STUDY OF TRANSIENT FUEL GASES MIXING WITH AIR

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Study of Transient Fuel Gases Mixing with Air

by

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15376

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

SEPTEMBER 2015

Universiti Teknologi PETRONAS,
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Perak

CERTIFICATION OF APPROVAL

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Approved by,

____

(Dr. Rajashekhar Pendyala)

UNIVERSITI TEKNOLOGI PETRONAS
BANDAR SERI ISKANDAR, PERAK
September 2015

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own expect 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.

KEE YUHANG

ABSTRACT

The leakage of the fuel gases can results in the dispersion of fuel gases in air and it will lead to explosion. The physical properties of fuel gases (odorless and colorless) are often become a threat to the industries. This project aim to study the pattern of transient dispersion behavior mixture of fuel gases when mixed with air in 3D simulation. By understanding on the properties and the pattern of dispersion behavior can had an early detection and is easily to prevent major accident if there is any fuel gas leakage. Mitigation guidelines can be developed from this simulation to prevent any major accident in the industries. The binary mixture of the fuel gases such as methane, hydrogen, ethane, propane, butane, carbon monoxide and acetylene had taken into account in this project. The simulation is performed in 3D enclosed geometries of a cylinder. Various transient behavior of binary mixtures are simulated using Computational Fluid Dynamics (CFD).

ACKNOWLEDGEMENT

First of all, I would like to express the gratitude towards the people who arrange this Final Year Project program. Secondly, I would like to thank my supervisor, Dr. Rajashekhar Pendyala for his guidance and supervision during this 2 semesters.

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CHAPTER 1

INTRODUCTION

The demand for energy in the world had increased drastically after the millennium year. Energy are consume everyday either in the industry or household daily usage. People usages energy to make their life more comfortable to live on such as charging their hand phones, generate air-conditional, driving cars.

Energy can be produced by oil, gas, coal, nuclear power, solar power and fuel gases. Fuel gas is one of the source of producing energy. Natural gas, ethane, hydrogen, acetylene are the examples of fuel gases. Fuel gases are often used in the gas turbine, gas engine, pipeline transport, compressor station and etc. Fuel gases possess two physical properties is colorless and odorless. This had been seen as a biggest threat in the industry. Any fuel gas leakage in the pipeline could easily catch a fire and it will lead to explosion in the plant.

With the help of Computational Fluid Dynamic (ANSYS Fluent), we can study the transient behavior of fuel gases when mixing with air by having the numerical simulation displays of the dispersion and the distribution of fuel gas. CFD tool can be used here as the accurate predictions of formation and decay of flammable zones are difficult with experiments and theoretical hand calculations [1].

1.1 Problem Statement

Fuel gases such as acetylene, propane are widely used in the cutting, heating, hardening processes. In these industries, it involves very high temperature operation reaction. The two main physical properties of a fuel gases are colorless and odorless. If one of the pipeline had burst and it will lead to the leakage of the fuel gases. The accumulation of fuel gases in a close surrounding such in the factory will lead to fire when it contact with sparks and mixed in air.

1.2 Objectives

1. To develop and study the pattern of transient dispersion behavior mixture of fuel gases when mixed with air in 3D simulation.

2. To develop and study the patterns demonstrated by the mixture of fuel gases mixing with air.

1.3 Scope of Study

The project will cover the study of flammability limits and transient dispersion of the combination from the typical fuel gases that are normally used in the industries as below:

1) Hydrogen
2) Methane
3) Ethane
4) Propane
5) Butane
6) Acetylene
7) Carbon Monoxide

TABLE 1.1 Binary Mixture of Fuel Gases

	Hydrogen	Methane	Ethane	Propane	Butane	Acetylene	Carbon Monoxide
Hydrogen		✓	✓	✓		✓	✓
Methane			✓			✓	✓
Ethane				✓	✓		
Propane					✓		
Butane							
Acetylene							
Carbon Monoxide							

With the 3D simulation of ANSYS Fluent 15.0, we could obtain the flammability limits and dispersion model of each binary mixture of the fuel gases. The geometry that will be used for the simulation:

1. Initial 10% binary mixture of fuel gas at the bottom and 90% air at the top of the geometry in a closed geometry.
2. Initial 10% binary mixture of fuel gas at the bottom and 90% air at the top of the geometry in an open top geometry.

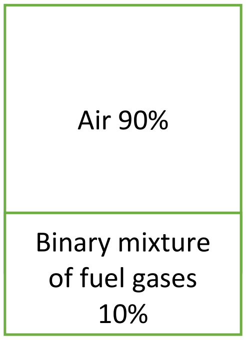


FIGURE 1.1 Proposed Geometry

CHAPTER 2

LITERATURE REVIEW

In this project, we are studying the behavior combination of various fuel gases when it mixed with air. It had a high hazard in performing fuel gases experiment, a numerical simulation is used to avoid it [2]. With the help of Computational Fluid Dynamics (CFD) software, it will help us to compute and predicts the pattern and the formation of flammable region that are difficult to be done with experiments and theoretical hand calculations [1]. It is easier to simulate using a CFD than to do it with experiments. The cost will be lower and there is no danger in performing the simulations. Studies had been carried out on studying the behavioral of fuel gases released in air e.g. hydrogen leakage from a fuel cell vehicle in an underground parking garage [3], underground gas pipeline explosion and fire [4], leakage in a nuclear containment model [5], leakage of natural gas from compressor stations [6], dispersion and behavior of hydrogen during a leak in a prismatic cavity [7], hydrogen diffusion cause by high pressured storage tanks failure [8].

In the present study, we investigated the dispersion of binary mixture of fuel gases for a model in a cylindrical shape with stationary, no slip and adiabatic wall boundary conditions are applied [9]. There are two objectives: (1) to develop and study the pattern of transient dispersion behavior mixture of fuel gases when mixed with air in 3D simulation and (2) to develop and study the patterns demonstrated by the mixture of fuel gases mixing with air. We performed a Computational Fluid Dynamics (CFD) by using ANSYS 15.0 (Fluent) to simulate transient mixing of fuel gases in air. According to Shravan K. Vudumu & Umit O. Koylu, they had perform the simulation in a simple cylindrical shape with a 1 meter height and 0.25 meter diameter was chosen (Figure 1.1) [9]. From Table 1, we perform a simulation by changing the combinations of the fuel gases. 10% of the cylinder is filled with binary mixture of fuel gases at the bottom of the cylinder and 90% of the cylinder is filled with air. Computational fluid dynamics is a branch of fluid mechanics that uses numerical analysis and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. CFD uses numerical methods to solve the fundamental nonlinear differential equations that describe fluid flow (the Navier-Stokes and allied equations) for predefined geometries and boundary conditions. Engineers can evaluate the performance of a wide range of HVAC/IAQ system configurations on the computer without the time, expense, and disruption required to make actual changes onsite.

- CFD predicts performance before modifying or installing systems.
- CFD provides exact and detailed information about HVAC design parameters.
- CFD Saves Cost and Time.
- CFD is Reliable.

Fuel gas is any one of a number of fuels that under ordinary conditions are gaseous. Many fuel gases are composed of hydrocarbons. Such gases are sources of potential heat energy or light energy that can be readily transmitted and distributed through pipes from the point of origin directly to the place of consumption. List of fuel gas:

- Acetylene
- Associated petroleum gas
- Butane
- Compressed natural gas
- Compressed hydrogen
- Liquefied natural gas
- Methane
- Natural gas
- Propane

Flammability limit is the amount of combustible gas in an air mixture when the mixture is flammable. Lower flammability limit (LFL) is the minimum amount of fuel that may cause burn or explode upon mixing with air. If there is too little fuel, the air/fuel mixture is considered too "lean" and will not a burn. Upper flammability limit (UFL) is the maximum amount of fuel that cause a burn or explode. If there is too much fuel, the air/fuel mixture is considered too "rich" and will not burn.

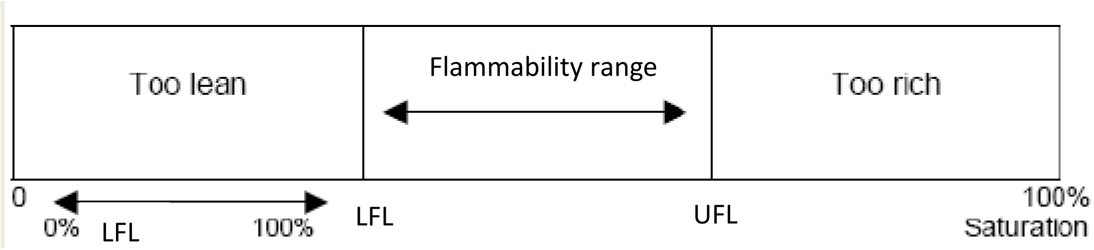


FIGURE 2.1 Graphic explanation of LEL and UEL

TABLE 2.1 Properties of Fuel Gases

Fuel gases	**Chemical formula**	**Molecular weight, g/mol**	**Density (kg/m^3)**	**LFL**	**UFL**
Hydrogen	H_2	2.01	0.0899	4.0	75.0
Methane	CH_4	16.04	0.66	5.0	15.0
Acetylene	C_2H_2	26.04	1.1	2.5	100
Carbon monoxide	CO	28.01	1.15	12.5	74.0
Air	-	28.97	1.225	-	-
Ethane	C_2H_6	30.07	1.28	3.0	12.4
Butane	C_4H_{10}	58.12	2.48	1.8	8.4
Propane	C_3H_8	44.10	493.00	2.1	9.5

The Navier–Stokes momentum equation can be derived as a particular form of the Cauchy momentum equation.

$$\frac{\partial}{\partial t}(\rho u) + \nabla . (\rho u u + pI) = \nabla . \tau + \rho g \qquad (1)$$

ρ is the density,

u is the flow velocity,

∇ is the del operator.

p is the pressure

I is the identity matrix

τ is the deviatory stress tensor, which has order two,

g represents body accelerations (per unit mass) acting on the continuum, for example gravity, inertial accelerations, electric field acceleration, and so on.

The transient mixing during leakage in most of the journals are using a laminar flow analysis. Rayleigh numbers which indicates the type of buoyant flow cause by the change of temperature and Reynolds number were always low enough to be in the laminar region [9]. Variables such as the temperature surrounding, weather conditions and direction of the wind is made as assumption. Nature of hydrogen in air are very high in diffusion coefficient, a fine mesh size which at a 0.1 mm is used to construct the geometry model. A time step of 0.01 s are used and the simulation is performed at 50 iterations. Walls of the enclosed cylinder is set as stationary, no-slip and adiabatic wall [9]. In our research study, we are using at a higher iterations of 500 to simulate more time steps for the fuel gases for being able to reach to the top of the cylinder.

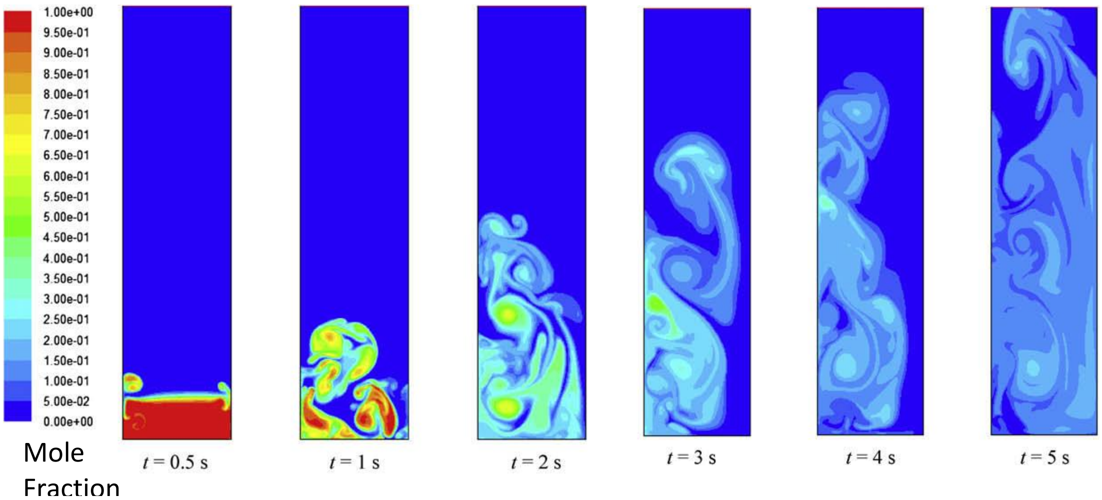


FIGURE 2.2 Open Top Cylinder

The contour above is simulated result for hydrogen mole fraction disperse into air region at a different time. The hydrogen diffuses into the air region at a very short amount of time. Buoyancy and molecular diffusion is the key of the hydrogen concentration distribution. As the hydrogen rapidly disperse into the region of air, the concentration of hydrogen decay from initial mole fraction of 1 into a smaller value. At a time = 5s, the hydrogen had reached to the top of the enclosed cylinder.

Knowledge of transient dispersion behavior for binary fuel gases are not yet been studied. The novelty of this project is to study the transient dispersion behavior for different binary mixtures. Limited studies are available on the transient dispersion behavior of fuel gases.

CHAPTER 3

RESEARCH METHODOLOGY

3.1 Work Process Flow

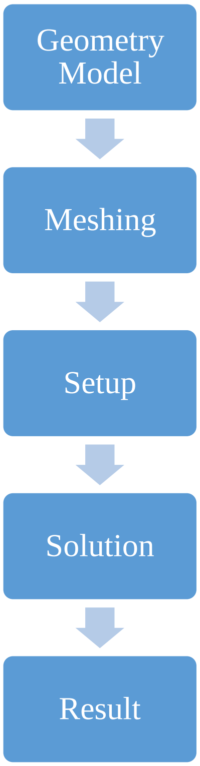
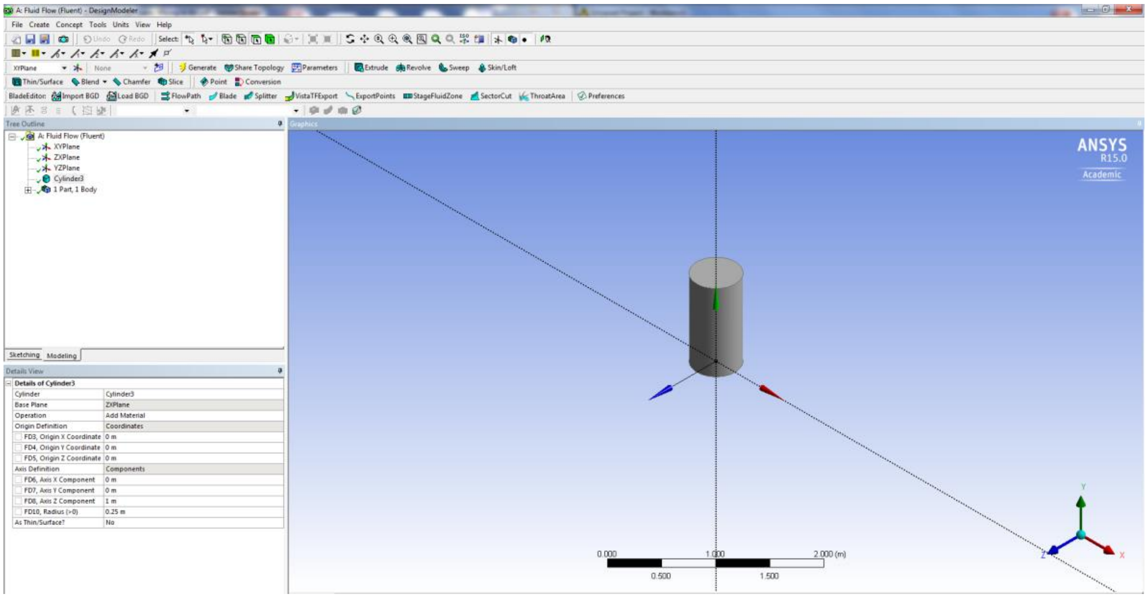


FIGURE 3.1 Simulation of ANSYS

Computational Fluid Dynamics (CFD) had used in this project to develop and study the behavior of transient mixing binary mixture of fuel gases with air. In ANSYS 15, the geometry model is been created and meshed. In this project, a simple geometry of 0.25 meter diameter cylinder with 1 meter height. The binary mixture of fuel gases is put at rest at the bottom of the cylinder at t = 0s. The binary mixture of fuel gases is then mixed with the 90% of air in three different situation open top cylinder, partially open top cylinder and fully closed top cylinder. The geometry is then mesh and divided into my parts. After that, the boundary condition of the geometry is setup physics. Finally the software will compute itself and come out to the result in the form of graphs and displays.

3.2 Preparation for simulation

3.2.1 Geometry Modeling

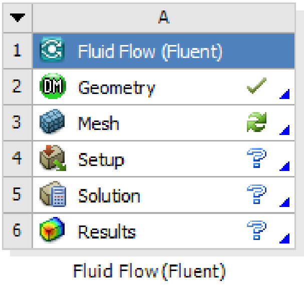


Details of Cylinder3	
Cylinder	Cylinder3
Base Plane	ZXPlane
Operation	Add Material
Origin Definition	Coordinates
☐ FD3, Origin X Coordinate	0 m
☐ FD4, Origin Y Coordinate	0 m
☐ FD5, Origin Z Coordinate	0 m
Axis Definition	Components
☐ FD6, Axis X Component	0 m
☐ FD7, Axis Y Component	0 m
☐ FD8, Axis Z Component	1 m
☐ FD10, Radius (>0)	0.25 m
As Thin/Surface?	No

FIGURE 3.2 Geometry Modeling

The shape of the geometry had been decided and cylinder with 0.25m diameter and 1m height had used. The geometry can proceed for meshing.

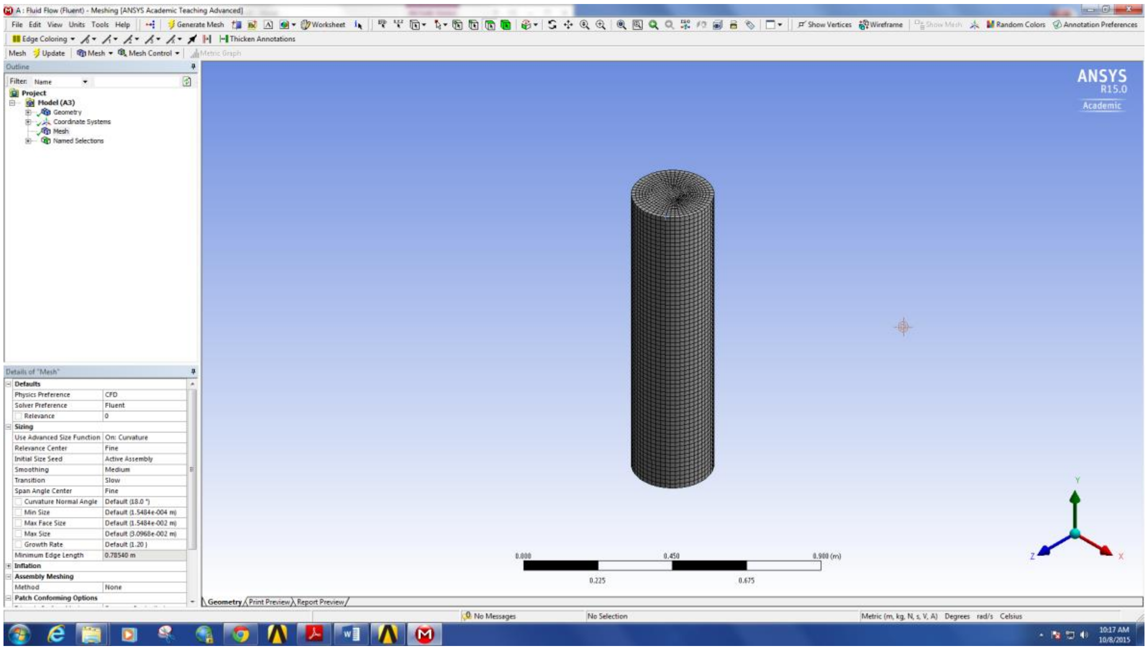
3.2.2 Meshing



	A
1	Fluid Flow (Fluent)
2	Geometry ✓
3	Mesh
4	Setup
5	Solution
6	Results

Fluid Flow (Fluent)

FIGURE 3.3 Meshing



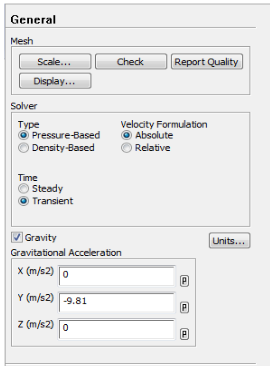
Details of "Mesh"

Defaults	
Physics Preference	CFD
Solver Preference	Fluent
☐ 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	Default (18.0 °)
☐ Min Size	Default (1.5484e-004 m)
☐ Max Face Size	Default (1.5484e-002 m)
☐ Max Size	Default (3.0968e-002 m)
☐ Growth Rate	Default (1.20)
Minimum Edge Length	0.78540 m
Inflation	
Assembly Meshing	
Method	None
Patch Conforming Options	

FIGURE 3.4 Geometry Meshing

In the meshing part, it will divide the geometry into smaller parts to calculate for more accurate results. In this project, curvature and fine mesh was used.

3.2.3 Setup physics



General

Mesh

Solver

Type
● Pressure-Based
○ Density-Based

Velocity Formulation
● Absolute
○ Relative

Time
○ Steady
● Transient

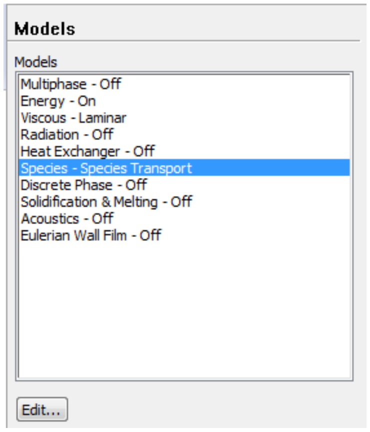
☑ Gravity

Gravitational Acceleration

X (m/s2) 0
Y (m/s2) -9.81
Z (m/s2) 0

FIGURE 3.5 Laminar Model Setup

The time setup is set as transient and there is a gravitational acceleration of -9.81 m/s^2.



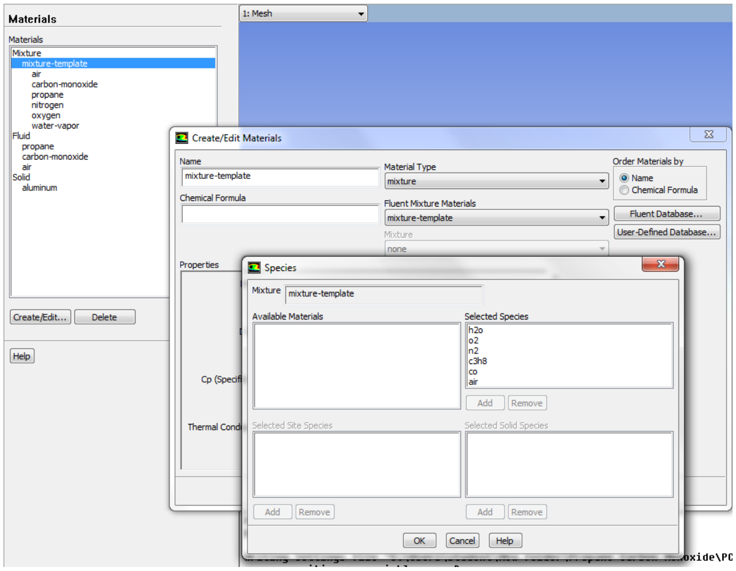
Models

Models

Multiphase - Off
Energy - On
Viscous - Laminar
Radiation - Off
Heat Exchanger - Off
Species - Species Transport
Discrete Phase - Off
Solidification & Melting - Off
Acoustics - Off
Eulerian Wall Film - Off

FIGURE 3.6 Models

Navier Stokes-related equations which comprise of energy equation had been selected. Laminar flow was chosen on the viscous and the mixture material of the fuel gases is selected in the species transport.


Materials

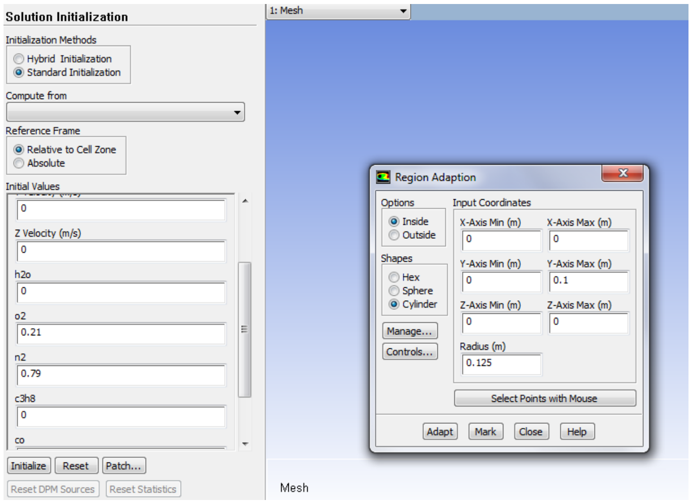
Materials
Mixture
mixture-template
air
carbon-monoxide
propane
nitrogen
oxygen
water-vapor
Fluid
propane
carbon-monoxide
air
Solid
aluminum

Name: mixture-template
Chemical Formula:
Material Type: mixture
Fluent Mixture Materials: mixture-template
Mixture: none
Order Materials by: ● Name ○ Chemical Formula

Species
Mixture: mixture-template
Available Materials:
Selected Species:
h2o
o2
n2
c3h8
co
air

FIGURE 3.7 Materials mixture-template

Inside the mixture-template, this is where we are choosing on the mixture of fuel gases. For this case, we are choosing on the binary mixture of propane and carbon monoxide.

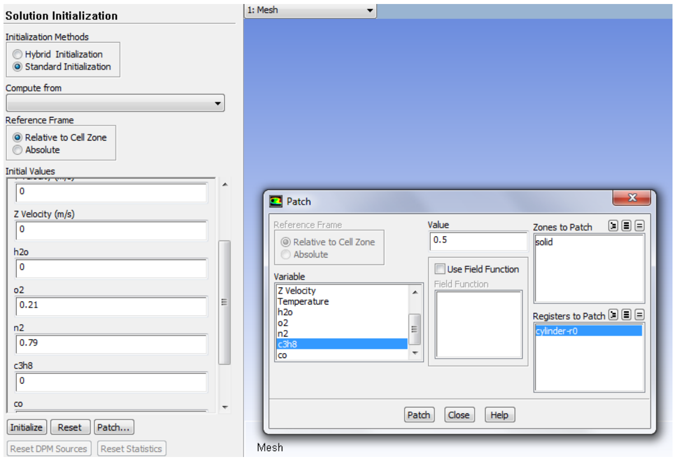

Solution Initialization

Initialization Methods: ○ Hybrid Initialization ● Standard Initialization
Compute from:
Reference Frame: ● Relative to Cell Zone ○ Absolute
Initial Values
0
Z Velocity (m/s): 0
h2o: 0
o2: 0.21
n2: 0.79
c3h8: 0
co

Region Adaption
Options: ● Inside ○ Outside
Shapes: ○ Hex ○ Sphere ● Cylinder
Input Coordinates
X-Axis Min (m): 0
X-Axis Max (m): 0
Y-Axis Min (m): 0
Y-Axis Max (m): 0.1
Z-Axis Min (m): 0
Z-Axis Max (m): 0
Radius (m): 0.125

FIGURE 3.8 Solution initialization & Region Adaption

In the figure above, oxygen and nitrogen is prompted inside the cylinder at an intial value of 0.21 oxygen and 0.79 nitrogen. This to illustrated the composition of air. Now the whole cylinder is filled with air. Region adaption is to assign the fuel gases at the bottom of the cylinder. For this case, cylinder is chosen and 10% of the geometry is set.


Solution Initialization

Initialization Methods
○ Hybrid Initialization
● Standard Initialization

Compute from

Reference Frame
● Relative to Cell Zone
○ Absolute

Initial Values
0
Z Velocity (m/s): 0
h2o: 0
o2: 0.21
n2: 0.79
c3h8: 0
co

Patch

Reference Frame
● Relative to Cell Zone
○ Absolute

Value: 0.5

☐ Use Field Function

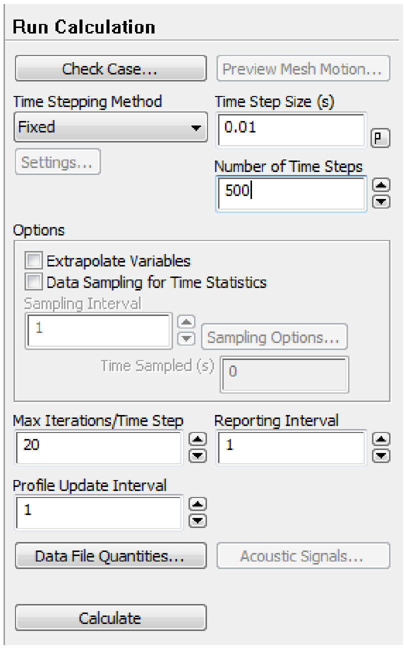
Variable: Z Velocity, Temperature, h2o, o2, n2, c3h8, co (c3h8 selected)

Zones to Patch: solid

Registers to Patch: cylinder-r0 (selected)

FIGURE 3.9 Patching

After the region adaption had set, patching is done to assign the fuel gases inside the region that we had set. For this case, propane and carbon monoxide is patch inside the region at a mol fraction composition value of 0.5 and 0.5.


Run Calculation

Time Stepping Method: Fixed

Time Step Size (s): 0.01

Number of Time Steps: 500

Options
☐ Extrapolate Variables
☐ Data Sampling for Time Statistics

Sampling Interval: 1

Time Sampled (s): 0

Max Iterations/Time Step: 20

Reporting Interval: 1

Profile Update Interval: 1

FIGURE 3.10 Run Calculation

After the setup has been done, time step size is use at 0.01s and 500 time steps in order to determine the how far the fuel gases can reach to the top.

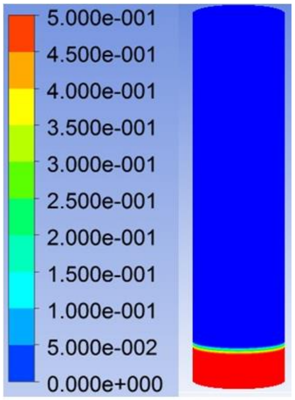


FIGURE 3.11 Initial Setup

From the contours, we can display the mole fraction concentration of fuel gases inside the cylinder. For this case, the blue color area is the air area that we prompt 0.21 oxygen and 0.79 nitrogen in it. The red color part is where the fuel gases where situated which is 0.5 mole fraction.

FIGURE 3.12 Plane

XZ plane was used to compare the changes of the mole fraction of the fuel gases. The coordinate at (0, 0.1, 0) is used to compare the concentration changes of the fuel gases.

TABLE 3.1 Gantt chart for FYP 1

No	Details	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of Project Title		✓												
2	Preliminary Research Work and Literature Review			✓	✓	✓	✓	✓	✓	✓					
3	Submission of Extended Proposal							✓	✓						
4	Preparation for Proposal Defense							✓	✓						
5	Proposal Defense									✓					
6	Simulation Work							✓	✓	✓	✓	✓	✓	✓	
7	Submission of Interim Report													✓	

TABLE 3.2 Gantt chart for FYP 2

No	Details	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Project Work Continues	✓	✓	✓	✓	✓	✓	✓								
2	Submission of Progress Report							✓								
3	Project Work Continues								✓	✓	✓	✓	✓			
4	Pre-SEDEX										✓					
5	Submission of Draft Final Report											✓				
6	Submission of Dissertation (soft bound)												✓			
7	Submission of Technical Paper												✓			
8	Viva													✓		
9	Submission of Project Dissertation (Hard Bound)															✓

CHAPTER 4

RESULT AND DISCUSSION

An enclosed cylinder geometry with a diameter of 0.25m and 1m height containing of fuel gases and air is being simulated using the software ANSYS 15.0. At time = 0 s, the cylinder is filled with 10% of binary mixture of fuel gases and 90% of air. The fuel gases at the bottom of the cylinder is let to mix with the air at the top. Technically, fuel gases such as hydrogen, methane acetylene and carbon monoxide will disperse faster in air because of its density is lower than air. While fuel gases such as ethane, propane and butane will disperse slowly in air as its density is higher than air. Hydrogen is the least dense fuel gas while propane is the most dense fuel gases in this project.

Fuel gases	**Chemical formula**	**Molecular weight, g/mol**	**Density (kg/m^3)**
Hydrogen	H_2	2.01	0.0899
Methane	CH_4	16.04	0.66
Acetylene	C_2H_2	26.04	1.1
Carbon monoxide	CO	28.01	1.15
Air	-	28.97	1.225
Ethane	C_2H_6	30.07	1.28
Butane	C_4H_{10}	58.12	2.48
Propane	C_3H_8	44.10	493.00

TABLE 4.1 Properties of Fuel gases

The dispersion study had been taken out at a time step of 0.01s and 500 iteration had been carried out. After the simulation, the shortest time that the fuel gases reach the top of the cylinder will be taken compare with other fuel gases. These simulation had divided into three parts which is mixture of light gases only, mixture of heavy fuel gases only and mixture of heavy and light fuel gases. Mixture of light gases which consists of hydrogen, methane, acetylene, carbon monoxide; mixture of heavy fuel gases consists of ethane, butane and propane as shown in Table 5.

4.1 Mixture of light fuel gases only

It is observed that the mixture of light fuel gases disperse in the air more rapidly compare to heavy fuel gases. The light fuel gases started to disperse as soon as the simulation starts. It is due to the low density ratio between the air and fuel gases. Fuel gases such as hydrogen, methane, acetylene and carbon monoxide had a density lower than air. They disperse very fast into the air region and reached the top of the cylinder with a short amount of time.

4.1.1 Mixture of Hydrogen & Methane

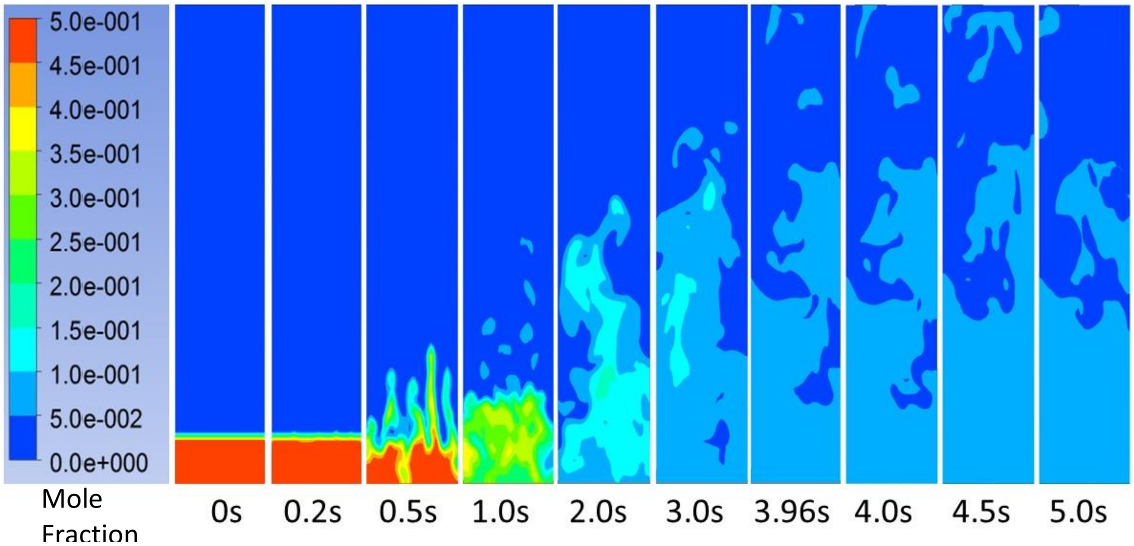


FIGURE 4.1 Mole Fraction of Hydrogen & Methane

In this simulation, the mixture of hydrogen and methane is the fastest fuel gases that reach the top at a time of 3.96s as in Figure 4.1. At time = 0.5 seconds, the mixture of hydrogen and methane already started to disperse through the air. At the time = 1.0 second, the mixture of hydrogen and methane had filled half of the cylinder. This is due to the buoyancy of the hydrogen and methane that are lighter than air. It tends to disperse into the air at faster rates. This combination of fuel gases is the fastest as the density of both mixture together is the lowest among of all. The dispersion of fuel gas will be fast as the buoyancy is lower. If the simulation is done by prompting the fuel gas at the top of the cylinder, the jet momentum is opposite direction of buoyancy force, with thus, the mixture of fuel gases will actually harder to diffuse into the region of the air in the bottom of the enclosed cylinder. [9]

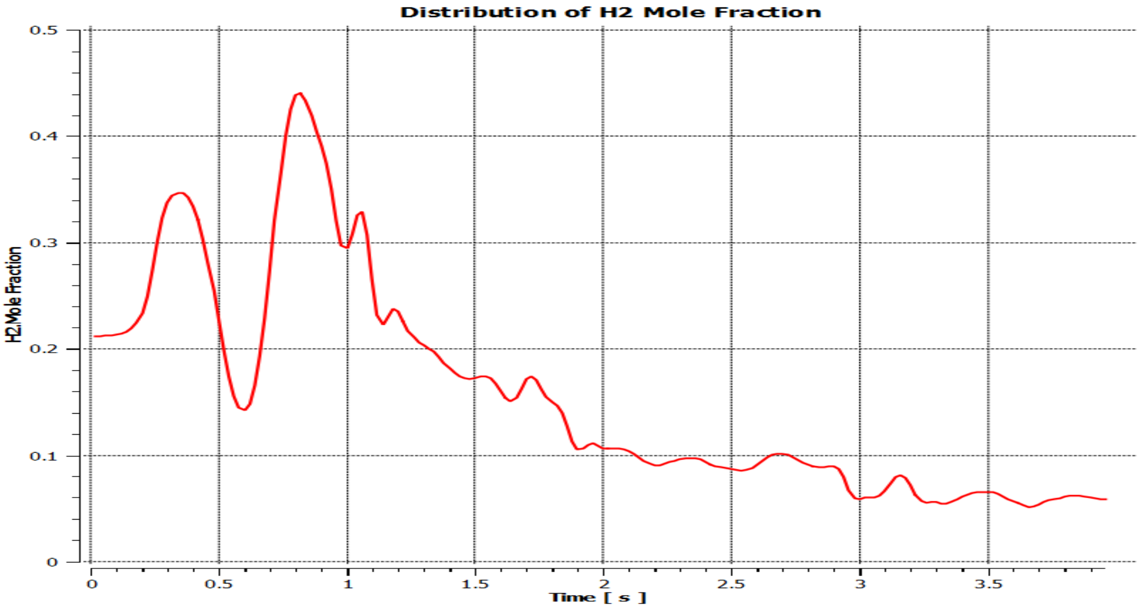


FIGURE 4.2 Distribution of hydrogen mole fraction

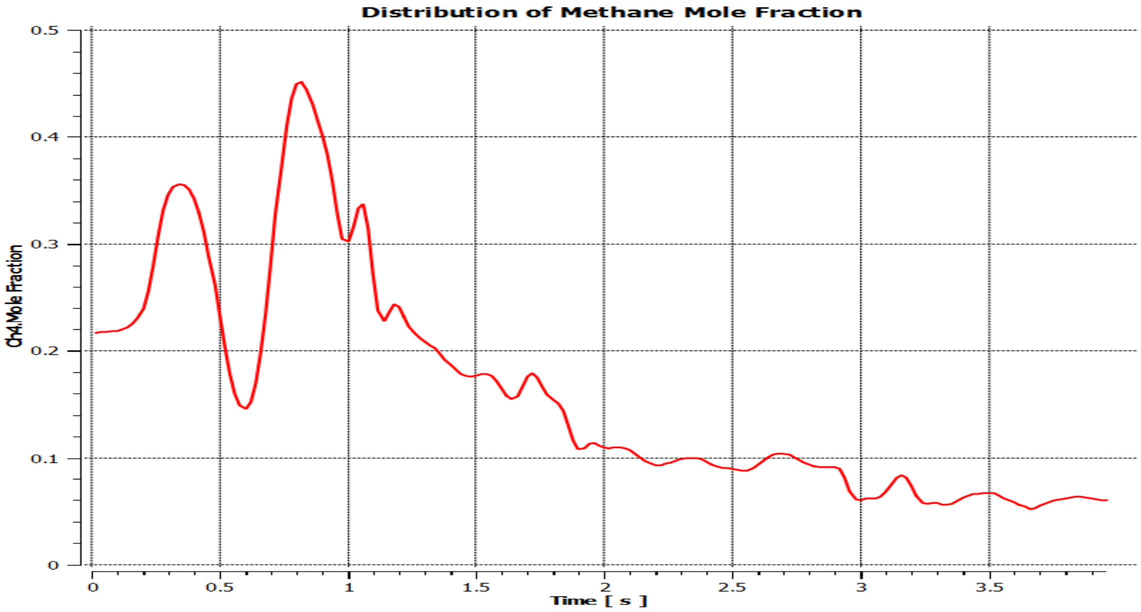


FIGURE 4.3 Distribution of methane mole fraction

Figure 4.2 and Figure 4.3 shows the distribution of hydrogen and methane mole fraction at the point of (0, 0.1, 0) in the mixture of hydrogen and methane. The distribution of hydrogen and methane had increases from 0s to 0.3s. This is due to the fast dispersion of fuel gases inside the cylinder. Then the mole fraction of fuel gases increase until the peak which we can see at time = 0.7s and it drop down as the fuel gases had disperse evenly into the whole enclosed cylinder.

4.1.2 Mixture of Hydrogen & Acetylene

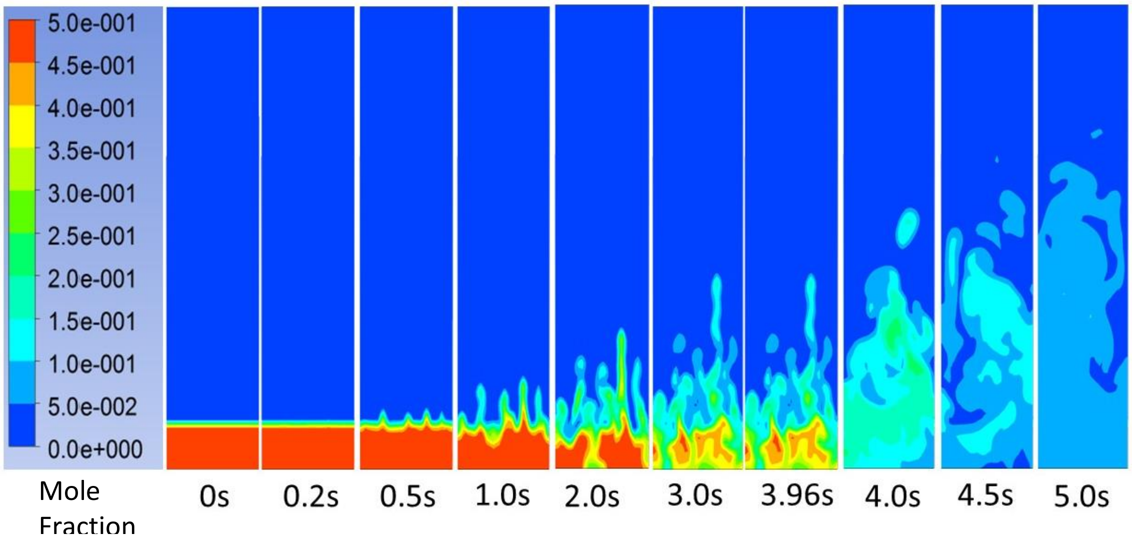


FIGURE 4.4 Mole Fraction of Hydrogen & Acetylene

Figure 4.4 shows the contour of mole fraction for hydrogen and acetylene. Likewise, it started to disperse into the air region at the time of 0.5 second. At the time of 4.5 seconds, the cylinder half filled with the fuel gases. This is also due to the buoyancy of hydrogen and acetylene is lesser than air. If the simulation had done to 10 seconds and above, the contour of the mixture of hydrogen and acetylene will disperse more and eventually will reached to the top of the cylinder. The mixture of hydrogen and acetylene will filled up all the cylinder. Comparing the contour for mixture of hydrogen and methane, it is slightly slower than hydrogen and methane as the density of hydrogen and acetylene is higher than hydrogen and methane.

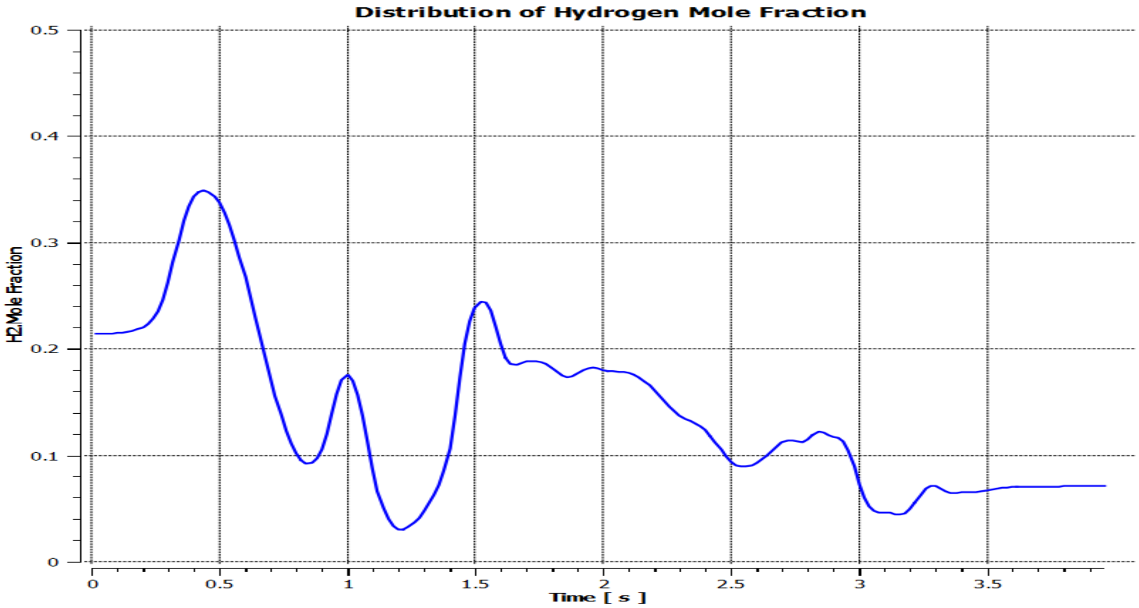


FIGURE 4.5 Distribution of hydrogen mole fraction

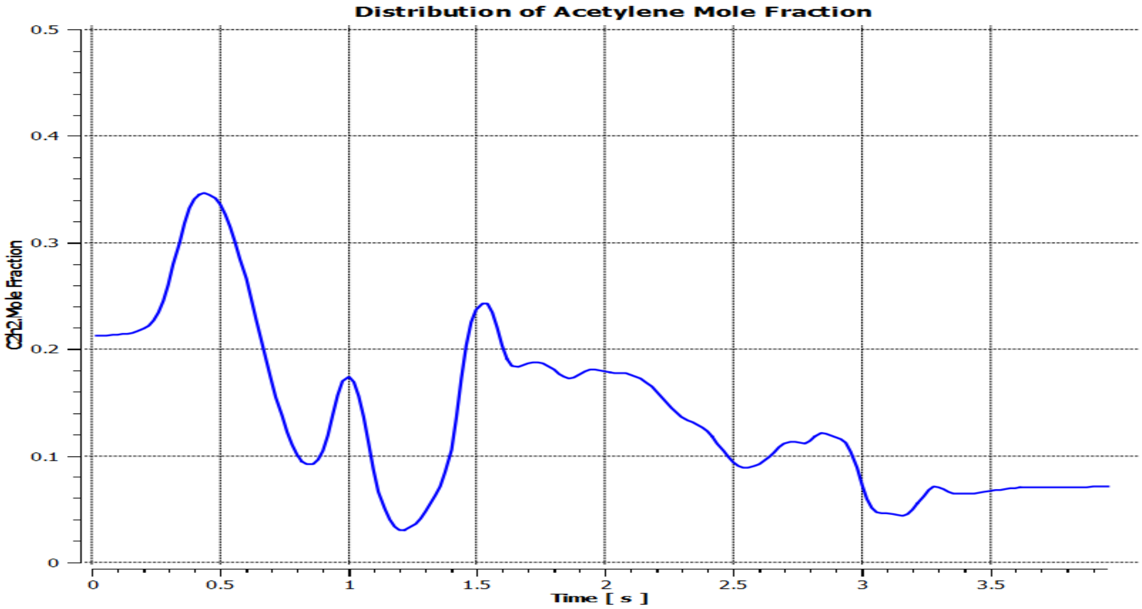


FIGURE 4.6 Distribution of acetylene mole fraction

Figure 4.5 and Figure 4.6 shows the distribution of hydrogen and methane mole fraction at the point of (0, 0.1, 0) in the mixture of hydrogen and methane. The distribution of hydrogen and methane had increases from 0s to 0.3s. The distribution reached to the peak at time = 0.3 s. Then the distribution started to disperse into the air region even until it reach at a constant mole fraction at 3.5s.

4.1.3 Mixture of Hydrogen & Carbon Monoxide

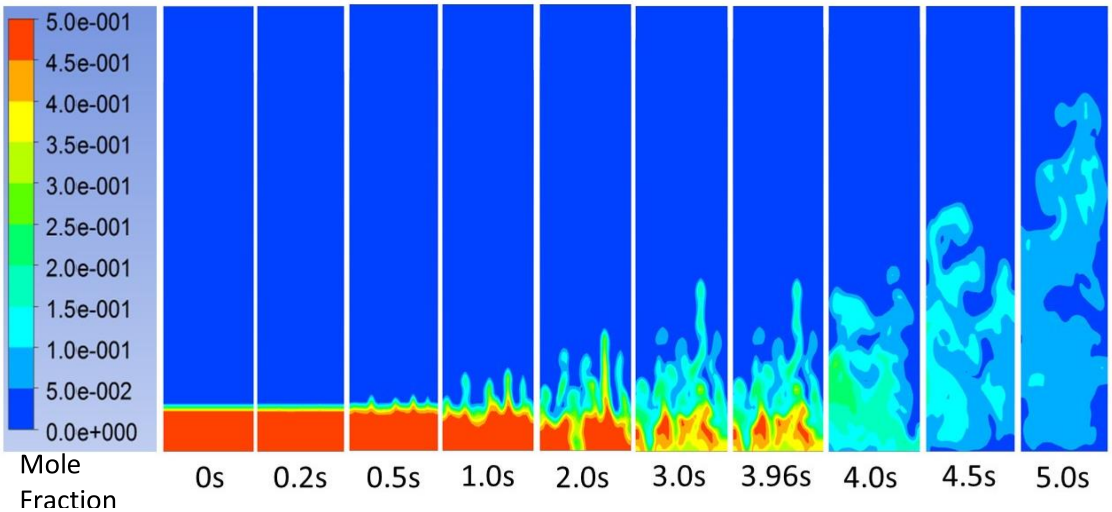


FIGURE 4.7 Mole Fraction of Hydrogen & Carbon Monoxide

Figure 4.7 shows the mole fraction of hydrogen and carbon monoxide. Both of the fuel gases are less dense than air. At a time = 1.0 second, the mixture of hydrogen and carbon monoxide started to disperse into the air region. Comparing at a time = 3.96 second, hydrogen and carbon monoxide only disperse until almost half of the cylinder. For contour of hydrogen and methane, it actually reaches the top of the enclosed cylinder.

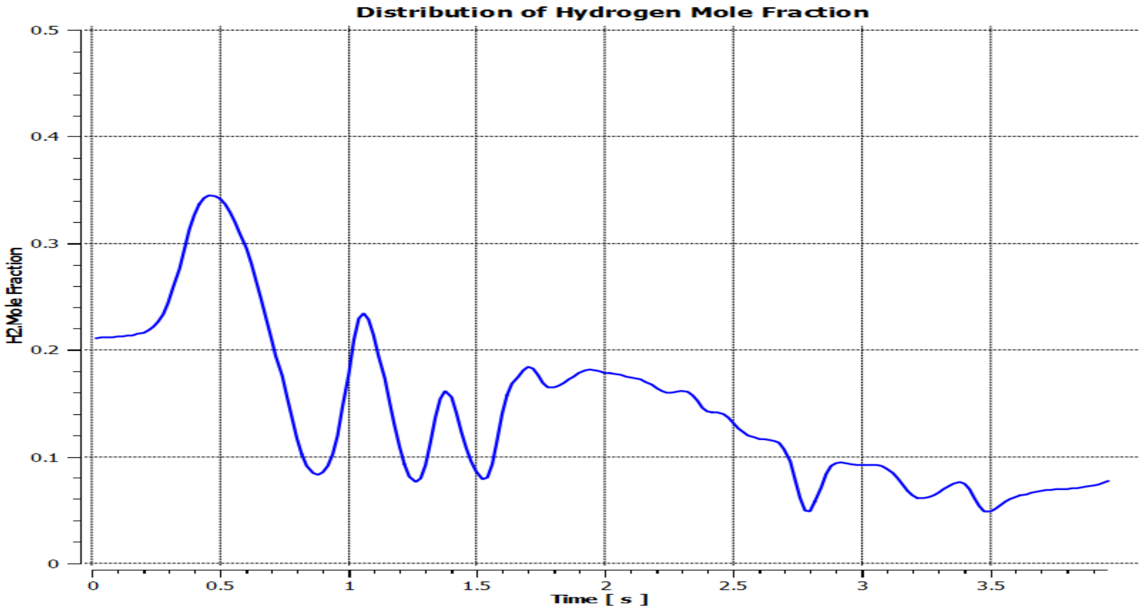


FIGURE 4.8 Distribution of hydrogen mole fraction

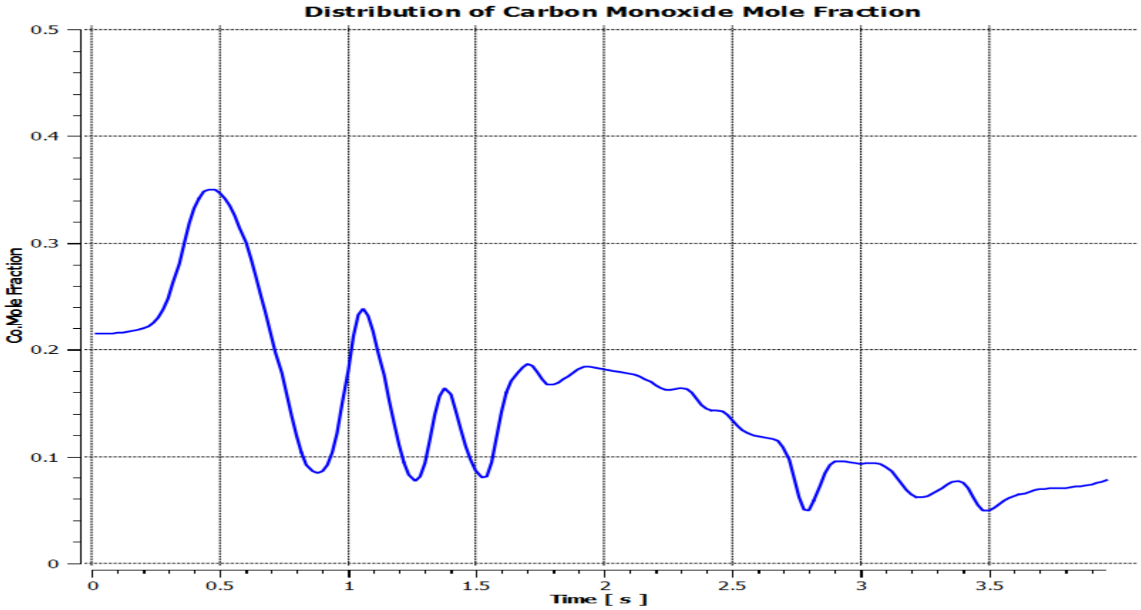


FIGURE 4.9 Distribution of carbon monoxide mole fraction

Figure 4.8 and Figure 4.9 shows the distribution of hydrogen and carbon monoxide mole fraction at the point of (0, 0.1, 0) in the mixture of hydrogen and carbon monoxide. The distribution of hydrogen and carbon monoxide had increases from 0s to 0.4s at a fast rate. The distribution reached to the peak at time = 0.4 s. Then it started to decrease in mole fraction.

4.1.4 Mixture of Methane & Acetylene

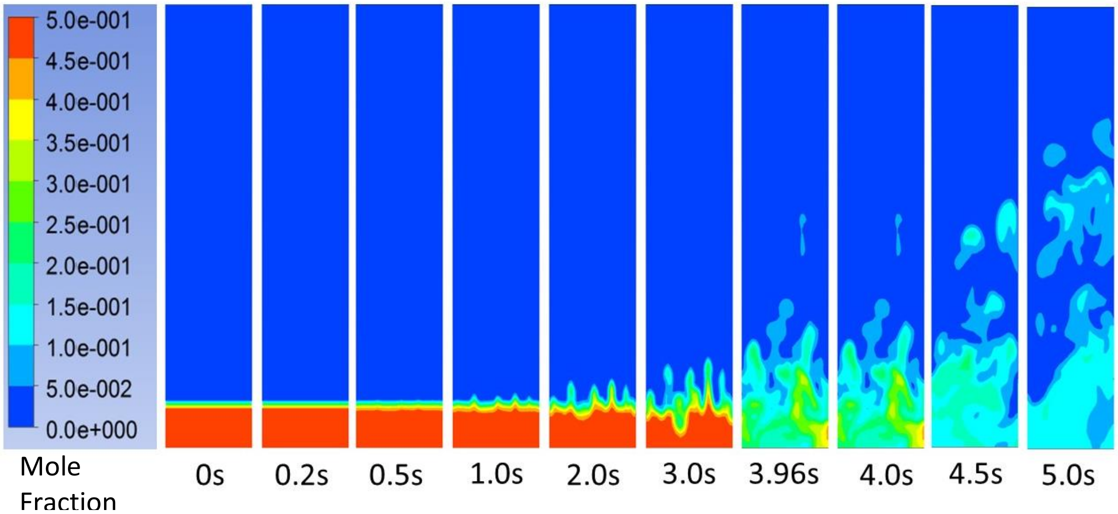


FIGURE 4.10 Mole Fraction of Methane & Acetylene

Figure 4.10 shows the mole fraction of methane and acetylene. In this simulation, the mixture of methane and acetylene disperse slowly into air region. At the time of 2.0 second, it only started to disperse. At the end of the simulation which is at 5 second, it actually reach more than 50% of the cylinder.

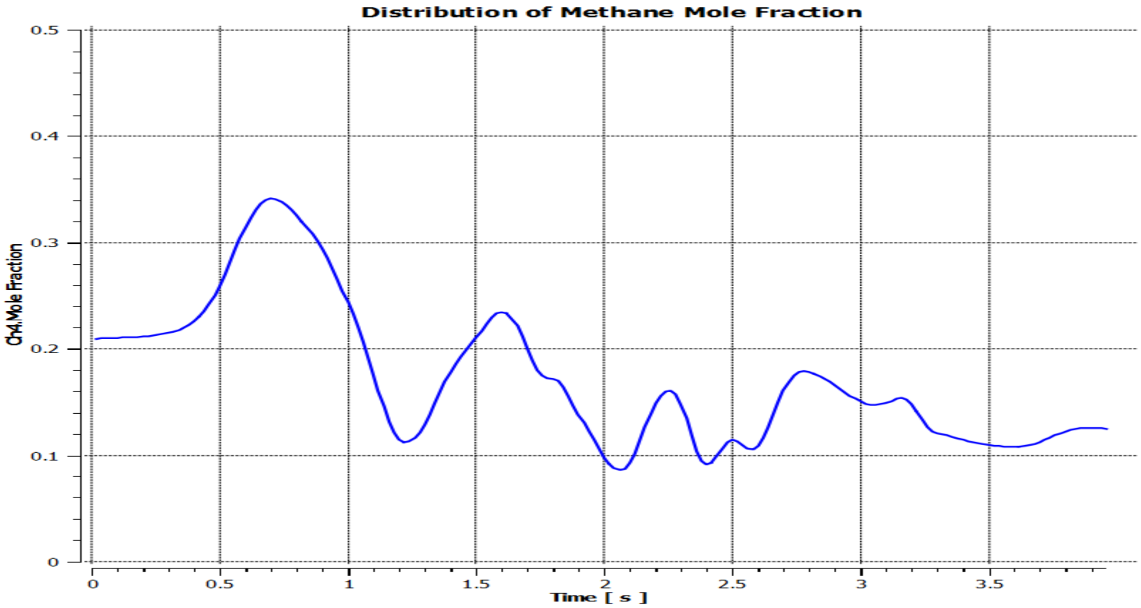


FIGURE 4.11 Distribution of methane mole fraction

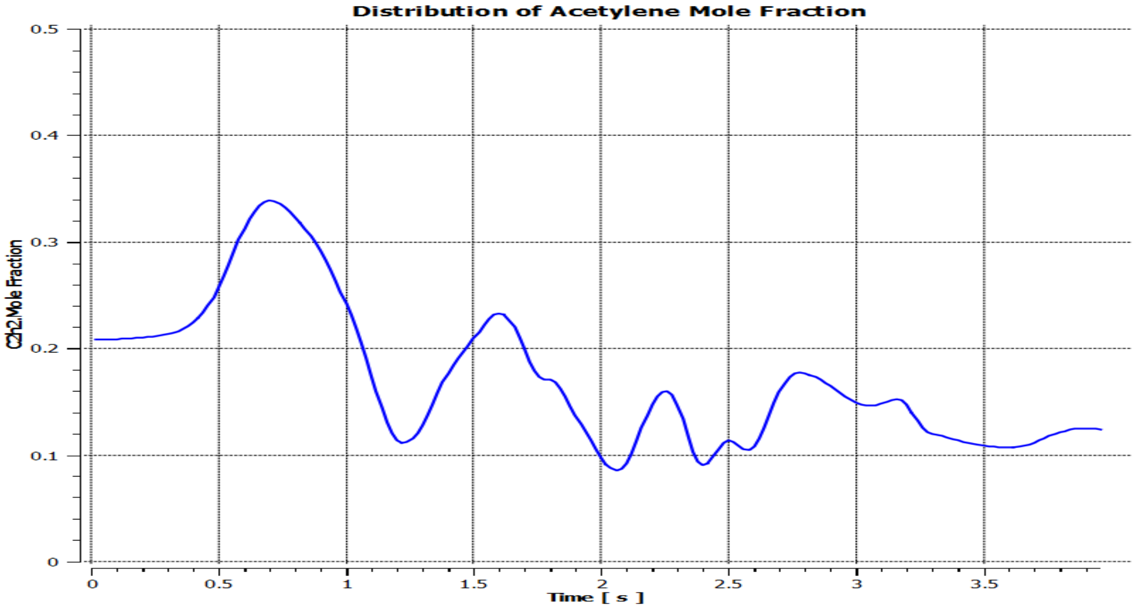


FIGURE 4.12 Distribution of acetylene mole fraction

Figure 4.11 and Figure 4.12 shows the distribution of mole fraction for methane and acetylene in mixture of methane and acetylene. The mole fraction of methane and acetylene increases from 0s and it reached to the peak at 0.7s. The peak mole fraction is shown as 0.34.

4.1.5 Mixture of Methane & Carbon Monoxide

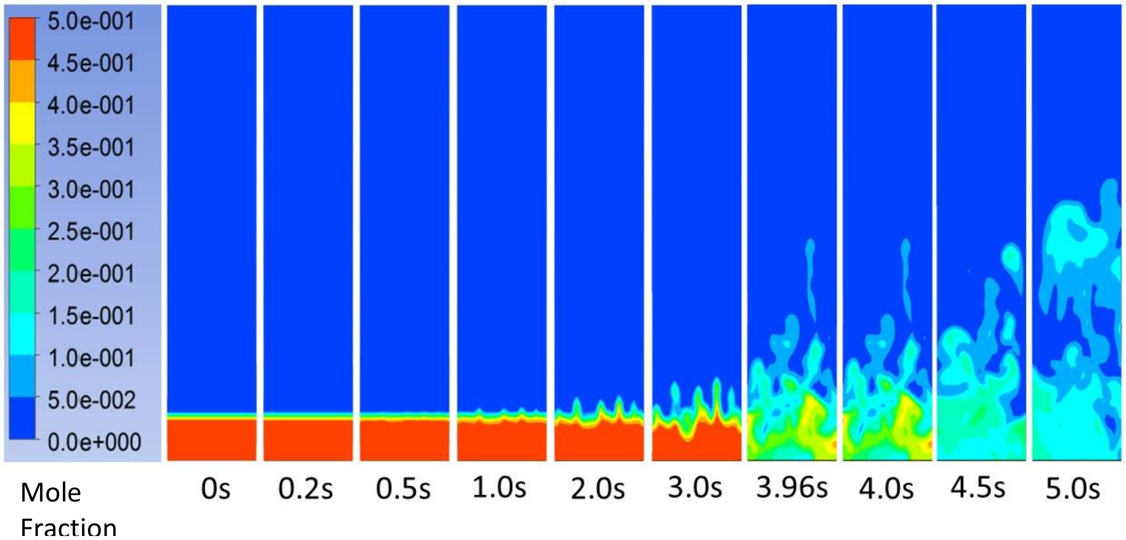


FIGURE 4.13 Mole Fraction of Methane & Carbon Monoxide

Figure 4.13 shows the mole fraction of methane and carbon monoxide. Comparing the contour with the mixture of methane and acetylene, both of the mixture started disperse at the time of 2.0 seconds. But for the mixture of methane and carbon monoxide, it disperses at a much slower rate. This can be seen from the density difference between the fuel gases. Density for mixture of methane and carbon monoxide is higher than the mixture of methane and acetylene. But if the simulation continues, the mixture would eventually reach to the top of the cylinder.

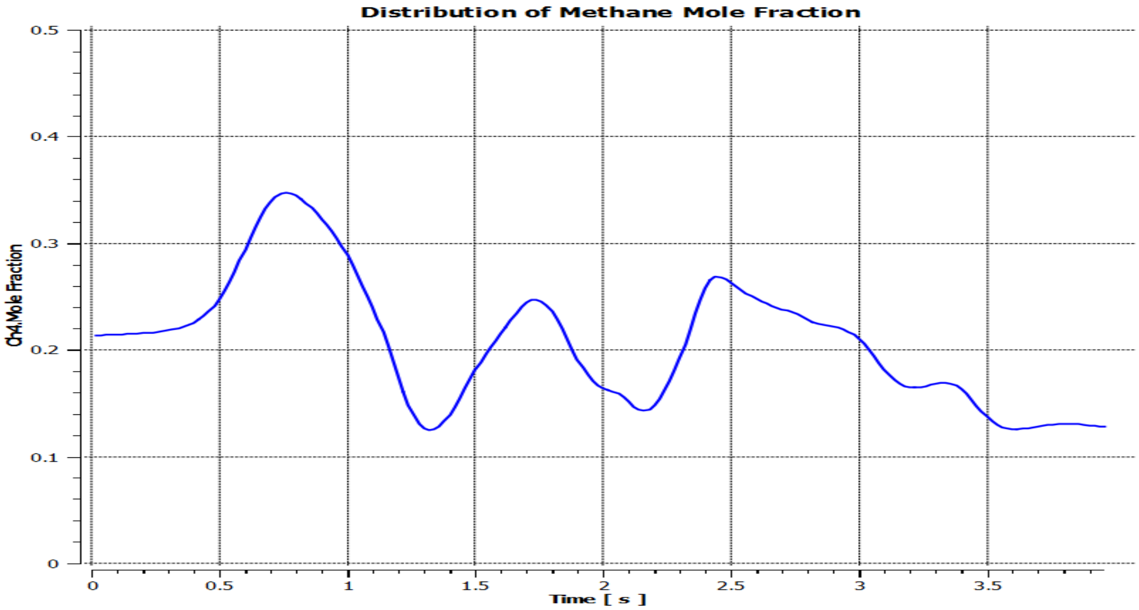


FIGURE 4.14 Distribution of methane mole fraction

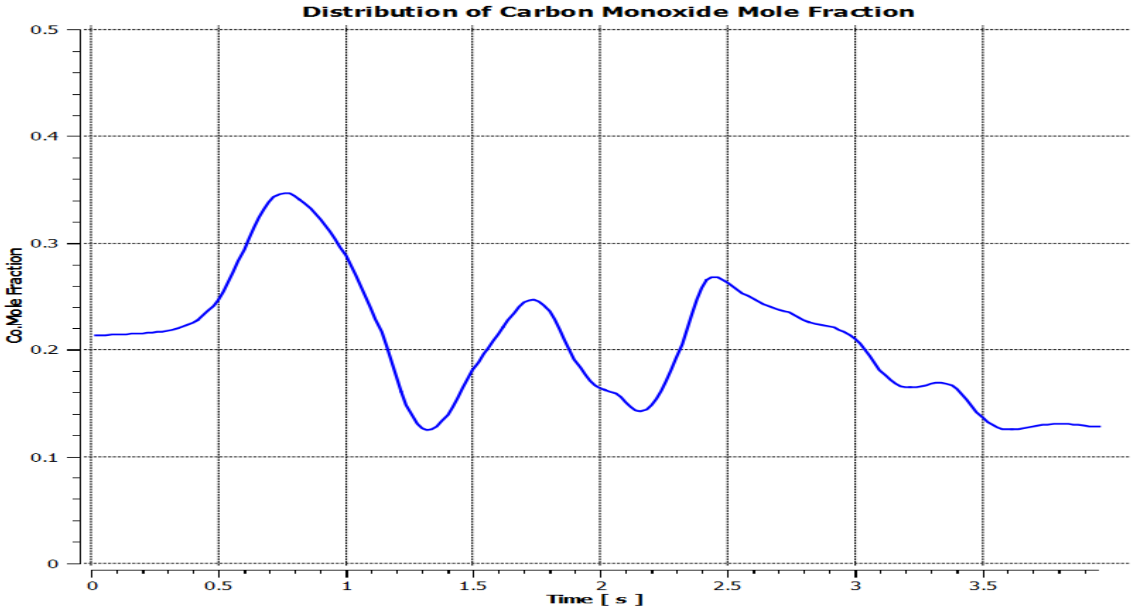


FIGURE 4.15 Distribution of carbon monoxide mole fraction

4.2 Mixture of heavy fuel gases only

It is observed that for the mixture of heavy fuel gases disperse in the air at a slower pace. The heavy fuel gases is let to disperse in air and it is not much of the difference comparing to the initial contour at t = 0s. This is caused by the higher density ratio between air and the fuel gases. Fuel gases such as ethane, propane and butane had a higher density compare to air. They did not reached to the top of the cylinder after the convergence.

4.2.1 Mixture of Butane & Propane

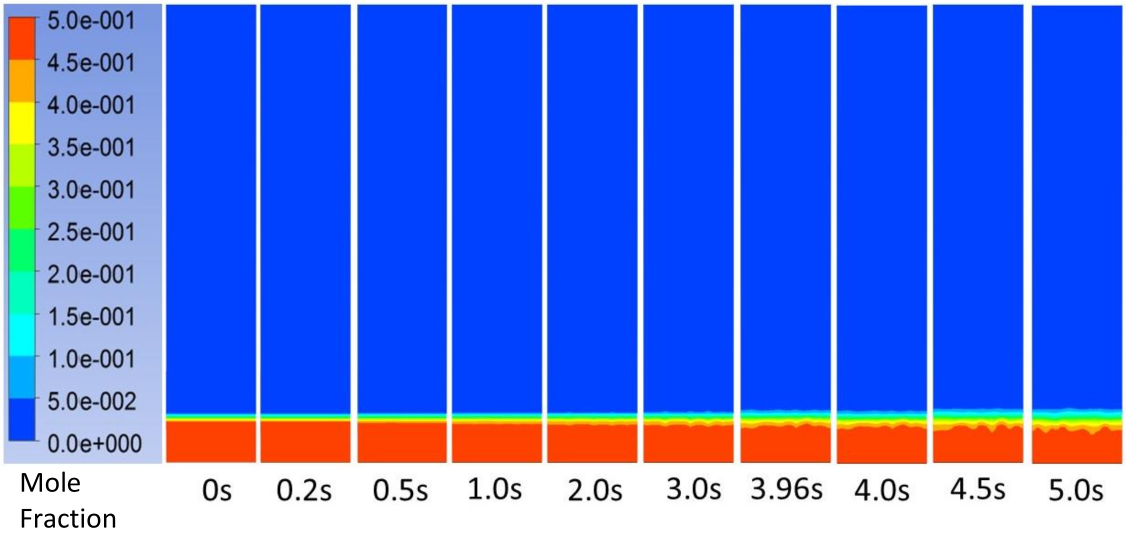
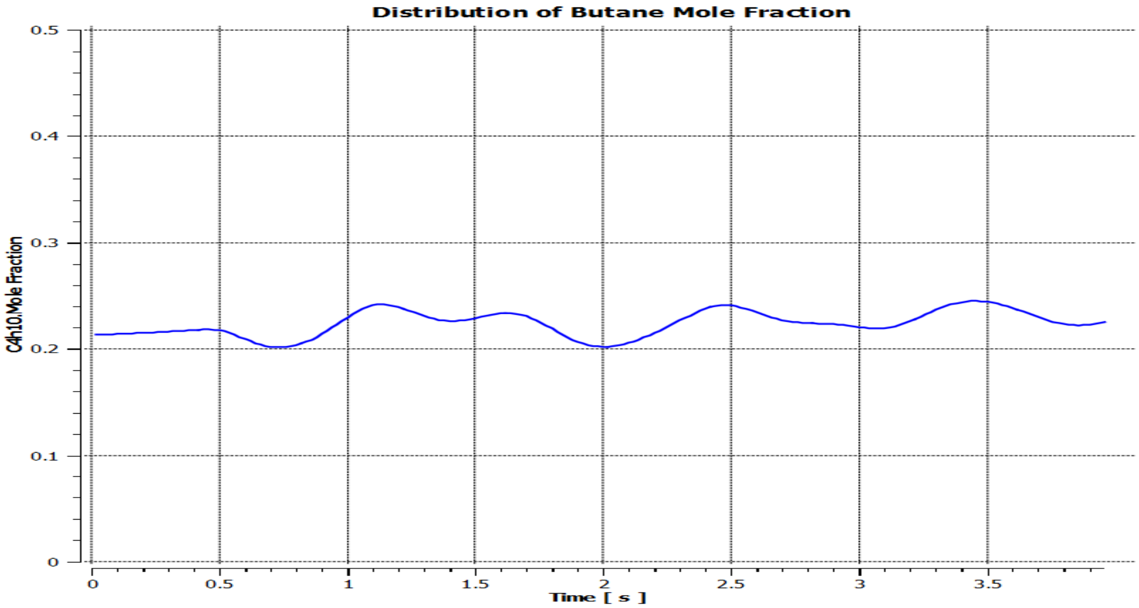
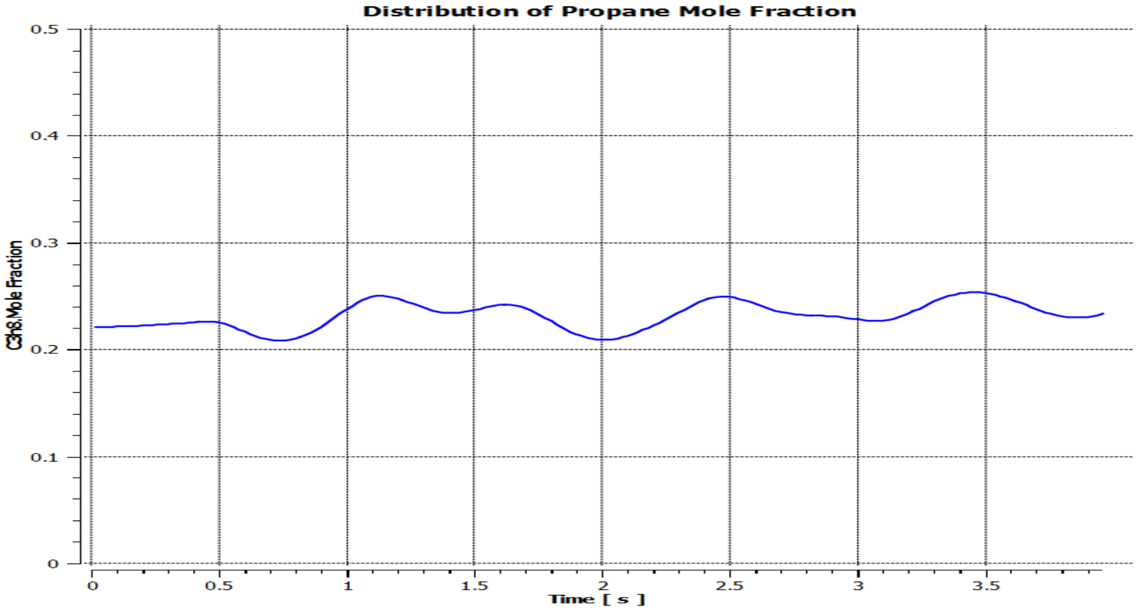


FIGURE 4.16 Mole Fraction of Butane & Propane

The slowest dispersion can been seen from the combination of butane and propane as in Figure 4.15. The combination of butane and propane had the highest density among all the simulations. At time = 4.0 second, the mixture started to disperse. But at the end of the simulation, it only disperse a little into the region. If the simulation is done prompting the fuel gas at the top of the cylinder, the buoyancy force will actually help to diffuse into the air region even better.



. FIGURE 4.17 Distribution of butane mole fraction



. FIGURE 4.18 Distribution of propane mole fraction

Figure 4.16 and Figure 4.17 shows the distribution of butane and propane mole fraction for mixture of butane and propane. It didn't defer much from the initial value as the dispersion of butane and propane is very slow.

4.2.2 Mixture of Ethane & Propane

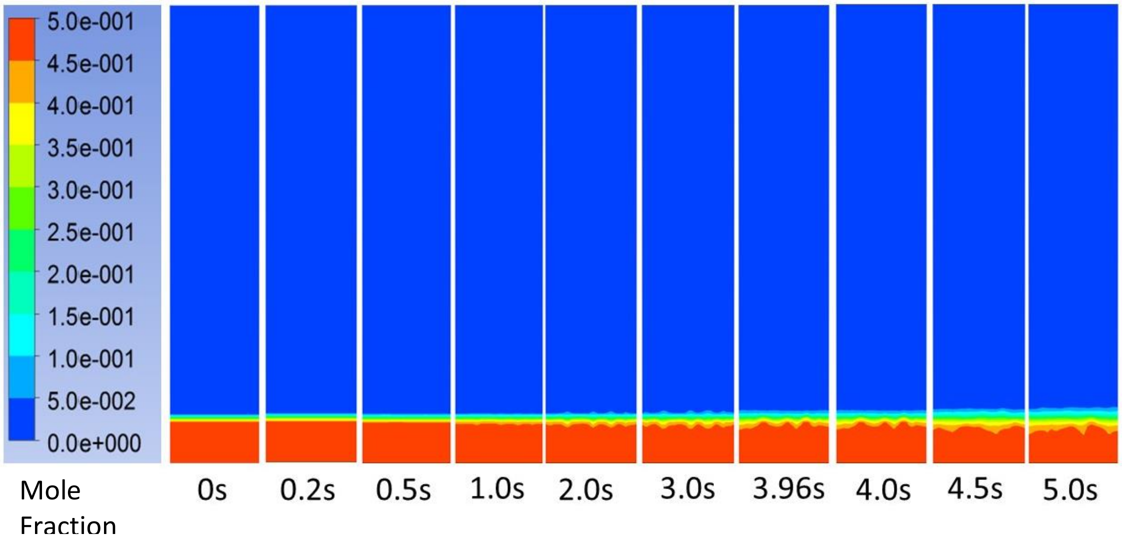


FIGURE 4.19 Mole Fraction of Ethane & Propane

Comparing the contour with the mixture of propane and butane, the combination of ethane and propane diffuse faster. This is due to the density for mixture butane and propane is higher than ethane and propane. At a time of 3.0 second, it started to disperse, but it disperse at a very slow rate. It will not reach the top even the simulation done it more than 10 seconds.

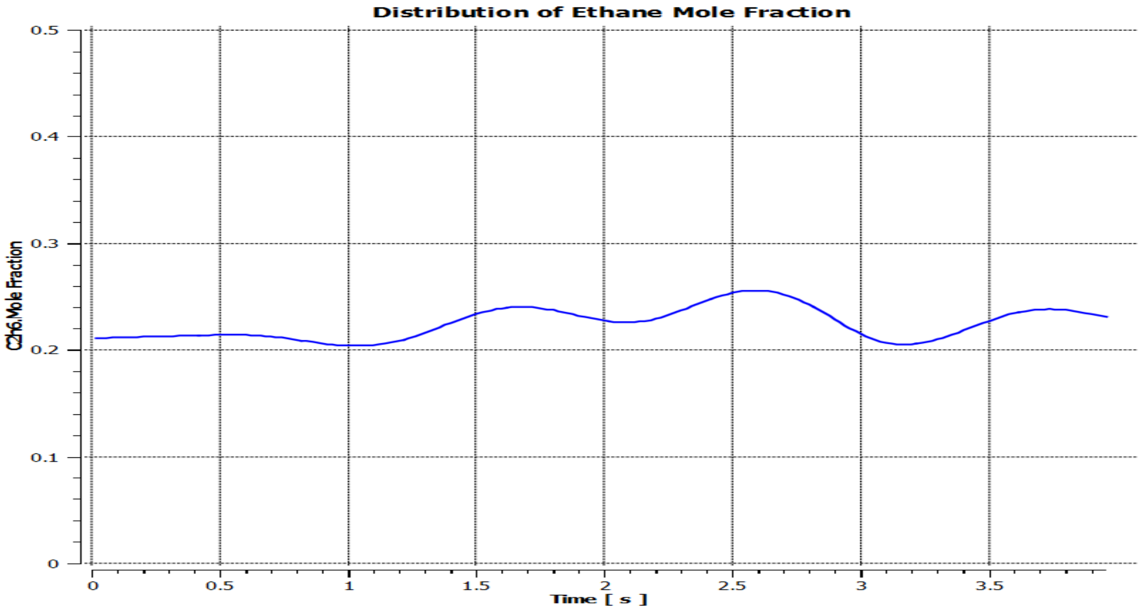


FIGURE 4.20 Distribution of ethane mole fraction

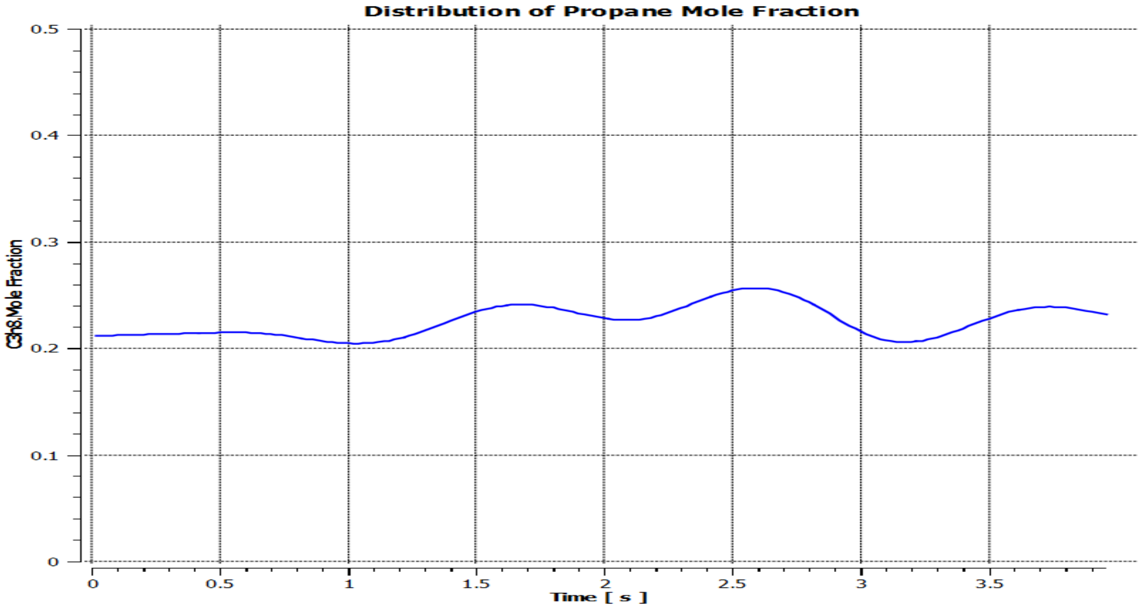


FIGURE 4.21 Distribution of propane mole fraction

Figure 4.19 and Figure 4.20 shows the distribution of ethane and propane mole fraction for mixture of ethane and propane. The pattern of the graph is alike as the mixture of butane and propane. This is because the dispersion of ethane and propane in mixing with air is very slow. At the point of (0, 0.1, 0), the mole fraction of ethane and propane does not differentiate much from the initial value.

4.2.3 Mixture of Ethane & Butane

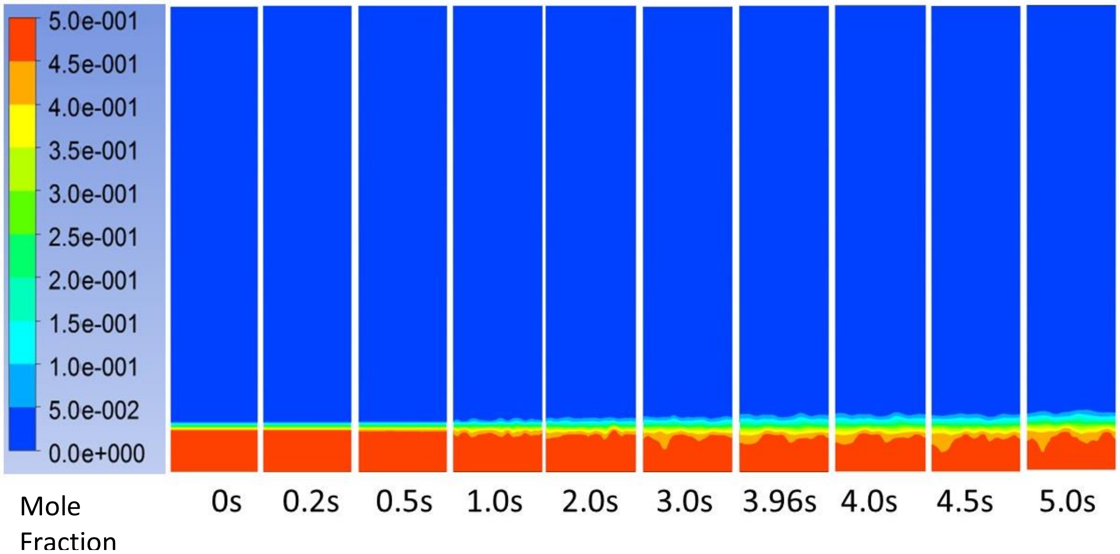


FIGURE 4.22 Mole Fraction of Ethane & Butane

Comparing the contour for mixture of ethane and propane, the mixture of ethane and butane disperse faster into the air region. This is due to the density for mixture ethane and propane is higher than ethane and butane. At a time of 2.0 second, it started to disperse, but it disperse at a very slow rate.

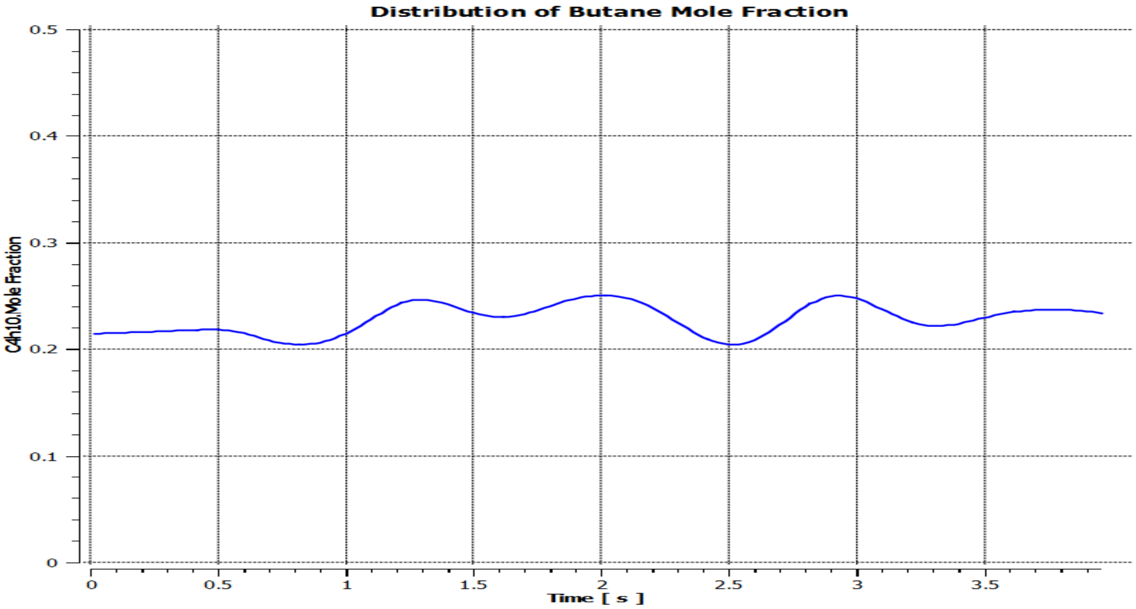


FIGURE 4.23 Distribution of butane mole fraction

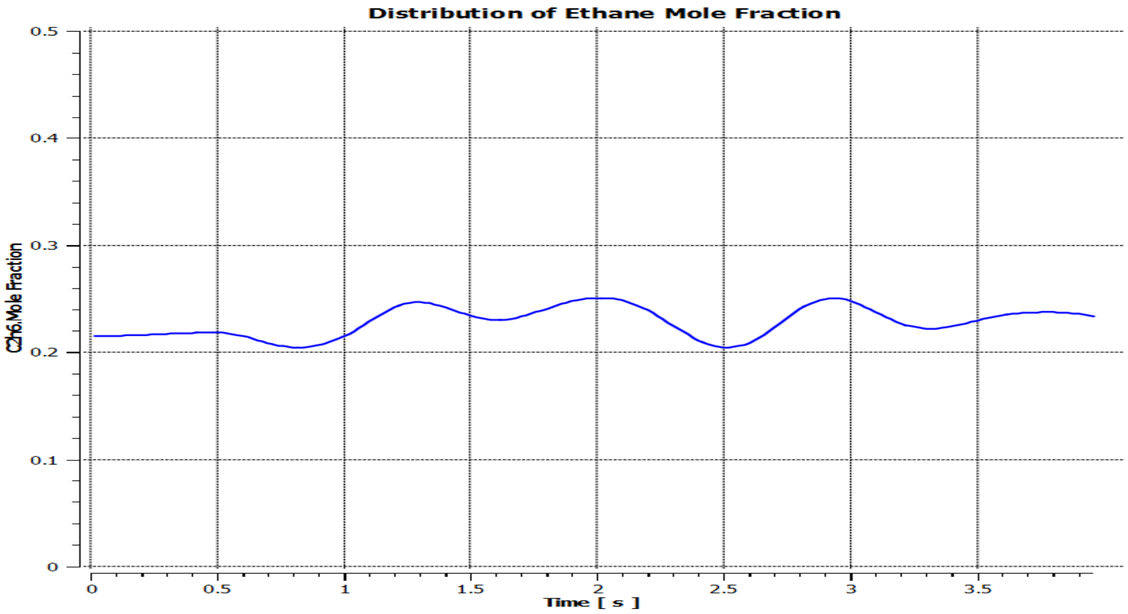


FIGURE 4.24 Distribution of ethane mole fraction

The distribution of the mole fraction for butane and ethane in mixture of butane and ethane shows similar pattern with the mixture for butane and propane. It does not differ much even the iteration of simulation had finished.

4.3 Mixture of heavy & light fuel gas

It is observed that for the mixture of heavy gas and light gas disperse in the air at a higher pace. Despite there is a heavy gas in the cylinder, the light gas will disperse very quickly into the air region in the cylinder. It will reach the top of the cylinder as fast as the mixture of light gases.

4.3.1 Mixture of Hydrogen & Ethane

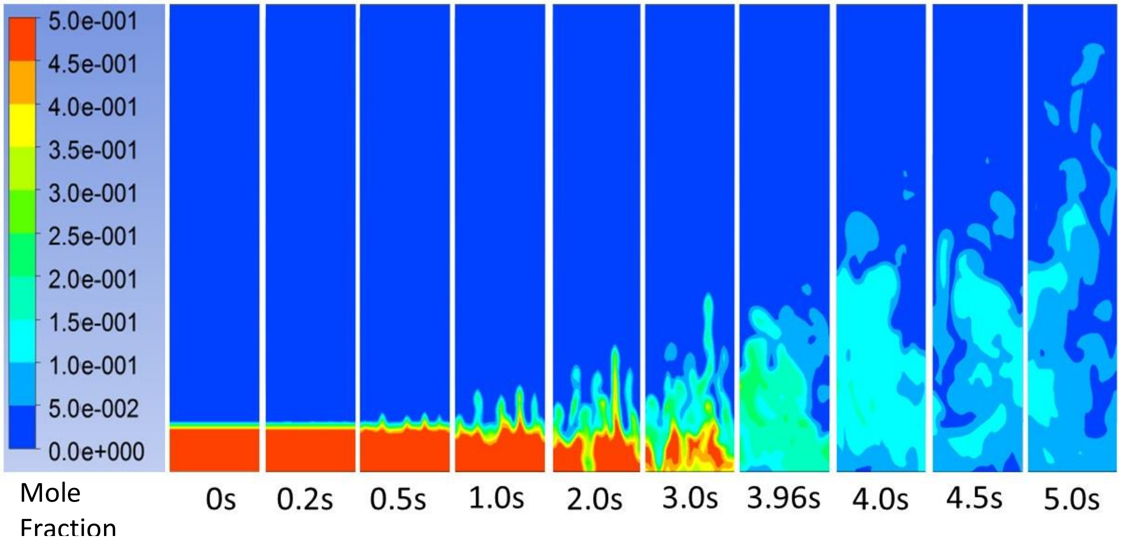


FIGURE 4.25 Mole Fraction of Hydrogen & Ethane

Even though the heavy gas which is the ethane is mixing with the light fuel gas hydrogen and prompt at the bottom of the cylinder. The hydrogen will tend to disperse out into the air region at a very fast rate. At the time of 1.0 second, it actually started to disperse into the air region. The dispersion is almost as fast as the mixture of light fuel gases only. At the time of 5.0 seconds, it almost reached the top of the cylinder.

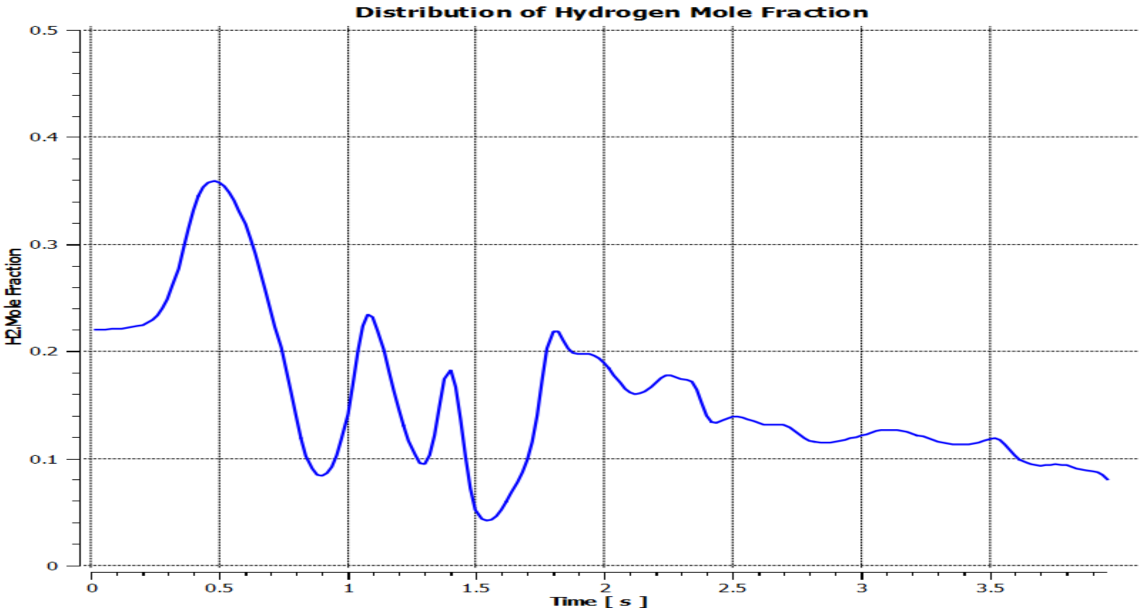


FIGURE 4.26 Distribution of hydrogen mole fraction

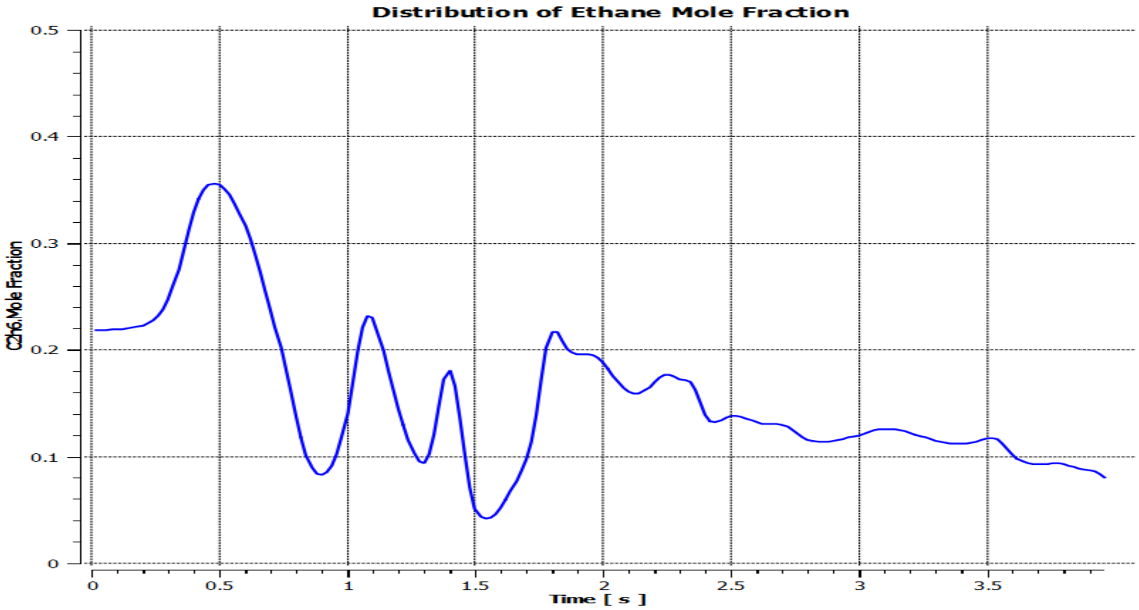


FIGURE 4.27 Distribution of ethane mole fraction

Figure 4.24 and Figure 4.25 shows the distribution of hydrogen and ethane mole fraction for mixture of hydrogen and ethane. The pattern of the graph is alike as the mixture of light gas only. This is because the dispersion of hydrogen in mixing with air is very fast.

4.3.2 Mixture of Hydrogen & Propane

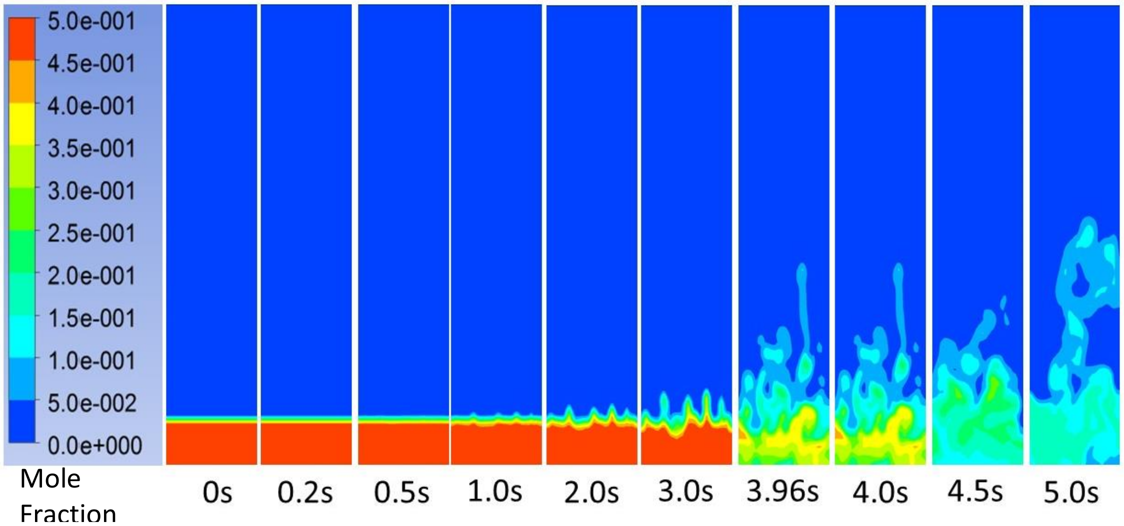


FIGURE 4.28 Mole Fraction of Hydrogen & Propane

At the time = 1.0 second, it started to disperse into the air region. The mixture of hydrogen and propane disperse slowly as compare to mixture of hydrogen and ethane as the density of propane is higher than ethane. It would eventually reach to the top of the cylinder is the simulation is done with more iterations.

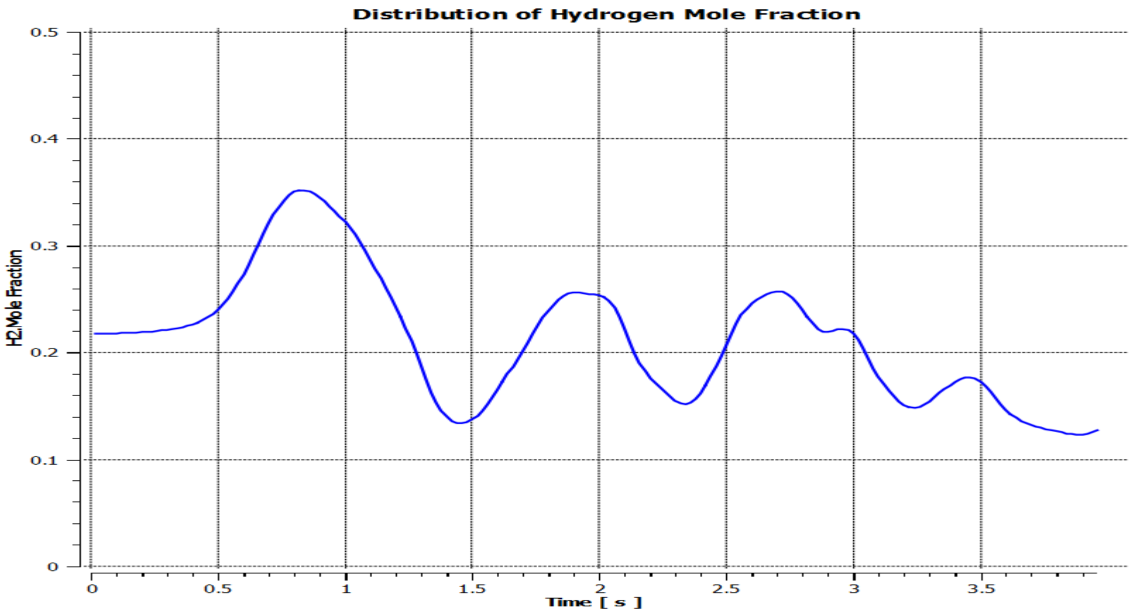


FIGURE 4.29 Distribution of hydrogen mole fraction

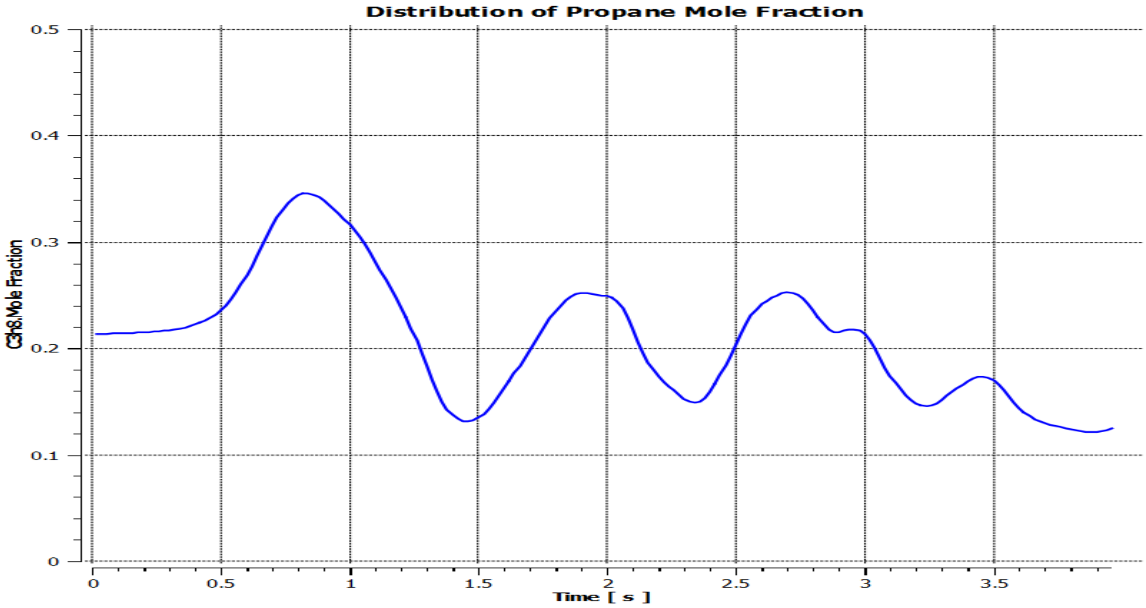


FIGURE 4.30 Distribution of propane mole fraction

Figure 4.27 and Figure 4.28 shows the distribution of hydrogen and propane mole fraction for mixture of hydrogen and propane. The mole fraction will increases at the point of (0, 0.1, 0) from 0. Mole fraction to the peak which is 0.34 mole fraction. After that it will start to decrease in mole fraction.

4.3.3 Mixture of Methane & Ethane

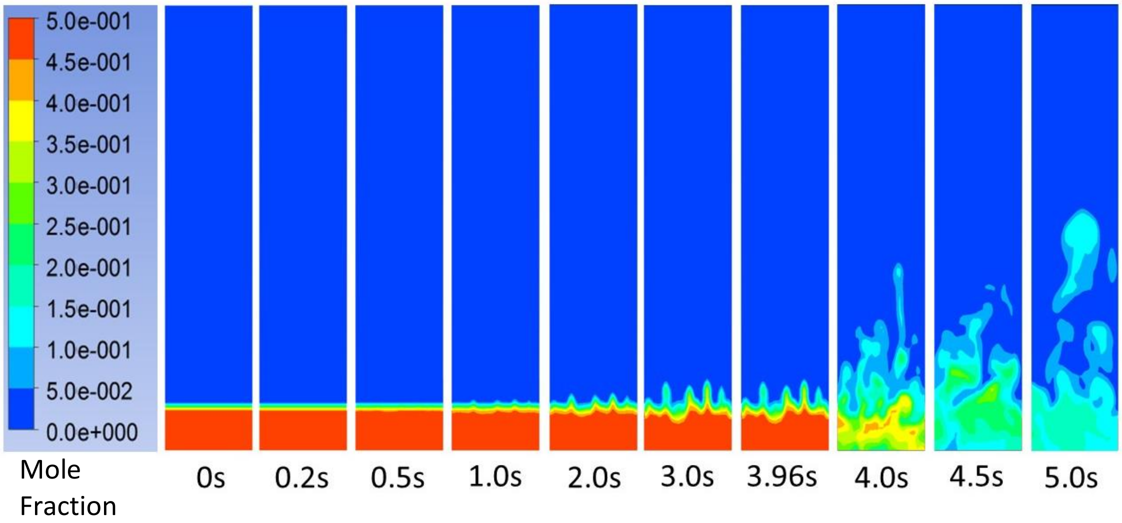


FIGURE 4.31 Mole Fraction of Methane & Ethane

For this contour, the mixture of methane and ethane started disperse at time = 2.0 seconds. After that, at the time of 4.0 seconds, it actually reaches almost half of the cylinder. If the simulation proceed to more than 10 seconds, it would reach the top of the cylinder.

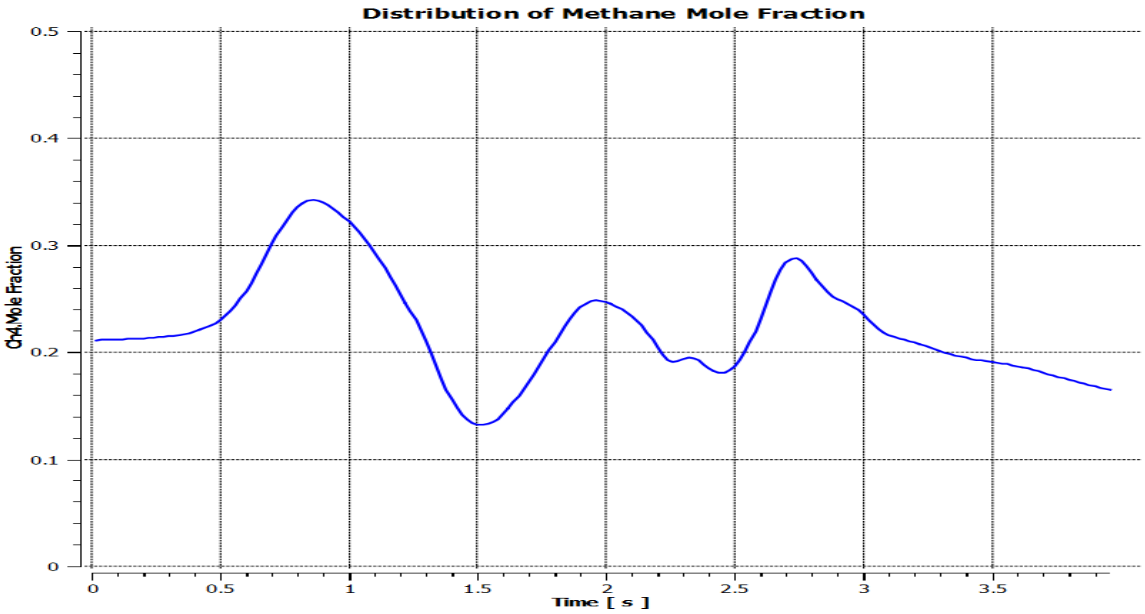


FIGURE 4.32 Distribution of methane mole fraction

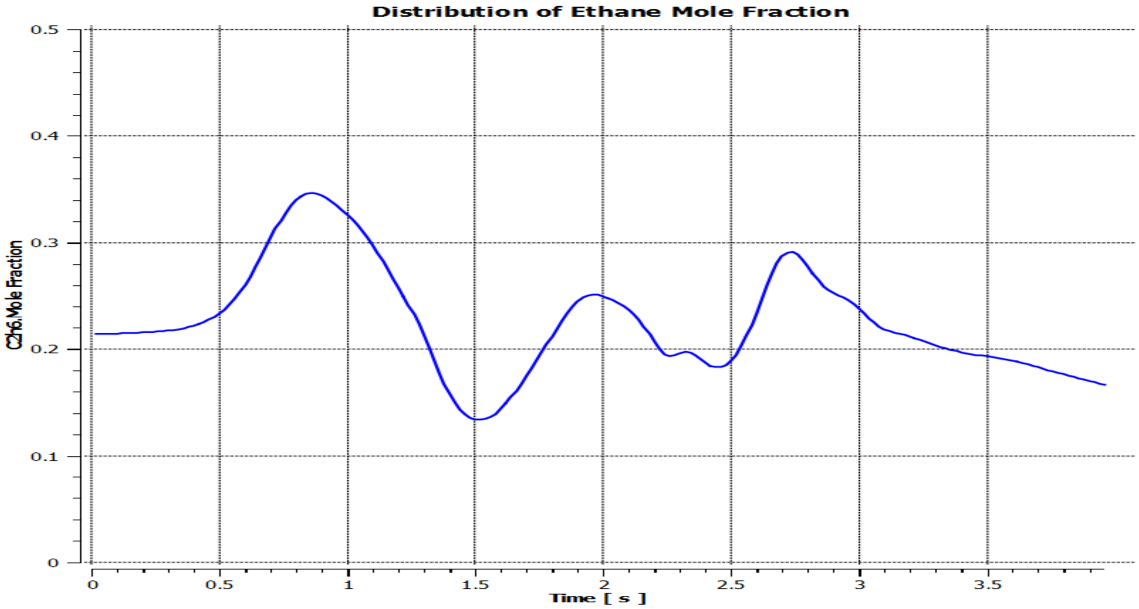


FIGURE 4.33 Distribution of ethane mole fraction

Figure 4.30 and Figure 4.31 shows the distribution of methane and ethane mole fraction for mixture of methane and ethane. The mole fraction will start to increase from 0s to 0.8s to reach the peak and it will start to decrease until 1.5s and it will increase again.

CHAPTER 5

CONCLUSION

As a conclusion, this project will be using Computational Fluid Dynamics to carry out the understanding and study of behavior of the binary mixture of the fuel gases. Simulation had been done by senior's project with just only one fuel gases is set at the bottom of the cylinder at a time. Fuel gases that consists of hydrogen, methane, ethane, propane, butane, acetylene and carbon monoxide. The 10% fuel gases had put it at stationary at t=0 and it will let to disperse into 90% of air inside the cylinder. The cylinder is 1 meter tall and 0.25 meter in diameter. The dispersion of fuel gases is conduct in enclosed cylinder. Simulations of transient fuel gases mixing in air are studied. The findings is important towards the development of safety and mitigation guidelines. The dispersion behavior is affected by the density of the fuel gases. Hydrogen and methane disperse very quickly in air in a short amount of time. It is very dangerous towards the industries that are operating with hydrogen and methane. Light fuel gases such as hydrogen, methane, acetylene and carbon monoxide tend to disperse very quickly in air. The fastest combination of all simulation is the mixture of hydrogen and methane. As the simulation started, it started to disperse in to the air and it reaches the top at fast rate of 3.96 seconds. Heavy fuel gases such as ethane, propane and butane had a low mixing behavior and does not reach the top of the cylinder even the simulation ends. This is because of the higher density of fuel gases comparing with air.

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