HYDRODYNAMICS BEHAVIOUR OF SIMULATION OF ONE-STEP UREA SYNTHESIS IN MICROREACTOR

By

Muhammad Nurdin Bin Othman

Dissertation submitted in partial fulfilment of

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(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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Approved by,

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(Dr.Anis Suhaila Binti Shuib)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

MAY 2013

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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MUHAMMAD NURDIN BIN OTHMAN

Abstract

Urea or Carbamide (NH_2CONH_2) functioned as nitrogen-rich fertilizers which is vital to the agriculture industry. Currently, the Urea synthesis involving two step conversions process; the initial steps are ammonia production through Haber - Bosch process through the reaction of Hydrogen (H_2) and Nitrogen (N_2) Gas in high temperature and pressure with the presence of Iron Oxide (Fe_2O_3) as the catalyst. The second step composed of reaction between ammonia (NH_3) and Carbon Dioxide (CO_2) in order to yield urea. Potential research of urea synthesis under the magnetic induction zone at ambient room temperature and pressure has been introduced as one alternative method of bypass the use of ammonia process as an intermediate.

At current state, the design of microreactor for one step urea synthesis is not available. This study will address on focusing the effect of geometry angle on the mixing efficiency of the reactant gases through the Microchannel. In this proposal, the fluid flow and molecular motion on the gas mixing were demonstrated using Ansys-Fluent (CFD modeling) through trial and error method. By varying the geometry / angle of the Microchannel, different degree of mixing can be observed in order to determine the optimum location of the catalyst input based on three governing parameters ; Mixing efficiency , Pressure Drop and length of Microchannel. The fluid flow can be obtained by solving the Eulerian equation and molecular motion can be calculated using the discrete phase model. Outcome throughout this simulation project was to propose an optimum Microchannel geometry condition based on mixing quality and retention time of the gas reactant spend in the microreactor.

ACKNOWLEDGEMENT

First and foremost, I'd like to express my utmost gratitude towards Allah S.W.T. It is due to His will that I have been able to conduct this project and successfully finish it within the given time.

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CHAPTER 1

INTRODUCTION

1.1 Background Of Study

The ammonia and urea industry is changing significantly as a new market for bio-fuels and NOx abatement emerges. A key driver of this fluctuation activity has been the cost of feedstock which is the natural gas that inflicts some production curtailments for major plant in North America and Western Europe. Access to low cost gas and processing technology has become a major priority for the plant to have upper hand on economic capability in order to produce low cost ammonia and urea.

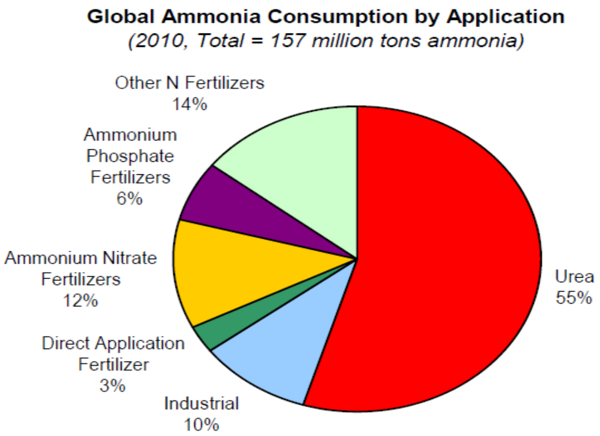


Figure 1: Global Ammonia Consumption by Application

Based on the figure 1 , the graph indicate that the urea continues to gain market share over another fertilizers , mainly due to the fact it contained high nitrogen content compared to ammonium nitrate and other fertilizers. Fertilizer production consumes approximately 1.2% of the world energy and responsible in contributing to the greenhouse effect. In detailed explanation, Urea is not stable as other solid nitrogenous fertilizers as it can be easily decomposed to N2O through ammonia volatilization, denitrification and leaching.

The loss contributes towards both economic and environmental problem. Currently, the urea technology exploit the ammonia as an intermediate raw material subsequently convert to urea. The Process synthesis involving two step conversions; the first steps are ammonia production through Haber - Bosch process through the reaction of Hydrogen (H_2) and Nitrogen (N_2) Gas in high temperature and pressure with the presence of Iron

Oxide (Fe_2O_3) as the catalyst. The second step composed of reaction between ammonia (NH_3) and Carbon Dioxide (CO_2) in order to yield urea. [1]

1.2 Problem Statement

Through the current method, the process run at high operating cost as it operates at high pressure and temperature (500°C & 150 Bar). Thus, the introduction of micro-reactor acts as an overview for new initiative of greener and economical chemical reaction for urea synthesis. Based on available patent [3], there is one-step-urea synthesis occur under magnetic induction which theoretically bypass the ammonia as an intermediate. This process directly converts into urea under ambient pressure and temperature .Currently, this study is not available in microreactor.

Good micro-mixing in the microreactor is a good solution for effective mixing and minimize the energy requirement. Practically, involve in straight microchannel. As it involves passive mixing, the fluid flow limited to low Reynolds number regime where the mixing rate occur at longer period and require more pressure to flow[4]. Hence, a shorter path and low pressure drop of microchannel will be ideal. Dependent on the geometry for microchannel, the mixing efficiency of each micro-mixer varies in term of the residence time, volume fraction of the reactant and degree of mixing. Therefore, the hydrodynamics behaviour of urea synthesis in microchannel has to be investigated.

1.3 Objective

The objective is:

1) To develop a numerical simulation of One-step urea synthesis in micro-reactor.
2) To investigate the effect of variation of configuration of microchannel on the volume fraction distribution and pressure drop.
3) To achieve optimum microchannel design for effective gas mixing.

1.4 Scope of study

This study will be encompassed on the approach of CFD modelling on the prediction of hydrodynamic behaviour of the flow mixing of the reactant gas; N_2, H_2 and CO_2 based different geometry configuration of micro-mixers. The volume fraction of the reactants is compared to each other to find the best reactive sites for the catalyst embodiment inside the microchannel. The parameters included in the prior study consist of the analysis of the mixing point displayed by the mixing efficiency.

CHAPTER 2

LITERATURE REVIEW

2.1 AMMONIA SYNTHESIS & FUNCTION

Ammonia serves as intermediate product for urea production and use primarily in fertilizers, chemicals, explosives, fiber & plastics and etc.

2.1.1 Ammonia synthesis by Haber - Bosch process

It is synthesised by the exothermic reaction of 3 volume of hydrogen (H_2) and 1 volume of nitrogen (N_2) at high temperature (400°C- 500°C) and pressure (150 bars – 300 bars) in the presence of the porous iron as a catalyst [1]. The reaction were initially proposed by Haber in 1909 and further commercialized into an industrial scale by Bosch.

N_2 (g) + $3H_2$ (g) $\rightleftharpoons$ $2NH_3$ (g) $\triangle$ **H = -92.4 kJ**

2.1.2 Ammonia synthesis by magnetic induction method

This ammonia synthesis reaction was carried out in microreactor covered in the electromagnetic induction (EM) at room temperature (28°C) and ambient pressure [2]. By manipulating the EM, it arouse the electron alignment and the catalytic activity occurred in the presence of nanocatalyst (manganese ferrite).The outcome from this invention has yield ammonia at 24.9%.

2.2 Urea synthesis by Basaroff Exothermic Liquid Extraction

Generally, urea is produced by reacting ammonia and carbon dioxide at high temperature and pressure. This is Basaroff exothermic liquid reaction $2NH_3 + CO_2 \rightarrow NH_2COONH_4$ and exothermic reaction $NH_2COONH_4 \rightarrow H_2O + NH_2CONH_2$ [5]. The scheme in Figure 3 explains the way to produce urea.

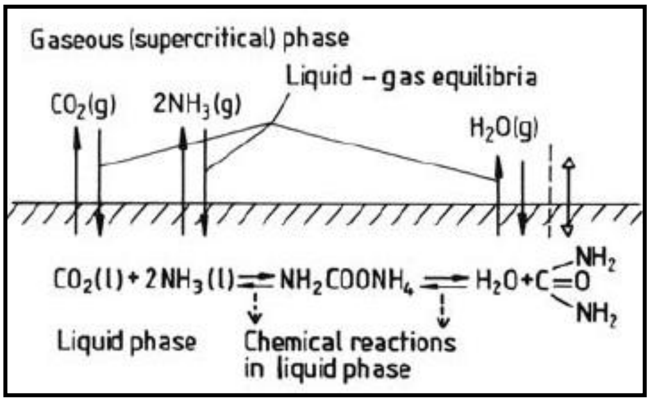


Figure 2 : Chemical and Physical equilibria equation

2.2.1 One-Step Urea production by magnetic induction

This method comprise of the mixing of three different gas reactant into a microreactor, a reactor chamber being disposed in the high density of electromagnetic flux with a catalyst/catalyst support microreactor systems to produce molten urea. The catalyst used is Fe-based nanocatalyst with catalyst supports made from Herrinbone Carbon nano fibre (CNF) structure and ZrO_2 tubes [3]. This one is the simpler method compared to the conventional method.

2.3 Microreactor

Microreactor is a device in which the chemical reaction take places in a confinement space with typical lateral dimensions micro-millimetre [6]. Mixing at micro state consists of active and passive mixing which in this case, it primarily involves passive mixing. However, mixing process at this stage face some difficulties as the fluid flow were constrained at low fluid regime i.e. laminar flow. Thus, it requires an alteration of the micro-mixers geometry until it achieve an optimum condition for passive mixing system through trial and error method based on mathematical modelling simulation.

2.4 Catalyst Used

Catalyst defined as a chemical substance that speed up the rate of reaction by lowering the activation energy required for the reaction to occur without changing the composition of product formed and the catalyst itself. The microchannel surface was embodied with nanowire and nanotubes that consist of nanocatalyst and nanocatalyst support that function to promote the rate of reaction. α-Fe_2O_3, Hematite is a nanowire which possesses catalytic activity for a number of chemical reactions. The iron oxide nanowire was grown by resistive heating under ambient temperature at diameter of 0.25 mm (Albert G.Nasibulin et.al, 2009) and grows to 1–5 μm long a temperature 700°C

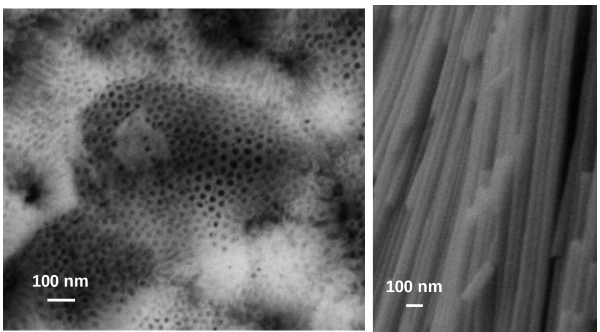


Figure 3: SEM images showmorphology of ZrO_2 nanotubes oxide [7]

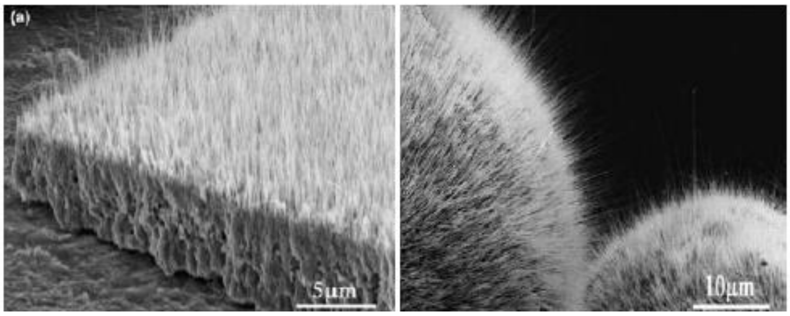


Figure 4: SEM images show the as-synthesized (a) α-Fe_2O_3 nanowires grow vertically from the substrate over a large flat area. (b) α-Fe_2O_3 nanowires grown on the spherical radial surfaces of iron particles [8]

2.5 Microchannel in Mixing Efficiency and Pressure Drop

Mixing efficiency and pressure drop has been characterized in various microchannel geometries. Table 1 shows the summary of pressure drop and mixing efficiency [10]

$$m_{eff} = \left(1 - \frac{\int_0^W |v - v_\infty| dx}{\int_0^W |v_0 - v_\infty| dx}\right) \times 100\% \quad \textbf{(1)}$$

Where m_{eff} = Mixing Efficiency, V= Volume fraction distribution across the transverse direction of outlet, V_o= Initial distribution of the volume fraction before mixing occurs, V_∞ = Volume fraction of complete mixing, W = the width of the micro-mixers

In cylindrical microchannel, **width** can be changed to **diameter.**

There are three literatures for comparing length, mixing and pressure drop in microchannel.

Table 1: Previous research in pressure drop and mixing efficiency of microreactor.

Microreactor type	Fluid	Pressure Drop (Pascal)	Mixing Efficiency	References
Wavy-wall	Newtonian fluid	Not Measured	x = 20 mm ; 89 %	Chen et.al [4]
Straight			x = 20 mm ; 20 %	
Zigzag	Fluid 1 : Gold Nanoparticles Fluid 2 :	x = 20 mm ; 58 Pa x = 32 mm ; 115	x = 20 mm ; 89 % x = 32 mm ; 95 %	Jeon et.al [9]

	$CuSO_4$	Pa		
Contraction-Enlargement		x = 20 mm ; 57 Pa x = 32 mm ; 98 Pa	x = 20 mm ; 70 % x = 32 mm ; 90 %	
Rhombic Baffles		x = 20 mm ; 65 Pa x = 32 mm ; 90 Pa	x = 20 mm ; 68 % x = 32 mm ; 88 %	
Circular Baffles		x = 20 mm ; 43 Pa x = 32 mm ; 88 Pa	x = 20 mm ; 54 % x = 32 mm ; 65 %	
Rectangular		x = 20 mm ; 41 Pa	x = 20 mm ; 40 %	

Based on the Jeon et.al research, the zigzag type indicates a higher mixing efficiency at 95 % compared to the micro-mixers with highest pressure drop: 115 Pa. Hence, the zigzag type is the most efficient geometry for micro-mixers. The length of the microchannel affects the pressure drop along the way in proportional in increase in high mixing efficiency. [9]

Pressure Drop

Microchannel's role is not only as microreactor but also like as long tube that have probability to decrease the pressure [11]. Friction factor (*f*) is used to indicate the pressure drop in a pipe [22]. It is defined as:

$$f = \frac{\Delta P \ x \ 2 \ x \ D}{\text{x} \ x \ \rho \ x \ u^2} \qquad (2)$$

Where ΔP = Pressure drop, D = Diameter of the pipe, x = Length of pipe, ρ = Density of the reactant, u = Velocity of the reactant flow in the pipe

2.6 Volume Fraction of Geometry in Microchannel

Volume fraction can be described in term of distribution of the molecule inside the microchannel which may consist of two or more species and subjected to changed dependent on the geometry of the microchannel applied.

Schematic Geometry	A	B	C	D
Type	Straight	Circular Baffles	Contraction-Enlargement	Zigzag

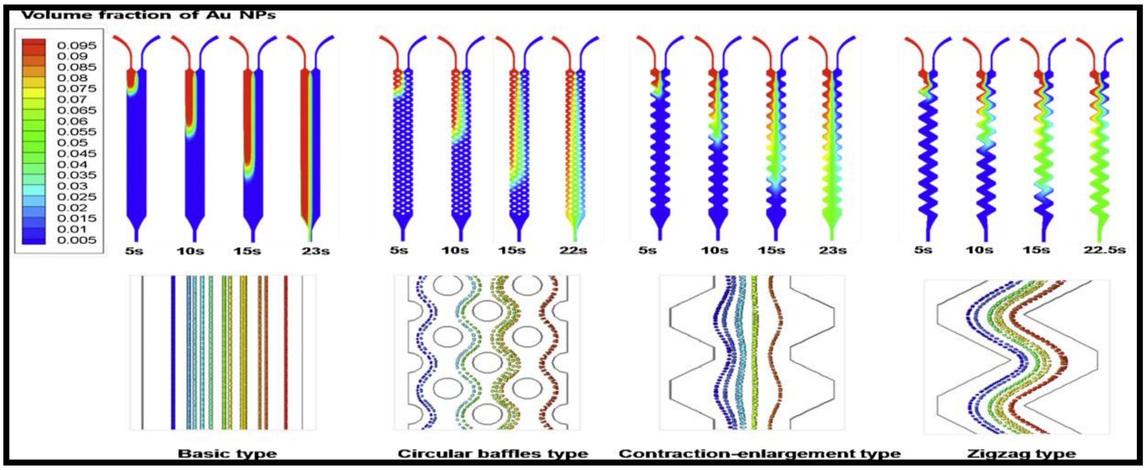


Fig 5: Contours of volume fraction and path line particles in different type of microchannel

* The green colour contour represents even distribution of reactant.

Based on the figure 3, Zigzag type shown most even distribution of the reactant as indicated by the green contour with lower residential time. The channel with curvature of 90° influences the velocity and flow direction at the inner and outer channel. Sudden change of flow direction induces flow instability that promotes more rigorous behaviour of reactant in the passive mixing performance. While the basic type, the fluid flow in a straight line without obstruction that powered by the capillary forces that originates between the microchannel wall and the gas which give it the ability to move along the channel [9]. In case of effective mixing, the red and blue colour from the counter should be vanished but it remains the same near the outlet for basic type.

2.7 Velocity Profile for different micro-mixers

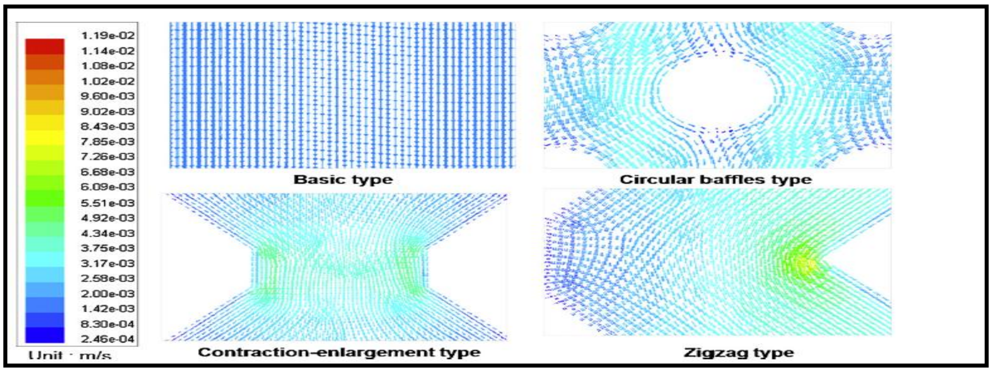


Figure 6: Velocity profile of different micro-mixers with vectors and contours. The velocity obstruction was observed near the obstructive location.

According to Jeon et.al research, the inner Boundary for microchannel was defined as no-slip condition near the surfaces of the baffles [9].

2.8 Hydrodynamics Theory

Eulerian equation is related to the conservation mass and momentum for gases flow phenomena.

<u>Mass conservation</u>

$$\frac{\delta\rho}{\sigma\tau} + \nabla(\rho\vec{u}) = 0 \qquad (4)$$

<u>Momentum conservation</u>

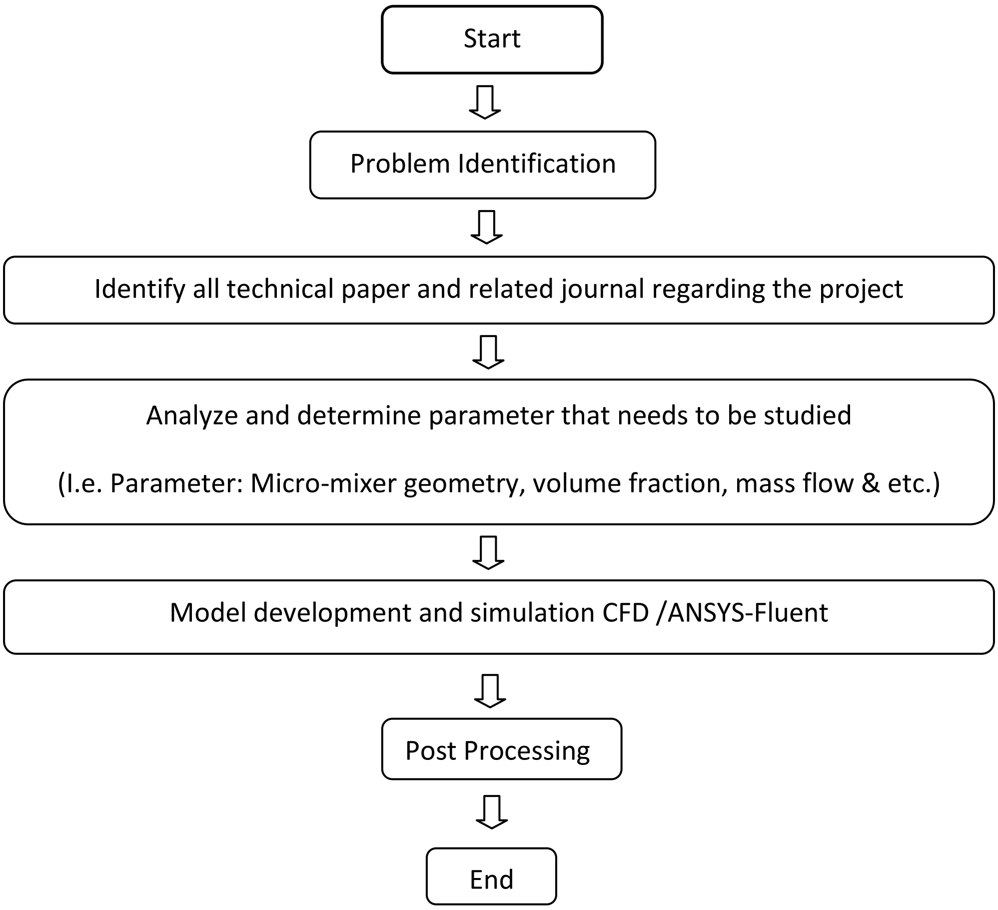
$$\frac{\sigma\rho u}{\sigma t} + \nabla(\otimes\, u(\rho\vec{U}) + \nabla\rho = 0 \qquad (5)$$

Where t = time, ρ = the fluid mass density, u = the fluid velocity vector (components u, v, and w), P = the pressure, ⊗ = denotes the tensor,ρ = Fluid density (kg.m^{-3}

CHAPTER 3
METHODOLOGY/ PROJECT WORK

3.1 RESEARCH METHODOLOGY

The hydrodynamic behaviour of urea mixing will be study by using Ansys CFD to determine the optimum geometry design suitable for the process specification. Computational Fluid Dynamic usually abbreviated as CFD, is a branch of of that uses numerical method and algorithm to solve and analyze problem that involves fluid flow. In this project, The Navier-Stokes equations are the basic governing equations for a viscous, heat conducting fluid and essential for CFD modelling for this project.



The core of the reaction will be assembled in the micro-reactor where the three reactant gas will be injected (i.e. N_2, H2, and CO2) into the system with the dimension as described in table 3.

Based on Yahya et.al research, two possible geometry of micro-mixers (i.e. zigzag and contraction enlargement type) was expected to have a best mixing performance. Initially, the ideal characteristic of micro-mixers structure was to achieve high mixing efficiency (%), low pressure drop (Pa) and short length of microchannel (nm). The zigzag type of micro-mixers had the best mixing performance which comes up with disadvantages, high pressure drop along the microchannel. Figure 6 display the configuration for trapezoidal with degree of inclination, 150°. As the length of microchannel determined to be 5.0 mm, the configuration can be extended to reduce the pressure drop across the microchannel.

Table 2: Basic configuration for the hydrodynamics solution.

Item	Symbol	Properties	Value
General	T	Ambient temperature (K)	298.15
	P	Ambient pressure (atm)	1
Microchannel	Q	Volumetric flow (mL/min)	3.33
	d	Diameter of microchannel (μm)	5.0
	l	Length of microchannel (mm)	7.0
	x_1	Cross-sectional of microchannel (nm)	1×10^6

3.1.1 Geometry Construction Using CFD

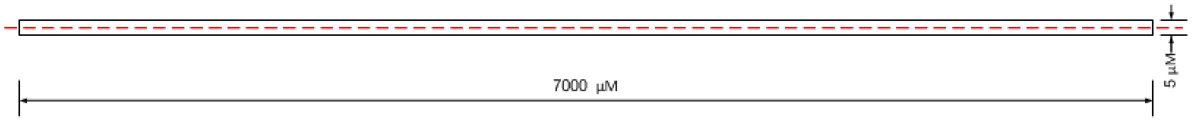
The modelling of the geometry of microchannel is the essence of this project. The 3D geometry construction is done using Design Modeller embedded in ANSYS 14 software. The default configuration as stated as follow;

Diameter	5 μm
Length	7000 μm

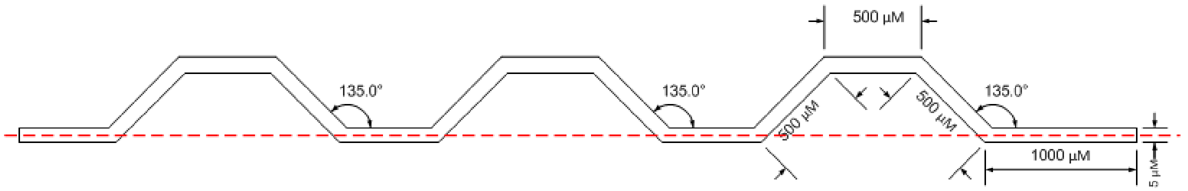
<u>2-Dimensional drawing of the proposed configuration of microchannel</u>

Three different configuration of microchannel were drawn 2-Dimensional to get an overview of design proposed;

Configuration 1



Configuration 2



Configuration 3

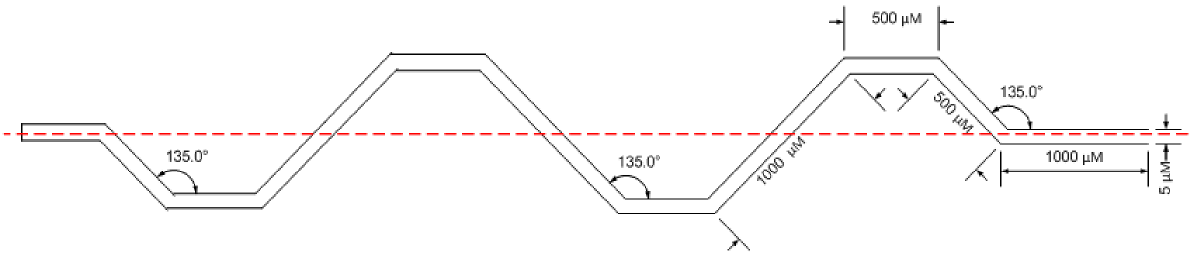
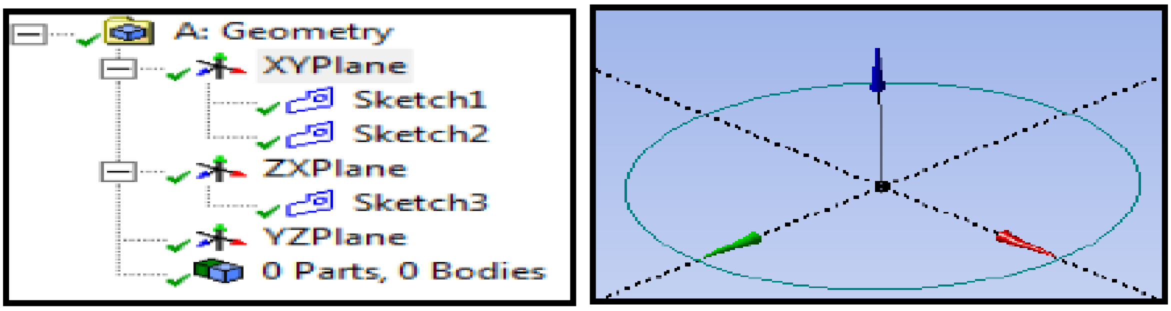


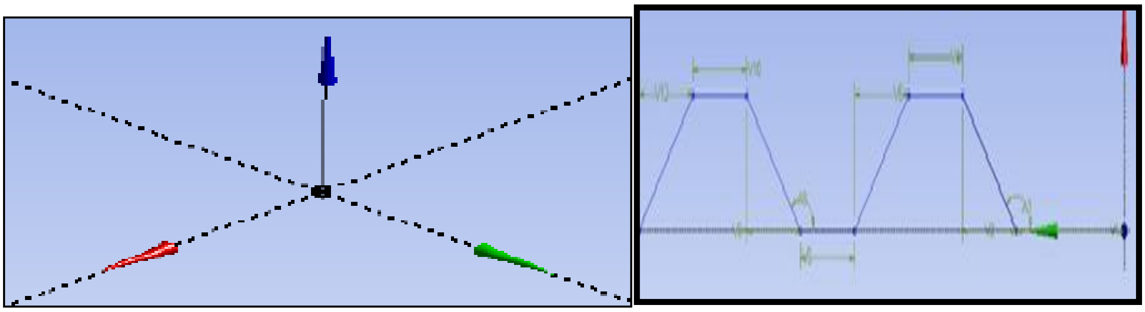
Figure 9: 2-Dimensional of the proposed configuration

Steps in geometry configuration as follow;

1) A circle is drawn with a diameter of 5µm 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.

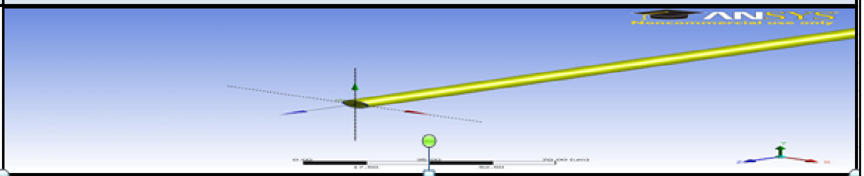
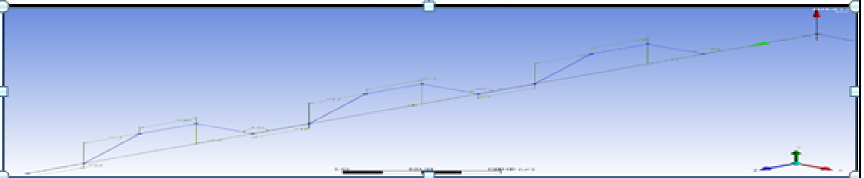
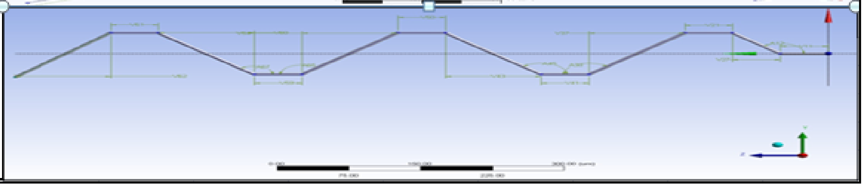
Geometry	Geometry Construction
Configuration 1	
Configuration 2	
Configuration 3	

Table 3: 3-D Generation of three different configurations

Based on the stated dimension, configuration is constructed in a straight line with a length of 7000 µm and a diameter of 5 µm. While, the configuration 2 is constructed with an initial length of 1000 µm and 500 µm for each cross sectional area. Angle of curvature of 135º is applied on the configuration 2 and configuration 3 that function as an obstruction to induce mixing.

3.1.2 Mesh Generation

The next step was to generate mesh that suits the geometry well. The term meshing illustrates the geometry domain that divided into smaller fragment which is called the grid or elements. The grids will be solved through discretization method based on the input parameter. The mesh quality is crucial in order to obtain an accurate simulation. A coarse mesh will cause large numerical errors, especially at the focus area of study from the geometry. The good quality mesh defined as it falls within correct range and from the orthogonal quality value. Meanwhile, the 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 100 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 proximity and curvature as the proposed model use angle as a focus point. Next is the relevance center adjusted from medium to fine. The function of relevance center is much alike the relevance in default parameter. Then the mesh is generated to see the preliminary result. Figure 10 shows the primary generated mesh, details of mesh and orthogonal quality. Basically, meshing model that has higher number of element is more complex to solve and offer more accurate and reliable simulation but time-consuming.

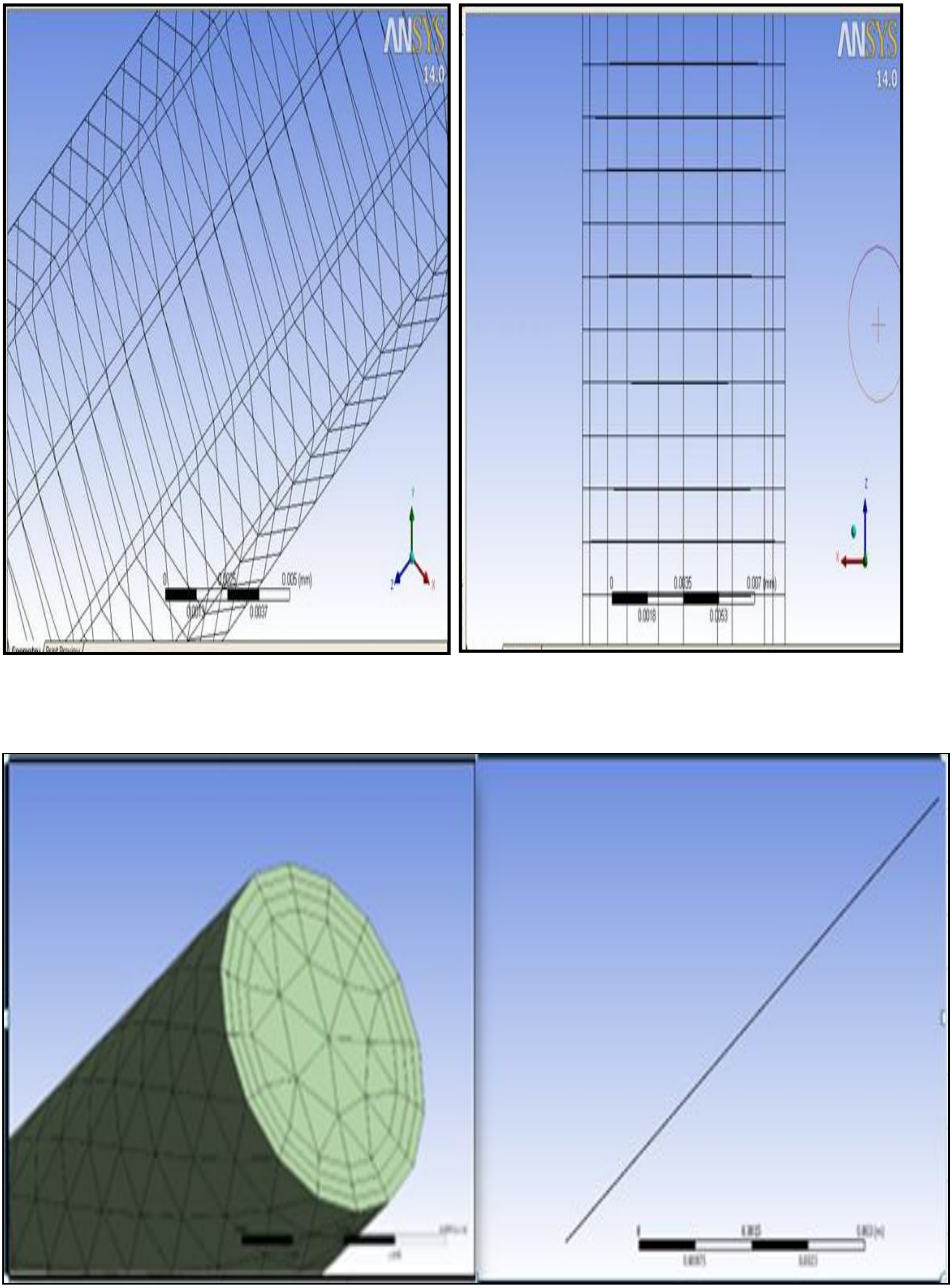


Figure 10: Mesh Generation for the configuration 1microchannel

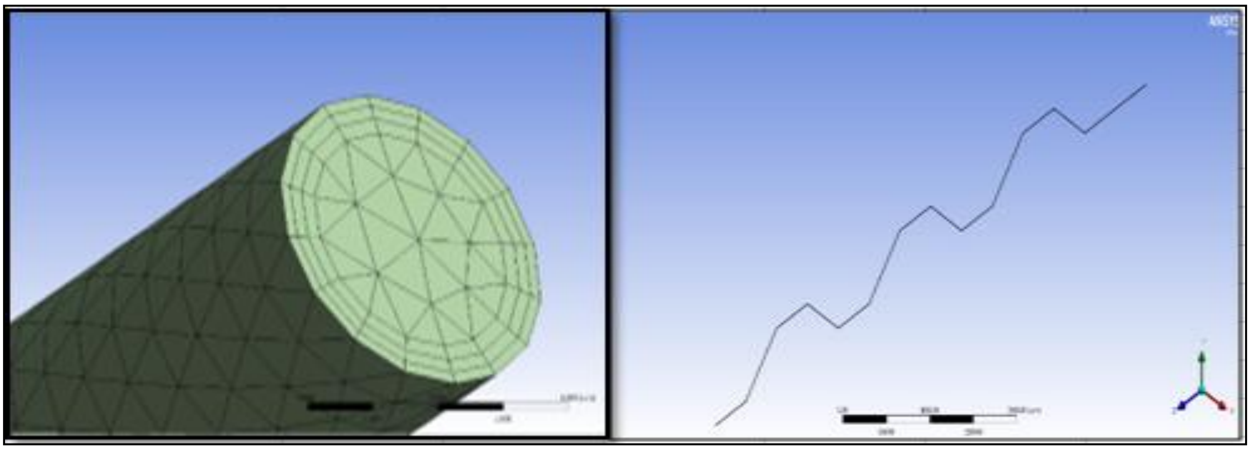


Figure 11: Mesh Generation for configuration 2 microchannel

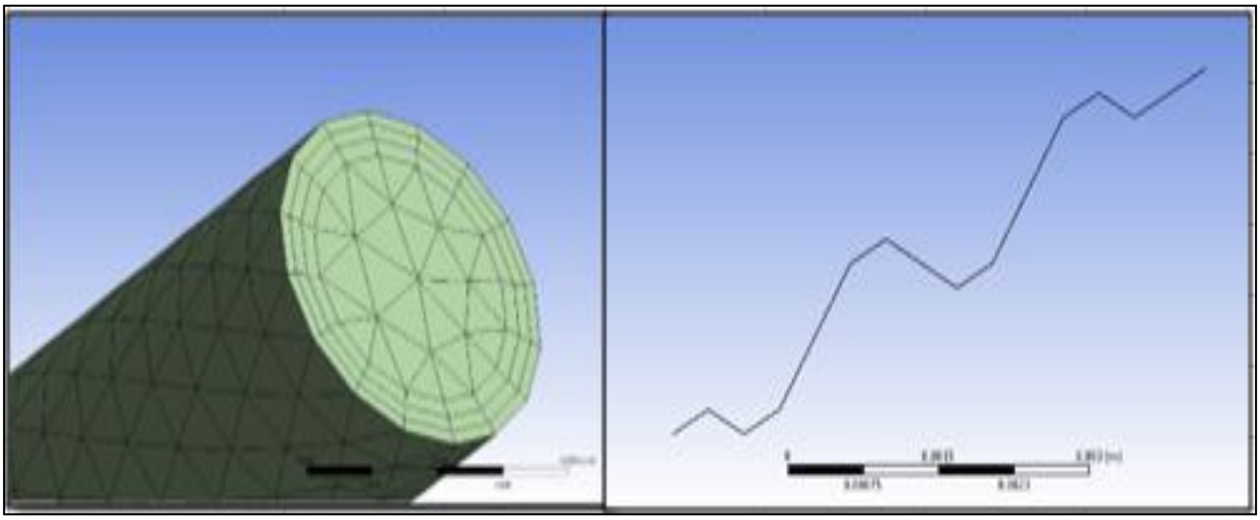


Figure 12: Mesh Generation for configuration 3 microchannel

Geometry Configuration	Nodes	Element
Configuration 1	**970596**	**1088355**
Configuration 2	**631449**	**1881852**
Configuration 3	**699322**	**1912487**

Table 4: Number of Nodes & Element for each configuration

Details of "Mesh"	
Defaults	
Physics Preference	CFD
Solver Preference	Fluent
Relevance	100
Sizing	
Use Advanced Size Fun...	On: Proximity and Curvature
Relevance Center	Fine
Initial Size Seed	Active Assembly
Smoothing	Medium
Transition	Slow
Span Angle Center	Fine
Curvature Normal A...	Default (12.0 °)
Proximity Accuracy	0.5
Num Cells Across Gap	Default (5)
Min Size	1.0 µm
Proximity Min Size	1.0 µm
Max Face Size	200.0 µm
Max Size	200.0 µm
Growth Rate	1.10
Minimum Edge Length	8.18070 µm

Figure 13: Applied setting on meshing process for three different configuration

Statistics	
Nodes	1088355
Elements	970596
Mesh Metric	Orthogonal Quality
Min	0.879075562194416
Max	0.997530883678584
Average	0.976125191771822
Standard Deviation	2.12938723478409E-02

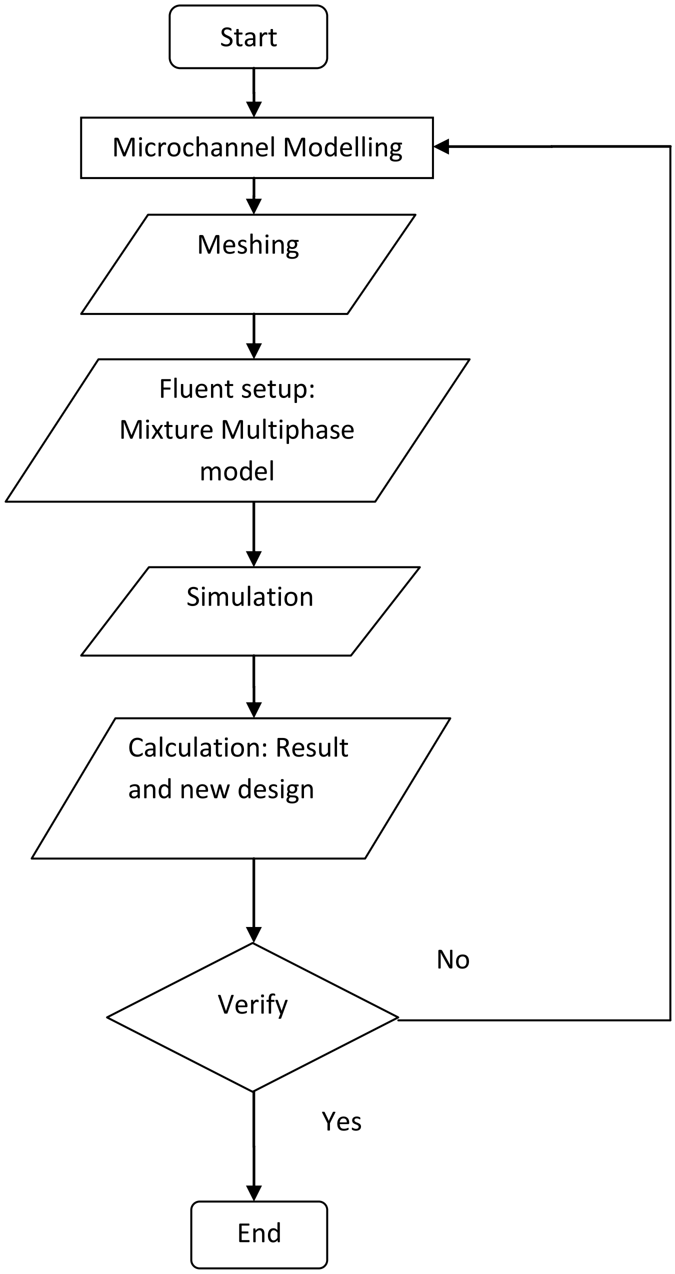
Defeaturing	
Statistics	
Nodes	631499
Elements	1881852
Mesh Metric	Orthogonal Quality
Min	0.160939608758049
Max	0.99743970000895
Average	0.905848686670006
Standard Deviation	7.80288739802258E-02

Figure 15: Orthogonal quality for straight & 135° upward configuration of microchannel

The orthogonal quality is one of the methods to evaluate the generated mesh. Generally, the range of orthogonal quality is between 1 and 0. The best value should be near to 1 and the worst is 0. The next step would be the fluent simulation of the movement of mixing of gas particle along the microchannel using a multiphase model. The concept of multiphase model here is applied on a broader system. Although hydrogen, Nitrogen and Carbon Dioxide are in one-phase component, even different-sized solid particles of the same material can be treated as different phases in Fluent

3.2 Hydrodynamic simulation (Pre-modelling micro-mixers for microchannel)

The simulation will be executed by using ANSYS fluent. The researcher initially constructed the micro-channel based on the Eulerian multiphase model.



3.2.1 Fluent Setting

After creating the model geometry, generates the grid, the next step will be directed to the solver setting which is in this case, Fluent is chosen. This section will give a general overview on the initialization of the setting applied to solve the flow problem.

3.2.2 General Setting

Double precision is chosen for Fluent option due to the nature of geometry which generally long and thin. The solver used is pressure-based type, absolute velocity formulation and steady time. In X-direction, the gravitational acceleration is 9.81 ms^{-1} by default. In this section, the meshing of the model need to be checked before the data input for boundary condition.

3.2.3 Model

At this stage, Multiphase model is chosen for the case since it involves the mixing of three different reactant gases (H2, N_2 & CO_2). The concept of multiphase model here is applied on a broader system. Although hydrogen, Nitrogen and Carbon Dioxide are in one-phase component, even different-sized solid particles of the same material can be treated as different phases in Fluent. In fluent, In ANSYS Fluent, there are multiphase model available dependent on the specific condition; Volume of Fluid (VOF), Eulerian and Mixture model. Mixture model is chosen due to the tendency to solve a set of momentum and continuity equation for each phase. Beside that, the mixture model is suitable for simulating two or more sorts of particles in liquids, and the phases are treated as an interpenetrating continua, The volume fraction represents the space occupied by each phase and the law of conservation mass and momentum are satisfied by each phase individually For Vicious model, a laminar flow is chosen since the microfluidic devices involve passive mixing.

The volume phase q;

$$V_q = \int a_q dv$$

Where;

$$\sum_{q=1}^{n} a_q = 1$$

Then, the effective gas density

$$\widetilde{P_q} = a_q p_q$$

3.2.4 Material

The component chosen for One-step Urea Synthesis is Hydrogen, Nitrogen and Carbon dioxide and aluminium serve as default component for the microchannel structure.

Component	Density (kg/m3)	Viscosity (kg/m.s)
Hydrogen	0.0819	8.41E-06
Nitrogen	1.138	1.66E-05
Carbon Dioxide	0.6099	1.24E-05

3.2.5 Boundary Condition

For microchannel configuration with a single point of entry, there are four named selection specified which is inlet, outlet, wall fluid and interior fluid. The inlet were specified as a velocity-inlet and directed for each phase in a single micro reactor. The inlet velocity was calculated theoretically based on the stoichiometry ratio of one step urea synthesis, H2: N2:CO2, 3:1:1. For the primary phase (H_2), the inlet velocity were set to 0.9 ms^{-1} and volume fraction of 0.6. While Secondary (N_2) and tertiary phase (CO_2), the inlet velocity was set to 0.32 ms-1 and 0.34 ms^{-1} under the identical volume fraction setting, 0.2.

3.2.6 Solution Method and Control

For multiphase model, pressure velocity coupling scheme which is phase-coupled simple and couple. The couple schemes were chosen as it able to solve the equation regarding the phase velocity correction and shared pressure correction simultaneously. Instead, the least square cell based is chosen for gradient and QUICK for momentum and volume fraction spatial discretization. To prevent premature of the convergence of the calculation, all the residual constraint are changed t from 0.001 (Default Value) to 1e-15 in order to avoid the program converge on its own. For each geometry, 400 iteration is applied for each parameter.

3.3 PROJECT MANAGEMENT & ACTIVITIES

3.3.1 Key Milestone

The key milestones are important agendas that need to be accomplished in time in order for this research project to be completed on Note that ●

NO	DETAIL WEEK	1,2	3,4	5,6	7,8	9,10	11,12	13,14	15,16	17,18	19,20	21,22	23,24	25,26	27,28
1	Confirmation of FYP topic														
2	Literature Review														
3	Extended Proposal				●										
4	Rough planning of project														
5	Secure the Information and parameter are needed for the project					●									
6	Detailed planning of Project														
7	ANSYS Fluent Software Training														
8	Pre-design of the microchannel and configuration														
9	Generate the microchannel design and data needed								●						
10	Run simulation and Data collection														
11	Analyse and interpret the results obtained														
12	Documentation of the whole project and presentation														●

represents the important milestones that need to be fulfilled on time.

3.3.2 Project Ga ntt chart

No.	Detail / Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14	15
	FYP 1																
1	Selection of project topic								Mid-Semester Break								
2	Preliminary Research Work																
3	Literature Review & Methodology																
4	Draft on extended proposal																
5	Submission of extended proposol																
6	Proposal defense																
7	Ansys training and computational setup																
8	Simulation work - Preliminary research 1) Micro-mixer 3D modelling 2) Generate grid size according the meshing																
9	Draft on the interim report																
10	Submission of the interim report																
	FYP 2																
1	Simulation Project continues																
2	Submission of the progress report																
3	Analysis of the data collected ; 1) Mixing efficiency (%) , Volume fraction , Pressure drop , Length of microchannel																
4	Pre-Sedex																
5	Submission of the draft report																
6	Submission of Dissertation (Soft bound)																
7	Submission of the technical paper																
8	Oral Presentation																
	Submission of Project Report (Hard bound)																

CHAPTER 4

RESULTS & DISCUSSION

4.1 Introduction

Three-dimensional Microchannel Simulation with FLUENT 14.5 offer an interested region of study the effect of angle of curvature and variation of configuration on pressure drop inflicted and the mixing efficiency of the volume fraction for each constituent inside the microchannel. In this mixing scheme of study, the interested areas are located for all the corner of the microchannel geometry to study the mixing pattern for each configuration. In the simulation, the total length of microchannel is 7000 µm, Diameter at the X-axis: 5µm and the applied angle is 135°. Meanwhile, the projects use three different configurations for a comparative analysis on the mentioned parameter. The straight microchannel configuration serves as a baseline in comparative with configuration 2 and 3.

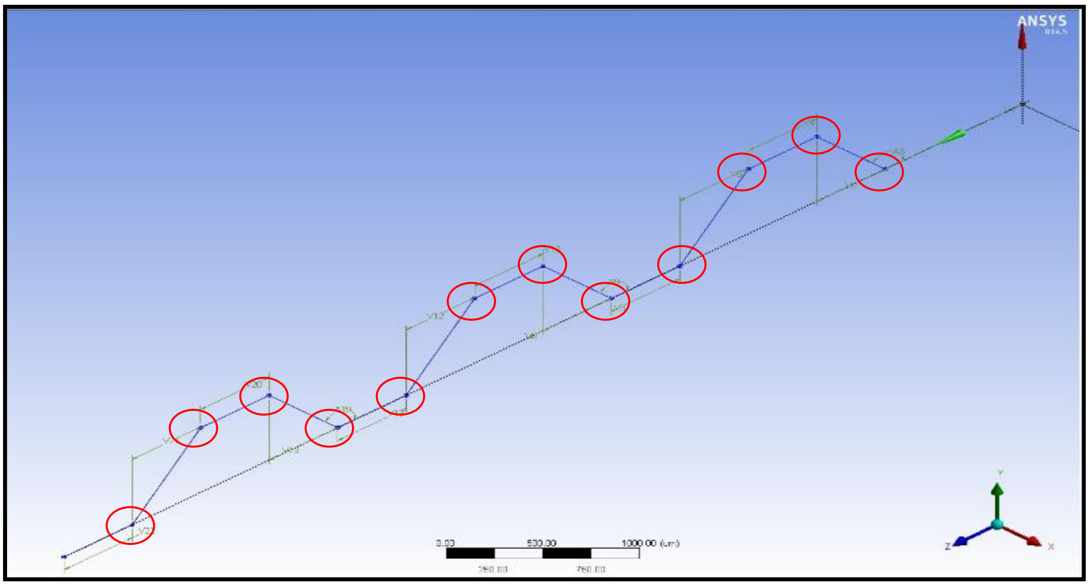


Figure 14: Focus area near all the corner of microchannel geometry

4.2. Volume fraction ratio for One-Step Urea Synthesis

$$N_2 + 3H_2 + CO_2 \rightarrow NH_2COONH_4 \rightarrow H_2O + CO(NH_2)_2$$

The Stoichiometric equation above explains on 1 mol of Nitrogen react with 3 mol of Hydrogen and 1 mol of Carbon Dioxide to produce 1 mol of Urea and water. The theoretical volume fraction can be calculated by using this formula;

$$\phi_i = \frac{V_i}{V}$$

Where V_I: Volume fraction of the constituents of the mixture, V: Volume fraction of the total mixture

Based on the theoretical ratio of number of mol N_2: H_2: CO_2 which is 1:3: 1 , the Stoichiometry mol fraction can be calculated ;

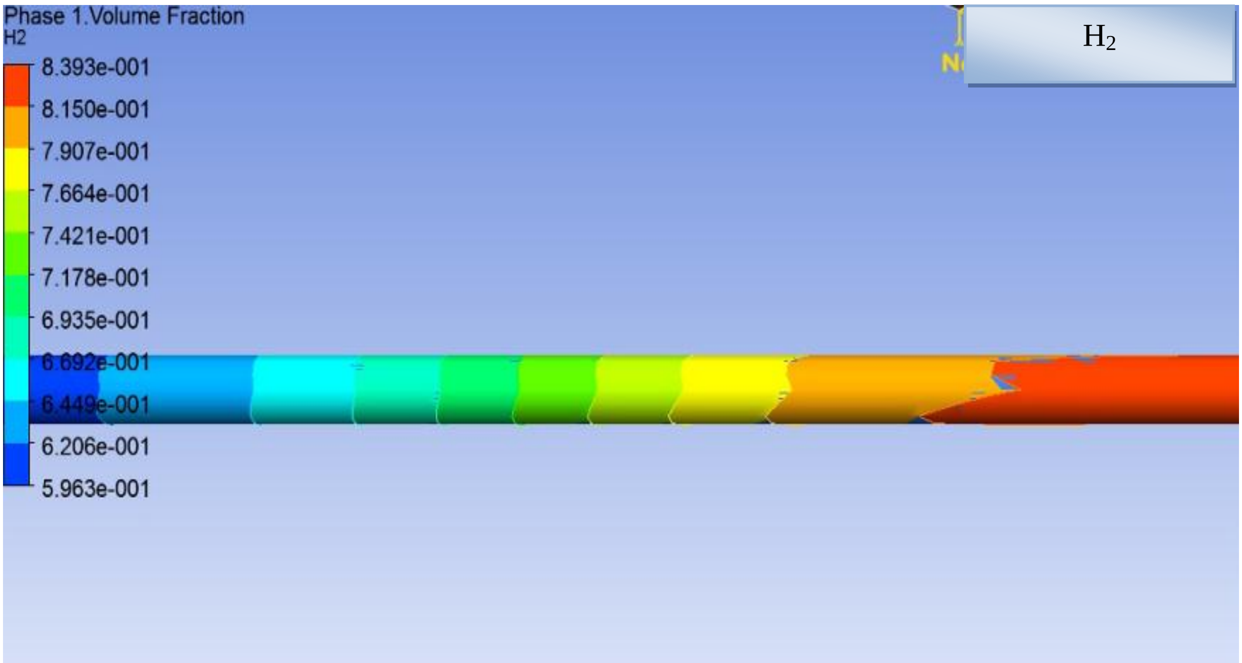
Component	Mole Ratio (%)
Hydrogen	60
Nitrogen	20
Carbon Dioxide	20

Table 5: Mole Ratio of the reactant mixture

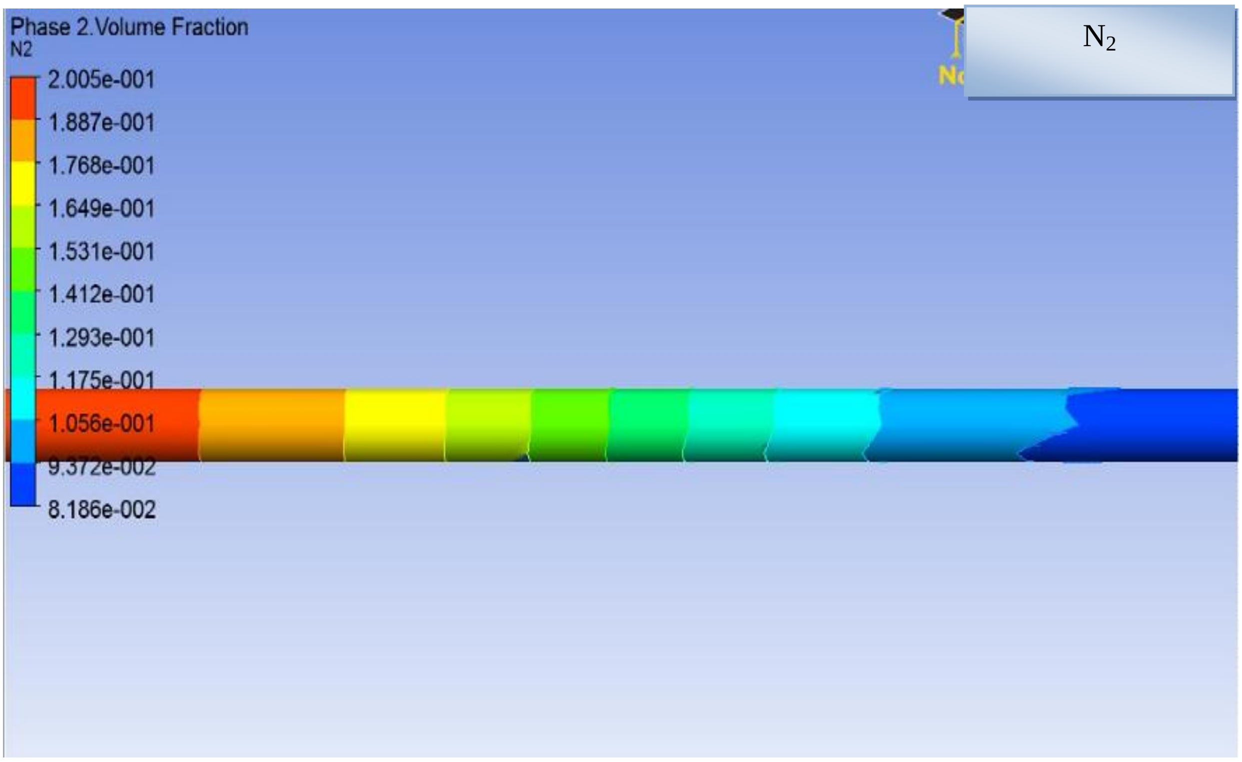
4.3 Effect of the microchannel configuration on the reactant volume fraction

In order to study the effect of various microchannel configurations on reactant volume fraction, the model is running with similar dimension (Length: 7000 µm, Diameter: 5 µm). Subsequently, the contour the volume fraction is drawn in order to acquire the mixing pattern exhibited by particular configuration. For this experiment, three different configurations have been proposed which is configuration 1, 2 and 3. The simulations commenced by examining the respective effects at the different configuration where the dynamic inlet flow behaviour are not steady state flow behaviours. To ensure a reasonable analysis, the contours were selected and compared at the point at time where the volume fraction for individual component exhibit even distribution that indicate a stoichiometric volume fraction is established

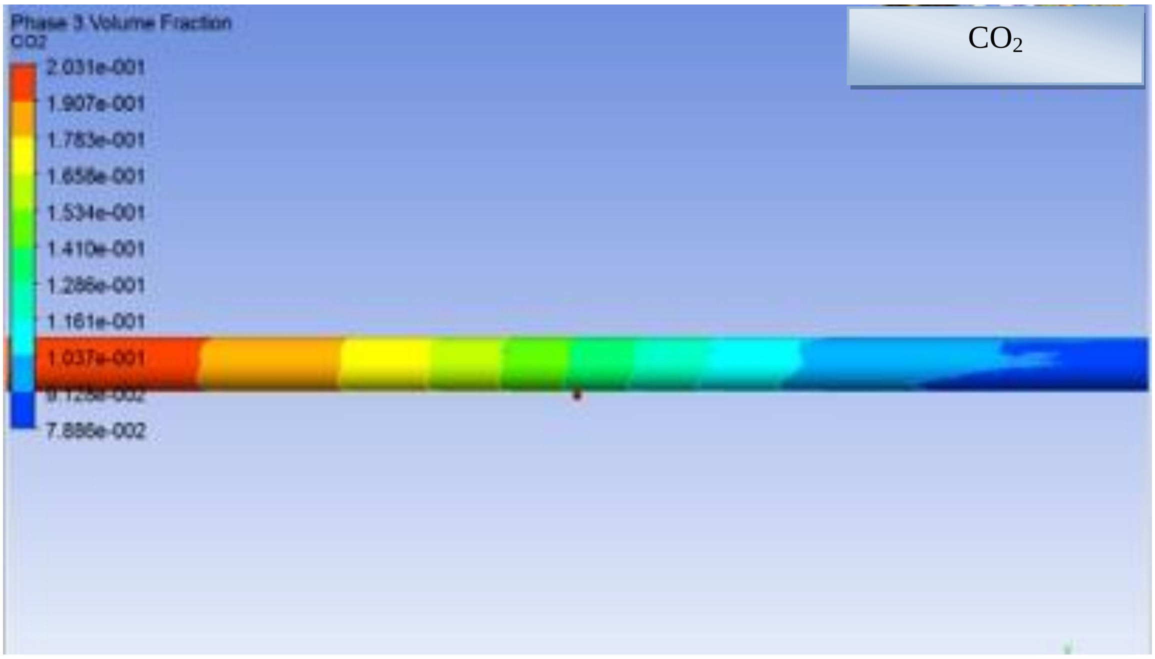
4.3.1 Configuration 1



Hydrogen volume fraction at length : 1000 µm

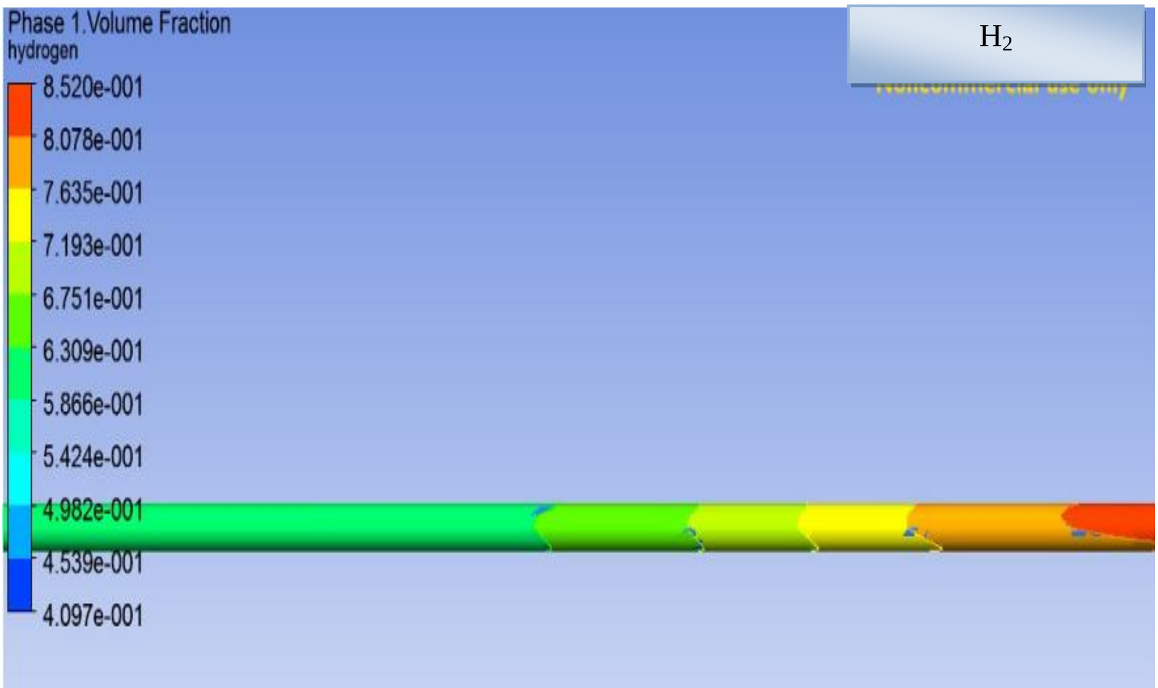


Nitrogen volume fraction at length: 1000 µm

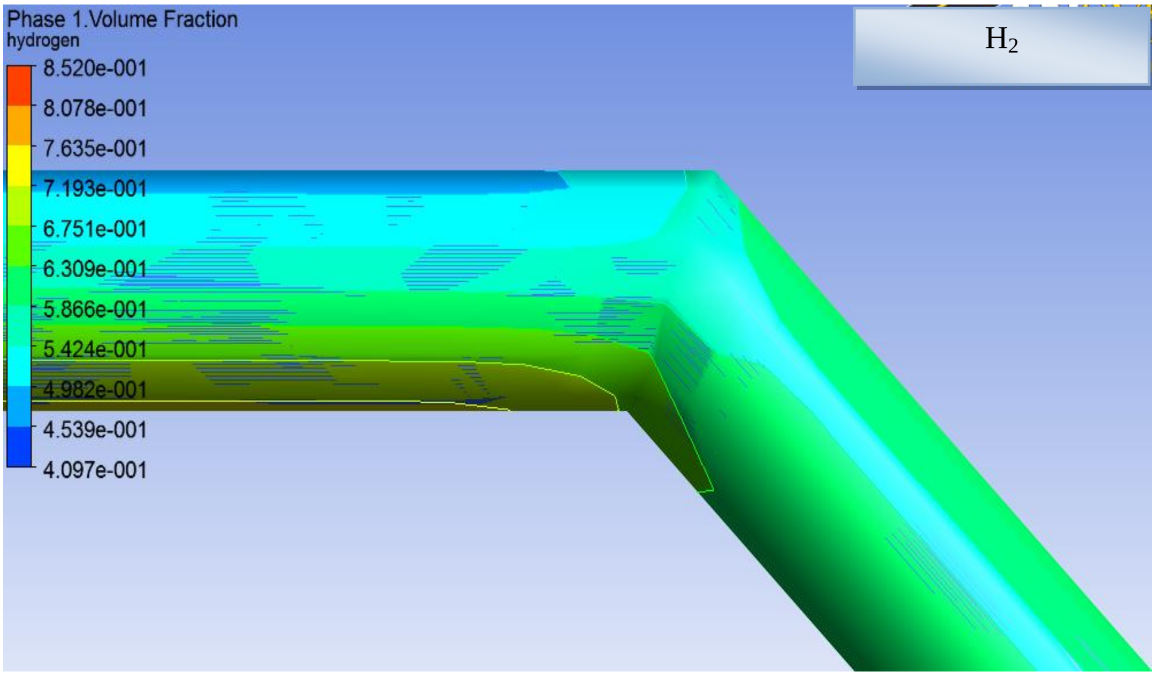


Carbon Dioxide volume fraction at length: 1000 µm

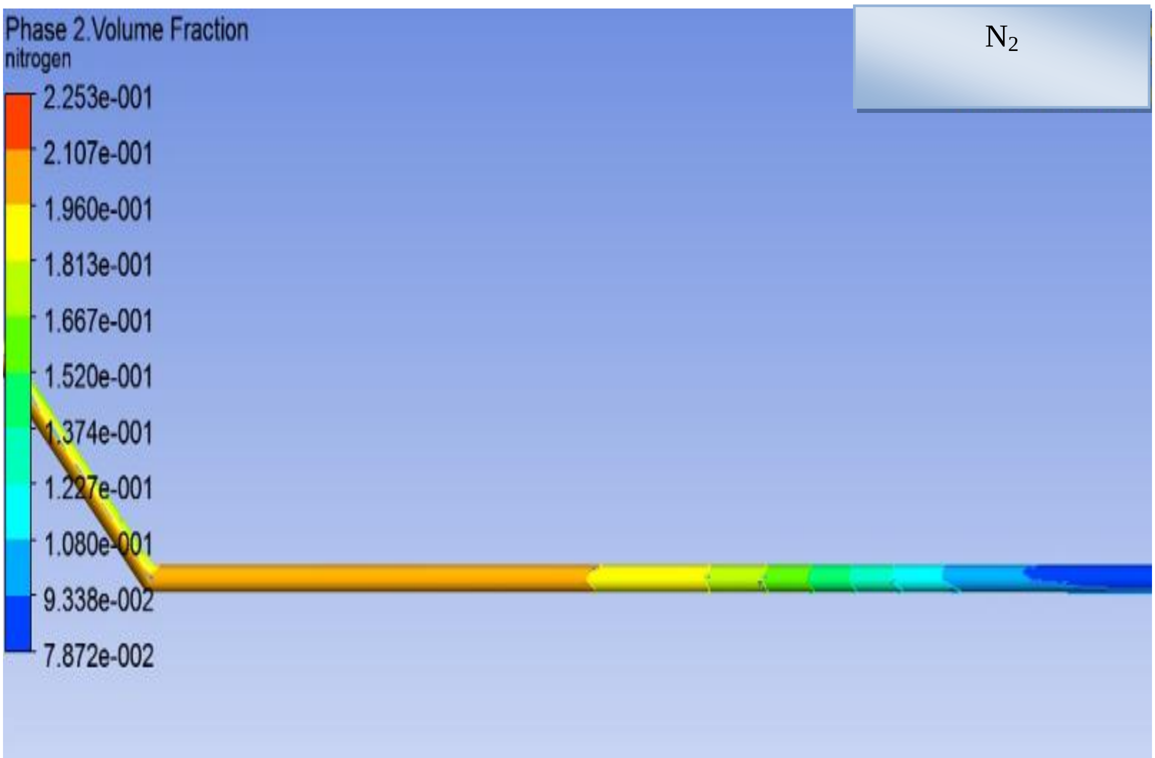
4.3.2 Configuration 2



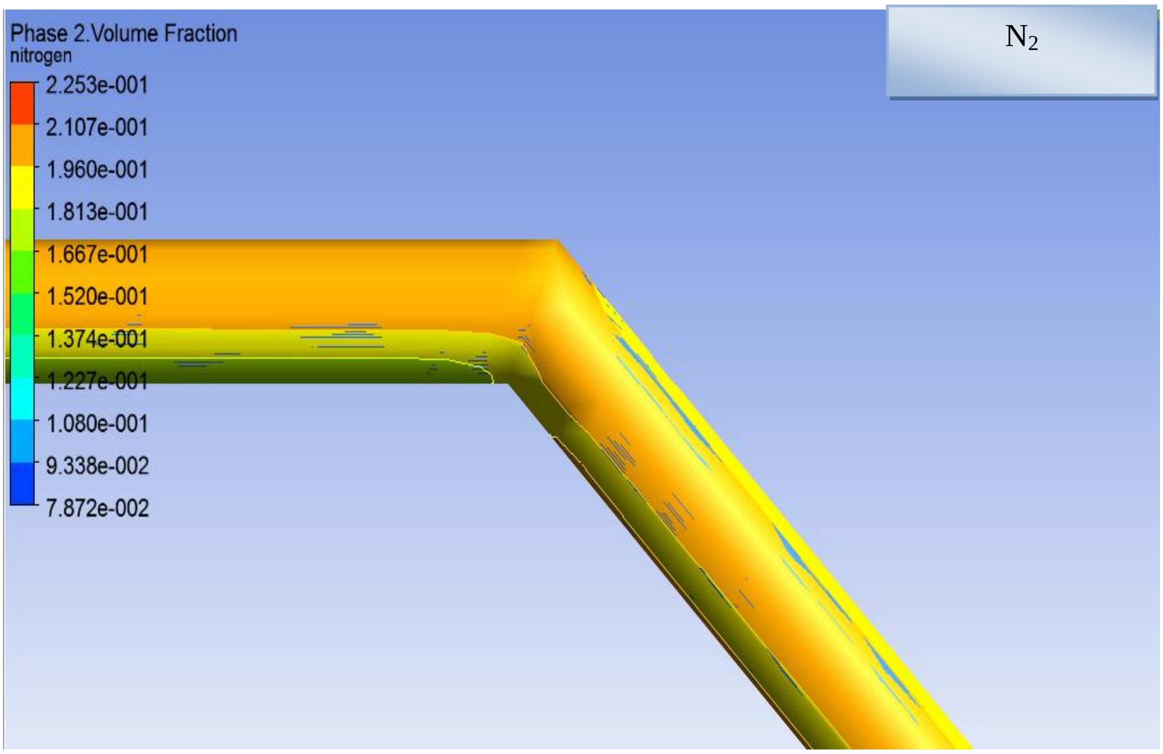
Hydrogen volume fraction at the inlet



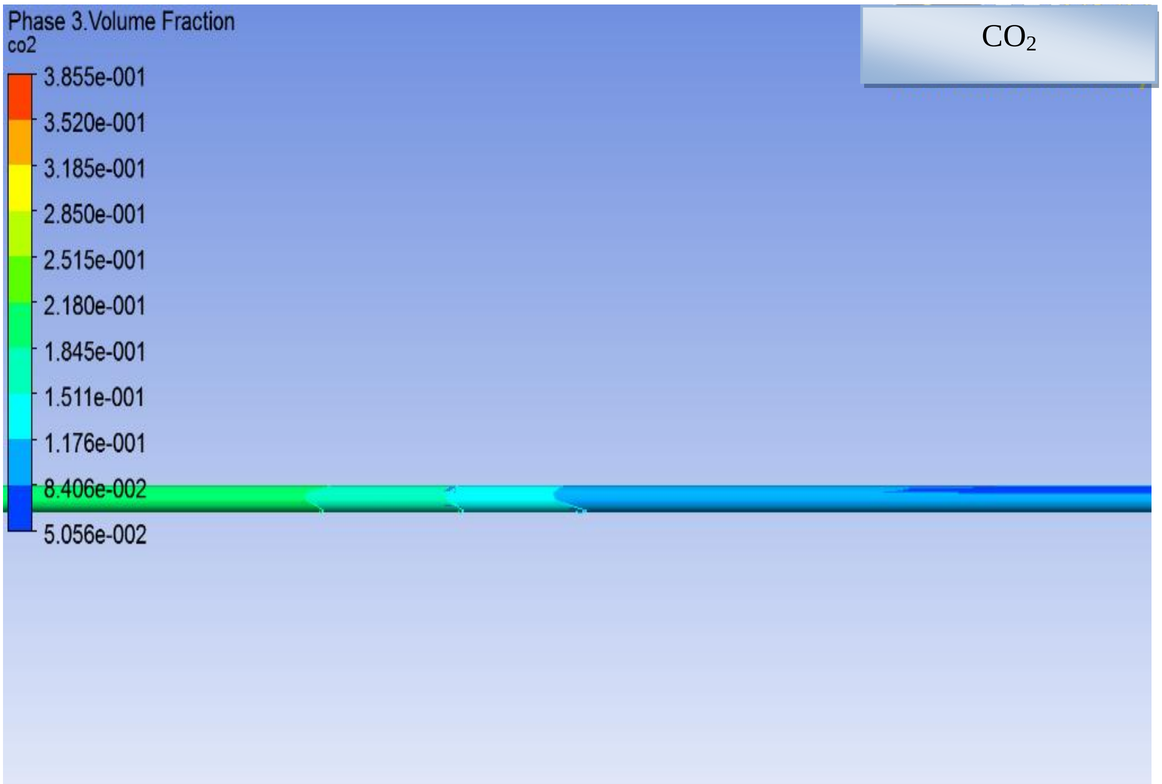
Hydrogen volume fraction at length: 3500 µm



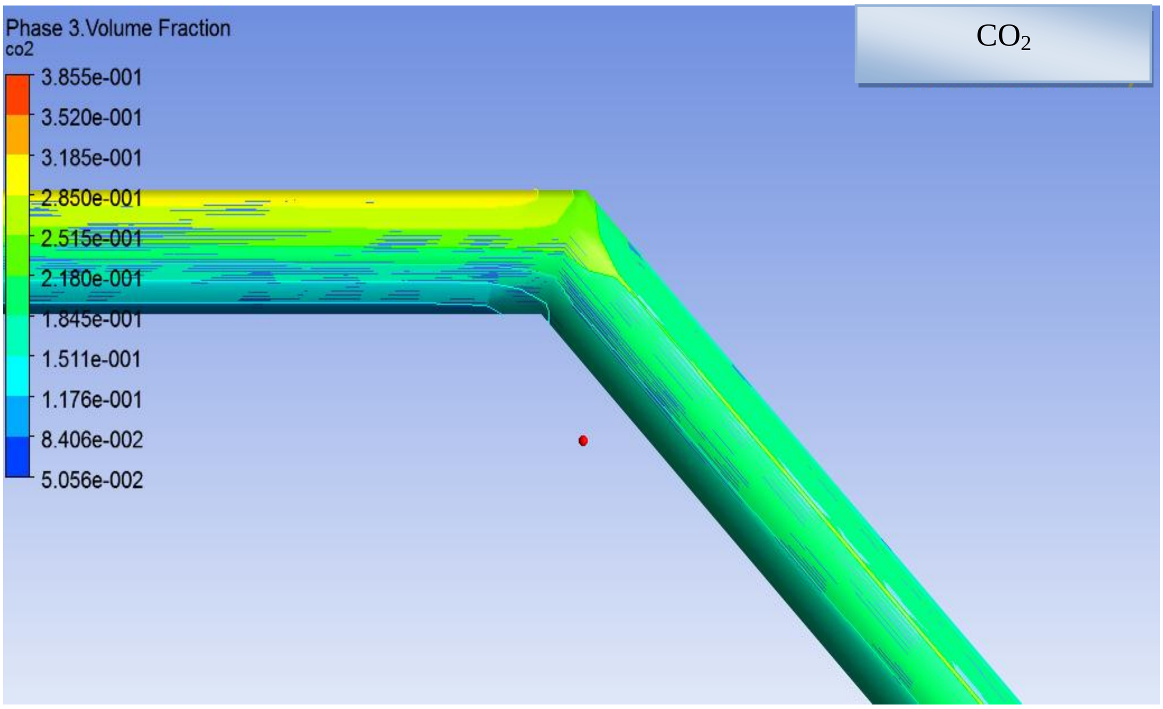
Nitrogen volume fraction at the inlet



Nitrogen volume fraction at length: 3500 µm

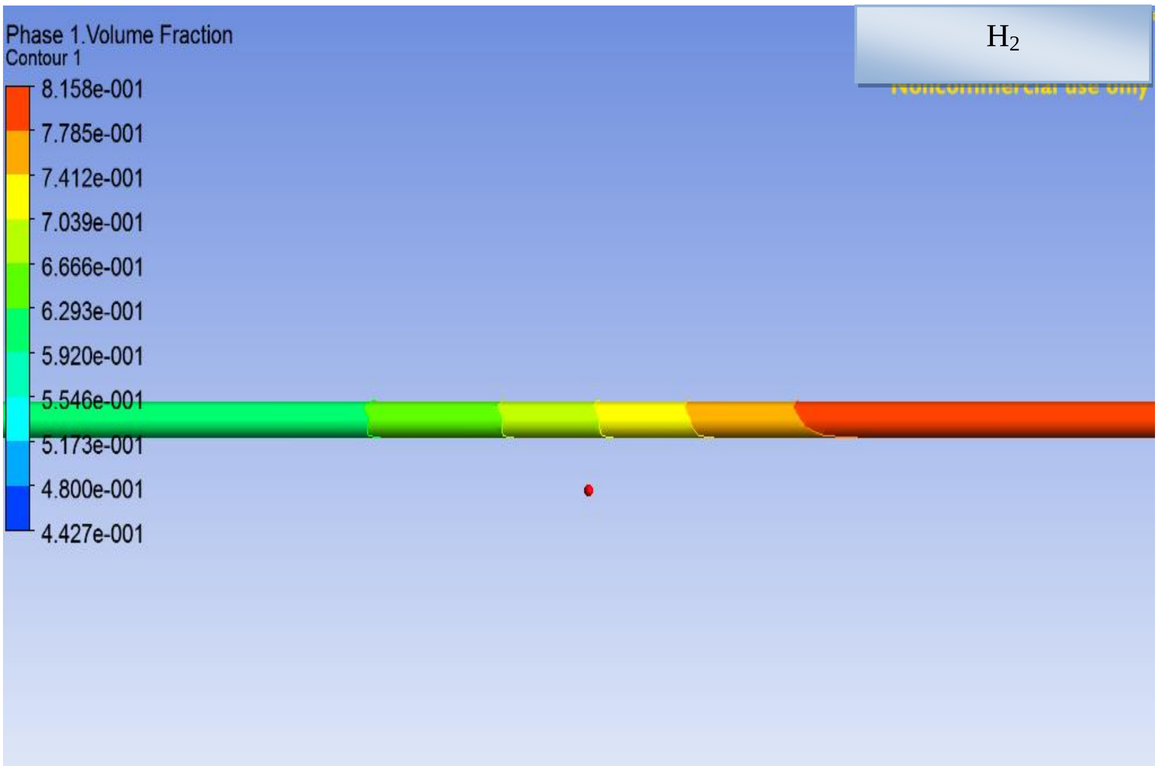


Carbon Dioxide volume fraction at the inlet

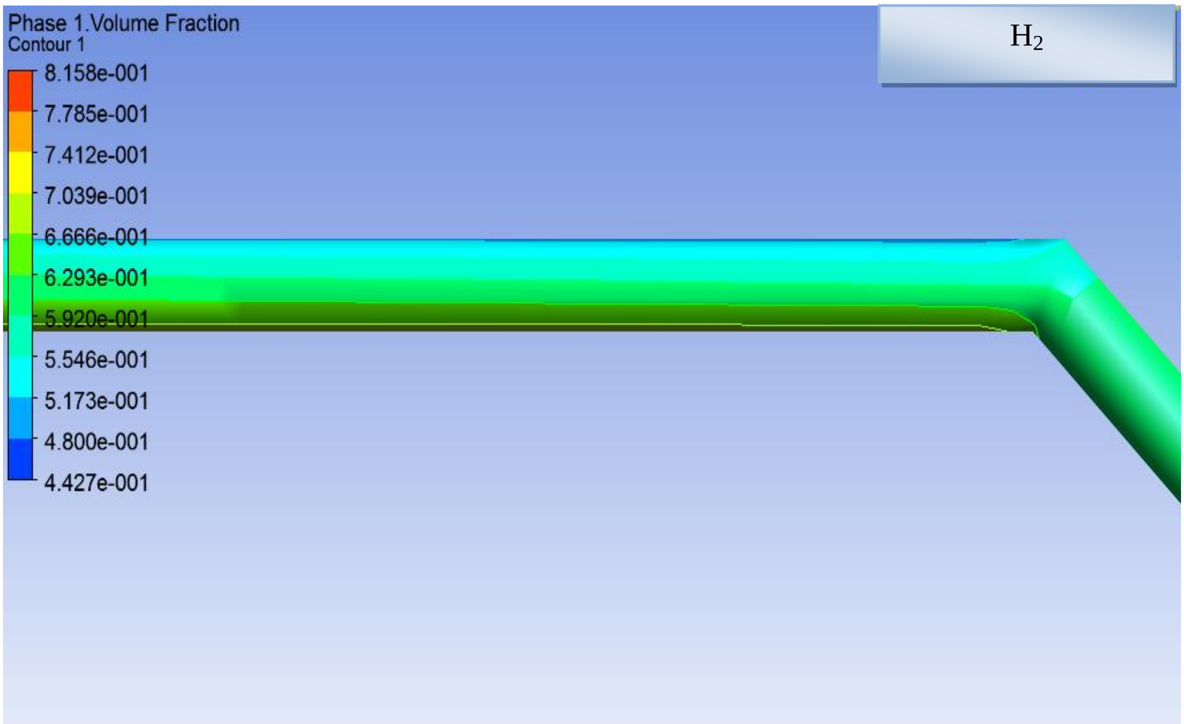


Carbon Dioxide volume fraction at length: 3500 µm

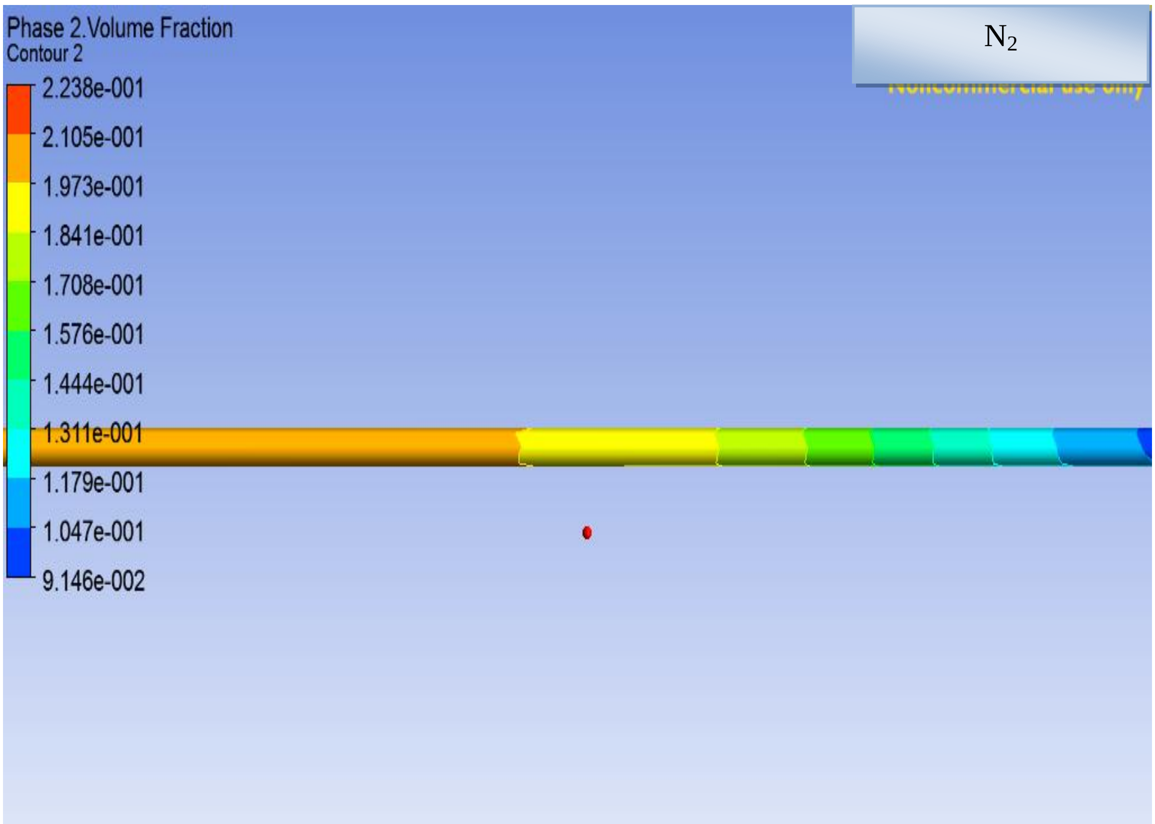
4.3.3 Configuration 3



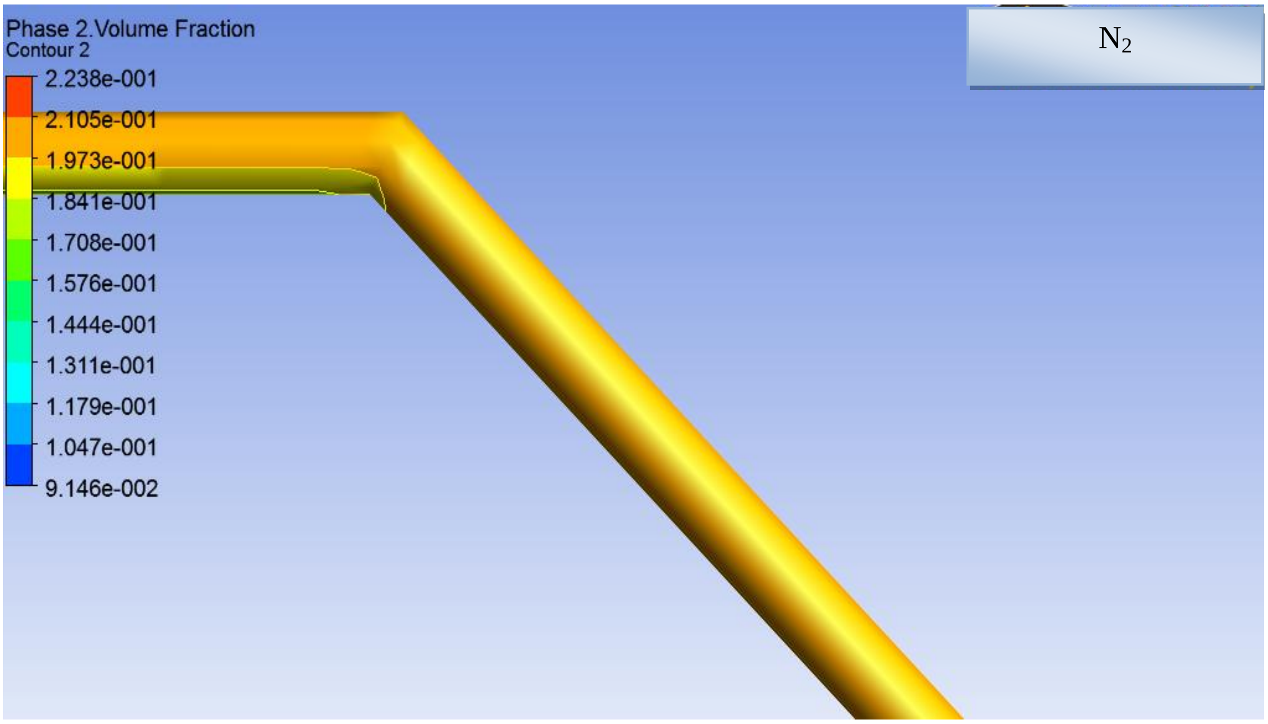
Hydrogen volume fraction at the inlet



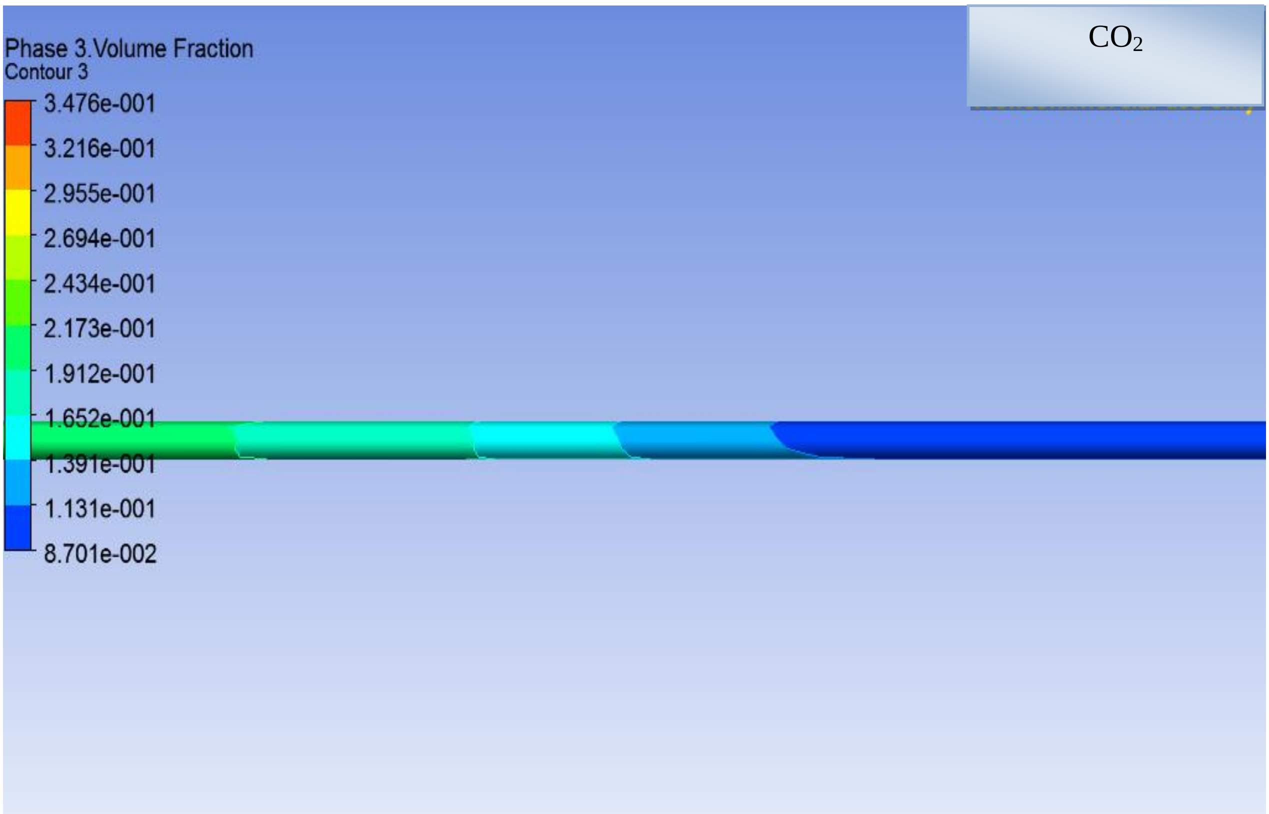
Hydrogen volume fraction at length: 4500 µm



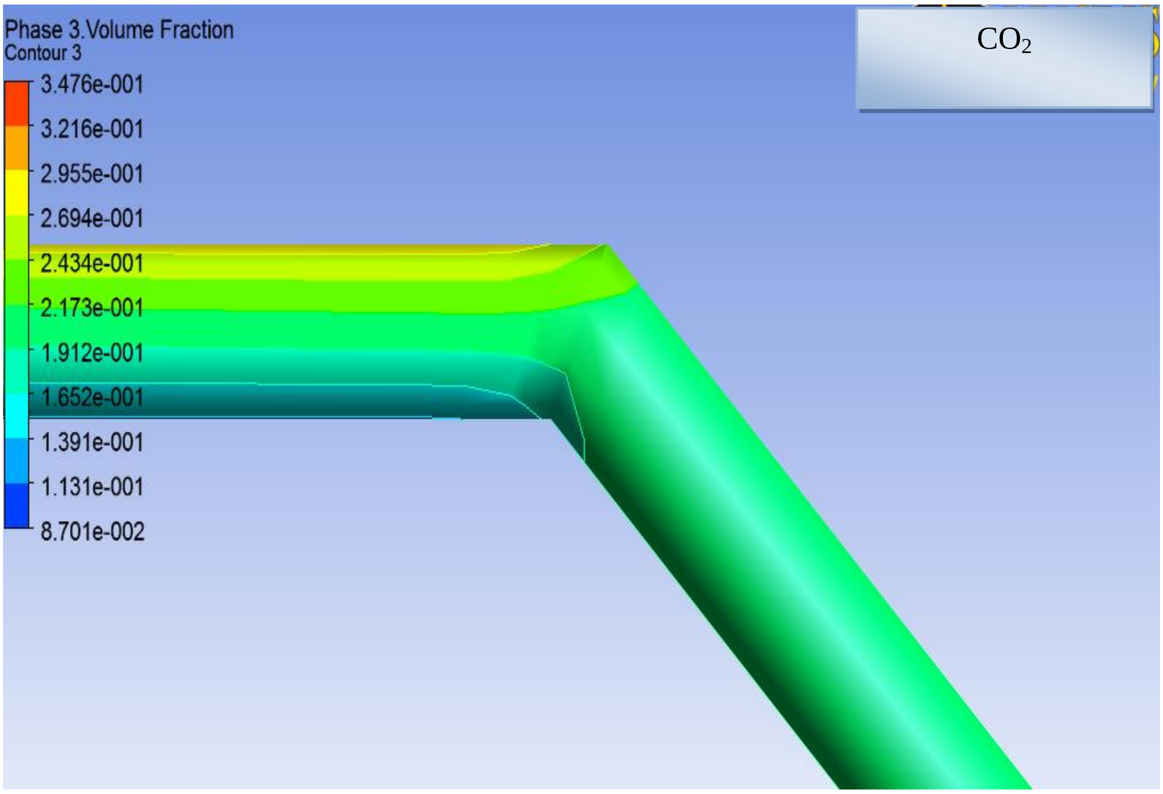
Nitrogen volume fraction at the inlet



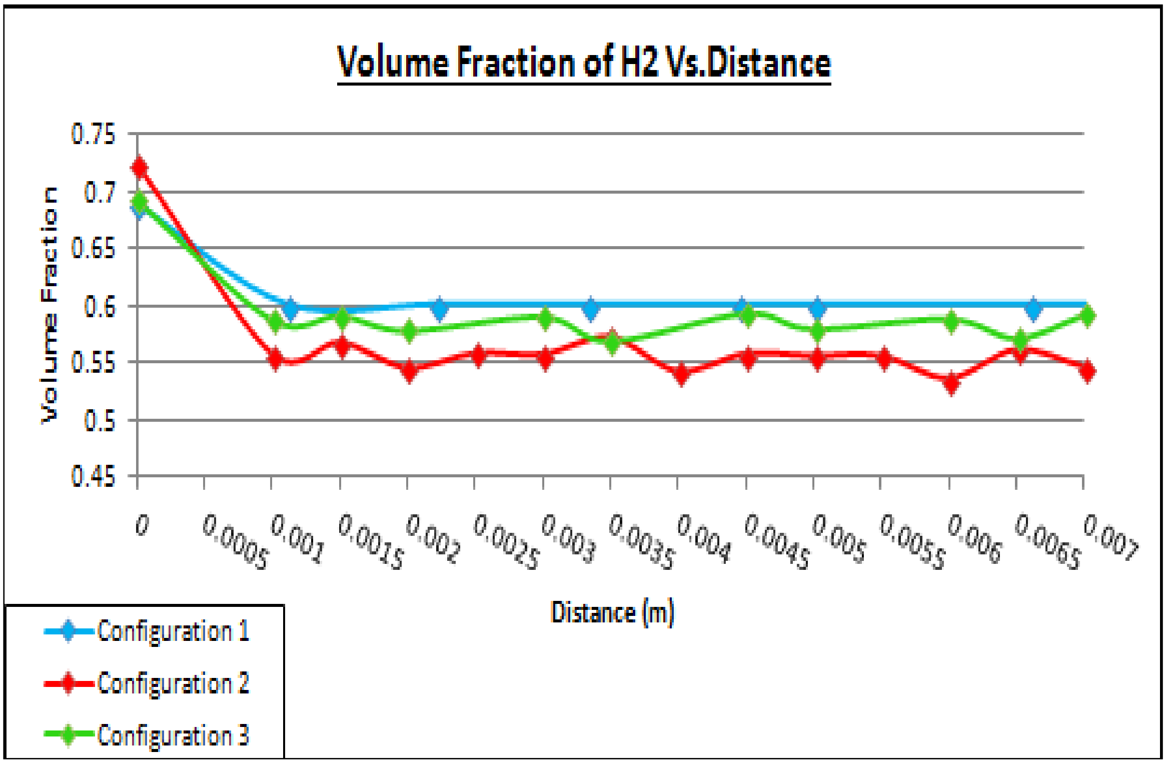
Nitrogen volume fraction at length of 4500µm

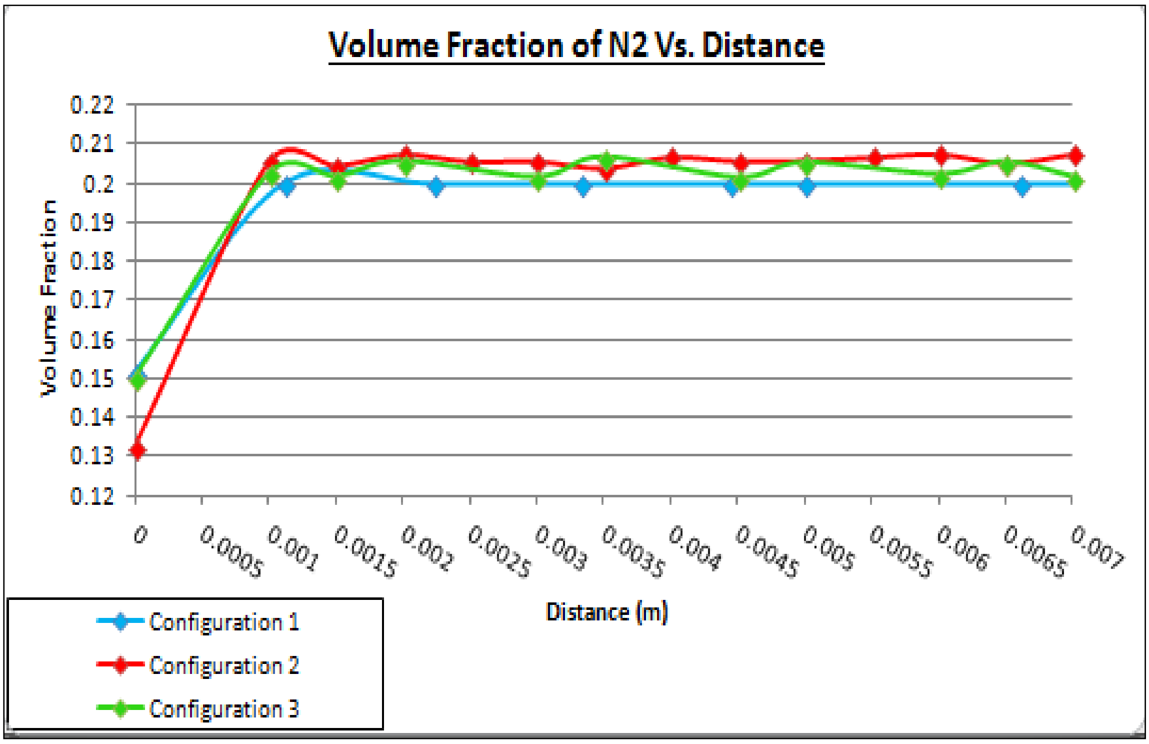


Carbon Dioxide volume fraction at the inlet



Carbon Dioxide volume fraction at length of 4500 µm





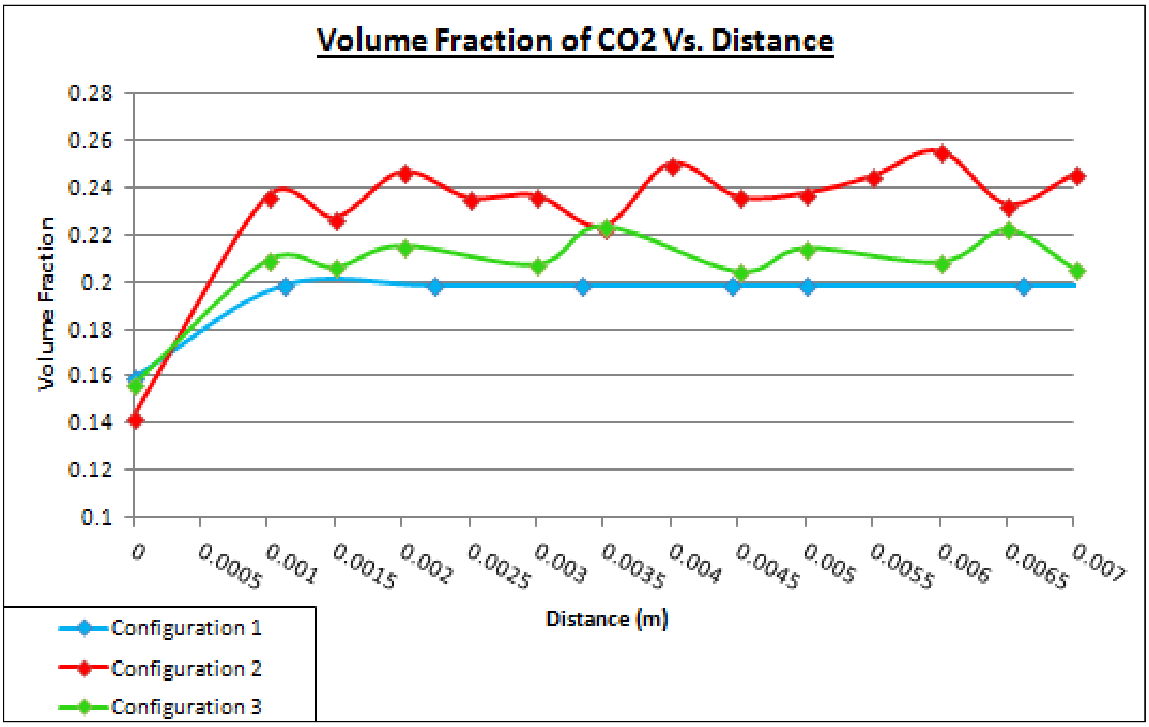
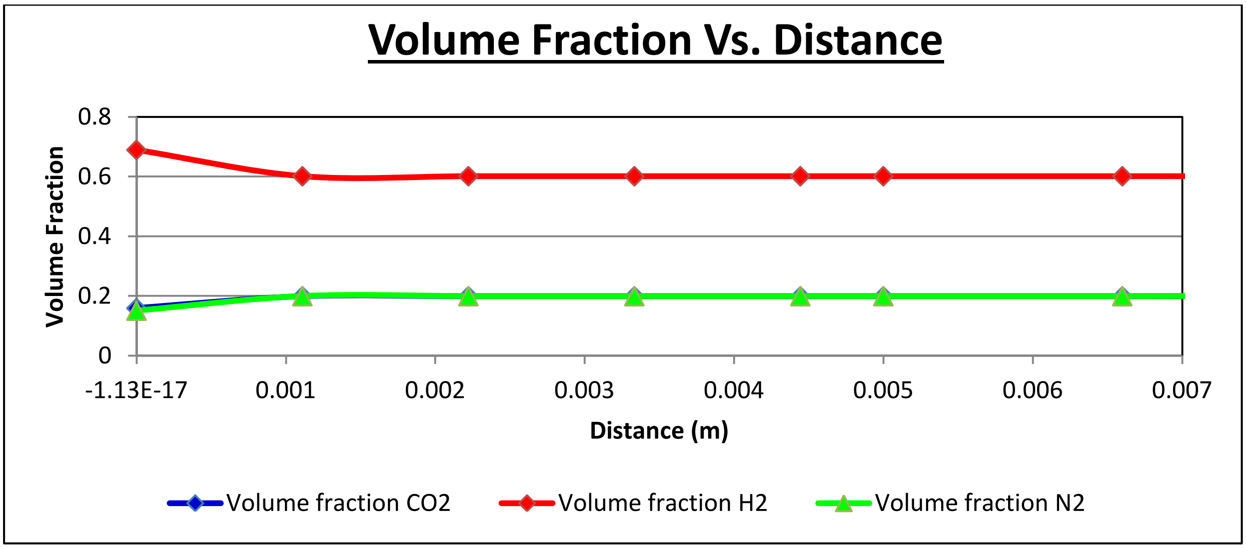
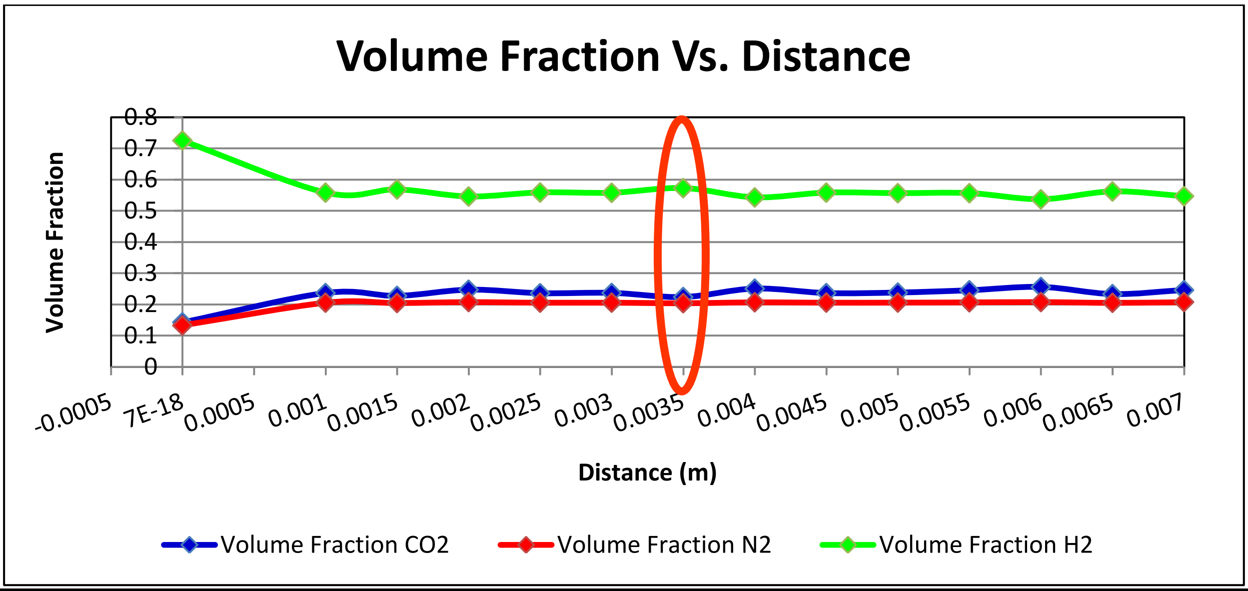


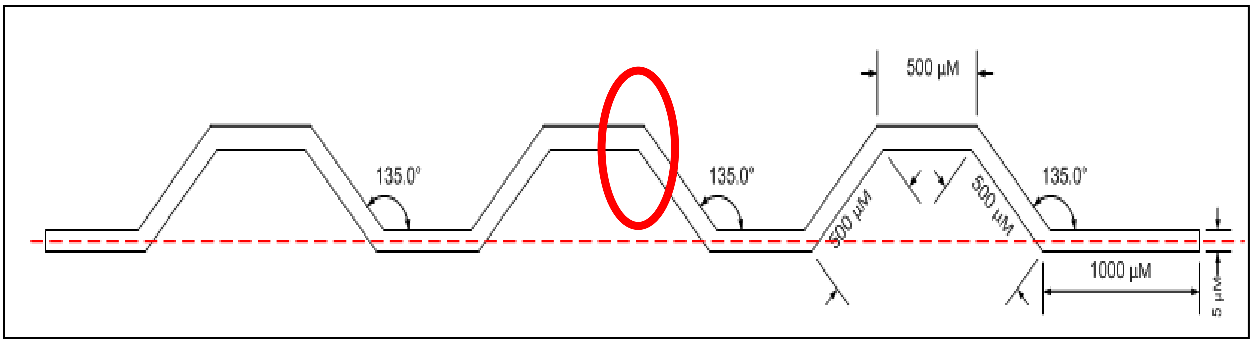
Figure: Graph for each Volume Fraction vs. Distance

Configuration 1

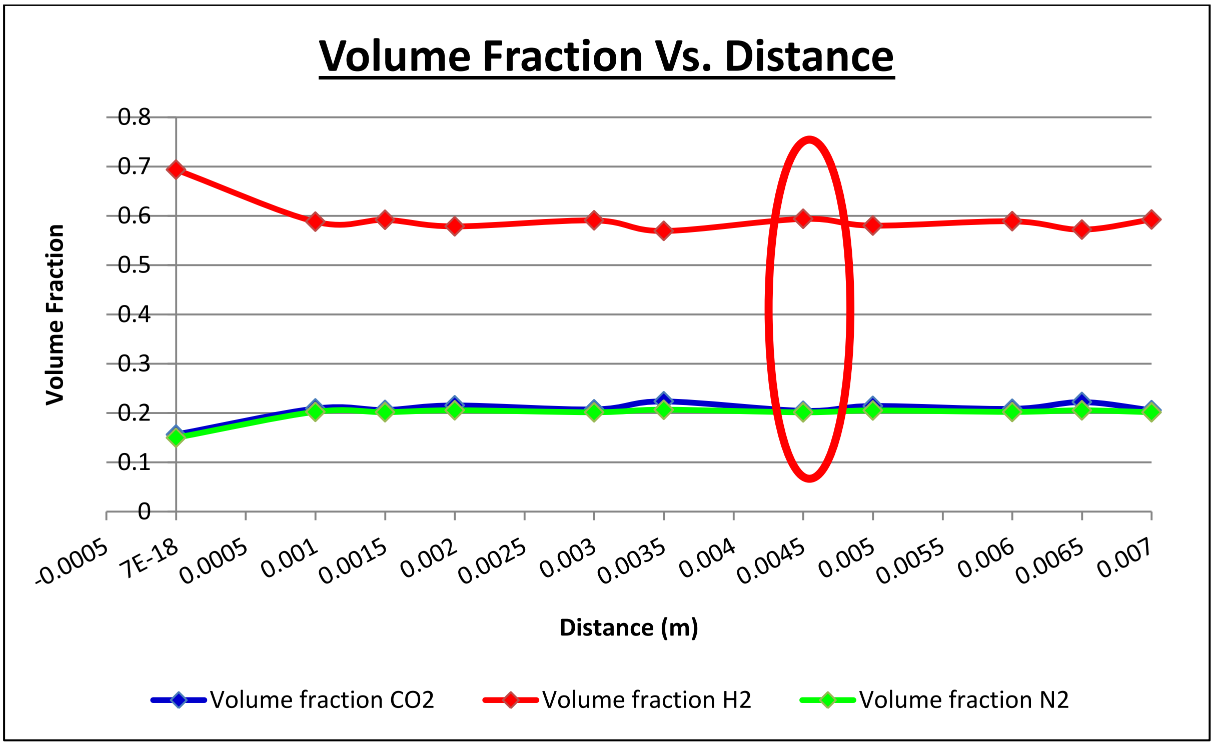


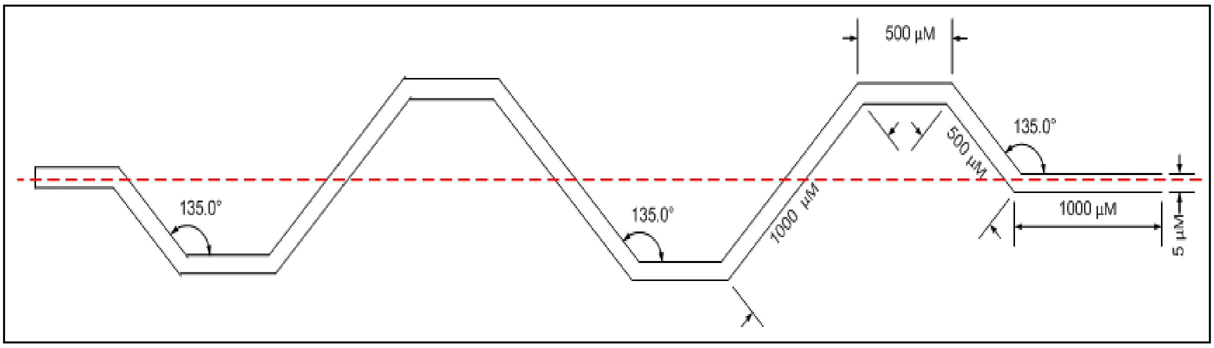
Configuration 2





Configuration 3





4.3.1 Discussion

The graph depicted the volume fraction for each reactant constituent inside the microchannel where the model simulated with three different microchannel configurations 1, 2, and 3. Based from the graph, straight microchannel show mixing of the gas reactant at the initial point of microchannel approximately at 1000 µm and progressing with constant value of volume fraction. Due to simple geometry, there was no mixing and the reactant just flow along the microchannel. In configuration 1, the species mixing occur as a result of diffusive mechanism. Consequently, the mixing distribution is poor by referring to the volume fraction contour and long channel lengths are required to obtain an acceptable volume fraction distribution result.

On the other hand, in the two microchannel configuration 2 & 3 with 135 º angle of curvature and trapezoidal where it incorporated a wavy-like concept that serve as an obstruction point to study the effect on the stoichiometric volume fraction distribution. The designs respectively cause more effective dispersion of the volume fraction of gas reactant compared to configuration 1. The two types of micro-mixers have distinct dispersion tendencies in their contour but with a slight difference in the curvature of the corner of microchannel. No slip boundary condition influenced the direction and velocity of the inner and outer wall of microchannel .While for configuration 2 and 3, the basic observation would be focused on the curvature point where the dispersion tendencies were predicted to be more intense due the introduction of obstruction. The driving force of volume fraction distribution is dependent on the variation of the flow direction. Referring the contour of configuration 2, the length of the microchannel required for established stoichiometric volume fraction is 3500 µm. While, configuration 3 established stoichiometric volume fraction at length of 4500 µm. The significance of the established location of the stoichiometric volume fraction in this paper denotes an even distribution of the volume fraction for each component that presumed a complete reaction of urea synthesis from mixing of H_2, N_2, and CO2 in the micromixers.

Among the various micro mixers, the configuration 1 included as the most homogenous green regions and thus this expected to established stoichiometric volume fraction at length of 1000 µm. Instead, for configuration 2, the stoichiometric volume fraction is established at the length of 3500 µm while configuration 3 established at 4500 µm. For configuration 3, the established volume fraction at l : 4500 µm . Since the recorded volume fraction at the circled point (N_2 : H_2 : CO_2 , 0.2014 : 0.594 : 0.2046)reach approximately the stoichiometric volume fraction (N_2 : H_2 : CO_2 , 0.2 : 0.6 : 0.2) , configuration 3 is chosen as the optimum model for One-Step Urea Synthesis.

4.4 Effect of microchannel configuration on pressure drop

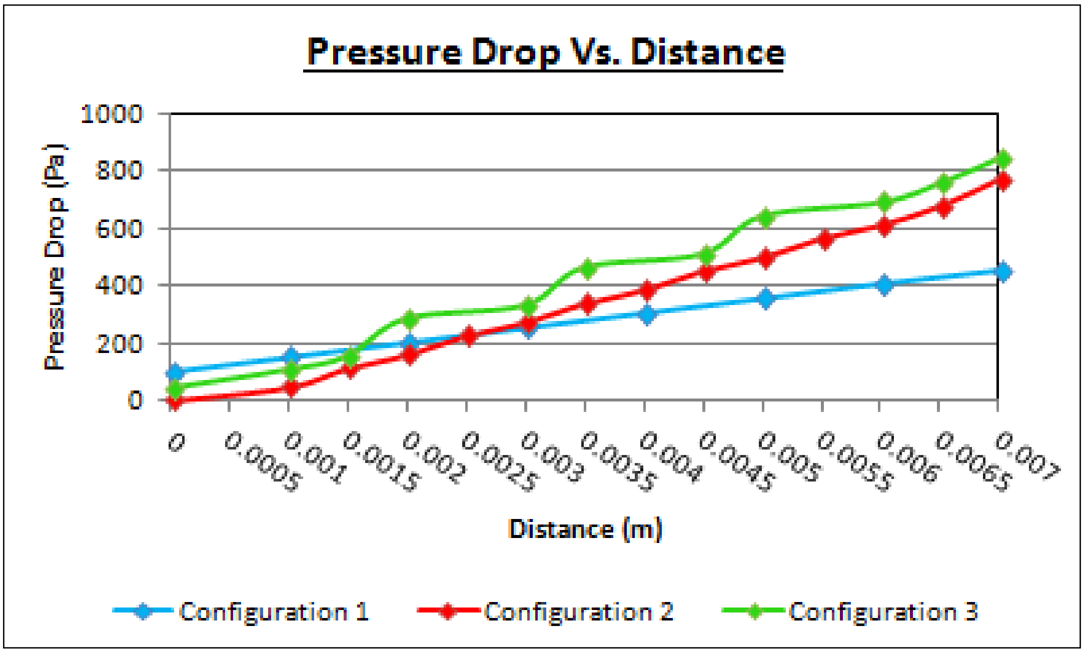


Figure 19: Simulation of pressure drop in different micromixers

In this project, the pressure drop across irregular geometry of microreactor channel is investigated using CFD approach. The pressure drop of three microreactor geometry with varying turning angle is sought.

Geometry	Pressure Drop (Pascal)
Configuration 1	455.5 Pa
Configuration 2	768.55 Pa
Configuration 3	845.89 Pa

Table 4: Pressure Drop recorded along the microchannel

From the three different micromixers, the pressure drop incurred in the configuration 1 yield the smallest due to its simple geometry. Instead, the other two configurations provided a larger pressure drop due to the modified structure relative to the introduction of obstruction along the microchannel. Among them, configuration 3 indicate larger pressure drop. The difference between the two configurations, 2 and 3 is based on the length of the cross-sectional, X_O and X_1. With an extra length of cross-sectional by 500 µm that occupied by configuration 3, the pressure drop increases proportional to the frictional shear forces within the pipe network.

CHAPTER 5

CONCLUSION & RECOMMENDATION

5.1 Conclusion

In this study, the mixing model of passive scheme of micromixers with different configuration was investigated by the simulation .The primary objective of the simulation is to predict the hydrodynamic behaviour of the gas reactant in the microreactor under variation of different microchannel configuration. The presence of obstruction in the created model is to study the significance of the curvature on the volume fraction distribution .The simulation of the passive mixing in the microchannel was achieved using fluent 14.5.

As for conclusion, the three objectives of the study are achieved. For the first objective, the numerical model for One-step Urea Synthesis is successfully developed. As for the second objective, the effect of the different configuration of the microchannel on the volume fraction distribution and pressure drop is investigated. In this study, the effective volume fraction distribution of passive micromixers with different configuration is investigated by the simulation. The obstructive structure induces the mixing of the gas constituent in the simulation with ($Re < 1$).In configuration 1, the species mixing occur as a result of diffusive mechanism. Consequently, the mixing distribution is poor by referring to the volume fraction contour and long channel lengths are required to obtain an acceptable volume fraction distribution result. However, current numerical simulation have shown that the introduction of obstruction in which a wavy-wall section is incorporated in corner of microchannel design increase the interfacial contact area for mixing process between the three reactant gases. The results have shown that the configuration 3 yield an impressive result where the volume fraction distribution for each component approximately reaching the stoichiometric volume fraction distribution (N2: H_2: CO_2, 0.2:0.6:0.2) at length of 4500 µm. The configuration 3 is established as an optimum design for microchannel at length: 4500µm and identified as the suitable site for catalyst location

Configuration	Distance of Stoichiometric volume fraction established at
1	1000 μm
2	3500 μm
3	4500 μm

Table 5: Stoichiometric volume fraction established

5.2 Recommendation

For this section, there are three recommendations for room an improvement on the model construction. First recommendation would be on the meshing refinement that covers the overall geometry. One of the steps can be carried out by increasing the relevance scale and set the relevance centre to fine. However, there is a drawback on refining the meshing grid of microchannel where the simulation process will take on a longer period but the reliability of the simulation is high.

In this study, the focus is on the hydrodynamic behaviour of reactant mixture under different configuration which primarily concern on the computational simulation only limited to three microchannel model Therefore; the studies need to be extended to experimenting on a different shape and angle of curvature for different model. Next, the experimental work should be carried out parallel with the simulation process to determine on specific parameter and data that serves as input. By this way, the result obtained offer more reliable data acquisition as to validate the numerical results predicted using simulation.

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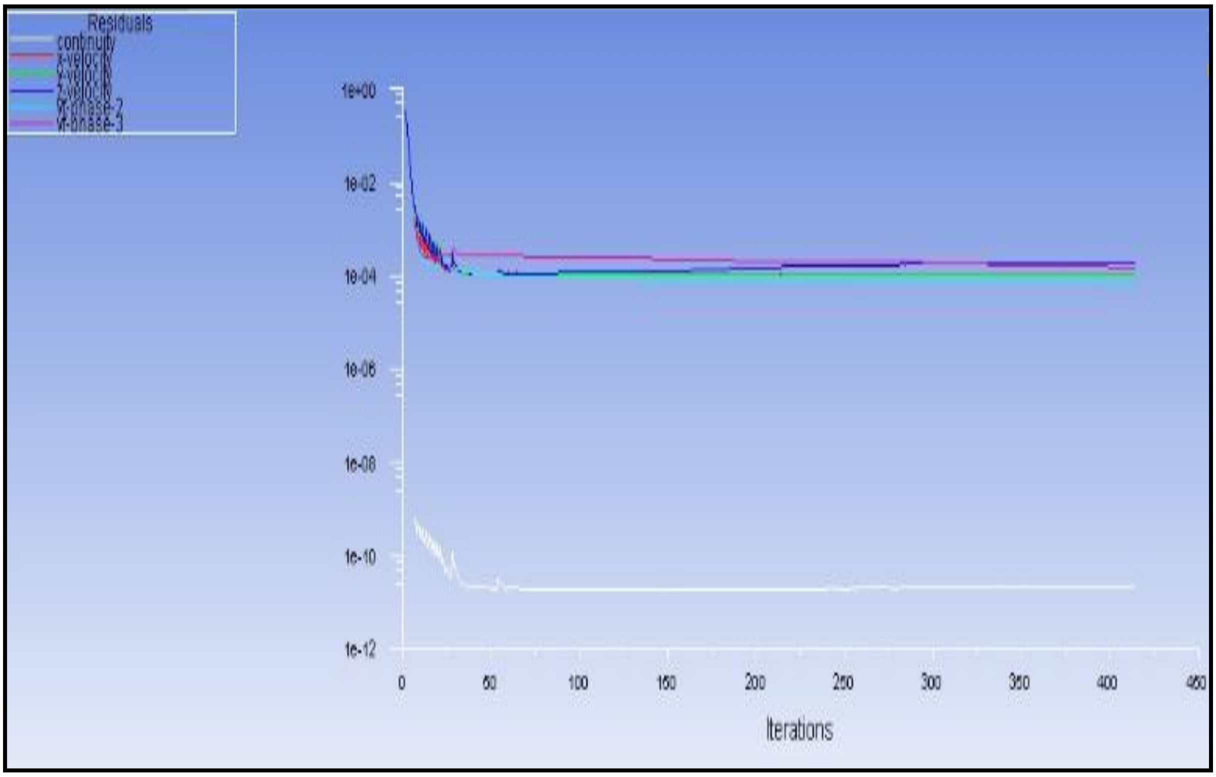
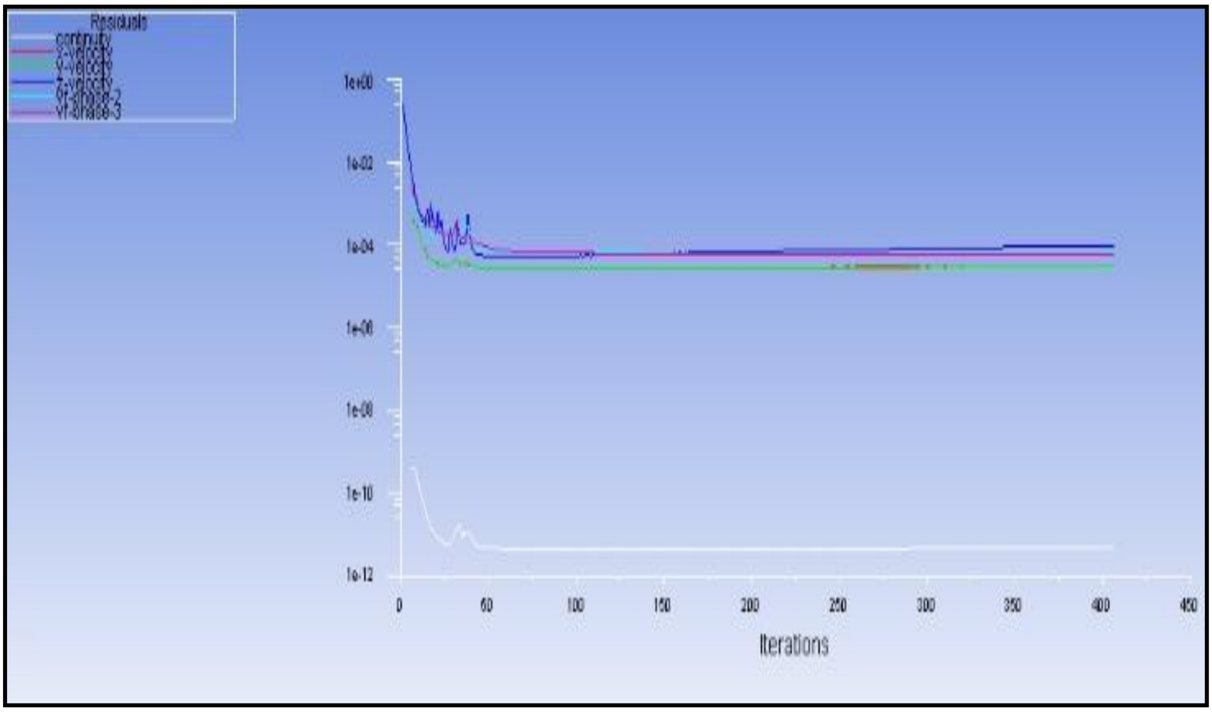
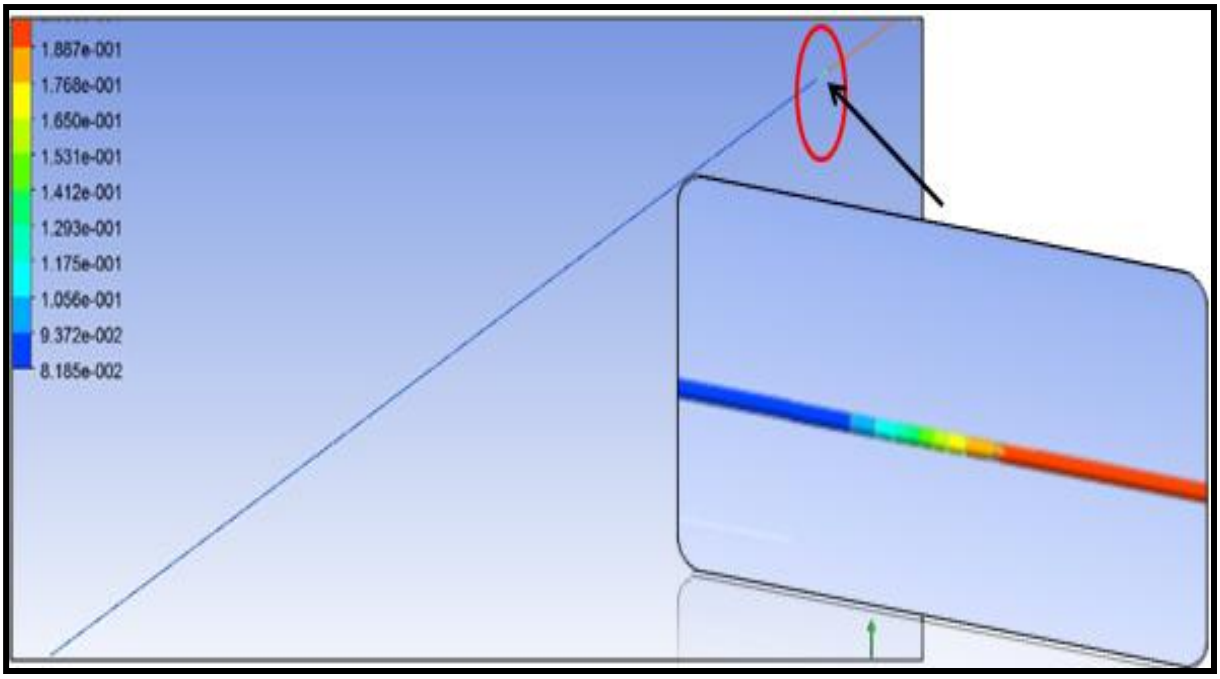
Appendices



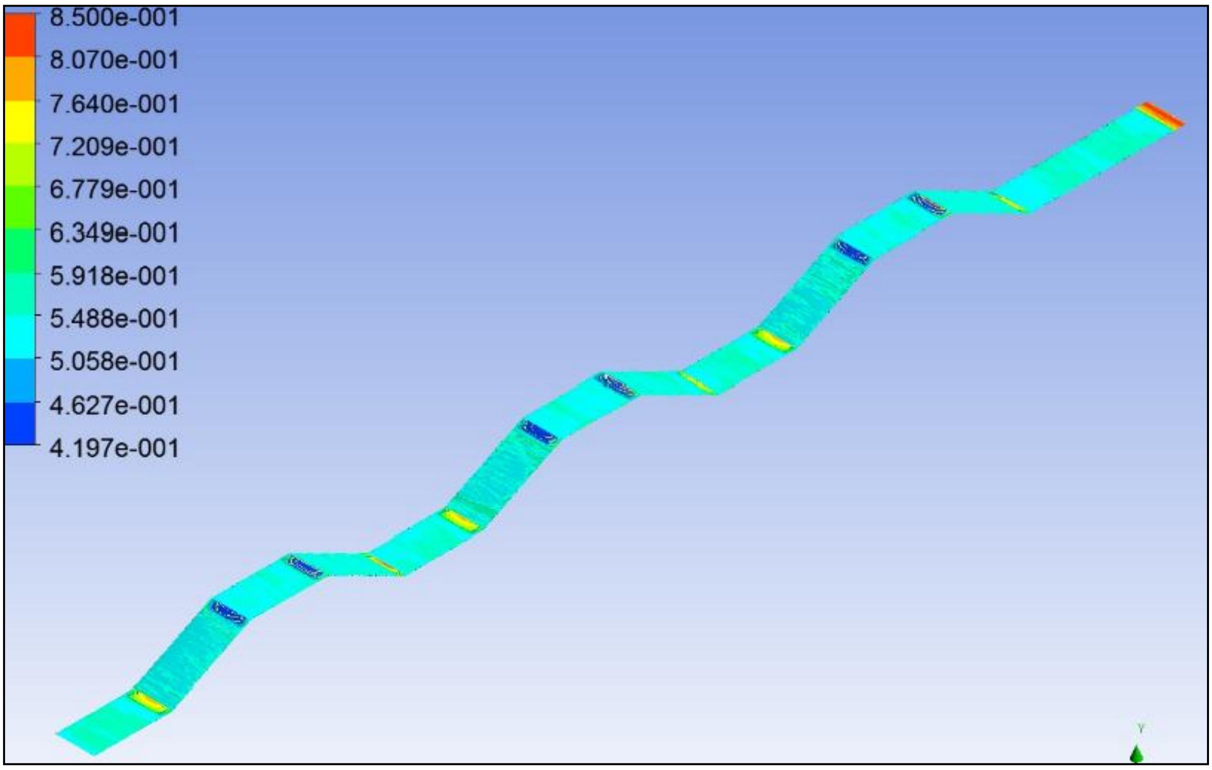
Residual graph for configuration 2 in fluent



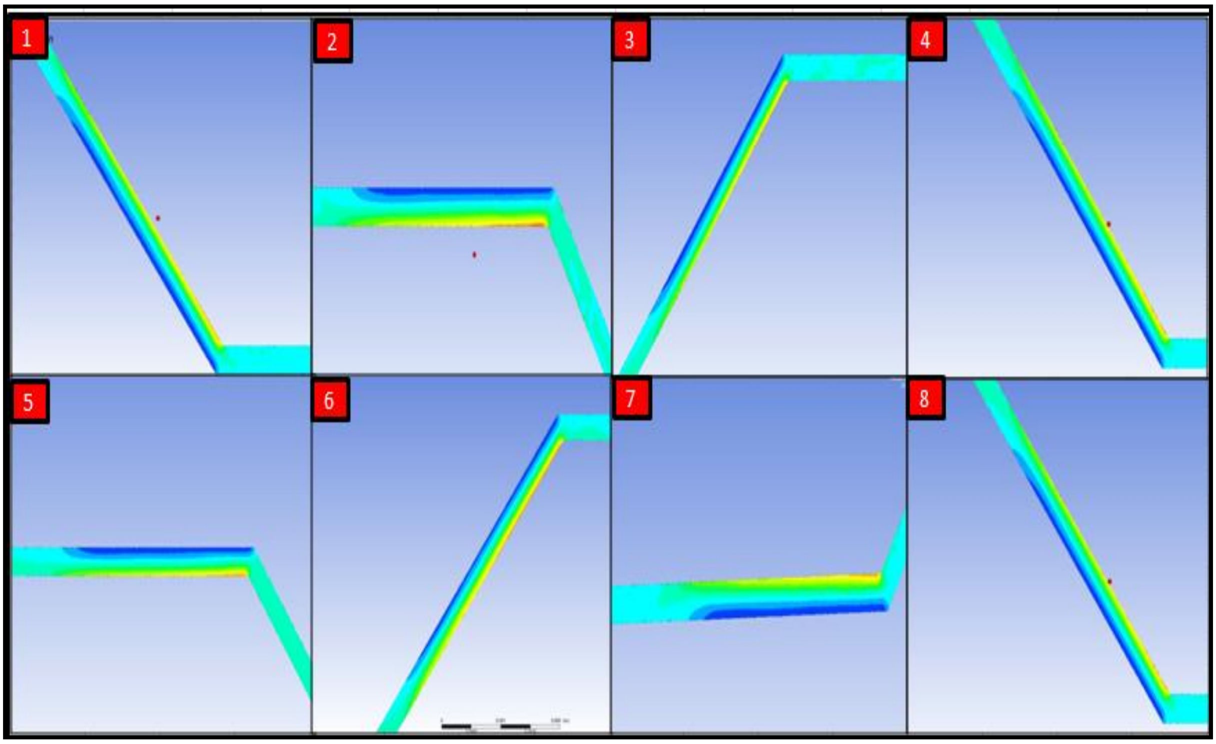
Residual graph for configuration 3 in fluent



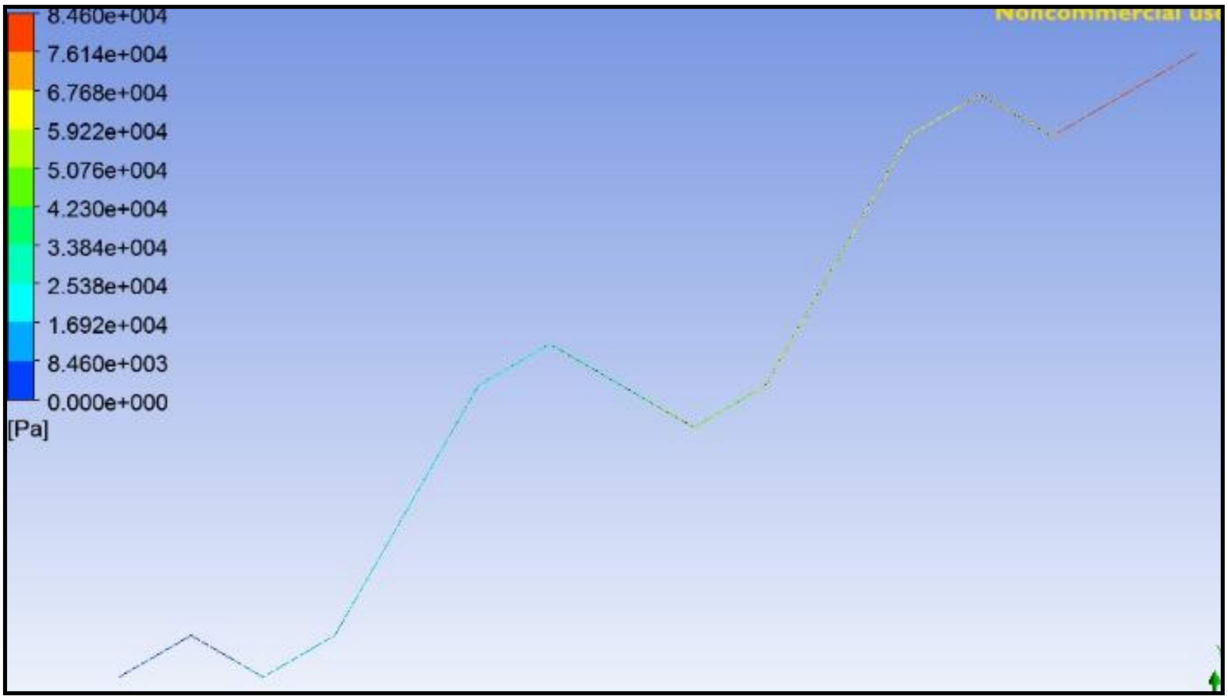
Overall Volume fraction contour for configuration 1



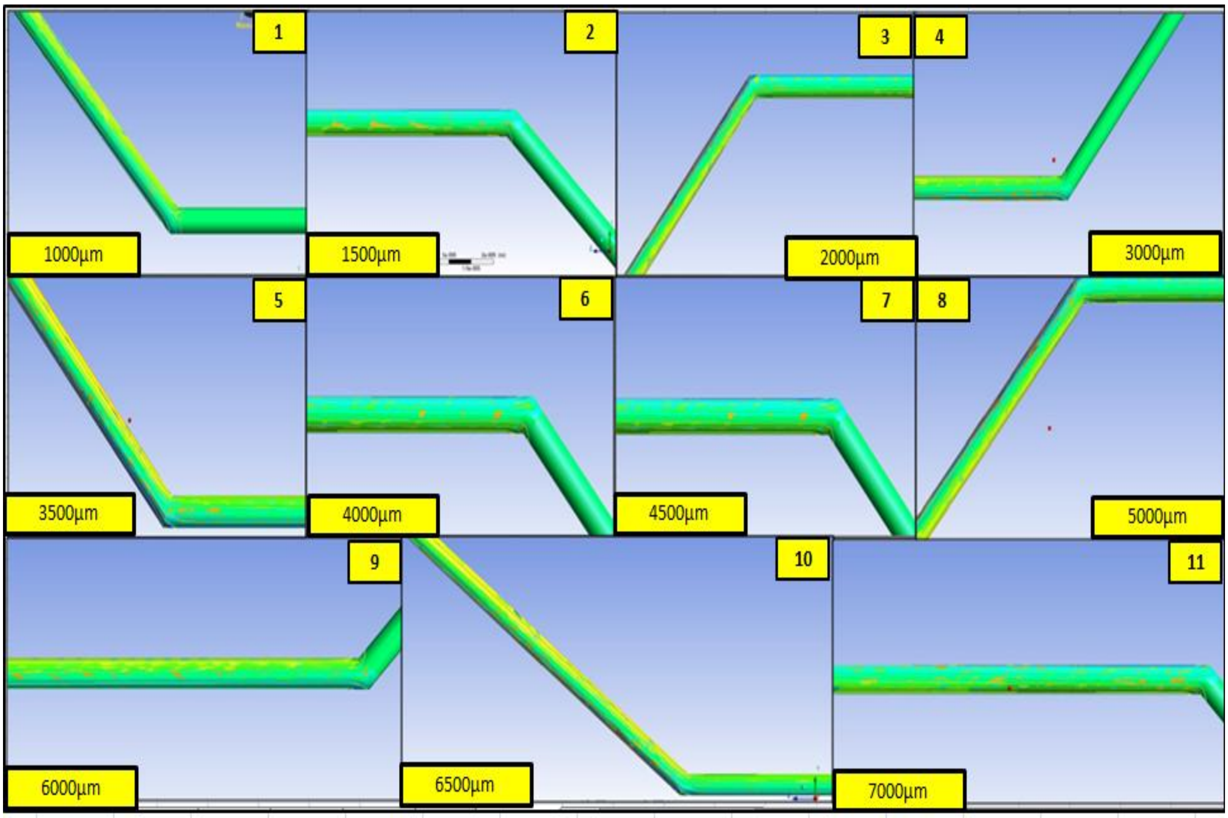
Overall Volume fraction contour for configuration 2



Detailed view on volume fraction of the overall gas constituent in microchannel



Overall Volume fraction contour for configuration 3



Detailed view on volume fraction of the overall gas constituent in microchannel