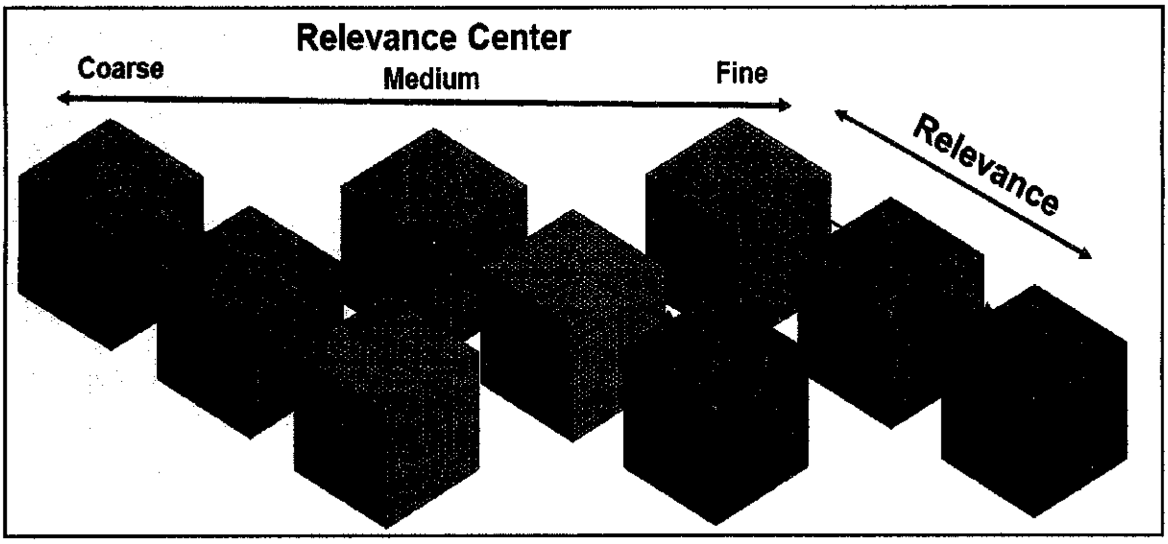
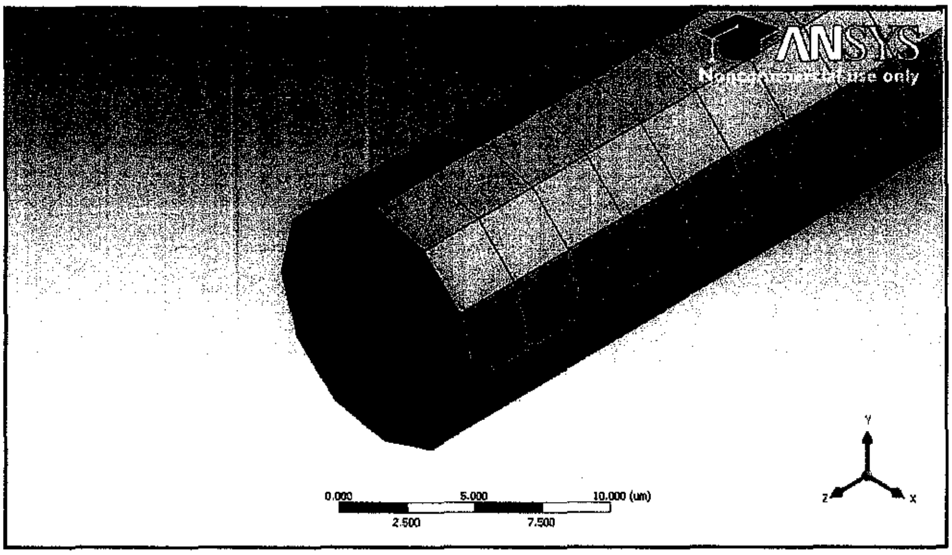


Figure 10: Relevance and Relevance Center

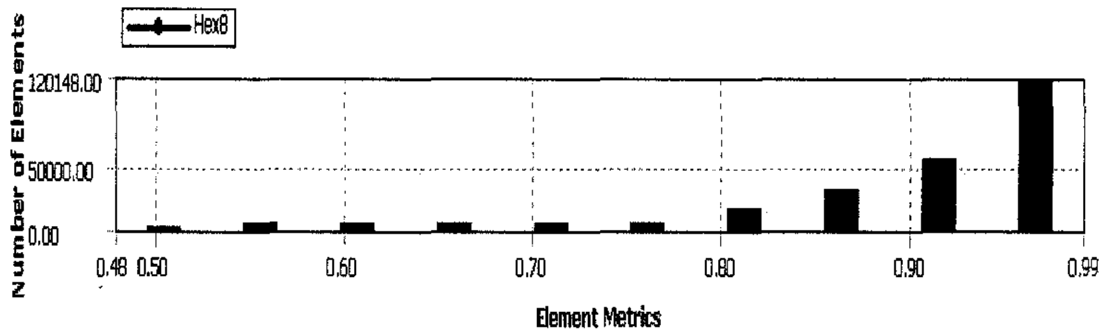
Then the mesh is generated to see the preliminary result. Figure 11 shows the primary generated mesh, details of mesh and orthogonal quality.



(a) Generated Mesh - preliminary

Details of "Mesh"	
Defaults	
Physics Preference	CFD
Solver Preference	Fluent
Relevance	25
Sizing	
Use Advanced Size Fu...	On: Curvature
Relevance Center	Fine
Initial Size Seed	Active Assembly
Smoothing	Medium
Transition	Slow
Span Angle Center	Fine
Curvature Normal ...	Default (15.3750 °)
Min Size	Default (2.69990 µm)
Max Face Size	Default (269.990 µm)
Max Size	Default (539.970 µm)
Growth Rate	Default (1.18440)
Minimum Edge Length	31.4160 µm
Inflation	
Assembly Meshing	
Patch Conforming Options	
Advanced	
Defeaturing	
Statistics	
Nodes	338182
Elements	247114
Mesh Metric	Orthogonal Quality
Min	0.478191463112144
Max	0.992569892386935
Average	0.901115135938566
Standard Deviation	0.102636045270494

(b) Details of Mesh - preliminary



(c) Orthogonal Quality - preliminary

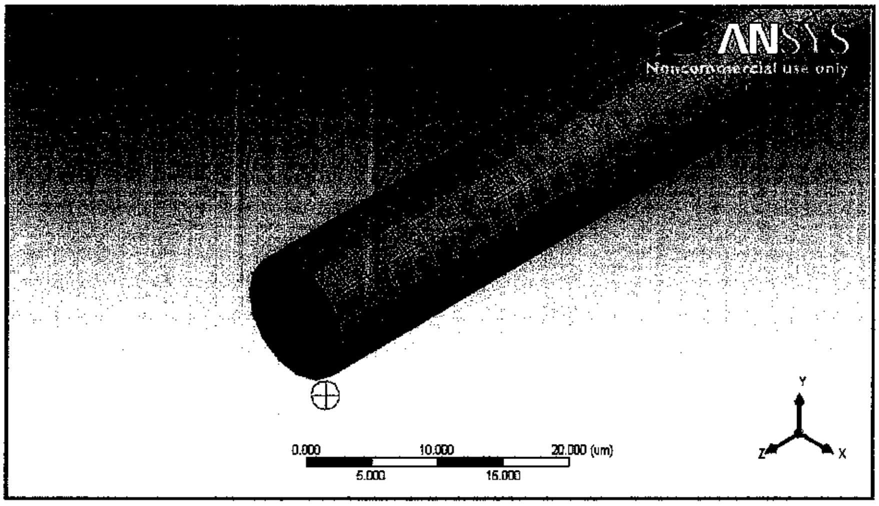
Figure 11: Preliminary Mesh Results

Orthogonal quality is one of the methods to evaluate generated mesh. It is derived directly from FLUENT solver discretization. To make simple, the best quality is 1 and the worse in 0. Due to the large ratio between the micro-channel diameter and length, the mesh generated is very coarse.

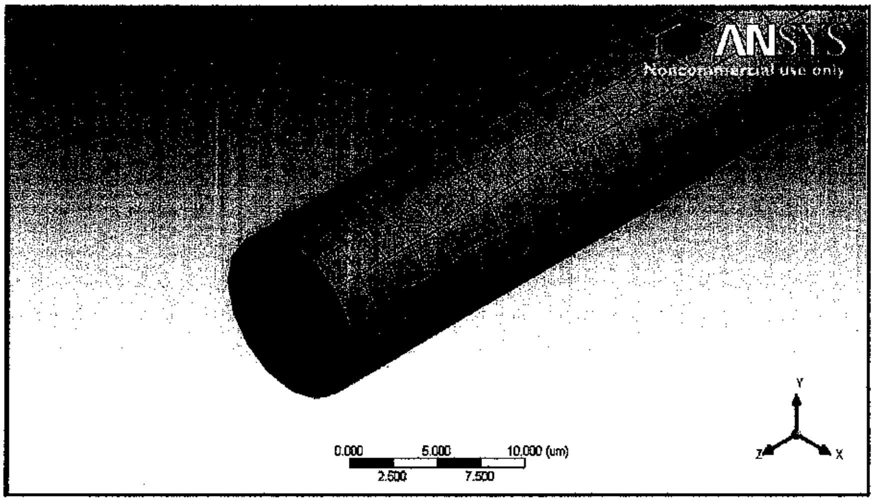
Unfortunately, there is constraint in number of cells/elements. Because the license of ANSYS 14 used is for education purpose only, the number of elements must not exceed 512,000 (APPENDIX A). The primary generated meshes already contain 247,114 numbers of elements. Therefore, the other mesh parameter (inflation, advanced, etc) is not changed from the default setting as it boosts up the number of element. In order to optimized the mesh generated the only parameter that is changed is the minimum size under sizing parameter. Table 4 show number of element for each minimum size and Figure 12 show the mesh generated.

Minimum Size (μm)	Number of elements
2.70 (preliminary)	247,114
2.20 (final)	**479,718**
2.15	567,168
2.10	567,136
2.00	680,544

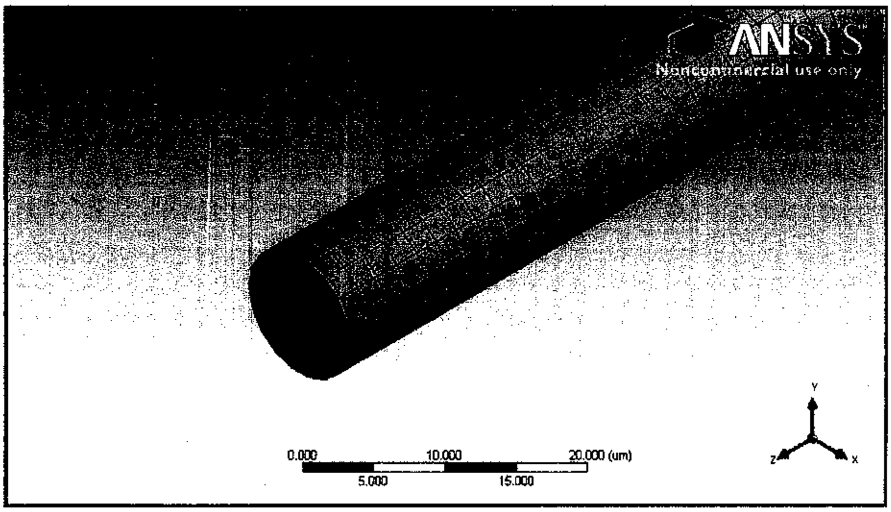
Table 4: Number of Element for Each Minimum Size



(a) Minimum size 2.15μm



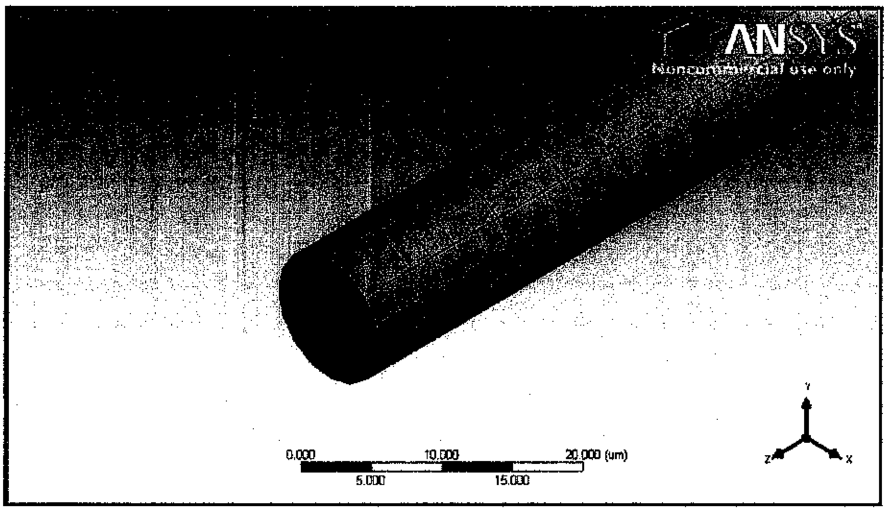
(b) Minimum size 2.10μm



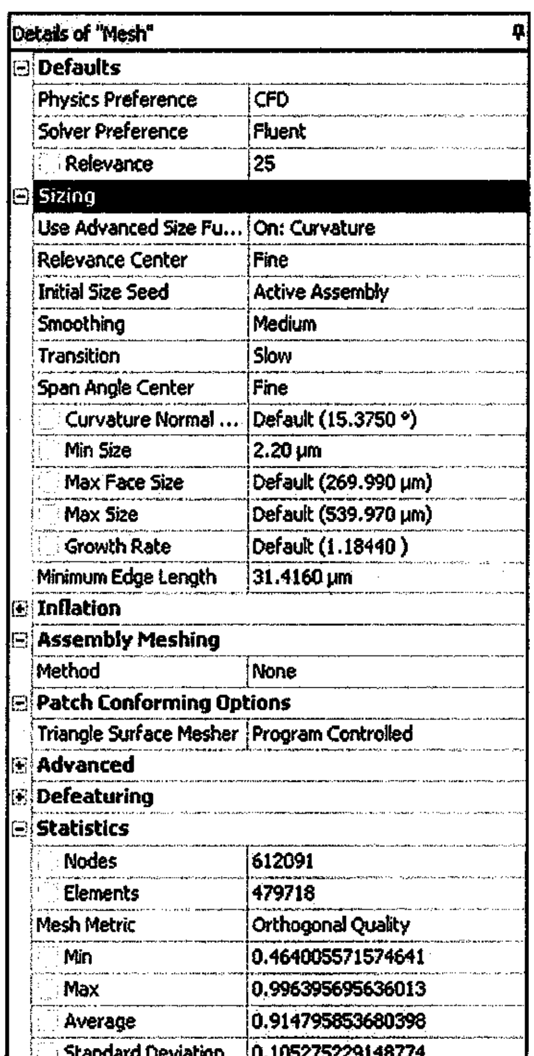
(c) Minimum size 2.10μm

Figure 12: Mesh for Each Minimum Size

The study show that meshes with minimum size of 2.2 μm is the optimal mesh can be achieved with the limitation. Figure 13 shows the final generated mesh, details of mesh and orthogonal quality.

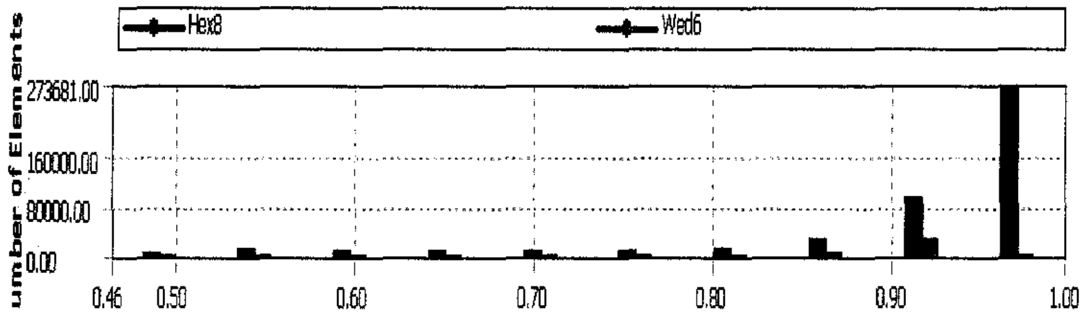


(a) Generated Mesh - final



Details of "Mesh"	
Defaults	
Physics Preference	CFD
Solver Preference	Fluent
Relevance	25
Sizing	
Use Advanced Size Fu...	On: Curvature
Relevance Center	Fine
Initial Size Seed	Active Assembly
Smoothing	Medium
Transition	Slow
Span Angle Center	Fine
Curvature Normal ...	Default (15.3750 °)
Min Size	2.20 μm
Max Face Size	Default (269.990 μm)
Max Size	Default (539.970 μm)
Growth Rate	Default (1.18440)
Minimum Edge Length	31.4160 μm
Inflation	
Assembly Meshing	
Method	None
Patch Conforming Options	
Triangle Surface Mesher	Program Controlled
Advanced	
Defeaturing	
Statistics	
Nodes	612091
Elements	479718
Mesh Metric	Orthogonal Quality
Min	0.464005571574641
Max	0.996395695636013
Average	0.914795853680398
Standard Deviation	0.105275229148774

(b) Details of Mesh - final



(c) Orthogonal Quality - final

Figure 13: Final Mesh Results

3.4 Solver Settings

In order to solve the problem, various parameters had to be specified. The solver chosen is FLUENT. This section will explain on every decision made in initializing the solution.

3.4.1 General Setting

The double precision is chosen for FLUENT option. Usually the single-precision solver is already sufficient, but for certain cases the use of double precision is needed. Since the micro-channel is very long and thin, the double precision needs to be enabled as single-precision calculations may not be adequate to represent the node coordinates. The solver used is pressure-based type, absolute velocity formulation and steady time. For gravity, the gravitational acceleration is -9.81 m/s^2 in X direction.

3.4.2 Model

The multiphase model is chosen for the case. Although the mixture contain only nitrogen and hydrogen gases (one phase), the concept of phase in multiphase flow system is applied in a broader system. In FLUENT, even different-sized solid particles of the same material can be treated as different phases. This is because each collection of particles with the same size will have similar dynamical response to the flow field.

In ANSYS FLUENT, there are three multiphase models available:

1) The Volume of Fluid Model (VOF)
2) The Mixture Model
3) The Eulerian Model

Each model is design for a specific condition. For this study, the Eulerian Model is used. This is because the dispersed phases are concentrated in some portion of the domain, for instance at the corner of the V-shape micro-channel. The Eulerian model will solve a set of n momentum and continuity equations for each phase. It also is a better choice for accuracy.

For viscous model, the laminar is chosen after calculating the Reynolds numbers. The density and viscosity for hydrogen gas are 0.0819 kg/m^3 and 8.411e^{-06} kg/m.s. Meanwhile, the density and viscosity for nitrogen gas are 1.1380 kg/m^3 and 1.663e^{-05} kg/m.s. By assuming 0.5 molar fraction for each phases, the mixture density and viscosity are 0.6099 kg/m^3 and 1.237e^{-05} kg/ms. Table 5 show the Reynolds number for each cases.

Diameter (μm)	N_{Re}
10	116
8	145
6	198

Volumetric Flow-rate (ml/min)	N_{Re}
3.33	348
2.22	186
1.11	116

Table 5: Reynolds Numbers for Each Parameter

3.4.3 Boundary Condition

For micro-channel geometry, there are four named selection specified which are inlet, outlet, interior solid and wall. In this model, the inlet is specified as velocity-inlet. Therefore, the velocity for each phases need to be specified in the inlet. The velocity is calculated by dividing the volumetric flow-rate with inlet surface area. The volume fraction of the secondary phase also needs to be determined. The value of 0.5 is used for the hydrogen, the secondary phase. Other than that, the static gauge pressure needs to be defined in the inlet and outlet. The gauge pressure of 0 atm is used for both inlet and outlet. Table 6 summarized the velocity for each case:

Diameter (μm)	Velocity (m/s)
10	236
8	368
6	654

Volumetric Flow-rate (ml/min)	Velocity (m/s)
3.33	707
2.22	471
1.11	236

Table 6: Inlet Velocity for Each Parameter

3.4.5 Solution Method and Control

There are only two options available for Eulerian multiphase model for Pressure-Velocity Coupling Scheme which are phase-coupled simple and coupled. The coupled scheme is chosen as it solves as all equations for phase velocity correction and shared pressure correction simultaneously. This method works very efficiently in steady state situations compared to phase-coupled simple that has proven to be robust. Meanwhile, the Least Squares Cell Based is chosen for gradient and QUICK for momentum and volume fraction spatial discretization. Other than that, premature convergence is avoided by changing the all the residual constraint into $1\text{x}10^{-12}$, which avoid the program to converge on its own. 500 iterations are done for each parameter and the residual graphs are attached in APPENDIX B.

CHAPTER 4: RESULTS & DISCUSSION

4.1 Introduction

The interested region of study for this micro-channel geometry is its corner as circled in Figure 14. The flow characteristic is observed here as there is a change in the flow direction through the bend. The focus is on the individual phase volume fraction and its velocity magnitude. The catalyst optimal location is identified. Next the effect of micro-channel diameter and inlet volumetric flow-rate toward reactants volume fraction and velocity is studied at the region.

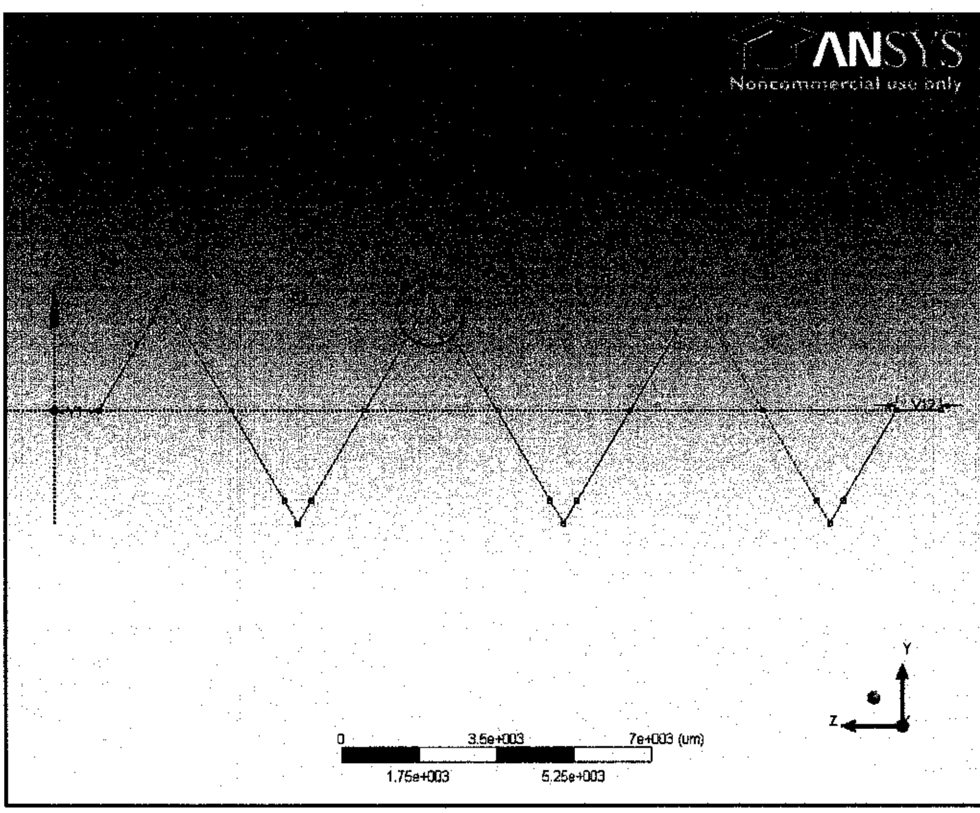


Figure 14: Micro-channel Corner - Top View

4.2 Catalyst Optimal Location

The ammonia reaction needs a catalyst to enhance the reaction. The catalyst use in 'One Baja' project is iron-based catalyst. The catalyst will be put on top of nanowire which will be plant along the micro-channel wall. Therefore the best positions for the nanowire need to be identified. The ammonia reaction equation is as follows:

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

The stoichiometric equation show that 1 mol of nitrogen gas will react with 3 mol of nitrogen gas to form 2 mol of ammonia gas. To find the corresponding volume fraction, the equation below is used:

$$\acute{\o}_i = \frac{z_i \, . \, x_i}{\sum_{k=1}^{N} z_k . x_k}$$

With:

$Z_{i,k,}$ = compression factor of component $x_{i,k,}$ at specified state condition (T & P)

$\acute{\o}_{i,k,}$ = volume fraction of component $x_{i,k}$

$x_{i,k,}$ = mole fraction of component $x_{i,k}$

N = number of component in the mixture.

Since the operating condition for this project is atmosphere pressure and room temperature, the compression factor can be assumed as 1. The resulting stoichiometric volume fraction calculated is 0.25 for nitrogen gas and 0.75 for hydrogen gas. The reaction rate will be optimized with this volume ration. The micro-channel with diameter 10μm and inlet volumetric flow-rate of 1.11 ml/min is used for the study of catalyst optimal location.

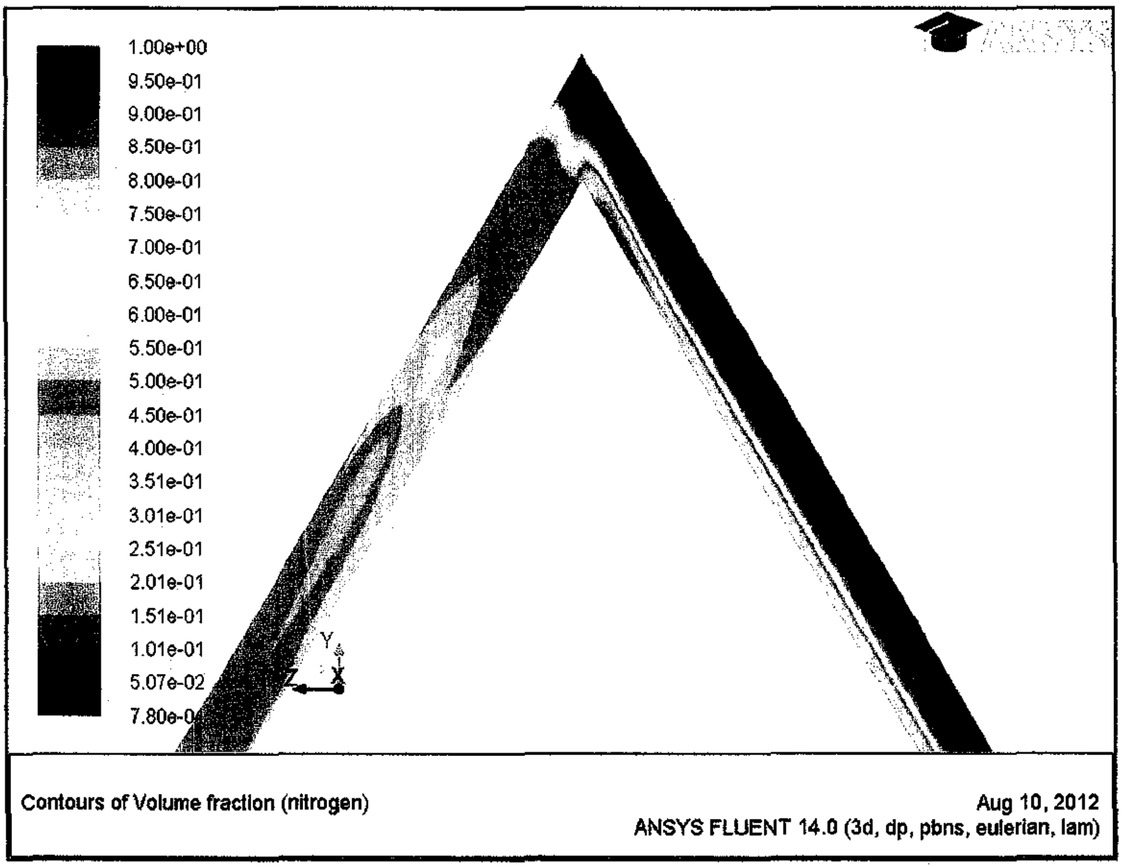


Figure 15: Volume Fraction of Nitrogen Gas - Top View

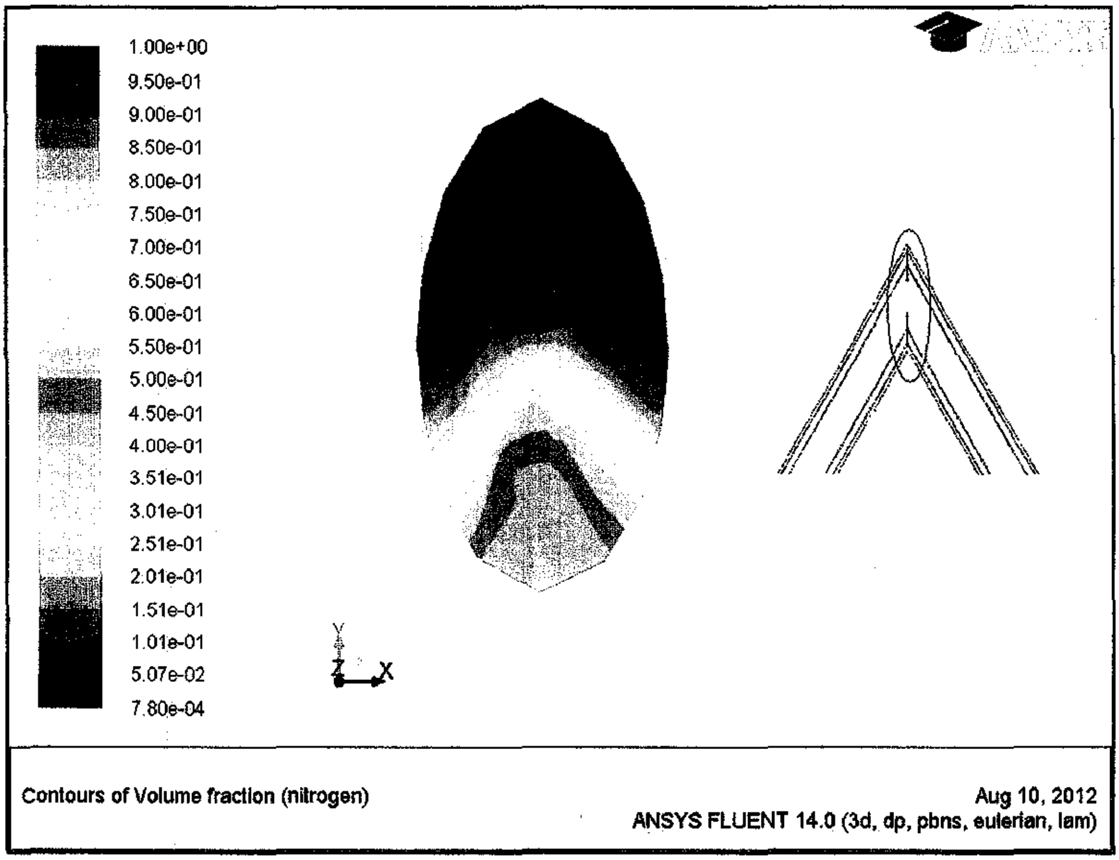
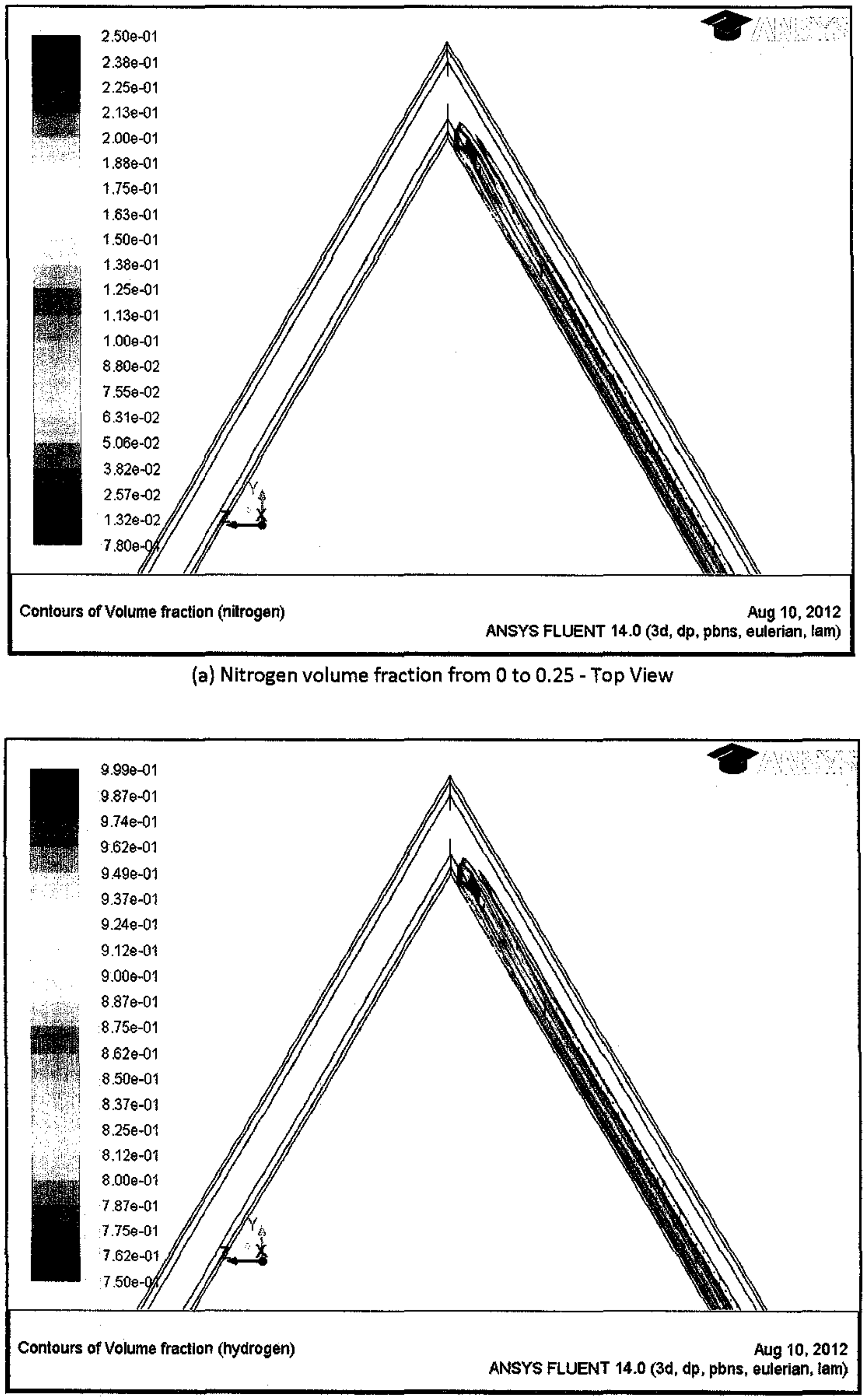


Figure 16: Volume Fraction of Nitrogen Gas at Cross Sectional Area



(a) Nitrogen volume fraction from 0 to 0.25 - Top View

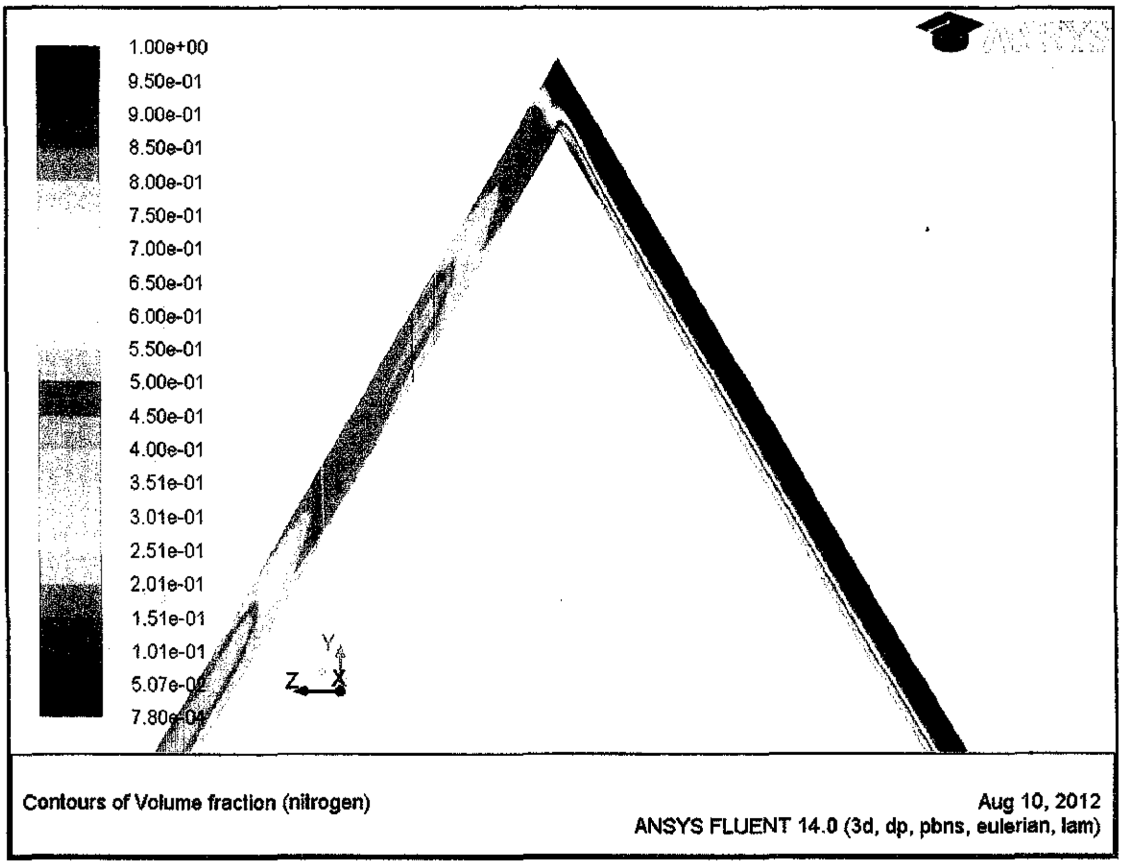
(b) Hydrogen volume fraction from 0.75 to 1 - Top View

Figure 17: Optimal location for catalyst

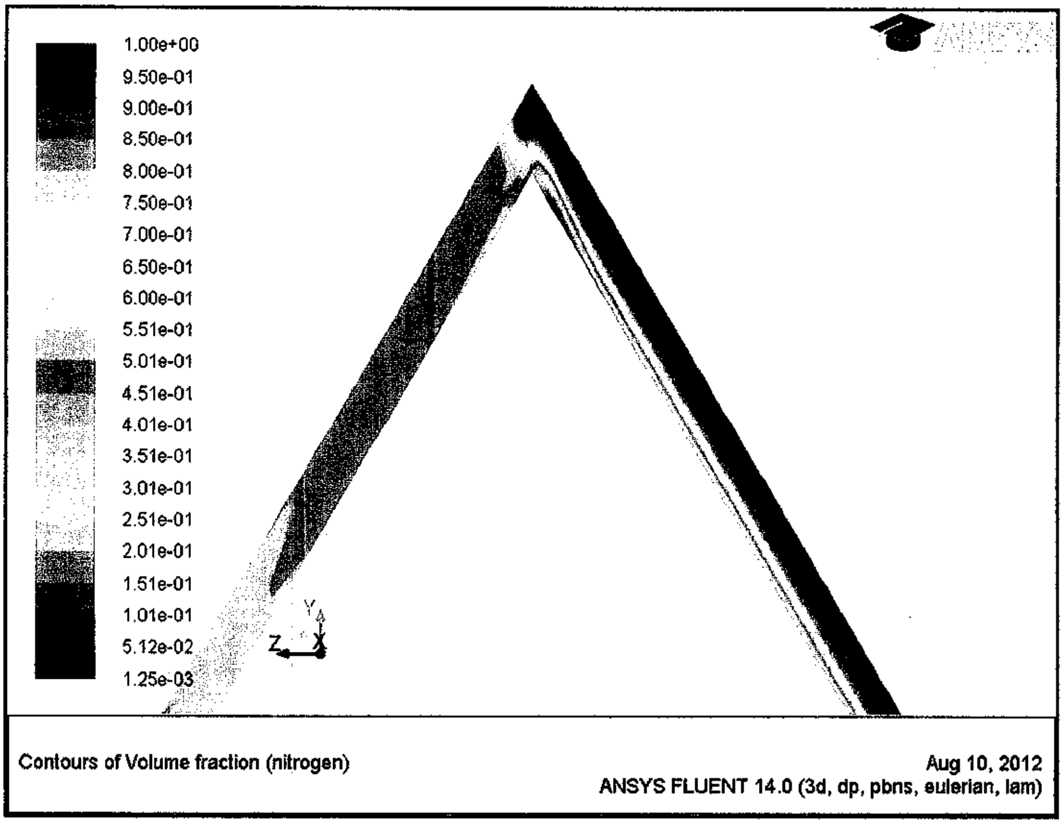
As observed in Figure 17, the catalyst optimal location will be at the inner side of the wall right after the corner. The outer site of the wall is not a best location as there are too much nitrogen gas accumulates. This phenomena is due to nitrogen gas density is heavier than hydrogen gas. Therefore, the amount of nanowire which carries the catalyst should be maximized at the inner side of the wall and minimized at outer side of the wall right after the corner.

4.3 The Effect of Micro-channel Diameter on Reactants Volume Fraction and Velocity

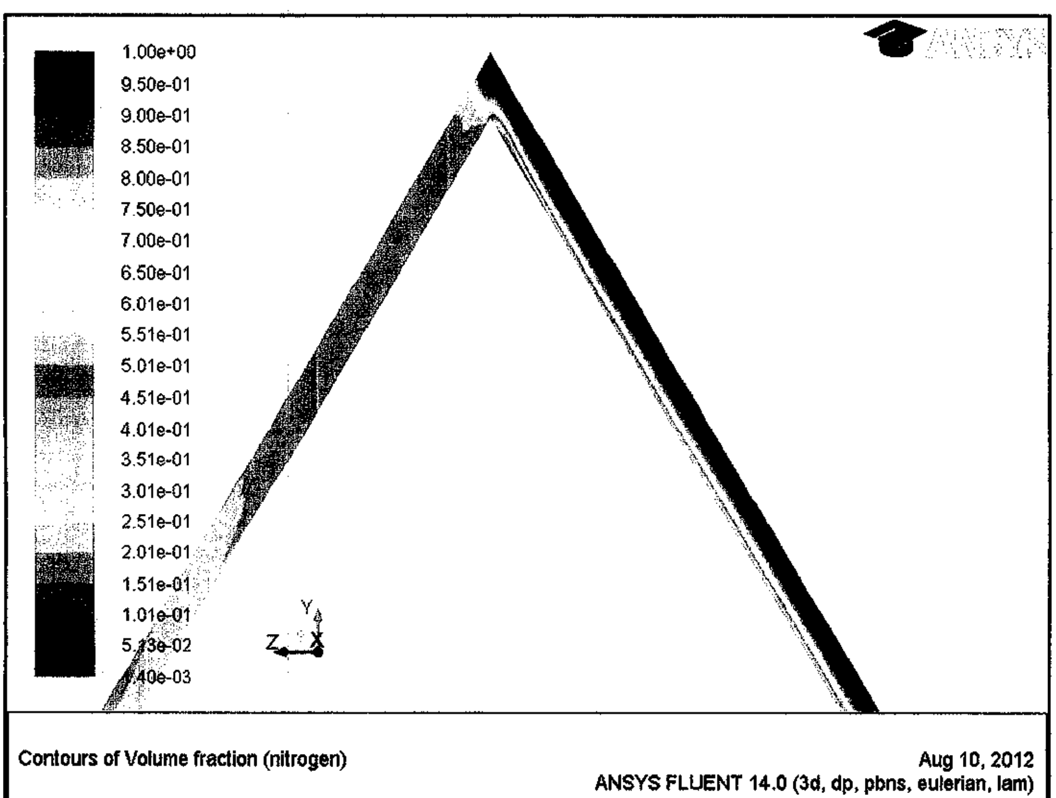
In order to study the effect of micro-channel diameter on reactants volume fraction and velocity, the model is run with three micro-channel diameter: 10, 8, and 6 μm. Then, the volume fraction and velocity contour is drawn in order to study the diameter effect towards the flow characteristic at the corner. For this experiment, the inlet volumetric flow-rate is kept constant at 1.11 ml/min. Figures 18 and Figures 19 show the comparison of volume fraction and velocity magnitude for parameter 1, which is micro-channel diameter.



(a) 10 μm

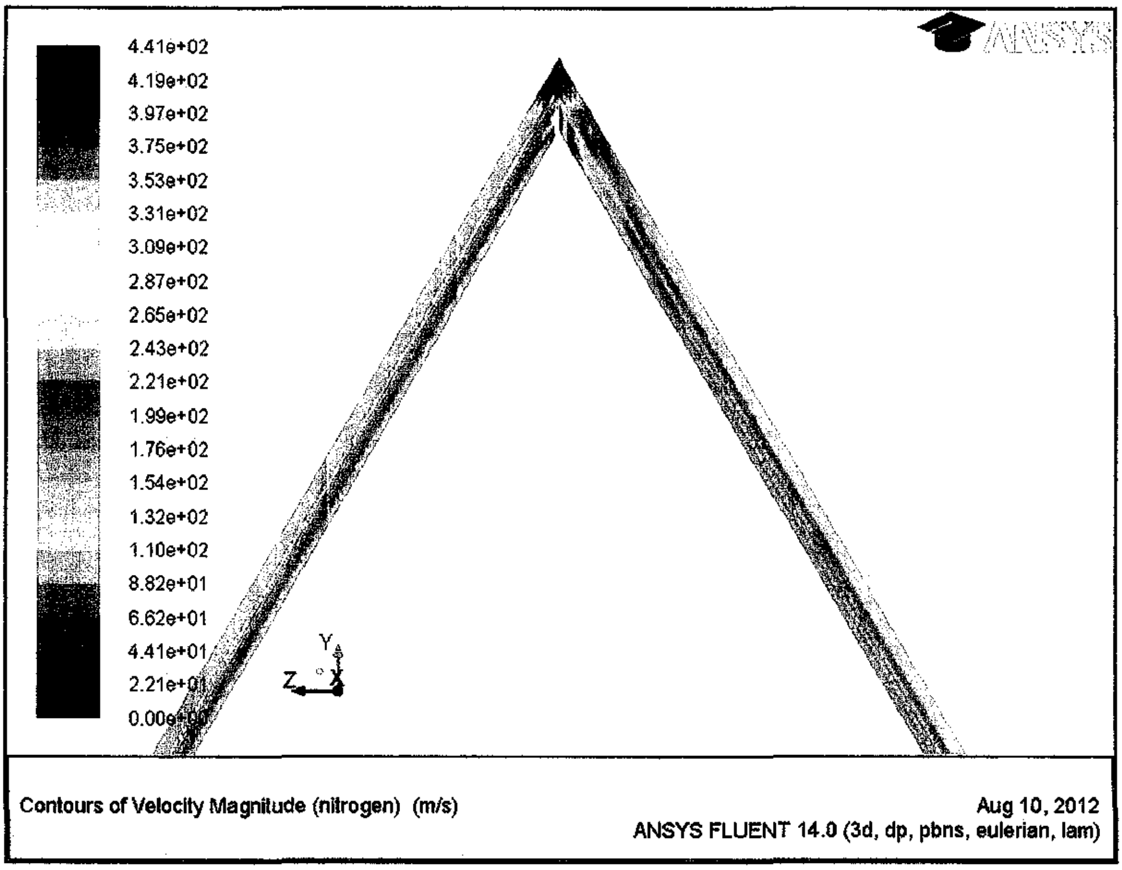


(b) 8 μm

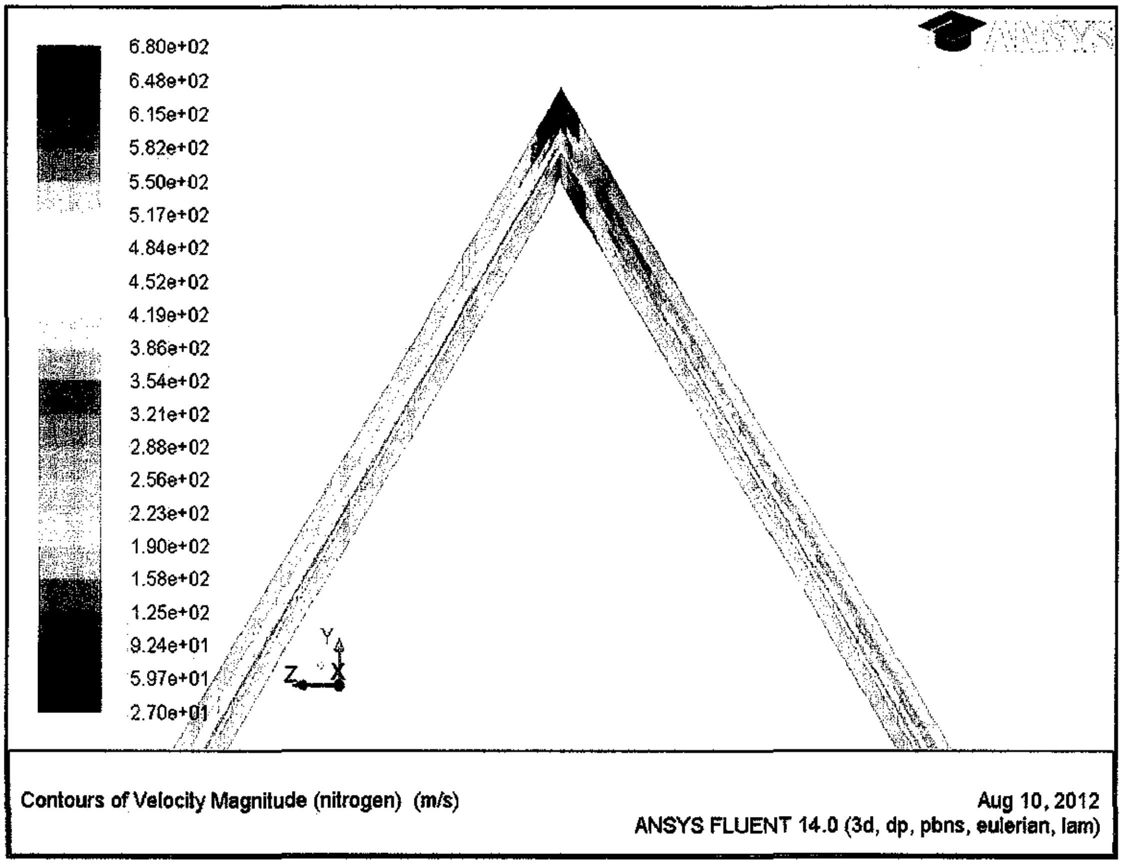


(c) 6 μm

Figure 18 Comparison of Volume Fraction for Parameter 1 (Diameter)


4.41e+02
4.19e+02
3.97e+02
3.75e+02
3.53e+02
3.31e+02
3.09e+02
2.87e+02
2.65e+02
2.43e+02
2.21e+02
1.99e+02
1.76e+02
1.54e+02
1.32e+02
1.10e+02
8.82e+01
6.62e+01
4.41e+01
2.21e+01
0.00e+00
Y
Z
X
Contours of Velocity Magnitude (nitrogen) (m/s)
Aug 10, 2012
ANSYS FLUENT 14.0 (3d, dp, pbns, eulerian, lam)

(a) 10 µm


6.80e+02
6.48e+02
6.15e+02
5.82e+02
5.50e+02
5.17e+02
4.84e+02
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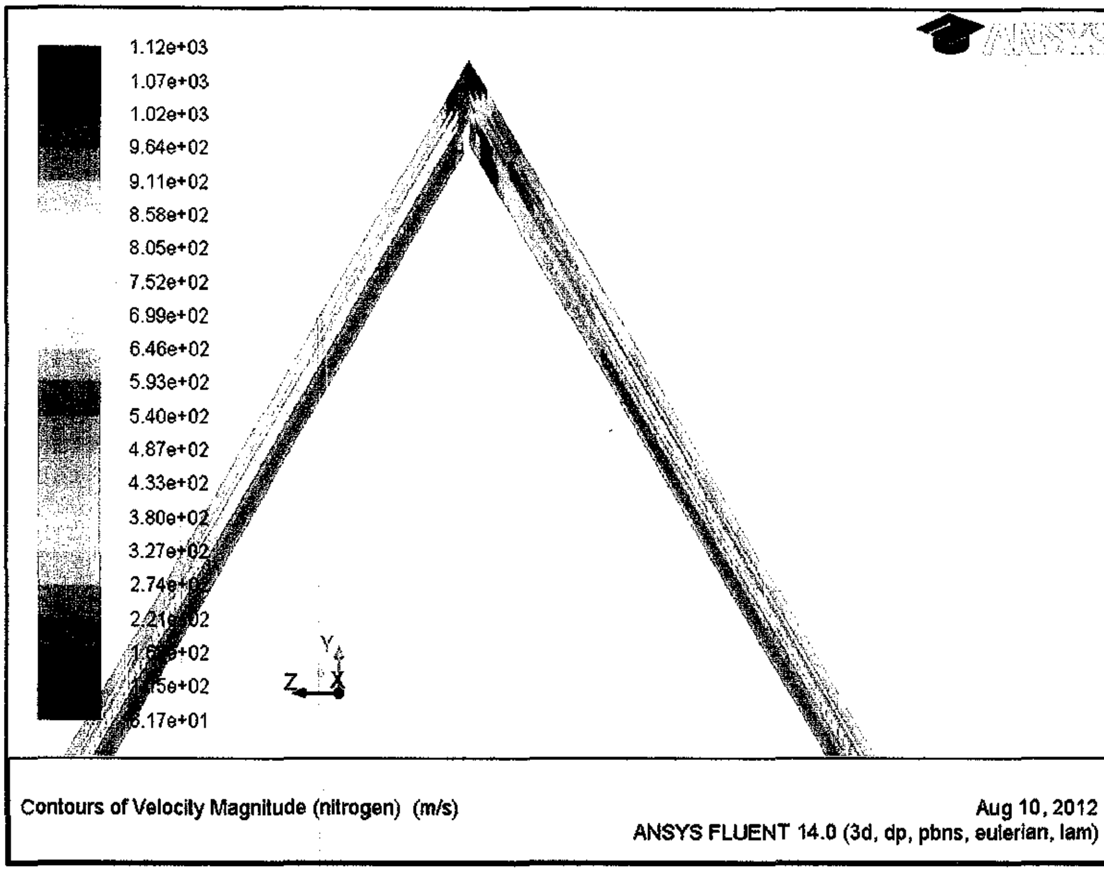
4.19e+02
3.86e+02
3.54e+02
3.21e+02
2.88e+02
2.56e+02
2.23e+02
1.90e+02
1.58e+02
1.25e+02
9.24e+01
5.97e+01
2.70e+01
Y
Z
X
Contours of Velocity Magnitude (nitrogen) (m/s)
Aug 10, 2012
ANSYS FLUENT 14.0 (3d, dp, pbns, eulerian, lam)

(b) 8 µm

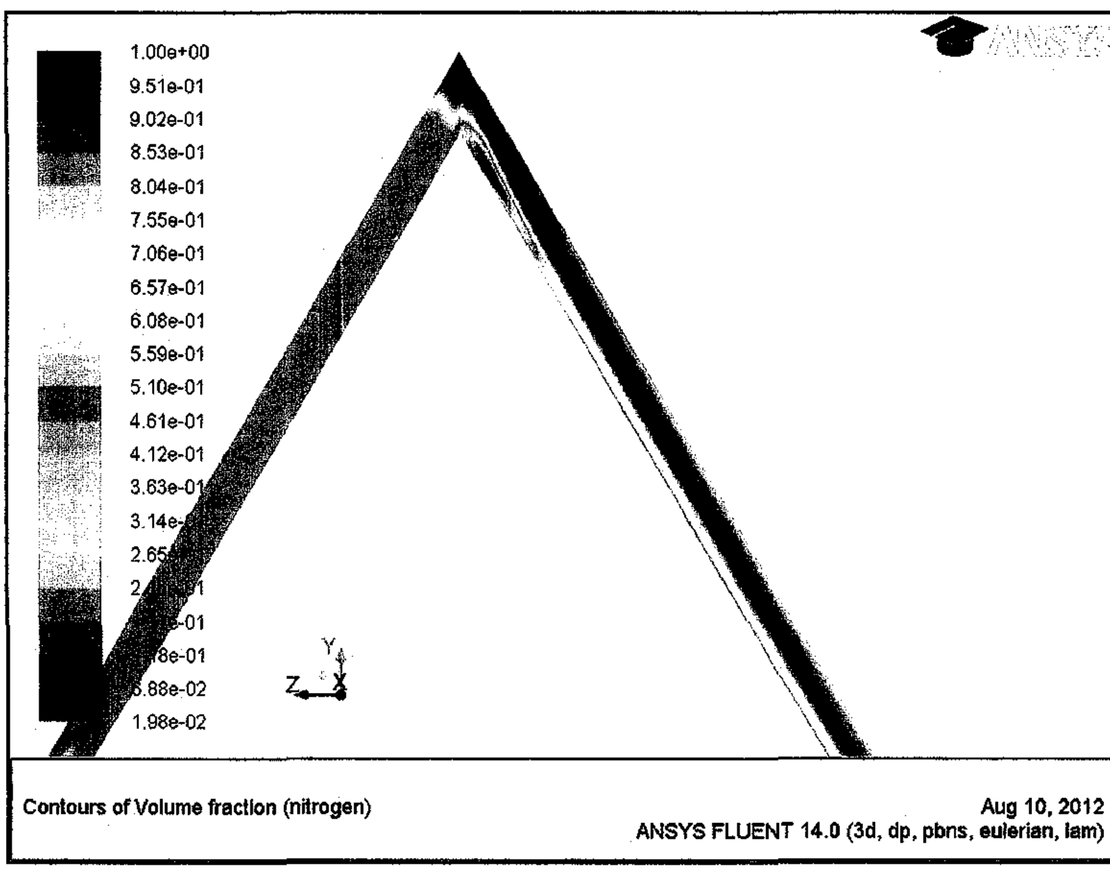


(c) 6 µm

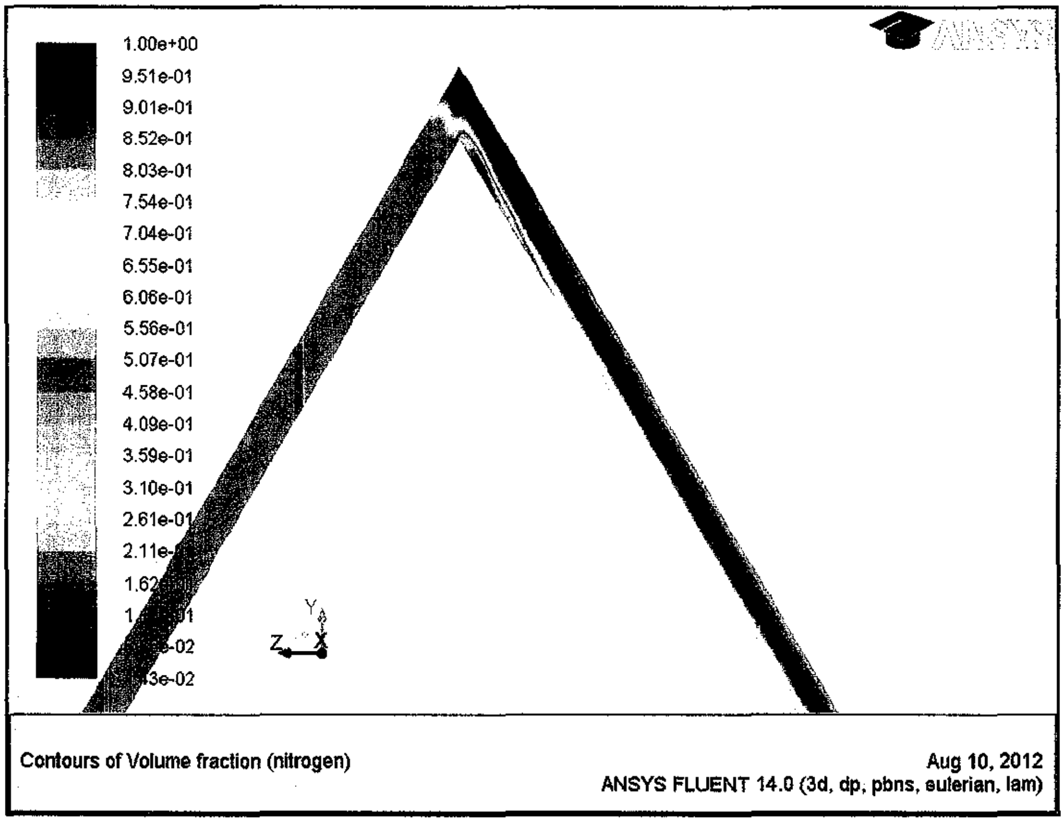
Figure 19: Comparison of Velocity Magnitude for Parameter 1 (Diameter)

4.4 The Effect of Inlet Volumetric Flow-rate on Reactants Volume Fraction and Velocity

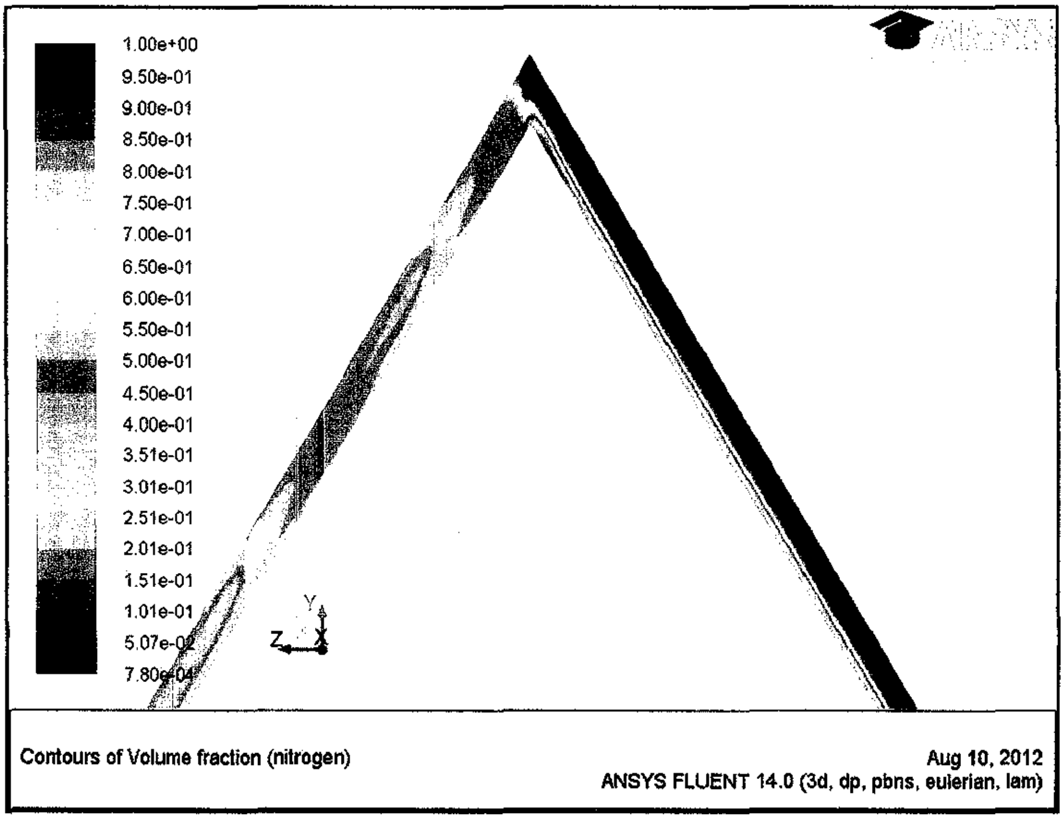
The last parameter that studied is the effect of inlet volumetric flow-rate on reactants volume fraction and velocity. For the simulation, the model is run with three inlet volumetric flow-rate: 3.33, 2.22, 1.11 ml/min. Then, the volume fraction and velocity contour is drawn in order to study the volumetric flow-rate effect towards the flow characteristic at the corner. For this experiment, the micro-channel diameter used is 10 μm. Figures 20 and Figures 21 show the comparison of volume fraction and velocity magnitude for parameter 2, which is inlet volumetric flow-rate.



(a) 3.33 ml/min

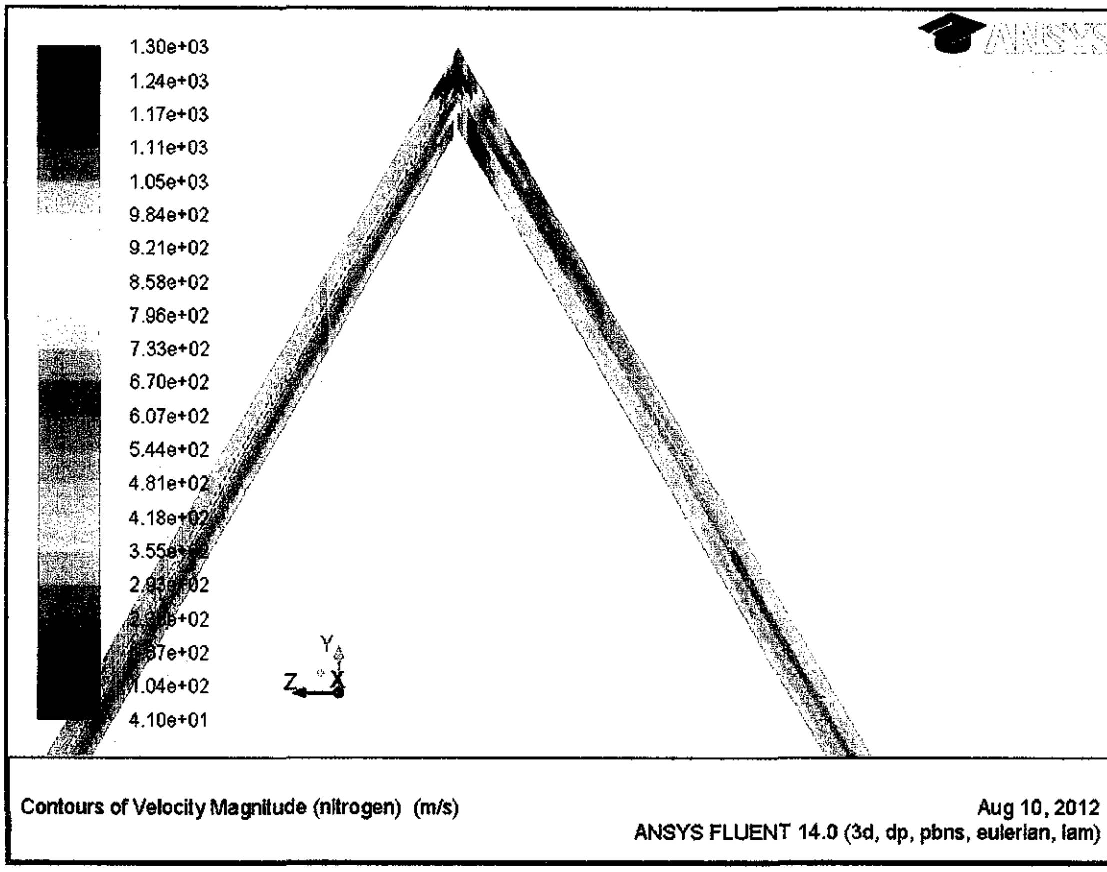


(b) 2.22 ml/min

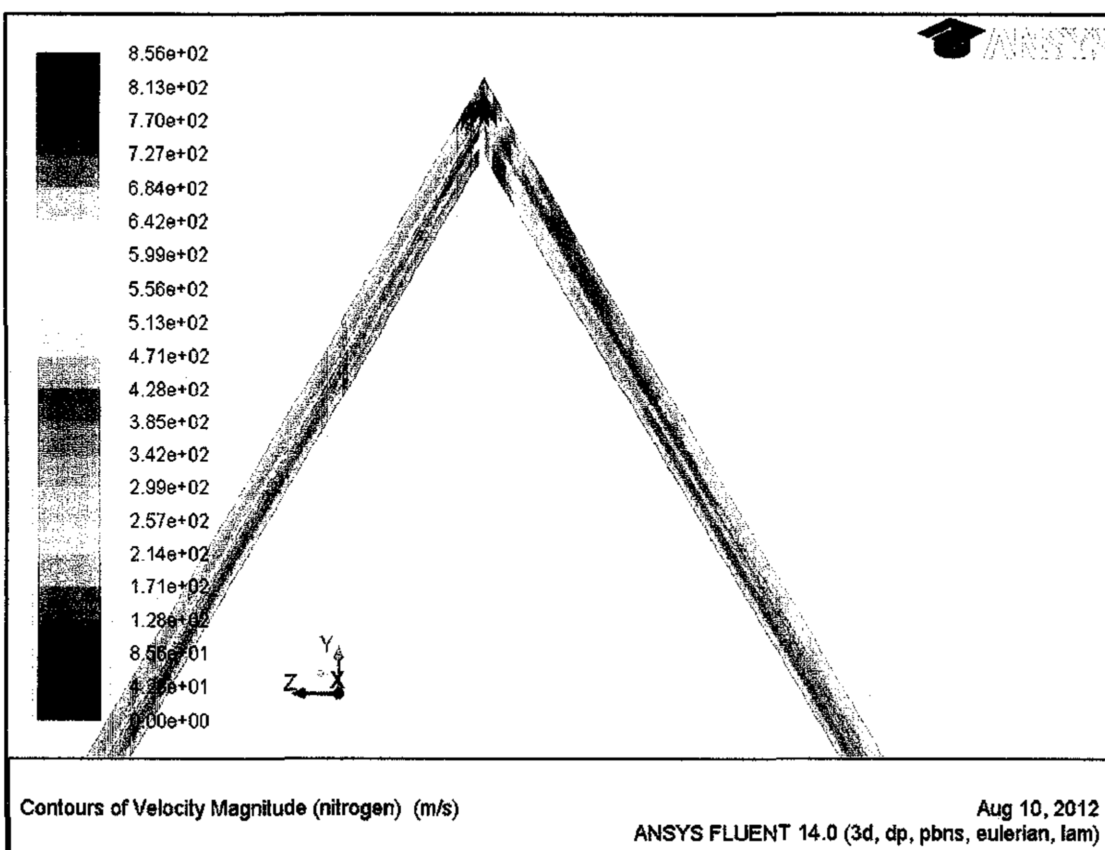


(c) 1.11 ml/min

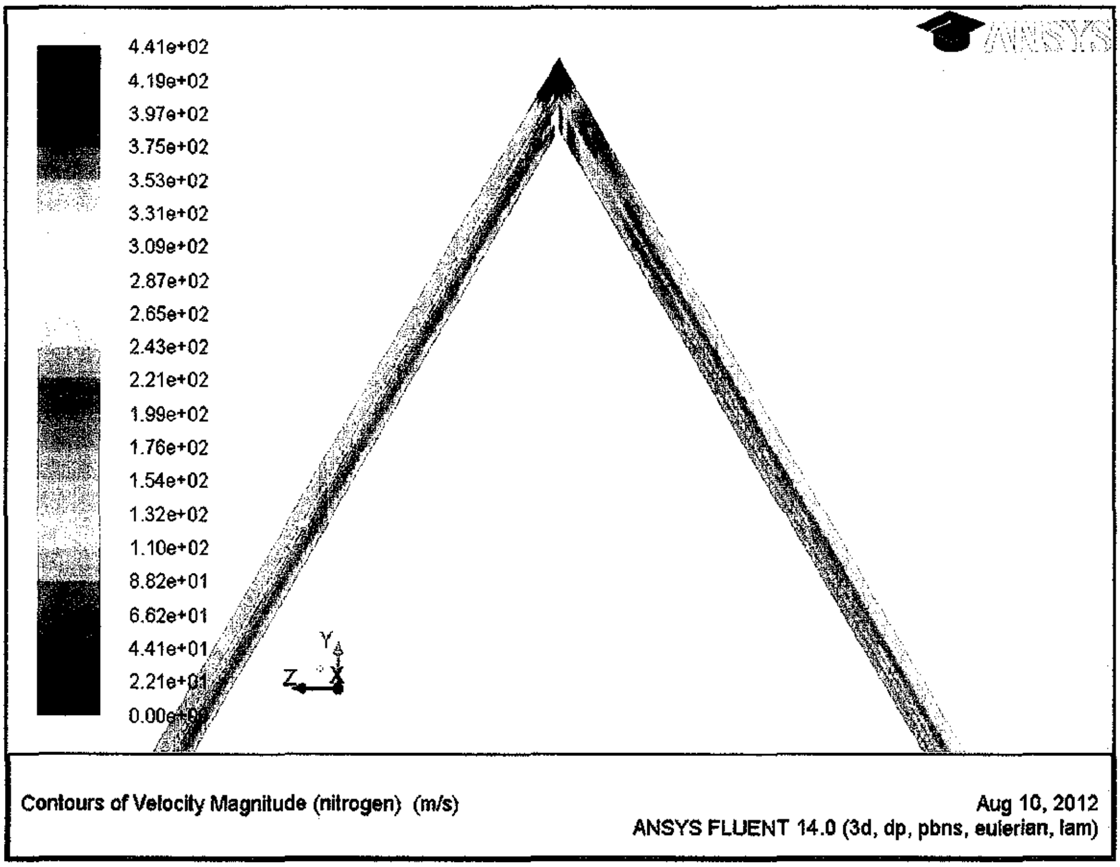
Figure 20: Comparison of Volume Fraction for Parameter 2 (Volumetric Flow-rate)



(a) 3.33 ml/min



(b) 2.22 ml/min



(c) 1.11 ml/min

Figure 21: Comparison of Velocity Magnitude for Parameter 2 (Volumetric Flow-rate)

4.5 Discussion

In identifying the catalyst optimal location, the study shows that the inner wall after corner is the best location.

In order to analyzed the result for parameter 1 (micro-channel diameter) and parameter 2 (inlet volumetric flow-rate), graphs of the parameters versus volume fraction and velocity are plotted. A single point is chosen from the domain which is the center of cross sectional area at the corner of the micro-channel. Then value for volume fraction of nitrogen and velocity is retrieved at the single point. Figure 22 shows the graph of micro-channel diameter versus volume fraction & velocity and Figure 23 shows the graph of inlet volumetric flow-rate versus volume fraction & velocity

Vector	Coordinate
X	$-5.27133e^{-08}$
Y	0.002500718
Z	-0.002500042

Table 7: Single Point Coordinate

Parameter 1 (μm)	VF (nitrogen)	Velocity (m/s)
10	0.86	184
8	0.84	280
6	0.83	519

Parameter 2 (ml/min)	VF (nitrogen)	Velocity (m/s)
3.33	0.90	557
2.22	0.88	380
1.11	0.86	184

Table 8: Nitrogen Volume Fraction and Velocity at Single Point Specified

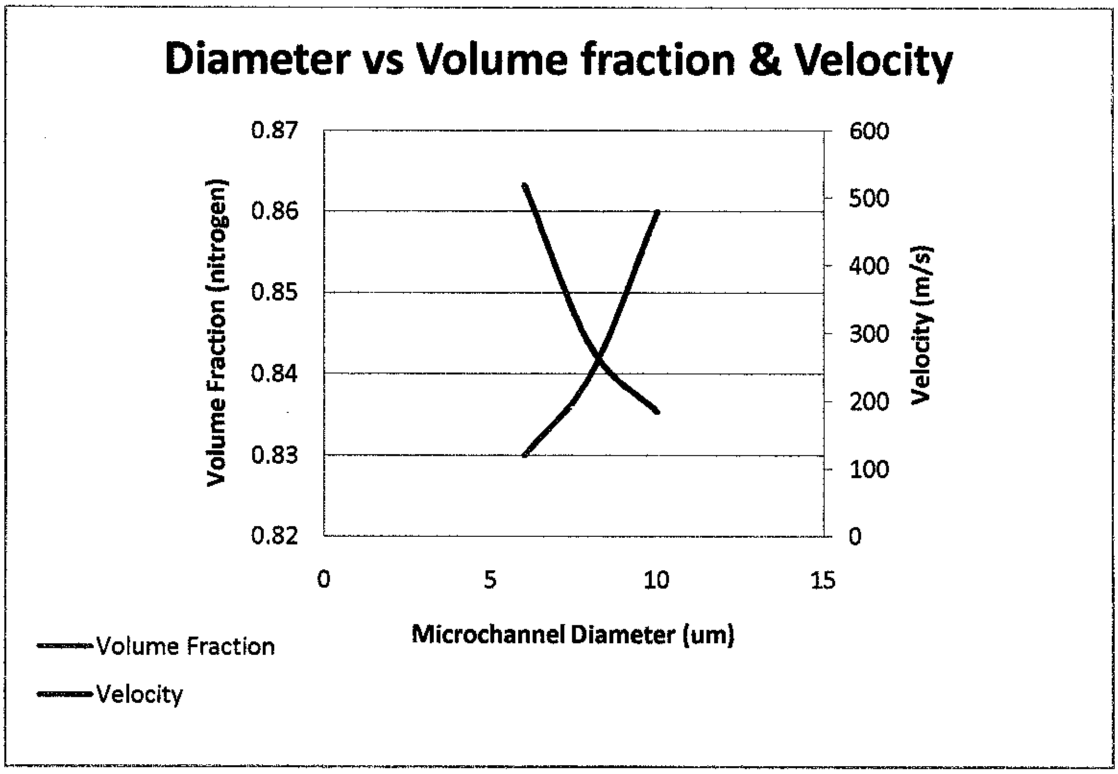


Figure 22: Micro-channel Diameter vs Volume Fraction & Velocity

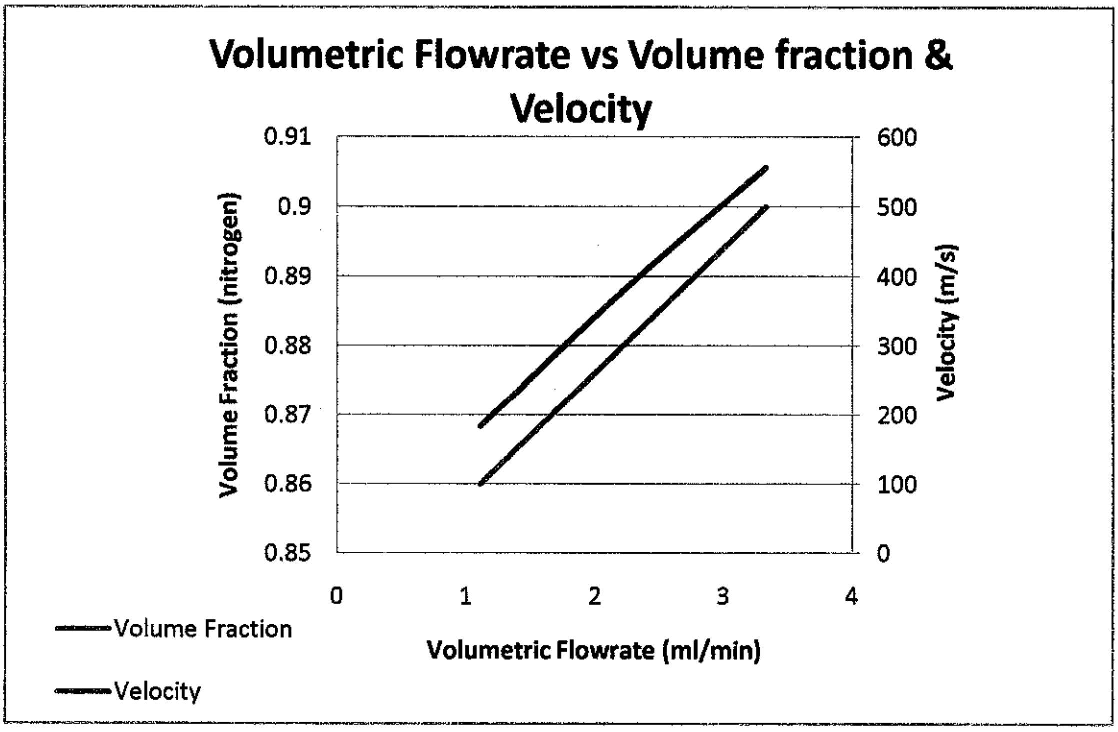


Figure 23 : Inlet Volumetric Flow-rate vs Volume Fraction & Velocity

CHAPTER 5: CONCLUSION & RECOMMENDATION

5.1 Conclusion

As conclusion, the three objectives of the study are achieved. For the first objective, the model for ammonia production in micro-reactor is successfully developed. As for the second objective, the optimal location for catalyst is identified. The optimal location is at the inner wall after corner as the mol fraction suit the stoichimetric ratio for ammonia reaction.

The last objective is the study of micro-channel diameter and inlet volumetric flow-rate toward volume fraction and velocity. The high volume fraction suggests a bad degree of mixing and high velocity is not preferable as it will decrease the reactants residence time.

For the first parameter, the graph shows that as micro-channel diameter increasing, the volume fraction of nitrogen at the specified point is increasing and the velocity is decreasing. Meanwhile for the second parameter, the graph shows that both volume fraction and velocity increasing as the inlet volumetric flow-rate increase.

After evaluating all the simulation, the best parameter is the simulation with micro-channel diameter of 10μm and 1.11 ml/min inlet volumetric flow-rate. This is because it produces a low nitrogen volume fraction, 0.86 and has a lowest velocity, 184m/s at the specified single point.

5.2 Recommendation

There are three recommendations for future studies. First is improvement in meshing as refinement should be done in order to obtain an accurate result. The full license of ANSYS 14 shall be obtained in order to do a better meshing quality for micro-channel geometry.

For this study, the focus only on hydrodynamics of fluid and the reaction to produce ammonia was not taken into consideration. Therefore, the study needs to be extended to consider the reaction in order to predict ammonia concentration and yield. Next, the residence time for ammonia reaction in micro-channel need to be determined in order to find the best inlet volumetric flow-rate for it.

The last recommendation is experiment have to be conducted in order to validate the numerical results predicted using the simulation. By this, the results will be much more accurate and convincing.

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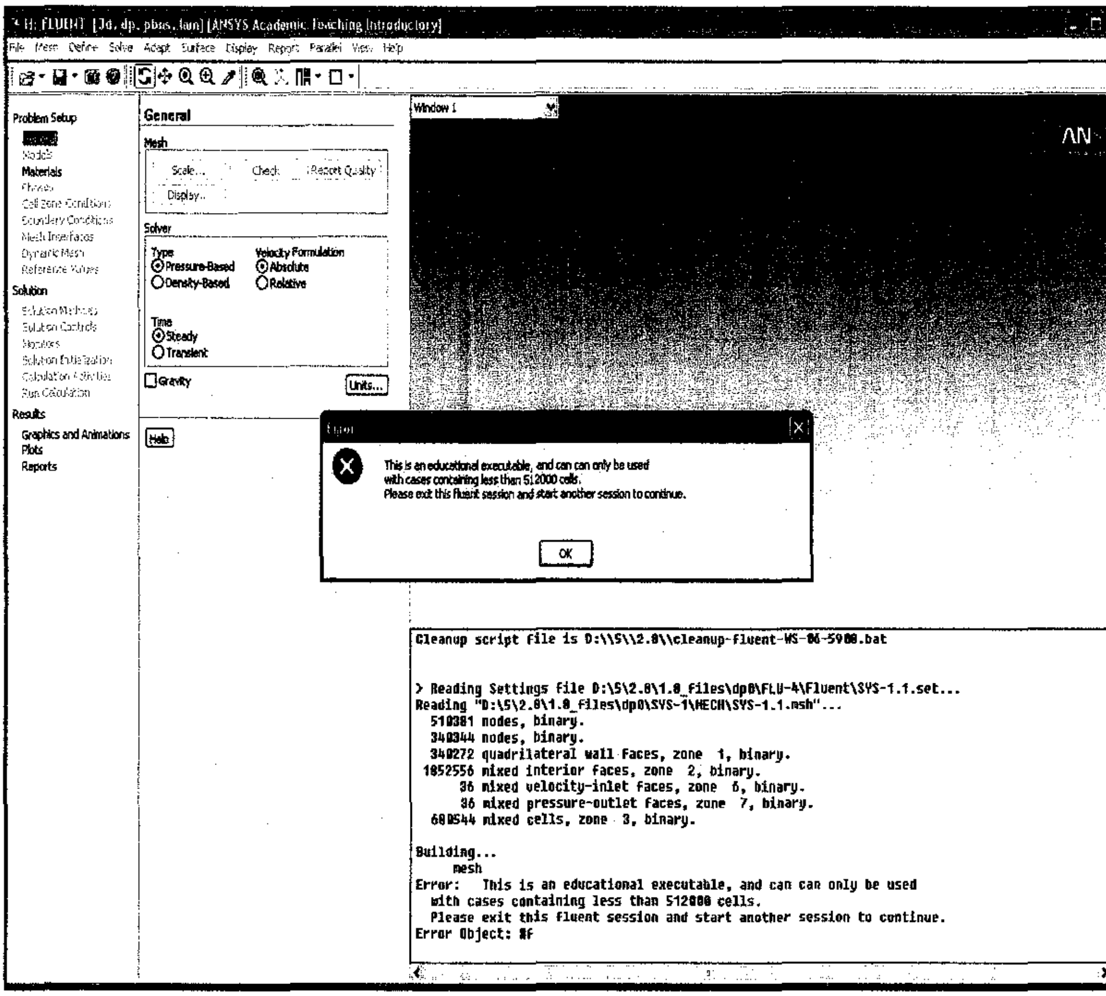
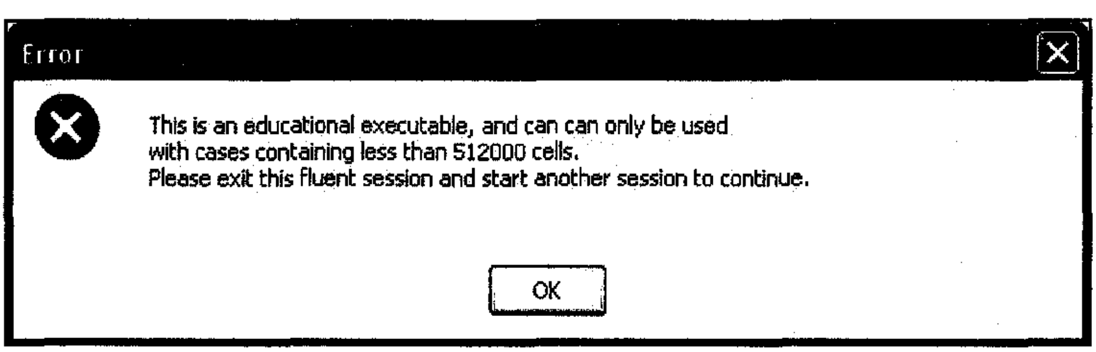
APPENDIX

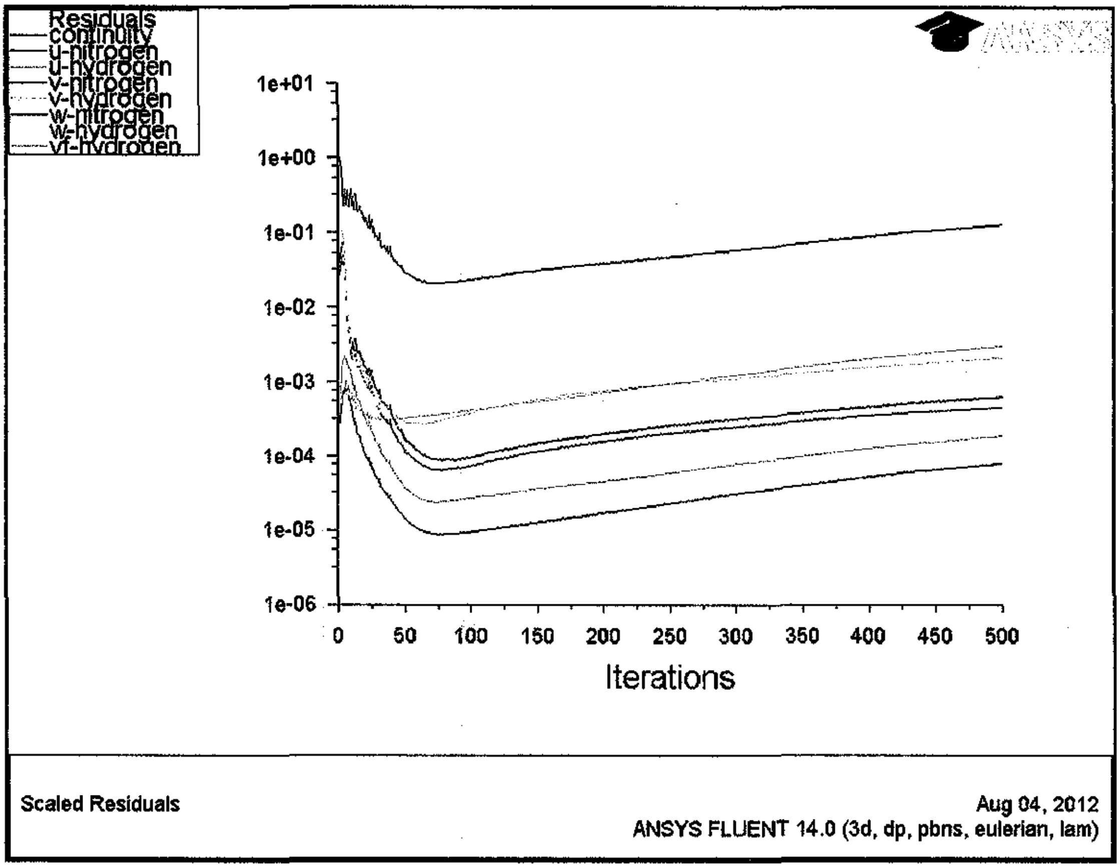
APPENDIX A - Educational License Cells Limitation



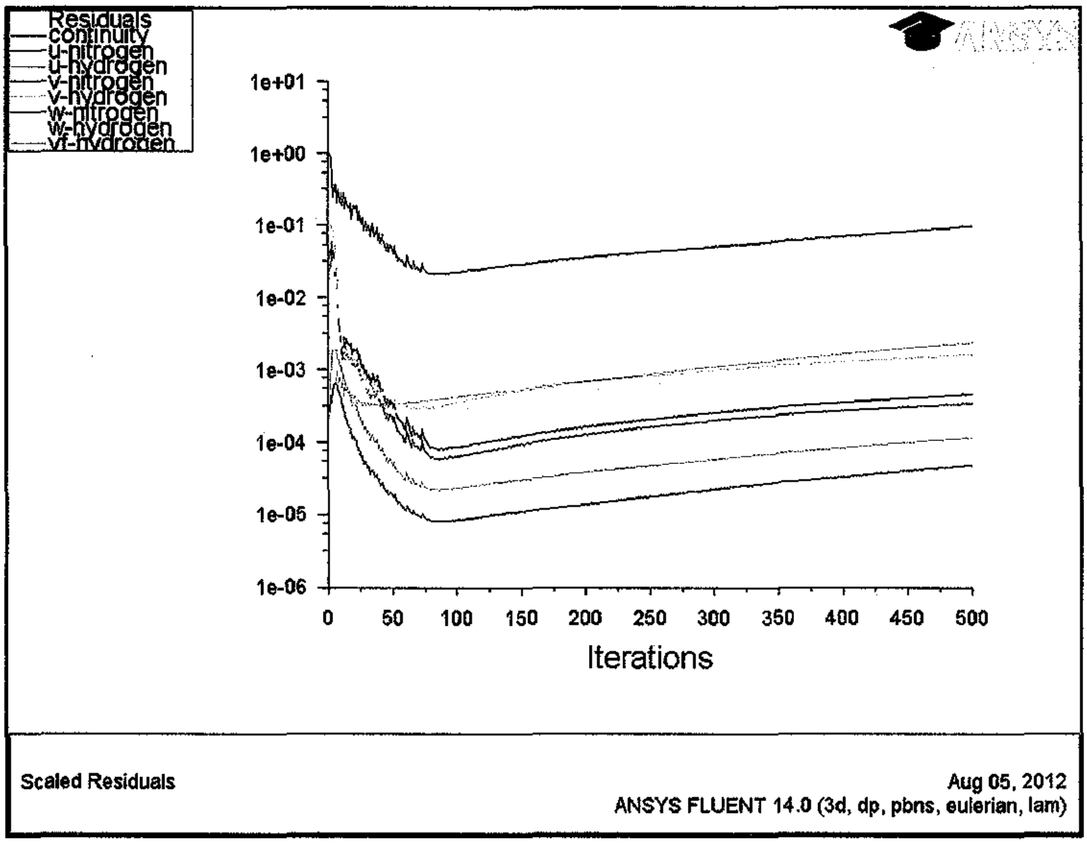


APPENDIX B - Residuals Graph

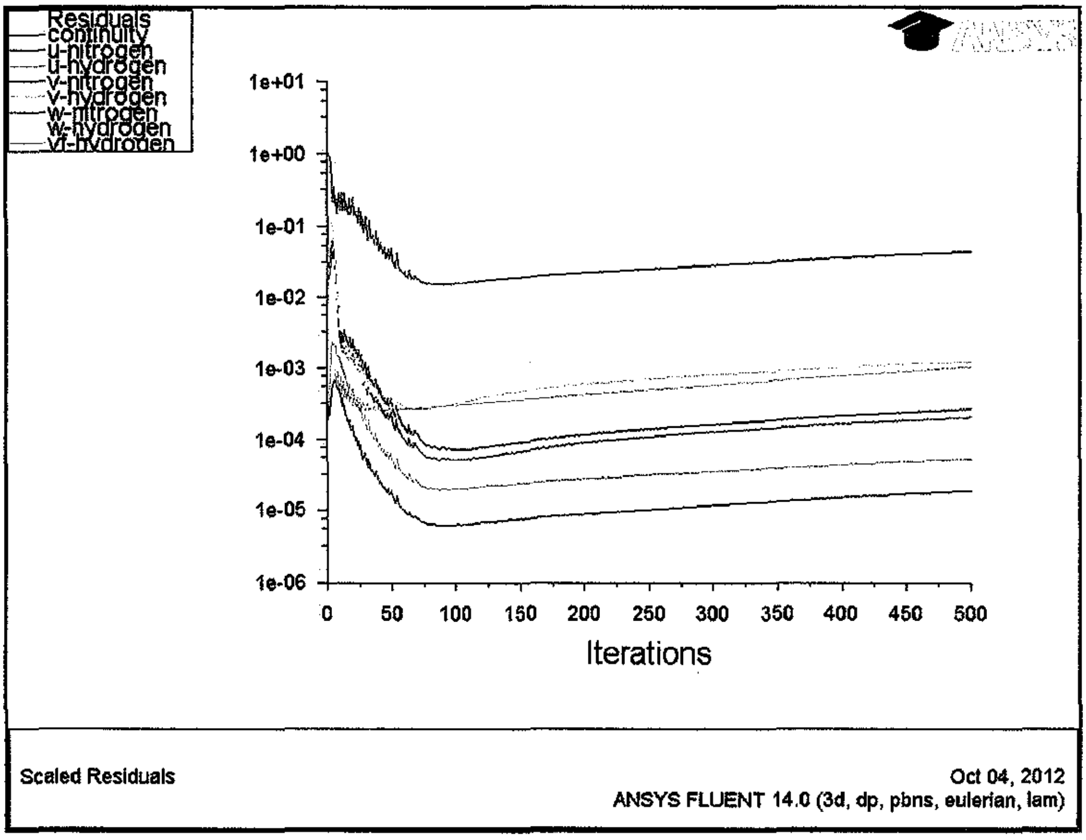
Residuals - 10μm, 1.11 ml/min



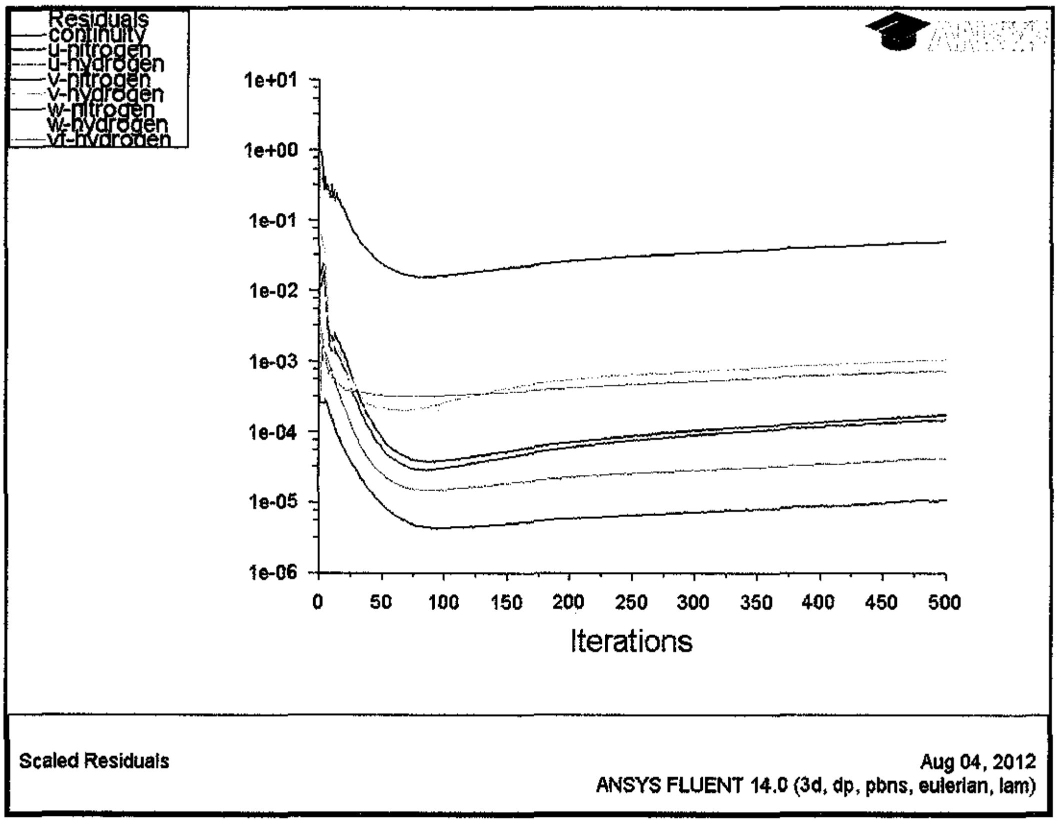
Residuals - 8μm, 1.11 ml/min



Residuals - 6μm, 1.11 ml/min



Residuals - 10μm, 3.33 ml/min



Residuals - 10μm, 2.22 ml/min