MATHEMATICAL MODELING ON THE EFFECT OF EQUIVALENCE RATIO IN EMISSION CHARACTERISTICS OF SPARK IGNITION ENGINE WITH HYDROGEN PEROXIDE ADDITION

DZAHIRUL AIMI BIN JAMIL

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

MATHEMATICAL MODELING ON THE EFFECT OF EQUIVALENCE RATIO IN EMISSION CHARACTERISTICS OF SPARK IGNITION ENGINE WITH HYDROGEN PEROXIDE ADDITION

DZAHIRUL AIMI BIN JAMIL

A report submitted
in fulfillment of the requirements for the degree of
Bachelor of Mechanical Engineering

Faculty of Mechanical Engineering

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

2022

DECLARATION

I declare that this project entitled "Mathematical Modeling on The Effect of Equivalence Ratio in Emission Characteristics of Spark Ignition Engine with Hydrogen Peroxide Addition" is the result of my own work except as cited in the references.

Signature : …………………………………..

Name : …………………………………..

Date : …………………………………..

APPROVAL

I hereby declare that I have read this project report and in my opinion this report is sufficient in terms of scope and quality for the award of the degree of Bachelor of Mechanical Engineering.

Signature : …………………………………..

Supervisor's Name : …………………………………..

Date : …………………………………..

ABSTRACT

The project of “Mathematical Modeling on the Effect of Equivalence Ratio on Emission Characteristics of Spark Ignition Engine with Hydrogen peroxide Addition” aims to investigate the effect of equivalence ratio on the emission characteristics of combustion product of a spark ignition engine. The fuel used is gasoline and it is mixed with hydrogen peroxide. Hydrogen peroxide acts as an oxidizing agent that helps to reduce the emission of harmful and toxic combustion products. Mathematical modelling is used to calculate the mole fraction for each combustion products and graphs on the effect of equivalence ratio to the emission characteristics will be generate. MATLAB simulation programme will be used to obtain the data.

ABSTRAK

Projek "Pemodelan Matematik terhadap Kesan Nisbah Kesetaraan terhadap Ciri-ciri Pelepasan Enjin Pencucuhan Percikan dengan Penambahan Hidrogen peroksida" bertujuan untuk menyiasat kesan nisbah kesetaraan ke atas ciri-ciri pelepasan hasil pembakaran enjin pencucuh percikan. Bahan api yang digunakan ialah gasolin dan ia dicampur dengan hidrogen peroksida. Hidrogen peroksida bertindak sebagai agen pengoksidaan yang membantu mengurangkan pelepasan produk pembakaran yang berbahaya dan toksik. Pemodelan matematik digunakan untuk mengira pecahan mol bagi setiap hasil pembakaran dan graf tentang kesan nisbah kesetaraan kepada ciri-ciri pelepasan yang akan dijana. Program simulasi MATLAB akan digunakan untuk mendapatkan data.

ACKNOWLEDGEMENT

First and foremost, I would like to take this opportunity to express my gratitude toward my supervisor, Dr. Adnan bin Roseli from the Faculty of Mechanical Engineering in Universiti Teknikal Malaysia Melaka (UTeM) for the guidance given in order for me to complete the project with the best outcome. All of the information, assistance and instructions given to me is used as best as I can to achieve my objective.

Besides, for my parents Mr. Jamil bin Ibrahim and Mrs. Aida binti Mawi, I would like to thank you for all of the motivations, support, and always being behind me supporting for what I has been dreaming for that is to become a successful person that can make both of my parents proud.

I will not forget all of my friends, lecturers and other people that always been helping me intentionally or unintentionally to complete the project and also the Degree. Thank you for believing me and supporting me through thick or thin. I will remember all the good deeds and I hope that I can return it back to them to as a token of my gratitude.

TABLE OF CONTENTS

PAGE

LIST OF TABLES

LIST OF FIGURES

LIST OF APPENDICES

LIST OF ABBREVITIONS

COx	-	Carbon Oxide
NOx	-	Nitrogen Oxide
COPD	-	Chronic Obstructive Pulmonary Disease
H_2O_2	-	Hydrogen Peroxide
SI	-	Spark Ignition
CI	-	Compressed Ignition
LNG	-	Liquid Natural Gas
RFG	-	Reformulated Gasoline
HC	-	Hydrocarbon
UHC	-	Unburned Hydrocarbon
CO_2	-	Carbon Dioxide
H_2O	-	Water (Hydrogen Dioxide)
N_2	-	Nitrogen gas
O_2	-	Oxygen gas
CO	-	Carbon Monoxide
H_2	-	Hydrogen gas
H	-	Hydrogen atom
O	-	Oxygen atom
OH	-	Hydroxide
NO	-	Nitrogen Oxide

CHAPTER 1

INTRODUCTION

1.1 Background

The world now lives in fear because of the pollution created by human themselves. This created problems that causing not only human, but all living things such as the animals, plants, and microorganism are affected by it. Various pollution exists but in the field of road transport, air pollution is the one that created the most problems. Common spark ignition engines produced toxic products such as Carbon Oxide (COx), Nitrogen Oxide (NOx), soot, and particulate matters and released it to the environment through the exhaust (Muhammad Saad Khan et al., 2009). The pollutant combined with the existing air composed of oxygen, hydrogen and other particle and created harmful gaseous that potentially enter the respiratory system of humans and animal and causing various type of diseases such as lung cancer, chronic obstructive pulmonary disease (COPD) and asthma (Jiang et al., 2016).

The higher the pollution level, the chances of getting sick by the polluted air is increased. For example, in Bandar Tun Razak, Kuala Lumpur, an experiment is conducted to study the average concentration of air pollutants recorded for a period of 2010-2014 because the city is congested with moving vehicles. From that long period of time, the result showed that amount of COx and NOx does not have the potential to decline. This means the probability of people getting sick due to the polluted air keep increasing and do not have an end to it. Numerous people will get sick if this problem still continues and it can also threaten the ecosystem. (Tajudin et al., 2019)

To solve the problems, engineers all around the globe try to undergo continuous changes and improvements to reduce the pollutants emitted by the vehicles. One of the ideas is by adding fuel additive to the existing fuel to create a safer product of combustion released by the engine. This brilliant idea does not focus only on the emission products but also the effect of the fuel additive to the fuel itself. Engineers wanted the fuel additive to give a boost to the fuel so it can burn efficiently without wasting any component. Hydrogen is one of the most suitable agents for the job. It is renewable, highly efficient, clean fuel, fast burning speed, high diffusion coefficient, wide firing range and low ignition energy that can bring a lot of advantages to the diesel-type engine. The same result also applied to hydrogen peroxide(H_2O_2) that it also gives the equal advantages just like the hydrogen. It also stated that hydrogen peroxide has led to a better combustion(Adnan et al., 2018). But not all vehicle using the same diesel-fuel type engine. Some other vehicle uses gasoline as it fuels and they give out the same problem just like the diesel-type vehicles, that is they emitted harmful gaseous to the atmosphere. Fortunately, hydrogen peroxide also works well as a fuel additive to the gasoline. With the help of hydrogen peroxide, the spark-ignition engine can work at its best and perform better compared to the engine when gasoline only is being used. The engine's peak pressure, thermal efficiency, indicated power and heat release rate showed that the engine give the best result when hydrogen peroxide is added into the fuel. (Adlan et al., 2018)

1.2 Problem Statement

When dealing with spark-ignition engine, it is not only about the power it gives to the vehicles, but also the product of the combustion that is released into the environment. This problem occurs because the transportation industry is getting bigger day by day and the numbers of vehicles on the road increases dramatically. Although at first the emission of toxic gaseous from the fossil fuel combustion such as NOx, COx and soot does not do much effect to the ecosystem, but eventually it will cause a lot of problems if it is not overcome immediately. Our respiratory system will face a great threat if air pollutants had entered the body through the respiratory organ. Studies have validated the relationship between traffic air pollution and chronic obstructive pulmonary disease. It has been shown that the damaged respiratory system is as dangerous as damages caused by ingestion of toxic chemicals(El Morabet, 2019). Researchers are trying to come out with the solution to improve the combustion products so the concentration of toxic components in combustion products will be lowered.(Adlan et al., 2018)

Studies had been made but the most of it is about compression ignition engine with injection of hydrogen peroxide. Only a few studies that are about spark ignition engine since it is not as hype as its brother. Although the fuel being used is different where compressed ignition engine uses diesel fuel while spark ignition engine uses gasoline for combustion, there is minor differences in term of combustion product as both fuels shares the same source of origin. Diesel powered vehicles have more torque while gasoline powered vehicles are suitable for city driving. With the help of hydrogen peroxide, each fuel improves the combustion process as stated that hydrogen-fuelled engine potentially create a low emission (Lee, 2001).

Studies has been made to proof the capability of hydrogen peroxide as a fuel additive practically but theoretically it has not yet been proven. Mathematical model can be used as the evidence to strengthen the researchers' studies of the hydrogen peroxide as fuel additives. The mathematical model can calculate the mole fraction for the emission products and from the simulation, we can see the effect of adding hydrogen peroxide on the emission of combustion products (Yusof et al., 2015).

1.3 Objective

The objectives of this project are as follows:

1. To construct a mathematical model to obtain mole fraction of each combustion products for spark ignition engine with hydrogen peroxide addition.
2. To study the effect of equivalence ratio to the mole fraction of the emission products.

1.4 Scope of The Project

The scope of the project that will be discussed are:

1. This project has been specific to the use of hydrogen peroxide as fuel additive that is used in spark-ignition engine.
2. This project is only required to obtain mole fraction for the combustion products of hydrogen peroxide mixed with gasoline.
3. All the calculation can be calculated manually by using every possible step that is needed in certain formula used to solve the equations.
4. MATLAB program can be used to solve all the calculation and graphs can be obtained from it that may help in the project purpose.

1.5 General Methodology

For the project, several methods will be used to achieve the objectives in this project and are listed below:

1. Literature review

   Journals, articles, or any suitable materials will be used as the guideline and references in order to complete the project. Most of the sources are related to the title of the project.

2. Calculation

   Method of calculation such as Newton Raphson method is conducted to obtain the mole fraction of the components of the combustion products of the project.

3. Simulation

   Computational simulation is generated to obtain the values of the combustion product will be made based on the calculation.

4. Report writing

   At the end of the study, a full complete report will be written

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction to Spark Ignition engine with Hydrogen peroxide Addition

New era of technologies is now focusing more on inventing various types of products that will create a better earth for the people. The sustainability of the earth can be well preserved if all products are created eco-friendly. From power generation, power consumption, and daily essential products should be used without giving harmful side effects to the environment. Countries such as India and United States of America have invested in the usage of geothermal energy resources from existing thermal spring of which there are found a lot in their country instead on generating power using old-fashioned way that is by using fossil fuels. This alternative way is very worthwhile as India is currently standing among top five countries whose uses maximum energy that is expected to increase by three times by 2023 (Kumar et al., 2019). Automobile industry has also created an alternative way to reduce the emission of harmful gaseous to the surrounding. Both spark-ignition (SI) engine and compressed-ignition (CI) engine has been releasing various hazardous gaseous since day one of the engines' usage until today that resulting in the thinning of the ozone layer and global warming. Greenhouse gases, carbon oxides, nitrogen oxides and other harmful gaseous are the reason of the problem. In China, the transport pollution has becoming a major threat to the air quality of the country and the problem may becoming even worse as the increase of ownership of personal vehicles (HE & QIU, 2016). More vehicles on the road will emit more amount of toxic emission to the environment and this will not only be affecting China but the whole world will also receive the effects of global warming.

So, renewable fuels such as bioethanol or biodiesel are produced to remove the side effect that has been the major problems to the existing fuels. Bioethanol is proven to reduce the emission of carbon dioxide of a compressed-ignition engine, giving the automobile industry a better hope in reducing air pollution. (Damyanov & Hofmann, 2019). However, the existing hydrocarbon fuels such as gasoline and diesel are still being used worldwide and there is no stopping sign on the usage of these fuels. Since the introduction of the biofuels to the automobile industry are still new, the popularity is still superiorly far compared with the existing hydrocarbon fuels. While the hydrocarbon fuels economy steadily increased and becoming one of the sources of national income, biofuels is known only by certain people. Thus, for now this is not the best answer to the global warming problems.

Another possible solution that might be as efficient as the usage of biofuels is by creating an eco-friendly combustion product for both CI engines and SI engines from existing fuels. This can be achieved by adding fuel additive to the existing fuel to create a new combustion product that will reduce or even better fully eliminate the emission of harmful gaseous to the environment. Hydrogen peroxide is one of the fuel additives that can be use besides formaldehyde (CH_2O) that can relate to the improvement of the autoignition (Manias et al., 2016). (Adnan et al., 2018) stated that gasoline with hydrogen peroxide addition perform better compared to gasoline alone. Better combustion is the result of mixed solution, creating an effective spark-ignition engine. With the mixed solution of gasoline and hydrogen peroxide with the suitable ratio of 95% of gasoline and 5% of hydrogen peroxide has created the best outcome in term of fuel consumption, indicated power, and heat release rate.

2.2 Hydrogen Peroxide

Hydrogen peroxide is not a natural source of energy that can be found inside the crust of the earth just like other minerals. it cannot be easily explored just by drilling into its core and treated to obtain the hydrogen peroxide. Hydrogen peroxide is first discovered by Alexander von Humbolt in his attempt to decompose air, but the compound is introduced to the world by Louis Jacques Thenard in 1818. Improved version of Thenard's hydrogen peroxide is created by the reaction of barium peroxide and nitric acid. with the reaction, hydrogen peroxide has been used commercially since 1880. With the help of modern technologies that are electrochemical processes and organic autoxidation process, the production of hydrogen peroxide is now simple and cost friendly. Hydrogen peroxide is widely used as an oxidizing agent, antimicrobial and chemical application in municipal wastewater and treatment plants. Although this liquid is widely used by everybody, but the odourless and colourless liquid is actually harmful to human body. (Abdollahi & Hosseini, 2014). Safety measures must be practiced, to prevent damages to the body. In automobile industry, today's research is mainly focusing on creating best result for the fuels emission products. When hydrogen peroxide is introduced, the research conducted found that the compound can improve the emission of combustion products for both CI and SI engines. With better efficiency while using the best mixed air/fuel ratio, vehicle usage is at their best ability (Francqueville et al., 2014).

2.2.1 Structural Formula

Hydrogen peroxide is famous for and its odourless and colourless liquid, but its true colour is light pale blue. Due to the very light visible colour that is hard to see with a normal naked eye, it is stated as colourless liquid. Hydrogen peroxide or also known as albone, dihydrogen dioxide, and perone is a chemical compound that consist of two elements that is hydrogen and oxygen. Each hydrogen atom is connected to the oxygen atom while the remaining oxygen bond are paired with each other(Abdollahi & Hosseini, 2014).

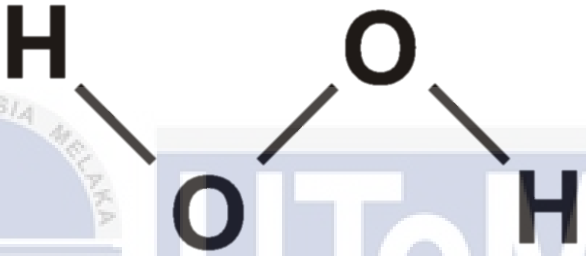


Figure 2.1: Hydrogen Peroxide Structural formula

2.2.2 Physical Properties

Table 2.1 shows the comparison of physical properties between hydrogen peroxide and water. Since water is the common liquid known by all, comparison made between the two compounds are relevant for the better understanding. The table shows that H_2O_2 is more viscous compared to water at both 0 ^{o} C and 20 ^{o} C (Oor et al., 2000). These physical properties of hydrogen peroxide helped in the reducing the emission of soot when it is injected into the combustion chamber of a diesel-powered engine (Born & Peters, 1998).

Table 2.1: Physical properties of hydrogen peroxide and water

Physical properties	Value	
	H_2O_2	H_2O
Melting point ^oC	-0.43	0
Boiling point (101.3 kPa) ^oC	150.2	100
Heat of fusion, J/g	368	334
Heat of vaporization, J/gK		
At 25 ^oC	1519	2443
At *bp*	1387	2258
Relative density, g/cm^3		
0 ^oC	1.4700	0.9998
20 ^oC	1.4500	0.9980
25 ^oC	1.4425	0.9971
Viscosity, mPa·s		
0 ^oC	1.819	1.792
20 ^oC	1.249	1.002
Critical temperature, ^oC	457	374.2
Critical pressure, MPa	20.99	21.44
Refractive index n_D^{20}	1.4084	1.3330

2.2.3 Chemical Properties

Dissociation

With a dissociation constant of 1.78×10^{-12} (pK 11.75) ant 20 ^{o}C, hydrogen peroxide is a weak acid if it is in an aqueous solution state. When it is put together with various type of metal, the solution will form salts due to its weak acid properties.

Oxidation and Reduction

Hydrogen peroxide also works as both oxidizing and reducing agent based on the way it is used.

Substitution

Hydrogen atoms in the chemical compound can be substitute with elements such as alkyl and acyl group, leading to the formation of compounds such as alkyl hydroperoxide (H-O-O-R) and diacyl peroxide (Ac-O-O-Ac).

2.3 Gasoline

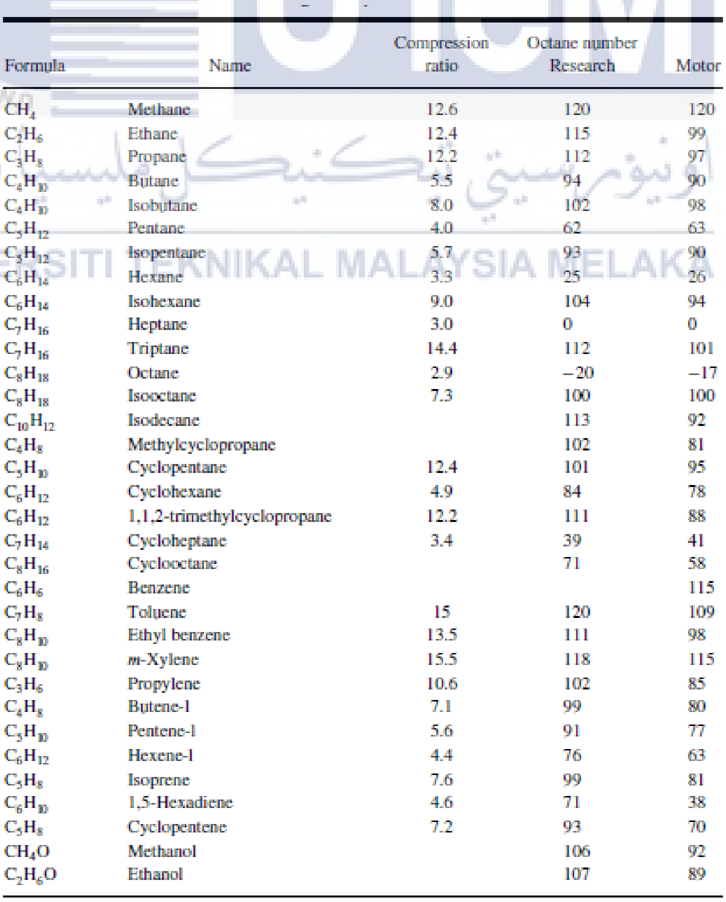
Fuels made from petroleum has been used for over a century ago and it still going on strong until now. Various type of transportation still loves to use the petroleum-based fuels and it covers all type of vehicles including the airplane, enormously massive cargo ship and a four-wheel drive. Since there are various types of transportation available, each of the transport requires different kind of fuel combustion for their engine to achieve the vehicle's full potential (Srivastava, S.P., Hancsok, 2014). Therefore, many types of fuels created in order to fulfil the needs of different types of engines. For aviation industry, the type of fuel used is liquid jet fuel (kerosene), which is more focusing on the high energy contents per unit volume. This is to gain as much energy produced by the fuels to move the turbines while at the same time does not taking a lot of space that created extra weight to the aircraft that can reduce its efficiency. Kerosene type fuel is a carefully refined, light petroleum, suited for the aircraft (Liu et al., 2013). While maritime industry recorded the increase of number of ships that uses liquid natural gas (LNG) as their fuels. LNG is a fuel that can significantly reduce the emission of SOx, NOx, and black carbon that are among the type of gaseous emitted from a ship's combustion process. This criterion made it the favourite choice for the ship fuels compared to conventional oil(Xu & Yang, 2020). For land transport, diesel is widely used for compression-ignition engine and it is designed for creating more torque for the vehicle to obtain more power and grip while gasoline is usually for spark-ignition engine is made for city driving or high acceleration involved vehicle (Lee, 2001). Although there are many options for fuels out there, engines technologist tends to focus on creating improvement or inventing a new powerful engine that uses gasoline or diesel. The technologies revolved around those two fuels compared to other available fuels(Srivastava, S.P., Hancsok, 2014). So, gasoline development is still a hot topic of conversation to design a world that is free from pollution since its users are abundance on the globe.

Gasoline or also known as petrol, is a mixture of a liquid hydrocarbon that is used as a fuel in a spark-ignition internal combustion. It is one of the fractions from crude oil and other petroleum liquids that is created via fractional distillation. Gasoline is preferred for the automobile fuel compared to kerosene because of its high energy combustion and capacity to be mixed with air in a carburettor. Nowadays, gasoline quality is improved by methods such as polymerization, alkylation, isomerization, and reforming (Encyclopedia, 2021).

2.3.1 Structural Formula

Gasoline is actually a mixture of different compounds that is called hydrocarbons. The hydrocarbon that exists in gasoline mixture varies in term of carbon number between 4 and 12. There is no exact structural formula for gasoline because its composition is depending on the crude oils used, overall balance of product demand, refinery processes available, and product specification. The structural formula typically used to characterize gasoline is C_8H_{15}, but (Ferguson & Kirkpatrick, 2016) stated that the chemical formula for gasoline that is commonly used as engine fuel is C_7H_{17}. Table 2.2 shows the single-component hydrocarbons that exist in a gasoline mixture.

Table 2.2: Knock Characteristics of Single-Component Fuels



Formula	Name	Compression ratio	Octane number Research	Motor
CH_4	Methane	12.6	120	120
C_2H_6	Ethane	12.4	115	99
C_3H_8	Propane	12.2	112	97
C_4H_{10}	Butane	5.5	94	90
C_4H_{10}	Isobutane	8.0	102	98
C_5H_{12}	Pentane	4.0	62	63
C_5H_{12}	Isopentane	5.7	93	90
C_6H_{14}	Hexane	3.3	25	26
C_6H_{14}	Isohexane	9.0	104	94
C_7H_{16}	Heptane	3.0	0	0
C_7H_{16}	Triptane	14.4	112	101
C_8H_{18}	Octane	2.9	−20	−17
C_8H_{18}	Isooctane	7.3	100	100
$C_{10}H_{12}$	Isodecane		113	92
C_4H_8	Methylcyclopropane		102	81
C_5H_{10}	Cyclopentane	12.4	101	95
C_6H_{12}	Cyclohexane	4.9	84	78
C_6H_{12}	1,1,2-trimethylcyclopropane	12.2	111	88
C_7H_{14}	Cycloheptane	3.4	39	41
C_8H_{16}	Cyclooctane		71	58
C_6H_6	Benzene			115
C_7H_8	Toluene	15	120	109
C_8H_{10}	Ethyl benzene	13.5	111	98
C_8H_{10}	*m*-Xylene	15.5	118	115
C_3H_6	Propylene	10.6	102	85
C_4H_8	Butene-1	7.1	99	80
C_5H_{10}	Pentene-1	5.6	91	77
C_6H_{12}	Hexene-1	4.4	76	63
C_5H_8	Isoprene	7.6	99	81
C_6H_{10}	1,5-Hexadiene	4.6	71	38
C_5H_8	Cyclopentene	7.2	93	70
CH_4O	Methanol		106	92
C_2H_6O	Ethanol		107	89

2.3.2. Properties of Gasoline

Since gasoline available in various type, properties of each gasoline may be varying due to the difference in the composition. Table 2.3 shows the comparison of properties between various gasolines and their properties are compared to each other. The gasoline listed for table 3 are industry average gasoline, gasoline oxygenated with ethanol (gasohol), phase 1 reformulated gasoline (RFG), and Phase 2 reformulated gasoline (RFG).

Table 2.3: Properties of Gasoline Fuels

	Industry average gasoline	Gasohol	Phase 1 RFG	Phase 2 RFG
Aromatic, vol%	28.6	23.9	23.4	25.4
Olefins, vol%	10.8	8.7	8.2	4.1
Benzene, vol%	1.60	1.6	1.3	0.93
Reid vapor pressure, kPa (S-summer W-winter)	60-S 79-W	67-S 79-W	50-S 79-W	46
T_{50}, K	370	367	367	367
T_{90}, K	440	431	431	418
Sulphur, mass ppm	338	305	302	31
Ethanol, vol%	0	10	4	0

2.4 Effect of Hydrogen Peroxide Addition into Hydrocarbon Fuels

Various research has been made to investigate the effect on adding hydrogen peroxide with hydrocarbon fuels for both spark ignition engine (SI) and compressed ignition engine (CI). Both engines use hydrocarbon fuels to run the engine, but the only differences are the chemical composition of the fuels. SI engines uses hydrocarbon fuels that has carbon range from 4 to 12 while diesel engine uses hydrocarbon fuel that has a carbon number between 12 to 20 (Ferguson & Kirkpatrick, 2016). The most popular hydrocarbon fuel for SI engine is gasoline while for CI engine is diesel. Since the automobile industry is focusing more on the development of those two types of engines, researchers try to improve the quality of combustion product since the use of it creating problems to the earth, that is air pollution. Combustion product for both engines is dangerous and possibly creating more harmful effect on the creatures of the earth. It is stated that transportation is reason of emission of 63% of CO, 34% of HC, and 38% of NO in the United States of America. While in European region, transportation industry is also responsible for the emission of 50%-70% of NO to the surrounding(Chaichan, 2015).

In order to save the earth from harmful gases emitted by the vehicles, fuel additives can be used. Fuels additives are obtained from non-petroleum resources that help to reduce the emission of toxic gaseous thus causing less pollution and most of them are renewable with low on cost production (Pourkhesalian et al., 2010). There are a lot of fuel additives that has been developed in order to create a better performance of fuel in the SI engine that improve in term of reduction of harmful gases, increase rate of fuel combustion, and knocking. Not all fuel additives can solve all of the existing problems that is faced especially by SI engine users but at least it can reduce some of the problems faced as not all of the problem occurred at the same period of time. So, different fuel additives such as ethanol, methanol, isopropyl alcohol, and hydrogen might give different result to the engine.

Hydrogen peroxide is one of the most known fuel additives that is used to improve the performance of the engine. Both SI engine and CI engine shows great result when hydrogen peroxide is mixed with fuels. When hydrogen peroxide is injected into the combustion chamber of a diesel engine, it can reduce the production of soot dramatically (Born & Peters, 1998). When n-butanol is used as a fuel for CI engine and hydrogen peroxide acts as fuel additive, it will be resulted in the low emission of NOx, a good sign for the environment (Zhou et al., 2019). For SI engine, with the addition of hydrogen peroxide into the petrol, (Adlan et al., 2018) had proven that the mixture of petrol and hydrogen peroxide produced better performance compared to petrol alone. The experiments are focusing on the chemical properties and the performance of the engine and graph was made based on the experimental result. Results showed that better performance when 10% of hydrogen peroxide mixed with petrol compared to petrol alone. Another experiment also carried out studying on the performance of SI engine when hydrogen peroxide is used as fuel additive when intake air temperature is the responding variable. From (Adnan et al., 2018) experimental result, the same output is given that is gasoline alone consume fuels more than mixed fuel with 5% hydrogen peroxide and 10% hydrogen peroxide at 3500 rpm and 60°C . once again, mixed gasoline and hydrogen peroxide beat gasoline fuel alone. With the use of fuel additive such as hydrogen peroxide, SI engine performance is lifted higher than before.

2.5 Air/Fuel Equivalence Ratio, ϕ

Equivalence ratio, ϕ is referring to the ratio between the fuel and air that is needed for the combustion process. There are three possible ratios that exist. First one is when $\phi < 1$, the combustion is considered lean. Lean combustion occurs when the value of fuel is lesser than the air. This will be resulted in the excess air in the combustion chamber during combustion. During this state, unburned hydrocarbon (UHC) will be emitted to the atmosphere, contamination of the soil and underground water will happen. Hydrocarbon that will be emitted are including methane, ethane, ethylene, acetylene, propylene and much more (Guo et al., 2018). Second case of air/fuel ratio is when the fuel is more than the air during the combustion. When $\phi > 1$, rich combustion will occur. Soot will be formed when rich combustion is occurred. Last case is when $\phi = 1$. This combustion process is called stoichiometric air fuel ratio when fuel and air are the same amount in the combustion chamber. This will create enough combustion process and all components will be fully used. Stoichiometric combustion emits mostly CO_2 and H_2O, non-toxic combustion product that is produce from complete combustion.

CHAPTER 3

METHODOLOGY

3.1 Introduction

This chapter will explain about the methodology used in order to find the mole fraction for each of the combustion product based on the given variables of a spark-ignition engine with hydrogen peroxide addition. For the combustion of fuel with hydrogen peroxide addition, fuel chosen is gasoline with structural formula of C_7H_{17}. There are 10 combustion product that was assumed and a total system of 11 nonlinear equation resulted from the derivation of the reaction combustion equation will be solved. By using Newton-Raphson methods, the 11 nonlinear equations can be solved. This report will explain the method of Newton-Raphson that will be used, and its solution will be explained in detail. Important values that will be used for simulation program will also listed and explained.

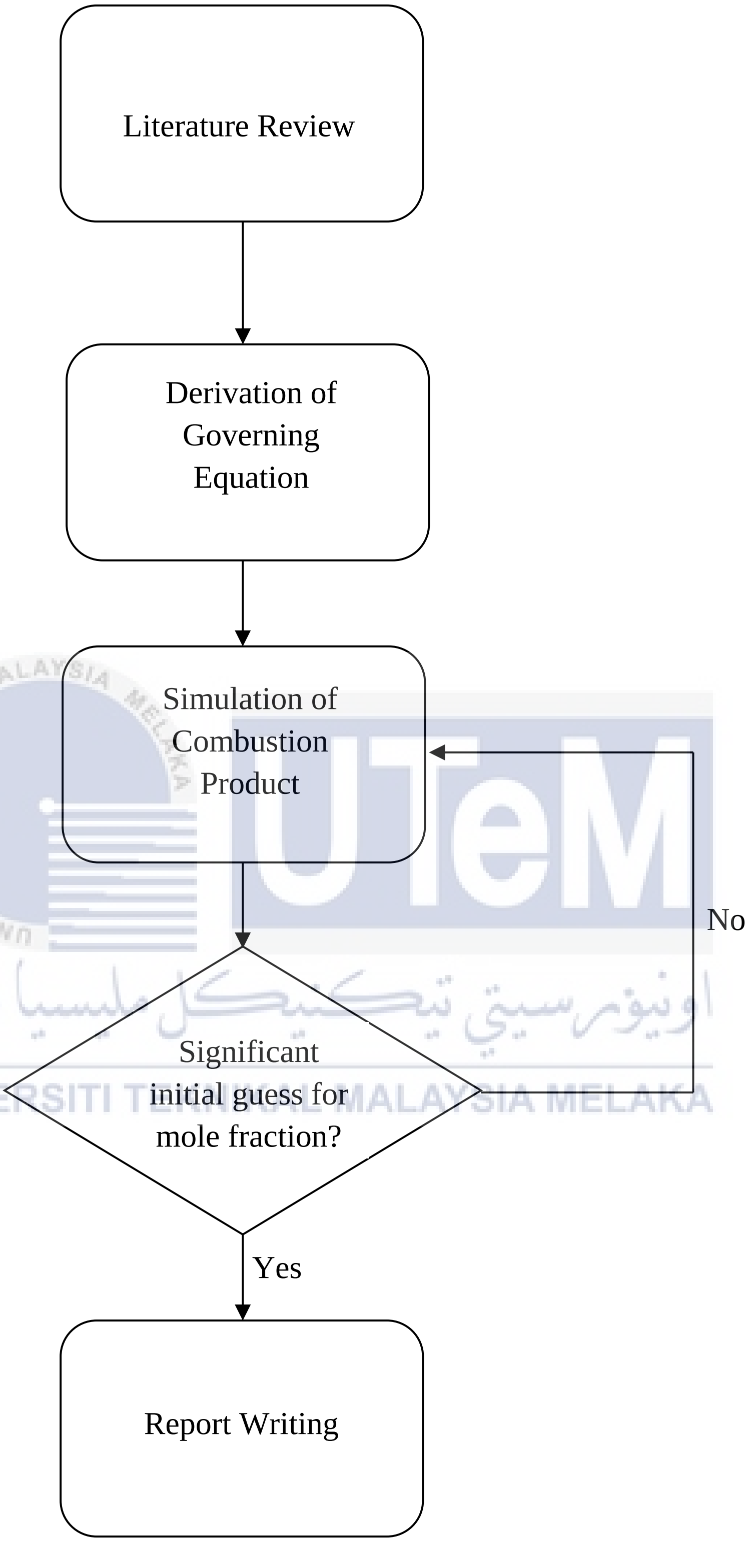


Figure 3.1: Flow chart of the methodology

3.2 Combustion Modelling Approach

In this project, it is mainly about the effect of equivalence ratio in emission characteristics of spark ignition engine with hydrogen peroxide addition. In order to obtain the result, combustion products of hydrogen peroxide addition with fuel will be assumed and total of 10 combustion products will be used. A system of 11 nonlinear equation will be obtained from the derivation of the governing equation. Mole fractions from the combustion product for fuel with hydrogen peroxide addition will be calculated using Newton-Raphson method and then the input will be key-in into MATLAB software to be run to validate the values obtained.

3.2.1. Governing Equations

Combustion products of hydrocarbon fuels varies depending on the temperature. There are two type of combustion that is lean combustion($\phi < 1$) and rich combustion($\phi > 1$) widely used and served different purpose (Schultze & Mantzaras, 2013). Lean combustion has excess air in the combustion chamber after the combustion process while rich combustion is vice versa. For SI engine, the product of combustion at temperature(T) below 1000K is CO_2, H_2O, N_2, and O_2 for lean combustion while CO_2, H_2O, N_2, CO, and H_2 for rich combustion at the same temperature(Adnan et al., 2011). For this project, 10 combustion products will be assumed as the result of combustion process of hydrogen peroxide addition mixed with gasoline in SI engine. The chemical reaction is written as below:

$$C_\alpha H_\beta + H_2O_2 + \left(\frac{a_s}{\phi}\right)(O_2 + 3.76N_2) \rightarrow (y_1CO_2 + y_2H_2O + y_3N_2 + y_4O_2 + y_5CO$$

$$+y_6H_2 + y_7H + y_8O + y_9OH + y_{10}NO)N \qquad (1)$$

For gasoline fuel used in this project the subscripts α and β are 7 and 17, respectively. Meanwhile the stoichiometric molar air-fuel ratio, a_s is written as below:

$$a_s = \alpha + \frac{\beta}{4} - \frac{\gamma}{2} \quad (1)$$

To find the value of mole fraction, y_i (i = 1,2, 3,…,10) of the combustion emission product and total number of moles, N in Eq. 1, the following condition can be applied:

I. The equilibrium of the concentration conditions. The summation of the mole fraction, y_i must be equal to unity so that this condition is correct. Concentration condition can be written as shown below:

$$\sum_{i=1}^{10} y_i = 1 \quad (2.1)$$

$$y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7 + y_8 + y_9 + y_{10} = 1 \quad (3.2)$$

II. Number of atoms must be balance on both side of Eq. (1). From this condition, four equations can be obtain as shown below:

Atom C: $$\alpha = (y_1 + y_5)N \quad (4.1)$$

Atom H: $$\beta = (2y_2 + 2y_6 + y_7 + y_9)N \quad (4.2)$$

Atom O: $$\gamma + \frac{2a_s}{\phi} = (2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10})N \quad (4.3)$$

Atom N: $$\delta + \frac{7.52a_s}{\phi} = (2y_3 + y_{10})N \tag{4.4}$$

III. Chemical equilibrium equation related to equilibrium constant K. six equation can be obtain from this condition as shown below:

$$\tfrac{1}{2}H_2 \rightleftharpoons H, \qquad K_1 = \frac{y_7\, p^{\frac{1}{2}}}{y_6^{\frac{1}{2}}} \tag{5.1}$$

$$\tfrac{1}{2}O_2 \rightleftharpoons O, \qquad K_2 = \frac{y_8\, p^{\frac{1}{2}}}{y_4^{\frac{1}{2}}} \tag{3.2}$$

$$\frac{1}{2}H_2 + \frac{1}{2}O_2 \rightleftharpoons OH, \qquad K_3 = \frac{y_9}{y_4^{\frac{1}{2}}\, y_6^{\frac{1}{2}}} \tag{5.3}$$

$$\frac{1}{2}O_2 + \frac{1}{2}N_2 \rightleftharpoons NO, \qquad K_4 = \frac{y_{10}}{y_4^{\frac{1}{2}}\, y_3^{\frac{1}{2}}} \tag{5.4}$$

$$H_2 + \frac{1}{2}O_2 \rightleftharpoons H_2O, \qquad K_5 = \frac{y_2}{y_4^{\frac{1}{2}} y_6\, p^{\frac{1}{2}}} \tag{5.5}$$

$$CO + \tfrac{1}{2}O_2 \rightleftharpoons CO_2, \qquad K_6 = \frac{y_1}{y_5\, y_4^{\frac{1}{2}}\, p^{\frac{1}{2}}} \tag{5.6}$$

The pressure mentioned in Eq. (5.1) until Eq. (5.6) are measured in atm. Value of equilibrium constant, K from the polynomial equation must be calculated. JANAF table has been created based on the curve-fit coefficient of equilibrium constants K_i(T) (Olikara & Borman, 1975). Table data are for temperature range from 600K to 4000K. The expression of K_i(T) can be express as shown below:

$$log_{10}K_i(T) = A_i\, ln\left(\frac{T}{1000}\right) + \frac{B_i}{T} + C_i + D_iT + E_iT^2 \qquad (4)$$

Then, to obtain the equation of mole number in term of y_3, y_4, y_5, and y_6 which are the mole fraction to combustion product species of N_2, O_2, CO and H_2, Eq (5.1) to (5.6) can be rearranged as written below:

$$y_7 = c_1\, y_6^{\frac{1}{2}} \qquad (7.1)$$

$$y_8 = c_2\, y_4^{\frac{1}{2}} \qquad (7.2)$$

$$y_9 = c_3\, y_4^{\frac{1}{2}}\, y_6^{\frac{1}{2}} \qquad (7.3)$$

$$y_{10} = c_4\, y_4^{\frac{1}{2}}\, y_3^{\frac{1}{2}} \qquad (7.4)$$

$$y_1 = c_5\, y_4^{\frac{1}{2}}\, y_5 \qquad (7.5)$$

$$y_2 = c_6\, y_4^{\frac{1}{2}}\, y_6 \qquad (7.6)$$

Where,

$$c_1 = \frac{K_1}{p^{\frac{1}{2}}} \tag{8.1}$$

$$c_2 = \frac{K_2}{p^{\frac{1}{2}}} \tag{8.2}$$

$$c_3 = K_3 \tag{8.3}$$

$$c_4 = K_4 \tag{8.4}$$

$$c_5 = K_5\, p^{\frac{1}{2}} \tag{8.5}$$

$$c_6 = K_6\, p^{\frac{1}{2}} \tag{8.6}$$

Total number of moles, *N* can be eliminated by dividing each Eq. (4.2). (4.3) and (4.4) with Eq. (4.1). With elimination method, numbers of unknown now reduced from 11 to 10. The result will be:

$$2y_2 + 2y_6 + y_7 + y_9 + \frac{\beta}{\alpha}y_1 - \frac{\beta}{\alpha}y_5 = 0 \tag{9.1}$$

$$\begin{aligned} 2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10} - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right)y_1 \\ - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right)y_5 = 0 \end{aligned} \tag{9.2}$$

$$2y_3 + y_{10} - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right) y_1 - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right) y_5 = 0 \tag{9.3}$$

Then, substitute Eq. (7.1) until Eq. (7.6) into Eq. (9.1), (9.2), (9.3) and Eq. (3.2). the equations are now in term of four unknown that is y_3, y_4, y_5, and y_6. Since there are four unknowns left, the equations seem like a nonlinear equation. Nonlinear equation can be solved by using Newton-Raphson iteration method. (Adnan et al., 2011), (Schultze & Mantzaras, 2013), (Ferguson & Kirkpatrick, 2016), and (Kayadelen & Ust, 2013) use this method in order to solve multiple nonlinear equation exist in their calculations. The nonlinear equation will be expressed as written below:

$$2\left(c_6\ y_4^{\frac{1}{2}}\, y_6\right) + 2y_6 + \left(c_1\, y_6^{\frac{1}{2}}\right) + \left(c_3\, y_4^{\frac{1}{2}}\, y_6^{\frac{1}{2}}\right) + \frac{\beta}{\alpha}\left(c_5\ y_4^{\frac{1}{2}}\, y_5\right) - \frac{\beta}{\alpha} y_5 = 0 \tag{10.1}$$

$$\begin{gathered} 2\left(c_5\ y_4^{\frac{1}{2}}\, y_5\right) + \left(c_6\ y_4^{\frac{1}{2}}\, y_6\right) + 2y_4 + y_5 + \left(c_2\, y_4^{\frac{1}{2}}\right) + \left(c_3\, y_4^{\frac{1}{2}}\, y_6^{\frac{1}{2}}\right) \\ + \left(c_4\ y_4^{\frac{1}{2}}\, y_3^{\frac{1}{2}}\right) - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right)\left(c_5\ y_4^{\frac{1}{2}}\, y_5\right) \\ - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right) y_5 = 0 \end{gathered} \tag{10.2}$$

$$2y_3 + \left(c_4\ y_4^{\frac{1}{2}}\, y_3^{\frac{1}{2}}\right) - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right)\left(c_5\ y_4^{\frac{1}{2}}\, y_5\right) - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right) y_5 = 0 \tag{10.3}$$

$$\begin{gathered} \left(c_5\ y_4^{\frac{1}{2}}\, y_5\right) + \left(c_6\ y_4^{\frac{1}{2}}\, y_6\right) + y_3 + y_4 + y_5 + y_6 + \left(c_1\, y_6^{\frac{1}{2}}\right) + \left(c_2\, y_4^{\frac{1}{2}}\right) + \\ \left(c_3\, y_4^{\frac{1}{2}}\, y_6^{\frac{1}{2}}\right) + \left(c_4\ y_4^{\frac{1}{2}}\, y_3^{\frac{1}{2}}\right) - 1 = 0 \end{gathered} \tag{10.4}$$

3.3. Newton-Raphson Iteration Method

Newton-Raphson iteration method is used to solve four nonlinear equation that exist in this project. This method can be used to find mole fraction of the combustion products. The nonlinear equation is as shown below:

$$\begin{aligned} f_1(y_3, y_4, y_5, y_6) &= 0 \\ f_2(y_3, y_4, y_5, y_6) &= 0 \\ f_3(y_3, y_4, y_5, y_6) &= 0 \\ f_4(y_3, y_4, y_5, y_6) &= 0 \end{aligned} \tag{11}$$

The system can also be expressed in a compact vector form as ***F(y)*=0**, where:

$$y = [y_1, y_2, y_3, y_4] \tag{12.1}$$

$$F(y) = \begin{bmatrix} f_1(y) \\ f_2(y) \\ f_3(y) \\ f_4(y) \end{bmatrix} \tag{12.2}$$

$$0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{12.3}$$

To solve nonlinear equations by using Newton-Raphson Method, evaluation of Jacobian Matrix is required. Jacobian Matrix is defined as:

$$\boldsymbol{J} = \frac{\partial(f_1, f_2, f_3, f_4)}{\partial(y_3, y_4, y_5, y_6)} = \begin{bmatrix} \frac{\partial f_1}{\partial y_3} & \frac{\partial f_1}{\partial y_4} & \frac{\partial f_1}{\partial y_5} & \frac{\partial f_1}{\partial y_6} \\ \frac{\partial f_2}{\partial y_3} & \frac{\partial f_2}{\partial y_4} & \frac{\partial f_2}{\partial y_5} & \frac{\partial f_2}{\partial y_6} \\ \frac{\partial f_3}{\partial y_3} & \frac{\partial f_3}{\partial y_4} & \frac{\partial f_3}{\partial y_5} & \frac{\partial f_3}{\partial y_6} \\ \frac{\partial f_4}{\partial y_3} & \frac{\partial f_4}{\partial y_4} & \frac{\partial f_4}{\partial y_5} & \frac{\partial f_4}{\partial y_6} \end{bmatrix} \tag{13}$$

By using Eq. (11), elements for the Jacobian Matrix, ***J*** for the combustion reaction equations that has been derived previously are as shown below:

$$J(1,3) = \frac{\partial f_1}{\partial y_3} = 0 \tag{14.1}$$

$$J(1,4) = \frac{\partial f_1}{\partial y_4} = 2\left(\frac{c_6 y_6}{2y_4^{\frac{1}{2}}}\right) + \left(\frac{c_3 y_6^{\frac{1}{2}}}{2y_4^{\frac{1}{2}}}\right) + \frac{\beta}{\alpha}\left(\frac{c_5 y_5}{2y_4^{\frac{1}{2}}}\right) \tag{14.2}$$

$$J(1,5) = \frac{\partial f_1}{\partial y_5} = \frac{\beta}{\alpha}\left(c_5 y_4^{\frac{1}{2}}\right) - \frac{\beta}{\alpha} \tag{14.3}$$

$$J(1,6) = \frac{\partial f_1}{\partial y_6} = 2\left(c_6 y_4^{\frac{1}{2}}\right) + 2 + \left(\frac{c_1}{2y_6^{\frac{1}{2}}}\right) + \frac{\beta}{\alpha}\left(\frac{c_3 y_4^{\frac{1}{2}}}{2y_6^{\frac{1}{2}}}\right) \tag{14.4}$$

$$J(2,3) = \frac{\partial f_2}{\partial y_3} = \left(\frac{c_4 y_4^{\frac{1}{2}}}{2y_3^{\frac{1}{2}}}\right) \tag{14.5}$$

$$J(2,4) = \frac{\partial f_2}{\partial y_4} = 2\left(\frac{c_5 y_5}{2{y_4}^{\frac{1}{2}}}\right) + \left(\frac{c_6 y_6}{2{y_4}^{\frac{1}{2}}}\right) + 2 + \left(\frac{c_2}{2{y_4}^{\frac{1}{2}}}\right) + \left(\frac{c_3 {y_6}^{\frac{1}{2}}}{2{y_4}^{\frac{1}{2}}}\right) + \left(\frac{c_4 {y_3}^{\frac{1}{2}}}{2{y_4}^{\frac{1}{2}}}\right) - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right)\left(\frac{c_5 y_5}{2{y_4}^{\frac{1}{2}}}\right) \tag{14.6}$$

$$J(2,5) = \frac{\partial f_2}{\partial y_5} = 2\left(c_5 {y_4}^{\frac{1}{2}}\right) + 1 - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right)\left(c_5 {y_4}^{\frac{1}{2}}\right) - \left(\frac{\gamma}{\alpha} + 2\left(\frac{a_s}{\phi\alpha}\right)\right) \tag{14.7}$$

$$J(2,6) = \frac{\partial f_2}{\partial y_6} = \left(c_6 {y_4}^{\frac{1}{2}}\right) + \left(\frac{c_3 {y_4}^{\frac{1}{2}}}{2{y_6}^{\frac{1}{2}}}\right) \tag{14.8}$$

$$J(3,3) = \frac{\partial f_3}{\partial y_3} = 2 + \left(\frac{c_4 {y_4}^{\frac{1}{2}}}{2{y_3}^{\frac{1}{2}}}\right) \tag{14.9}$$

$$J(3,4) = \frac{\partial f_3}{\partial y_4} = \left(\frac{c_4 {y_3}^{\frac{1}{2}}}{2{y_4}^{\frac{1}{2}}}\right) - \left(\frac{\delta}{\alpha} + \frac{7.52 a_s}{\phi\alpha}\right)\left(\frac{c_5 y_5}{2{y_4}^{\frac{1}{2}}}\right) \tag{14.10}$$

$$J(3,5) = \frac{\partial f_3}{\partial y_5} = \left(\frac{\delta}{\alpha} + \frac{7.52 a_s}{\phi\alpha}\right)\left(c_5 {y_4}^{\frac{1}{2}}\right) - \left(\frac{\delta}{\alpha} + \frac{7.52 a_s}{\phi\alpha}\right) \tag{14.11}$$

$$J(3,6) = \frac{\partial f_3}{\partial y_6} = 0 \tag{14.12}$$

$$J(4,3) = \frac{\partial f_4}{\partial y_3} = 1 + \left(\frac{c_4 {y_4}^{\frac{1}{2}}}{2{y_3}^{\frac{1}{2}}} \right) \tag{14.13}$$

$$J(4,4) = \frac{\partial f_4}{\partial y_4} = \left(\frac{c_5 y_5}{2{y_4}^{\frac{1}{2}}} \right) + \left(\frac{c_6 y_6}{2{y_4}^{\frac{1}{2}}} \right) + 1 + \left(\frac{c_2}{2{y_4}^{\frac{1}{2}}} \right) + \left(\frac{c_3 {y_6}^{\frac{1}{2}}}{2{y_4}^{\frac{1}{2}}} \right) + \left(\frac{c_4 {y_3}^{\frac{1}{2}}}{2{y_4}^{\frac{1}{2}}} \right) \tag{14.14}$$

$$J(4,5) = \frac{\partial f_4}{\partial y_5} = \left(c_5 {y_4}^{\frac{1}{2}} \right) + 1 \tag{14.15}$$

$$J(4,6) = \frac{\partial f_4}{\partial y_6} = \left(c_6 {y_4}^{\frac{1}{2}} \right) + 1 + \left(\frac{c_1}{2{y_6}^{\frac{1}{2}}} \right) + \left(\frac{c_3 {y_4}^{\frac{1}{2}}}{2{y_6}^{\frac{1}{2}}} \right) \tag{14.16}$$

In order to solve the Newton-Raphson iteration method, initial guess for the value of unknowns y_3, y_4, y_5, y_6 must be obtained first. So, in this project low combustion modelling is being used to find the mole fractions y_3, y_4, y_5, and y_6. Equation below shows the overall combustion reaction for low temperature combustion (T < 1000K):

$$C_\alpha H_\beta + H_2O_2 + \left(\frac{a_s}{\phi}\right)(O_2 + 3.76N_2) \rightarrow (y_1CO_2 + y_2H_2O + y_3N_2 + y_4O_2 + y_5CO + y_6H_2)\,N \tag{15}$$

The stoichiometric combustion in an assumed temperature of room temperature can be either lean combustion or rich combustion depending on the value of equivalence ratio, ϕ. If it is lean combustion, the emission combustion for CO and H_2 will be assumed zero while if it is rich combustion, emission combustion of O_2 is assumed zero. By applying this assumption, the initial value of mole fraction y_3, y_4, y_5, and y_6 can be approximately obtained. If $y=y_0$ represent the initial guess for the solution, approximation of the solution can be successively obtained from:

$$y_{n+1} = y_n - J^{-1}F(y_n) = y_n - \Delta y_n \tag{15}$$

Where J^{-1} can be obtained from the solution of Jacobian Matrix method as mentioned and Δy_n, is obtained from equation below:

$$\Delta y_n = y_n - y_{n+1} \tag{16}$$

3.4. MATLAB computer programming input

There is abundance of software created that can calculate the mole fraction of the combustion products for fuel with hydrogen peroxide addition in a spark-ignition engine just by key-in the required input and the software will help to calculate and find the unknowns available in the equation. The result will be automatically calculated with exact value for each mole fraction. Among the software that can help to calculate the mole fraction of combustion products are CHEMKIN, MATLAB, and POLYMATH. In this study, MATLAB computer programming has been chosen to compute the required mole fraction needed. This is because MATLAB is easy to be used and does not require much procedure to run and to develop computational codes. With MATLAB software also can help to validate the values of mole fraction obtained manually by using Newton-Raphson method. Variables can be manipulated easily as MATLAB can solve the equation for the combustion through simulation. Input can be changed to observe the effect of the input in the combustion product of hydrogen peroxide addition to obtain the best possible output from the equation. Input that can be key-in in MATLAB software are:

I. Temperature, T (in Kelvin)
II. Equivalence Ratio, ϕ
III. Pressure, P (in bar)

By inserting the input, exact value of mole fraction of combustion products can be obtained. Then the analysis of emission characteristics of different equivalence ratio for SI engine can be analysed based on the value obtained. Further discussion will be explained in detail later in chapter 4.

CHAPTER 4

RESULT AND DISCUSSION

In this chapter, MATLAB software has been chosen to solve the unknown value of mole fractions. MATLAB code has been developed successfully where the value of combustion product can be obtained just by key-in the manipulated variables such as temperature, equivalence ratio and pressure ‘s value as the input into the code. As this report is more focusing on the effect of equivalence ratio to the emission characteristics, other two manipulated variables were fixed that is temperature and pressure with values of 3000K and 30 bar respectively. While the values of equivalence ratio will be varying from 0.6 to 1.2 with increment of 0.1.Another study has been made by focusing on the effect of temperature to the mole fraction while equivalence ratio and pressure’s values will be fixed. Value of equivalence ratio is 1.2 while the pressure is at 30 bar. Values of temperature will be varying from 2000K to 4000K with increment of 400K.For third study, pressure will be the manipulated variables while mole fraction will be the responding variables. Values of equivalence ratio and temperature will be fixed that is 1.2 and 3000K respectively. The value of pressure is from 20bar to 50bar with increment of 10bar.

It is noted that this project is only simulation of the combustion process for a spark-ignition engine when hydrogen peroxide is used as fuel alternative. So, all the advantages and disadvantages when the mixed hydrogen peroxide and gasoline is used as the fuel for SI engine will be explained later in discussion part. Area of improvement will also be mentioned in the discussion part for further research use.

4.1 Mole fraction of every combustion product with variation of Equivalence Ratio, ϕ

In this study, the mole fraction for each combustion products will be recorded at different equivalence ratio in the range of 0.4 to 1.4 with the increment of 0.2. While temperature and pressure are kept constant at 3000K and 30 bar respectively.

4.1.1 Carbon Dioxide (CO_2)

Table 4.1.1: Mole fraction of CO_2 with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0478	0.0656	0.0792	0.0871	0.0846	0.0686

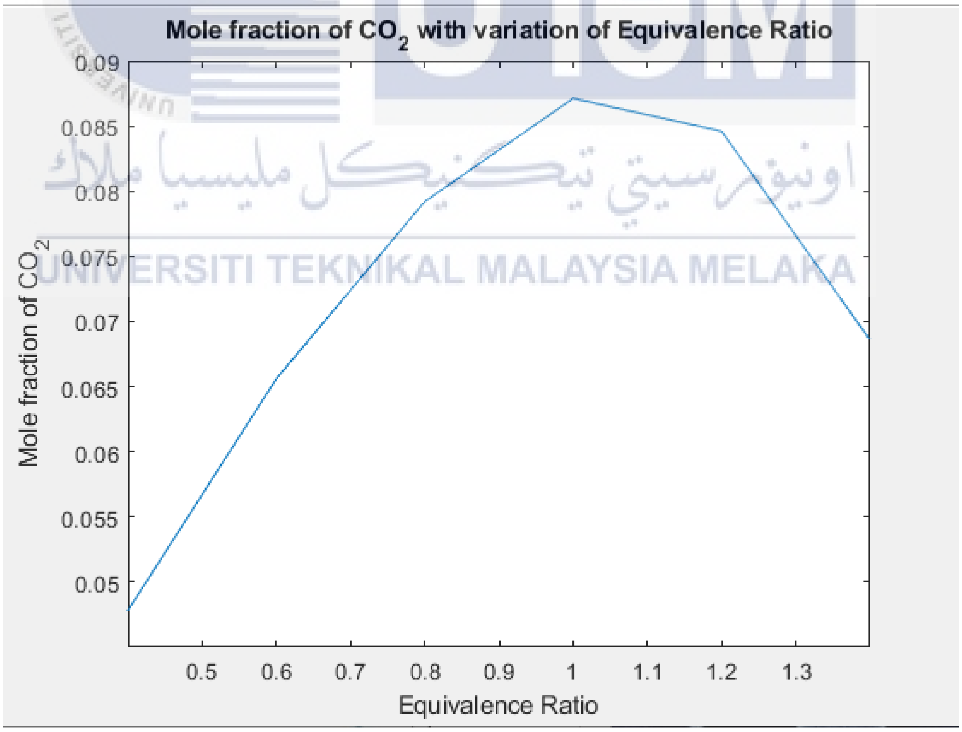


Figure 4.1.1: Mole fraction of CO_2 with variation of equivalence ratio

Based on figure 4.1.1, mole fraction of CO_2 increases during lean combustion ($\phi < 1$) but decreasing as it enter rich combustion ($\phi > 1$). Mole fraction of CO_2 is at it's peak during stoichiometric combustion ($\phi = 1$) that is 0.0871. During lean combustion, emission of CO_2 increase because of the increase of fuel that causing more complete combustion to occur. As it reaches stoichiometric combustion where amount of gasoline mixed with H_2O_2 is equal with the amount of air supplied, complete combustion process can occur a lot due to equal ratio of fuel and air, resulting in larger production of CO_2. And for rich combustion, the reason behind declining production of CO_2 is because of less combustion occur. It is caused by less amount of air supplied in the combustion chamber.

4.1.2 Water (H_2O)

Table 4.1.2: Mole fraction of H_2O with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0733	0.1028	0.1283	0.1498	0.1655	0.1710

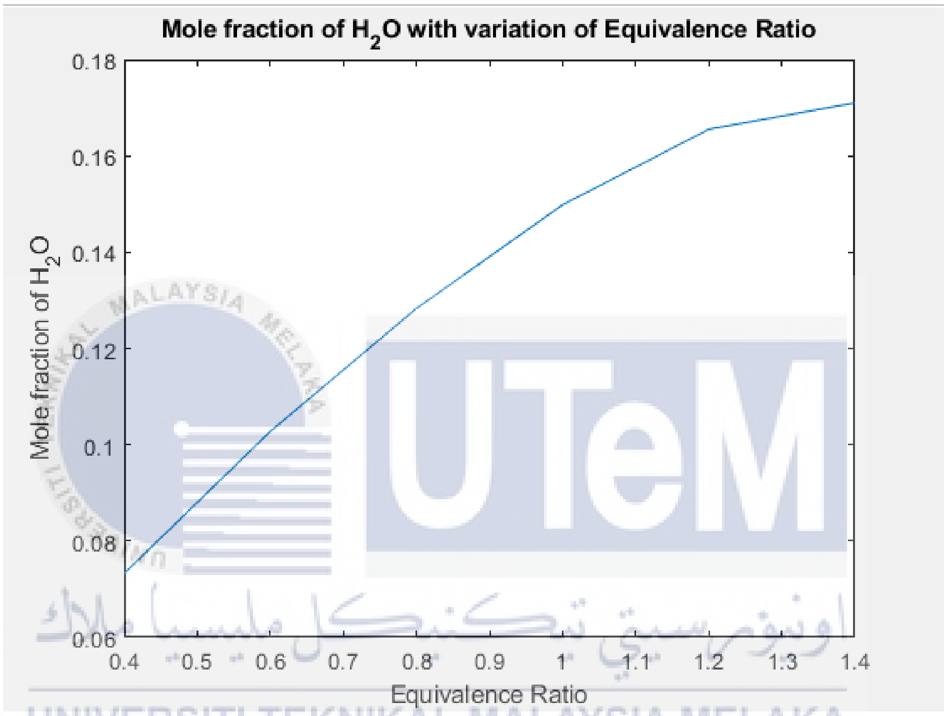


Figure 4.1.2: Mole fraction of H_2O with variation of equivalence ratio

From figure 4.1.2, we can see that the mole fraction of H_2O increases as the equivalence ratio increases up to 0.1710 at ϕ =1.4. With the help of H_2O_2 as oxidizing agent, more complete combustion can be produced resulting in the increase H_2O.

4.1.3 Nitrogen gas(N_2)

Table 4.1.3: Mole fraction of N_2 with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.8700	0.8169	0.7700	0.7281	0.6905	0.6567

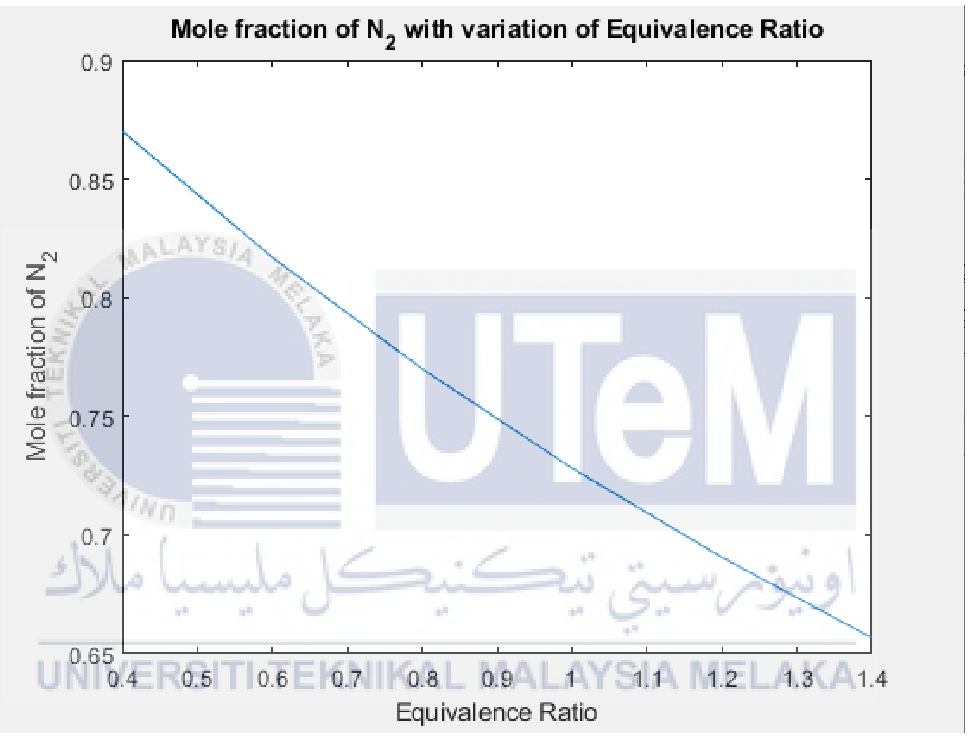


Figure 4.1.3: Mole fraction of N_2 with variation of equivalence ratio

From figure 4.1.3, value of N_2 is at the highest when equivalence ratio is 0.4 that is 0.8700 and it is decreasing as the equivalence ratio increases. This shows that the amount of nitrogen gas emitted is the lowest during rich combustion. Nitrogen is obtained from the air inside of the combustion chamber. The increase in equivalence ratio resulting in the smaller fraction of emission product representing N_2.

4.1.4 Oxygen gas(O_2)

Table 4.1.4: Mole fraction of O_2 with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.1512	0.1053	0.0662	0.0340	0.0117	0.0028

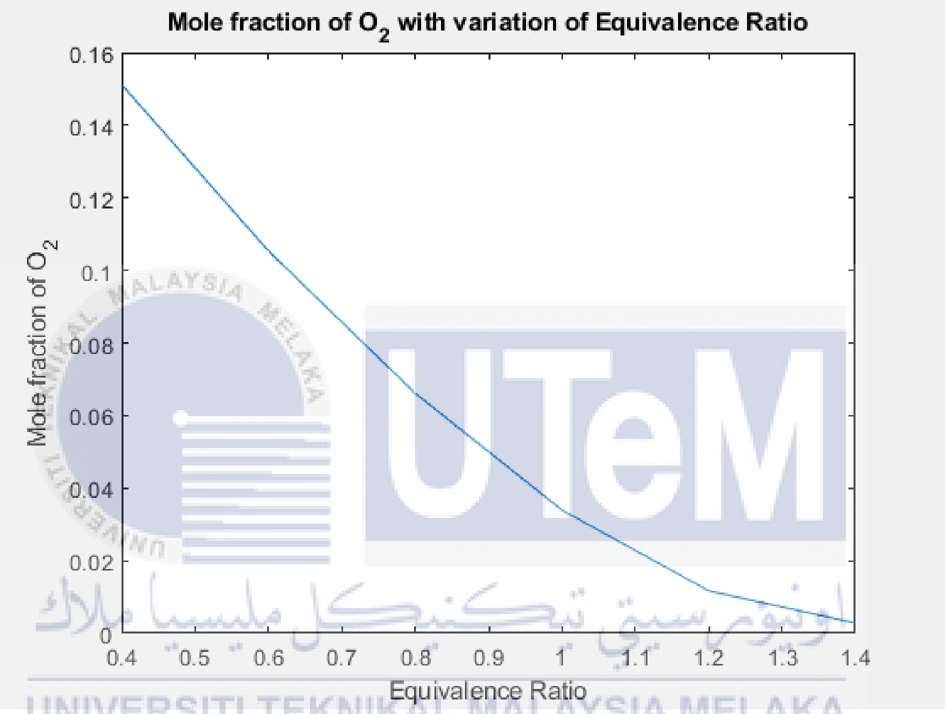


Figure 6: Mole fraction of O_2 with variation of equivalence ratio

During lean combustion (ϕ <1), the volume of air in combustion chamber is more than the volume of fuel so the mole fraction of O_2 obtained from the combustion product is high due to the abundance of oxygen. The equivalence ratio then increased towards rich combustion(ϕ >1). The increasement of equivalence ratio is because of the increase of volume of fuel into the combustion chamber. With the increase of volume of fuel, combustion process will take place and eventually used all the available air in the combustion chamber to form H_2O. Mole fraction of O_2 will decrease and approaching 0 during rich combustion as the amount of oxygen is fully utilized for the combustion process.

4.1.5 Carbon Monoxide (CO)

Table 4.1.5: Mole fraction of CO with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0073	0.0121	0.0184	0.0282	0.0467	0.0771

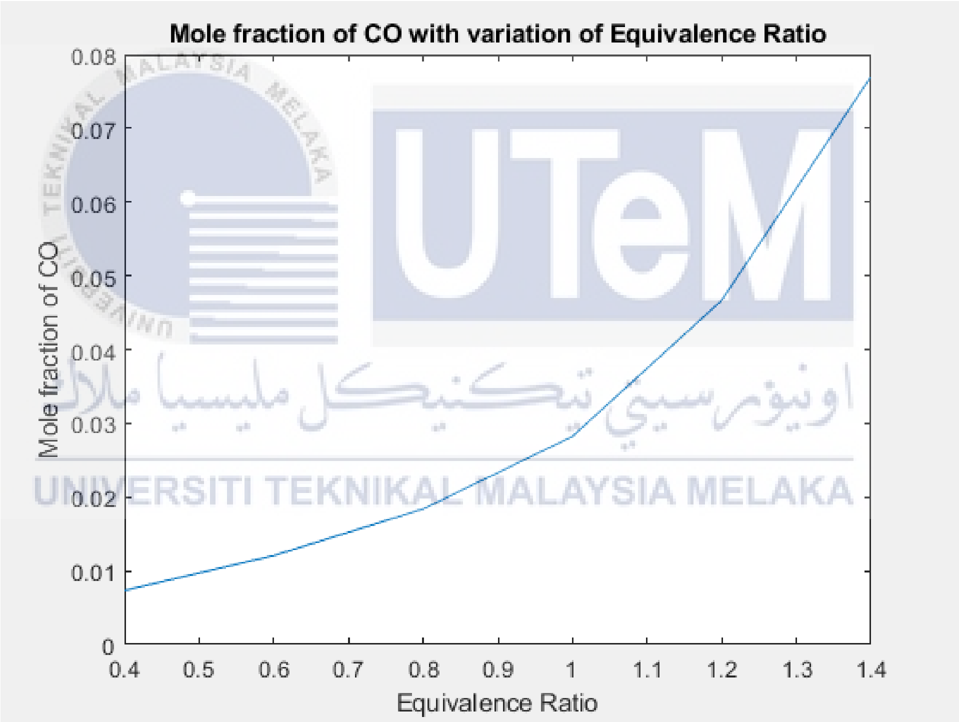


Figure 4.1.5: Mole fraction of CO with variation of equivalence ratio

Based on figure 4.1.5, mole fraction of CO increases as the equivalence ratio increases. During lean combustion (ϕ<1), the increasement of CO is about 0.005234 per 0.2 increment of equivalence ratio. The mole fraction of CO started to increase as it enters rich combustion where the peak value is at ϕ=1.4 that is 0.0771. This is because, during rich combustion, lack of oxygen provided for the combustion process, resulting in the incomplete of combustion reaction where CO is formed. The low access to oxygen will increase the formation of CO.

4.1.6 Hydrogen gas (H_2)

Table 4.1.6: Mole fraction of H_2 with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0016	0.0026	0.0041	0.0067	0.0127	0.0267

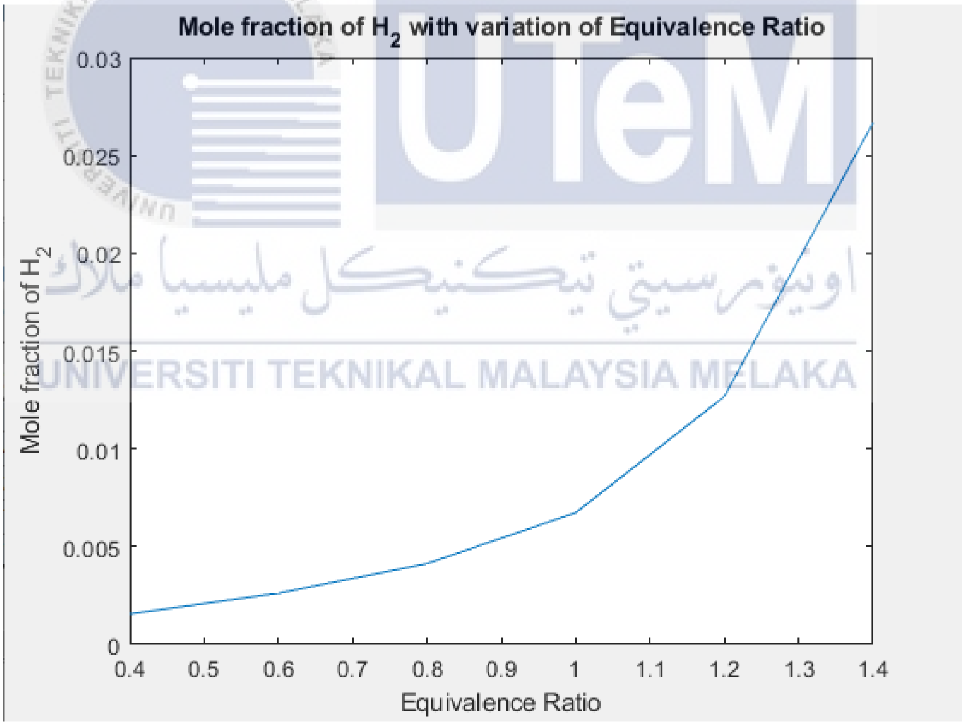


Figure 4.1.6: Mole fraction of H_2 with variation of equivalence ratio

As shown on figure 4.1.6, the graph of mole fraction of H_2 with variation of equivalence ratio has similar formation just like CO. Mole fraction recorded for H_2 is only 0.0016 at $\phi=0.4$, showing that the amount of H_2 in the combustion product during lean combustion is little. As it goes into rich combustion where the amount of fuel is now more than the amount of air, formation of H_2 has been greatly increased. Hydrogen element is supplied by the fuel. So, when the fuel is undergoing combustion, H_2O_2 will help to form water by oxidation oh hydrogen from the fuel, but there are still excess of hydrogen left. This is where H_2 will be formed. Mole fraction of H_2 recorded increase from 0.006735 at stoichiometric combustion ($\phi=1$) to 0.02667 at $\phi=1.4$, showing the increasement of 296%.

4.1.7 Hydrogen atom (H)

Table 4.1.7: Mole fraction of H with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0011	0.0015	0.0018	0.0024	0.0032	0.0047

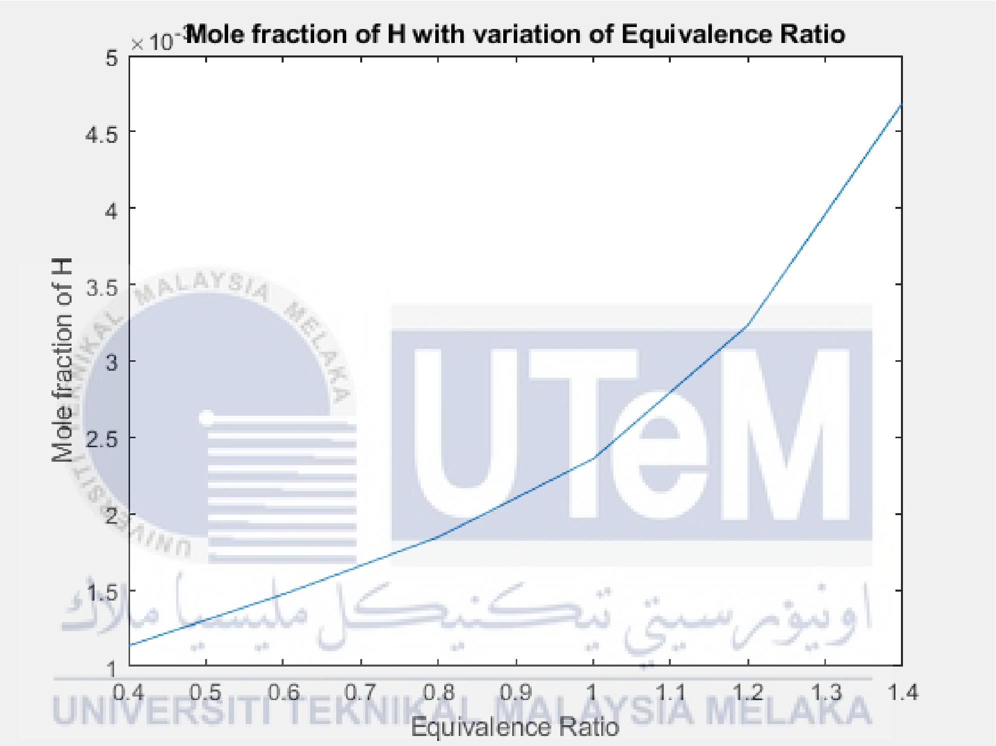


Figure 4.1.7: Mole fraction of H with variation of equivalence ratio

From figure 4.1.7, combustion product for Hydrogen atom is increasing as the equivalence ratio increases where peak emission of H is at ϕ=1.4, because of there are huge amount of hydrogen supplied. As the equivalence increase, the amount of oxygen supplied by the available air inside of the combustion chamber is not enough for the formation for all hydrogen to form H_2O, leaving hydrogen atom alone emitted from the combustion process. A huge production of Hydrogen atom is coming from the gasoline and H_2O_2 mixed fuel.

4.1.8 Oxygen atom (O)

Table 4.1.8: Mole fraction of O with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0080	0.0067	0.0053	0.0038	0.0022	0.0011

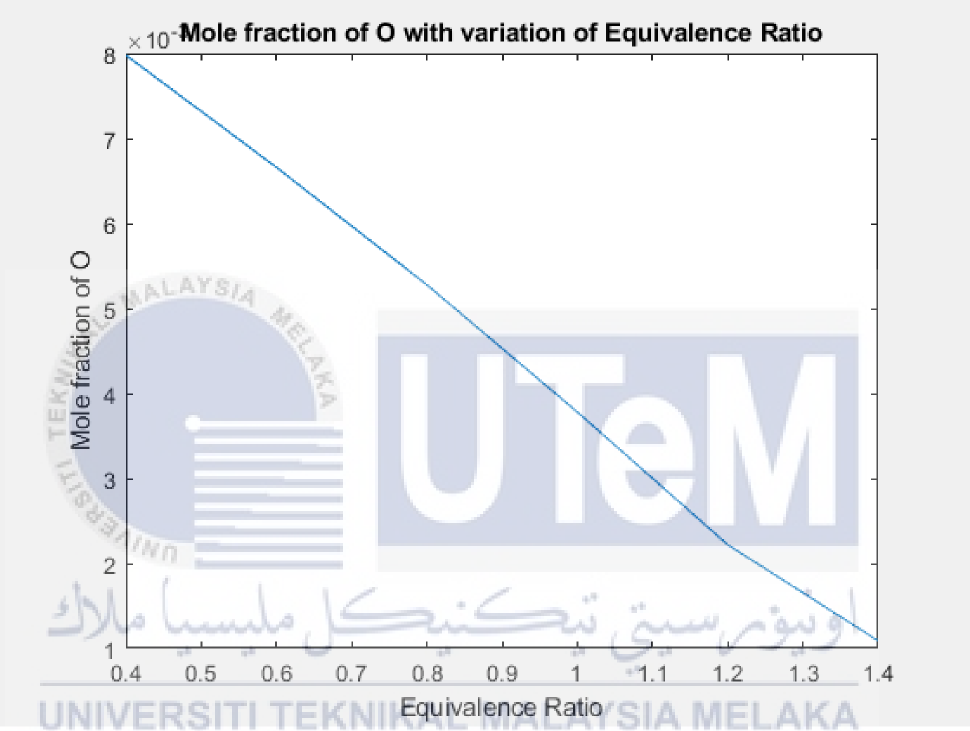


Figure 4.1.8: Mole fraction of O with variation of equivalence ratio

Oxygen atom can be found in the air in the combustion chamber. Starting at lean combustion (ϕ<1), the recorded mole fraction of oxygen atom in the combustion product shows a decreasing pattern and it continues as the equivalence ratio getting larger until it entered rich combustion (ϕ>1). Along with the decreasing volume of air supplied for the combustion process, most oxygen atom is used for the complete combustion, leaving a few oxygen atom that is not bonding with other element. This causing the amount of oxygen getting decrease and decrease until it is recorded only 0.001090 at ϕ=1.4.

4.1.9 Hydroxide (OH)

Table 4.1.9: Mole fraction of OH with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.4214	0.3409	0.2623	0.1827	0.1045	0.0500

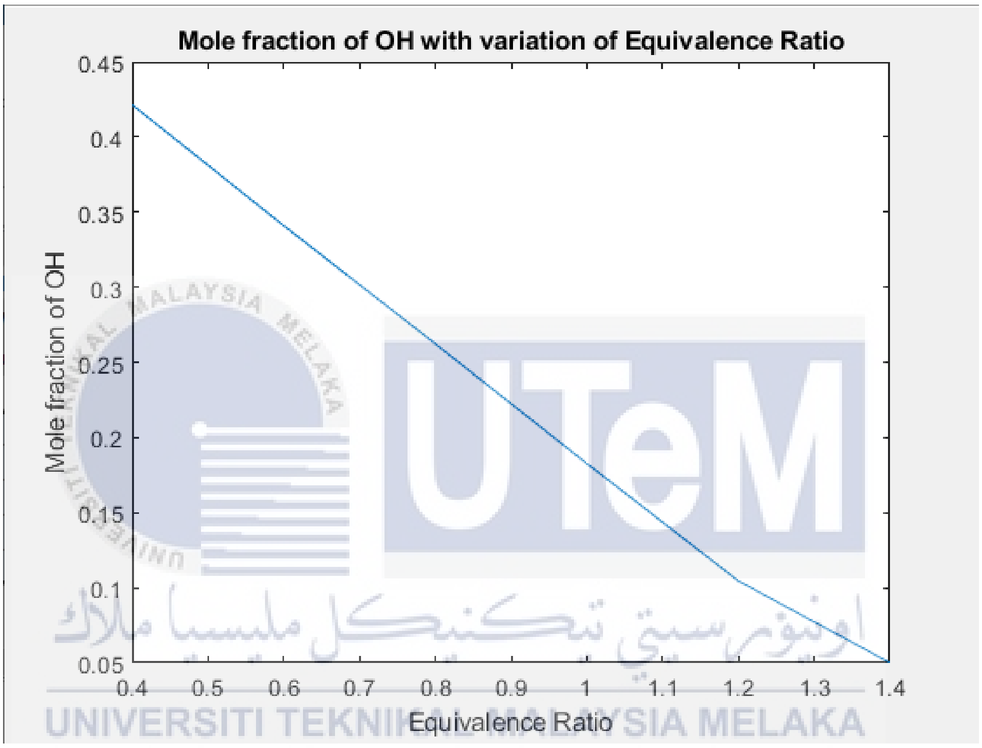


Figure 4.1.9: Mole fraction of OH with variation of equivalence ratio

When H_2O_2 is added into gasoline, the mole fraction of OH drastically decrease. This is because of the presence of H_2O_2 that improve the ability of fuel to oxidize, causing increase in complete combustion products. Since OH is not the product of complete combustion, mole fraction of OH decrease as the equivalence ratio increase because of oxygen is prioritize in the bonding of water compared to OH. Mole fraction of OH decrease uniformly from ϕ=0.4 to ϕ=1.2 and the slope slightly decrease when ϕ reaching 1.4.

4.1.10 Nitrogen Oxide (NO)

Table 4.1.10: Mole fraction of NO with variation of equivalence ratio

Equivalence Ratio (ϕ)	0.4	0.6	0.8	1.0	1.2	1.4
Mole Fraction	0.0443	0.0359	0.0276	0.0192	0.0110	0.0053

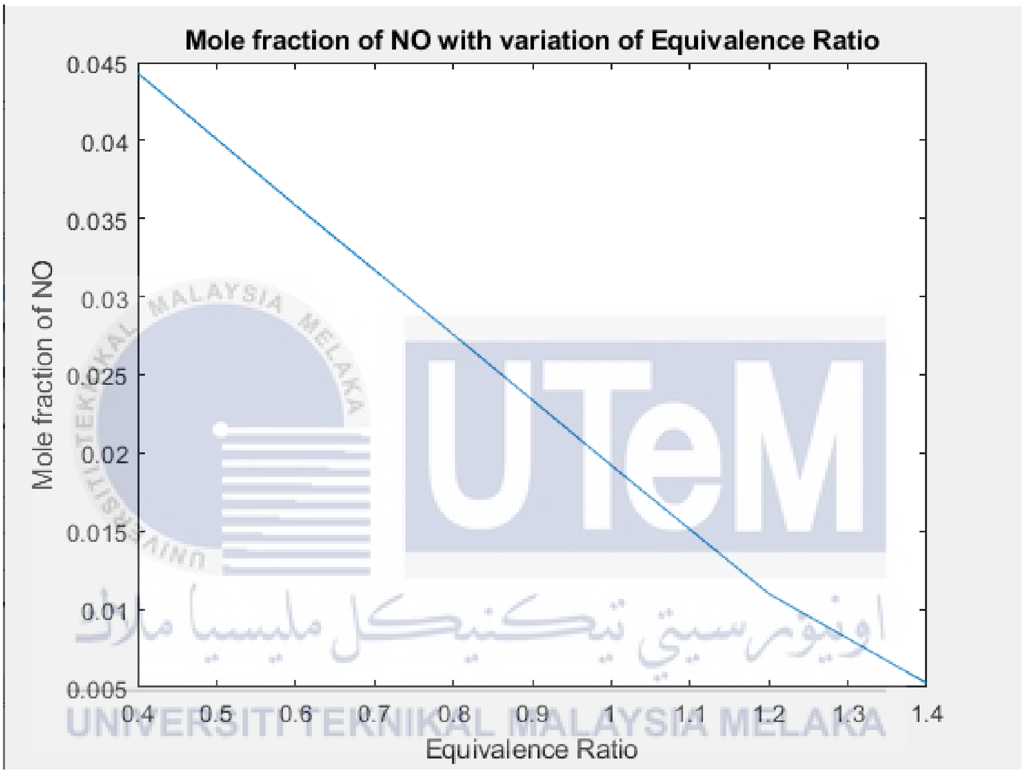


Figure 4.1.10: Mole fraction of NO with variation of equivalence ratio

Mole fraction that represents NO decrease as the equivalence ratio increase. The value of mole fraction of NO is approximately similar to the values obtained for OH, where at rich combustion (ϕ>1), the values for both OH and NO are reaching zero. From the observation in figure 4.1.10, we can tell the production of NO is not as much as during lower equivalence ratio due to insufficient element of oxygen inside of the combustion chamber that is used to form NO.

4.2 Mole fraction of every combustion product with variation of Temperature, T

In this study, the mole fraction for each combustion products will be recorded at temperature of combustion in the range of 1500K to 3000K with the increment of 500K. While for the equivalence ratio and pressure, the values are constant which is at ϕ=1.4 and 30 bar respectively.

4.2.1 Carbon Dioxide (CO_2)

Table 4.2.1: Mole fraction of CO_2 with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	0.1087	0.1048	0.1022	0.0846

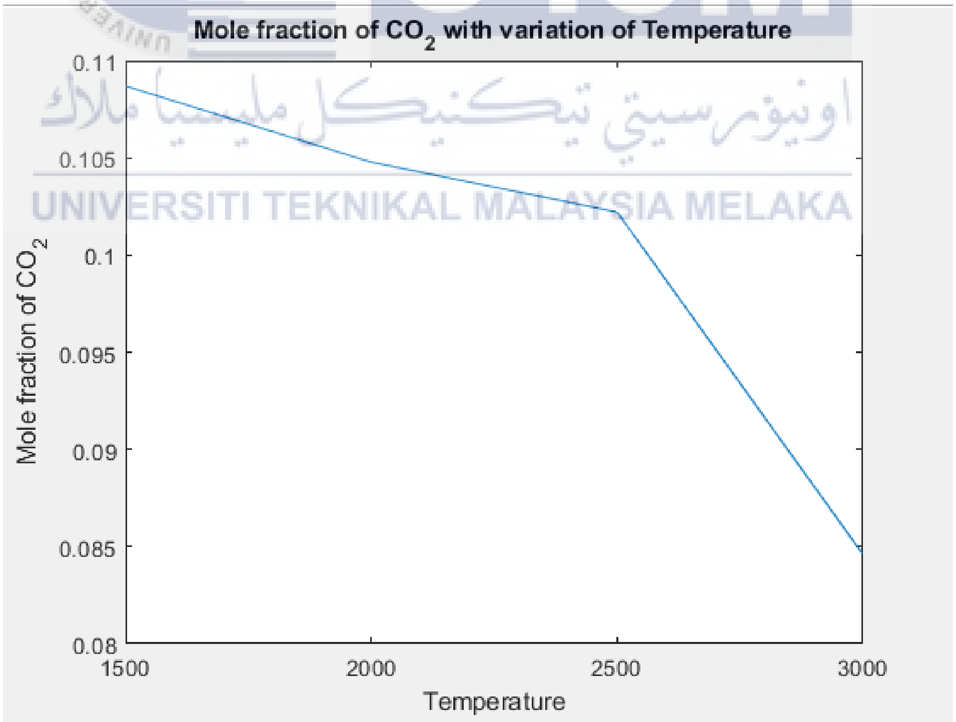


Figure 4.2.1: Mole fraction of CO_2 with variation of temperature

From Figure 4.2.1, we can see that the emission of CO_2 decrease when the temperature of combustion increase. The mole fraction representing CO_2 slightly decreases when the temperature increase from 1500K to 2500K . As the temperature increases from 2500K to 3000K, the mole fraction of CO_2 drastically drop to 0.0846 from 0.1022, with 17% of decrease percentage. The reason behind the huge difference is because at this temperature, although the emission of CO_2 still happen due to combustion, most of the compund will start to dissociate into carbon and oxygen ions. From the graph, we can proof that higher temperature of combustion is better as it can lower the emission of CO_2.

4.2.2 Water (H_2O)

Table 4.2.2: Mole fraction of H_2O with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	0.1648	0.1687	0.1702	0.1655

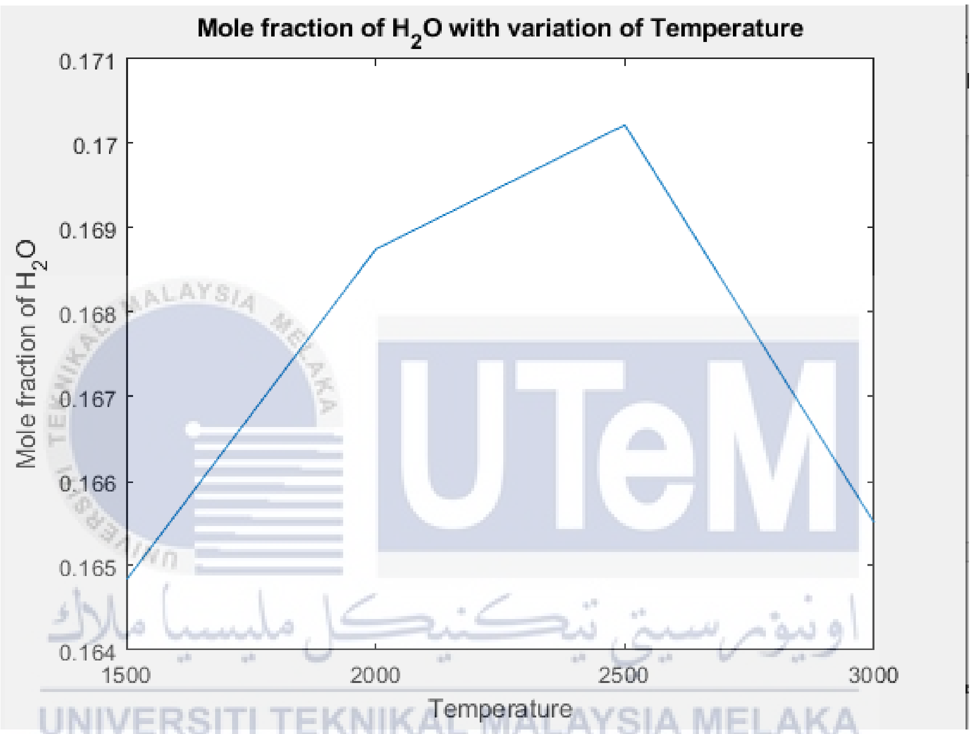


Figure 4.2.2: Mole fraction of H_2O with variation of temperature

From figure 4.2.2, the mole fraction of H_2O increases when temperature increase until it reaches 2500K. As it exceeds 2500K, the mole fraction of H_2O started to decrease. At this temperature, water splitting will start to occur. Water splitting is referring to the chemical reaction where H_2O will be broken down into oxygen and hydrogen. The higher the temperature of combustion, the larger the percentage of H_2O that will undergo water splitting, resulting in the decrease of mole fraction of H_2O in the combustion product.

4.2.3 Nitrogen gas(N_2)

Table 4.2.3: Mole fraction of N_2 with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	0.6905	0.6905	0.6905	0.6905

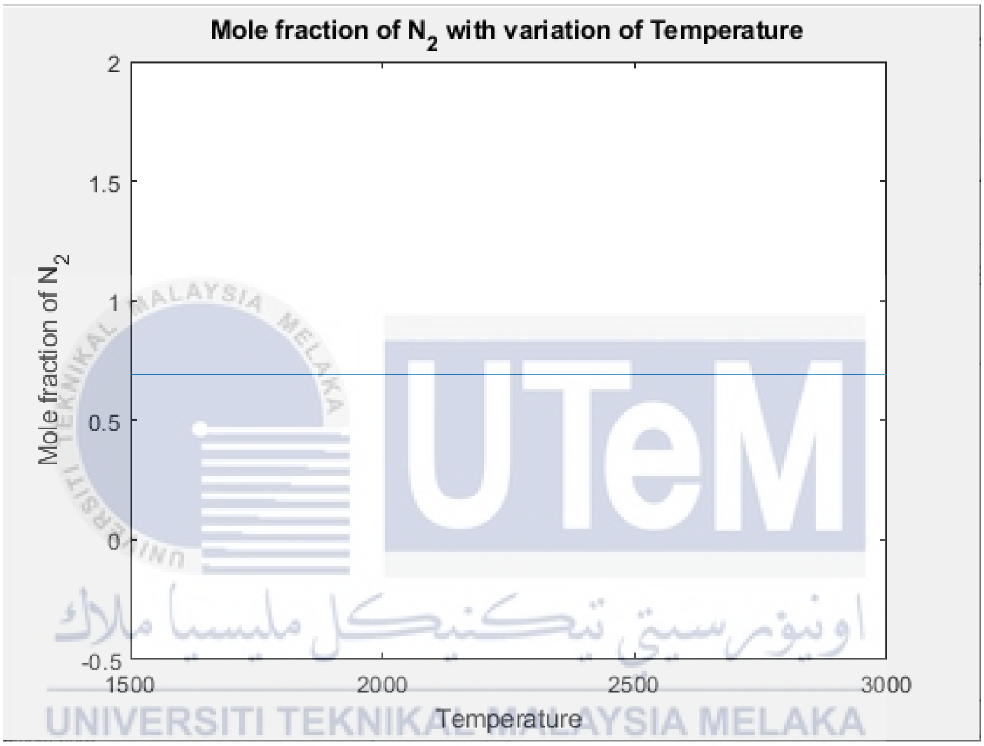


Figure 4.2.3: Mole fraction of N_2 with variation of temperature

From figure 4.2.3, mole fraction of N_2 is the same even when the temperature changes from 1500K to 3000K that is at 0.6905. This can conclude that temperature does not affecting the emission of N_2 for the combustion of H_2O_2 mixed gasoline fuel.

4.2.4 Oxygen gas(O_2)

Table 4.2.4: Mole fraction of O_2 with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	1.79E-11	8.86E-07	0.0005	0.0117

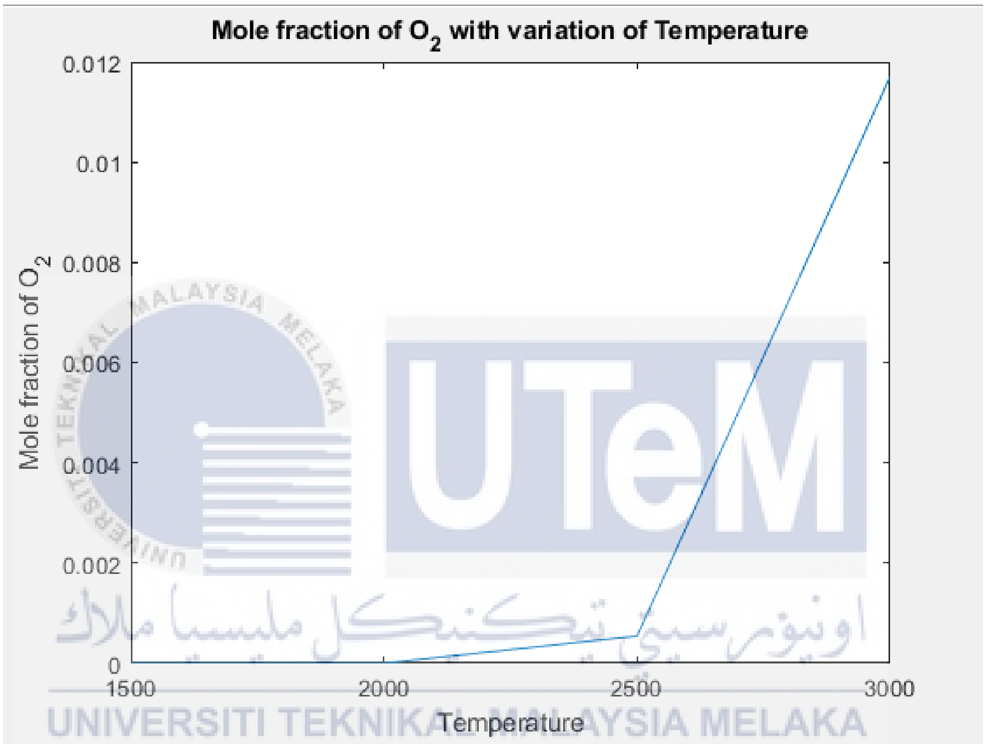


Figure 4.2.4: Mole fraction of O_2 with variation of temperature

During the temperature from under 2000K, the mole fraction recorded for O_2 is approximately 0 due to the O_2 forming is little during this temperature. The emission of O_2 started to occur at temperature 2000K and it increases slightly when the temperature increases to 2500K. During 2500K temperature, O_2 is formed due to the dissociation of compound such as CO_2 and H_2O, and also due to the incomplete combustion. The mole fraction increases superbly during the temperature is at 3000K as it goes from 0.0005 to 0.0117 with increase percentage of 2240%.

4.2.5 Carbon Monoxide (CO)

Table 4.2.5: Mole fraction of CO with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	0.0226	0.0265	0.0291	0.0467

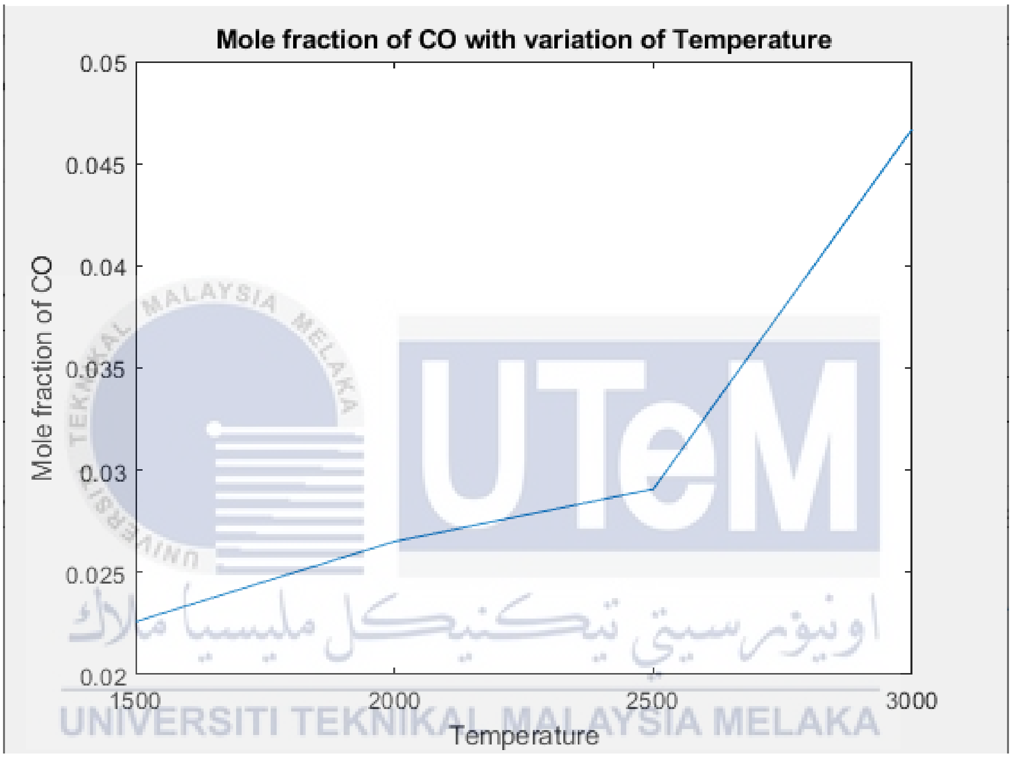


Figure 4.2.5: Mole fraction of CO with variation of temperature

The emission of CO during the combustion of H_2O_2 mixed gasoline fuel in SI engine has a percentage increase of 17% at temperature between 1500K to 2000K. As the temperature increases between 2000K to 2500K, the increase percentage has lowered to 10% only. However, as the temperature goes higher than 2500K, emission of CO has an increase percentage of 60%, due to the incomplete combustion that started to occur. Instead of forming complete oxidized compound such as CO_2 and H_2O, incomplete combustion increases the occurrence of incomplete oxidized compound such as soot and CO.

4.2.6 Hydrogen gas (H_2)

Table 4.2.6: Mole fraction of H_2 with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	0.0134	0.0094	0.0080	0.0127

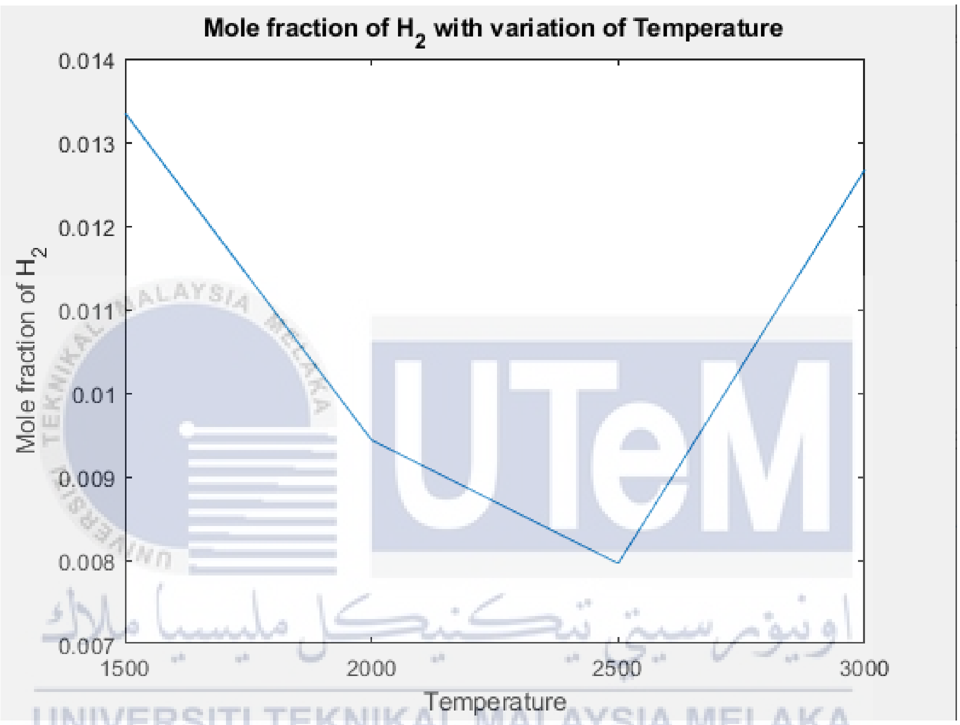


Figure 4.2.6: Mole fraction of H_2 with variation of temperature

Figure 4.2.6 shows the emission of H_2 is decreasing at the temperature between 1500K to 2500K because hydrogen elements will react with oxygen that will form H_2O. The higher the temperature, the more often the process will occur, resulting in the decreasing emission of H_2. As the temperature increases beyond 2500K, production of H_2O is decreasing due to dissociation, allowing the forming of H_2 . It is the reason why mole fraction of H_2 increase beyond 2500K temperature.

4.2.7 Hydrogen atom (H)

Table 4.2.7: Mole fraction of H with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	3.69E-07	2.87E-05	0.0004	0.0032

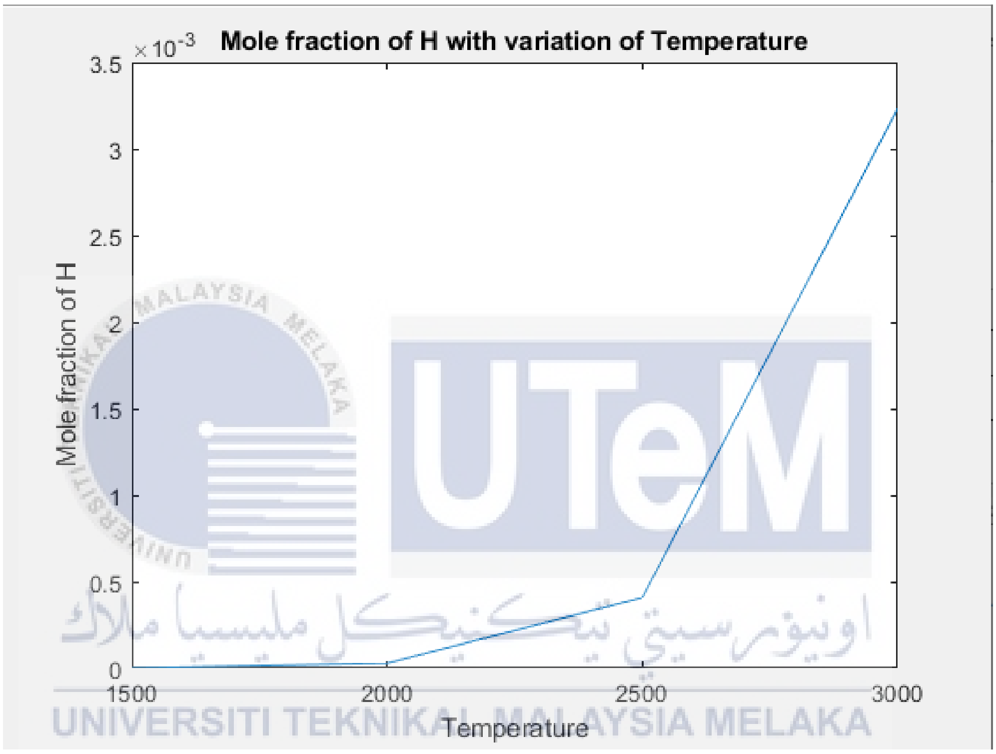


Figure 4.2.7: Mole fraction of H with variation of temperature

Mole fraction of hydrogen atom has an increase pattern during 1500K to 2000K temperature. However, the increase percentage is so little that the value can be assumed 0. As the temperature increase up to 2500K, the mole fraction increases dramatically, and the highest mole fraction recorded is during the temperature is at 3000K that is 0.0032. The increase of mole fraction of H is due to the decomposes of H_2O.

4.2.8 Oxygen atom (O)

Table 4.2.8: Mole fraction of O with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	3.11E-12	1.14E-07	6.13E-05	0.0022

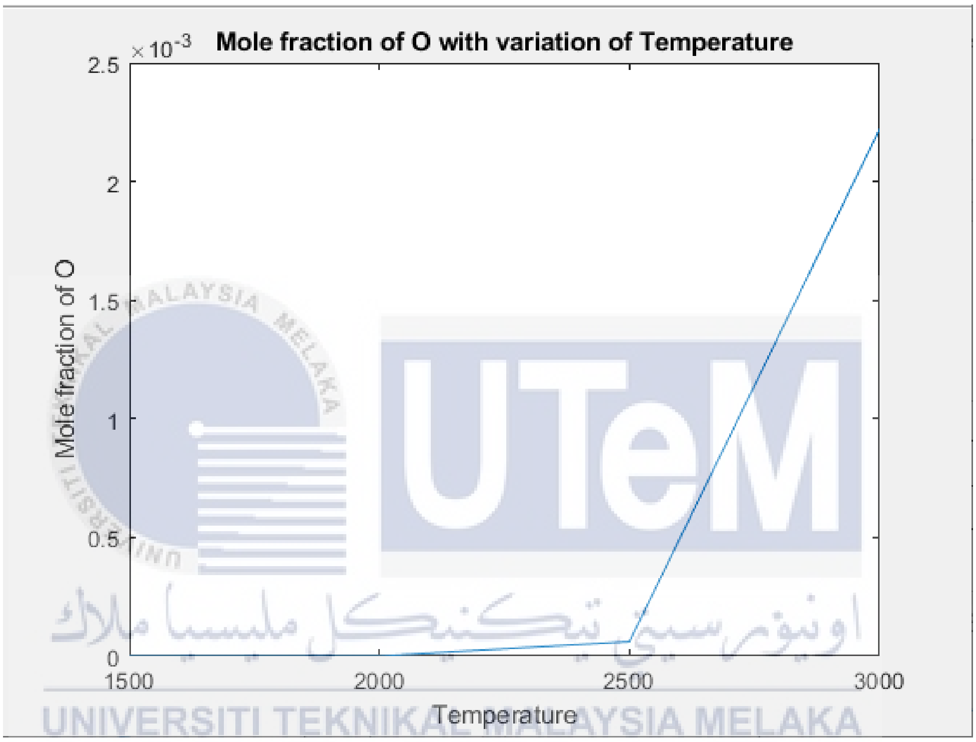


Figure 4.2.8: Mole fraction of O with variation of temperature

The same increasing pattern can be seen on figure 4.2.6, figure 4.2.7 and figure 4.2.8 but differs in the value of mole fraction of each combustion product. At the beginning of the combustion temperature at 1500K to 2000K, the mole fraction representing oxygen atom is very small, that can be neglected. The increase pattern starts to visualise as it goes beyond 2000K. At temperature of more than 2500K where incomplete combustion starts to occur, a huge increase on mole fraction of O can be seen on the graph. We can conclude that O is one of the products of incomplete combustion.

4.2.9 Hydroxide (OH)

Table 4.2.9: Mole fraction of OH with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	9.27E-07	0.0004	0.0169	0.1045

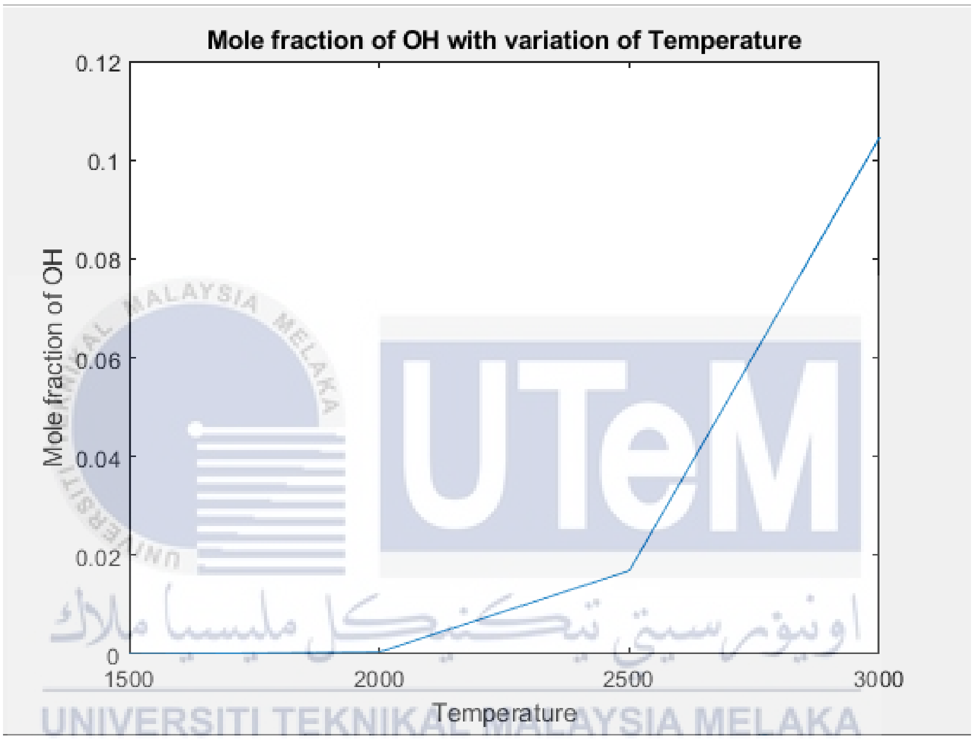


Figure 4.2.9: Mole fraction of OH with variation of temperature

Figure 4.2.9 has the exact same pattern as figure 4.2.8 that is increasing pattern, but it differs in the mole fraction it represents. During the value of temperature at 1500K to 2000K, mole fraction of OH does not has major increase or but as the temperature increases, the mole fraction of OH can be seen increase to a larger margin. We can say that the increase of temperature has an impact on the increase of hydroxide during combustion process.

4.2.10 Nitrogen Oxide (NO)

Table 4.2.10: Mole fraction of NO with variation of temperature

Temperature (K)	1500	2000	2500	3000
Mole Fraction	1.14E-08	1.56E-05	0.0012	0.0110

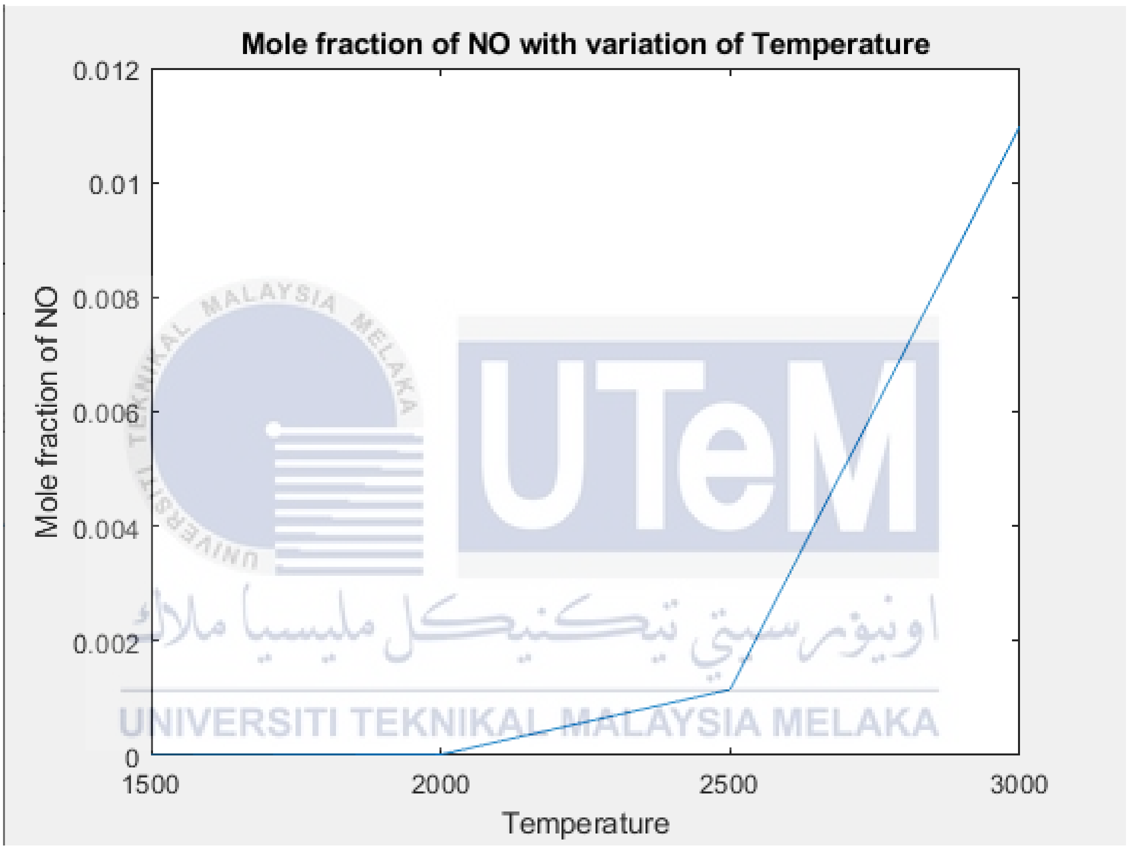


Figure 4.2.10: Mole fraction of NO with variation of temperature

The mole fraction of NO obtained is at the highest value when the temperature is at maximum value that is 0.0110 at 3000K temperature. The combustion temperature has a significant effect on the emission of NO. The increasement of NO can be clearly seen on figure 4.2.10 as H_2O_2 mixed with gasoline fuel is use as the fuel for the combustion process.

4.3 Mole fraction of every combustion product with variation of Pressure, P

For third study, the mole fraction for each combustion emission products will be observed at different pressure of combustion in the range of 20 bar to 50 bar with the increment of 10 bar. While for the equivalence ratio and temperature, the values are constant which is at ϕ=1.4 and 3000K respectively.

4.3.1 Carbon Dioxide (CO_2)

Table 4.3.1: Mole fraction of CO_2 with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.0812	0.0846	0.0868	0.0884

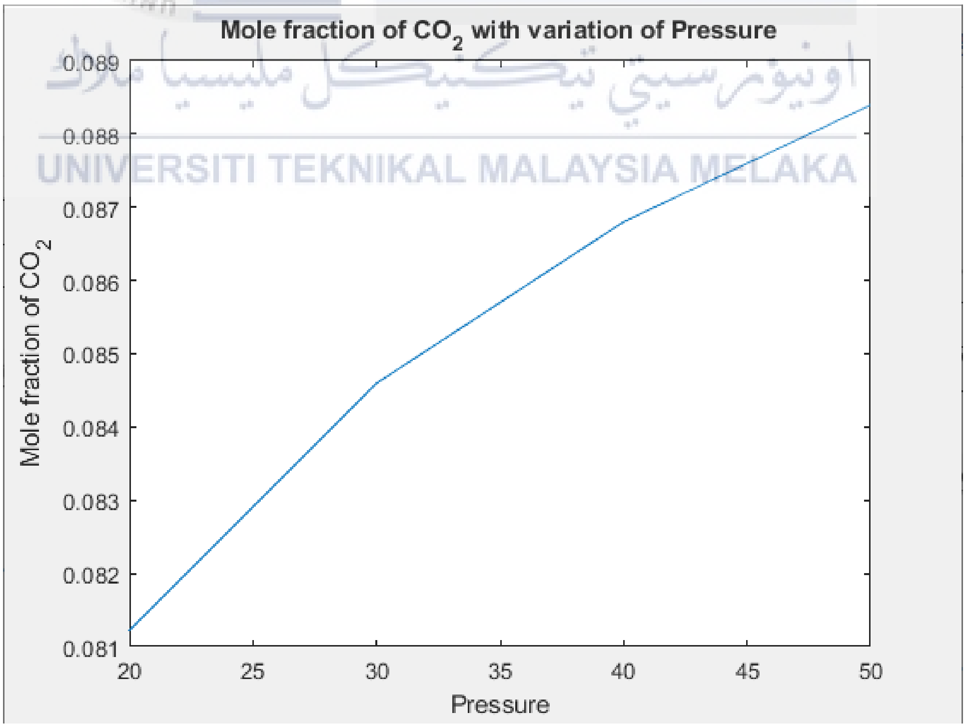


Figure 4.3.1: Mole fraction of CO_2 with variation of Pressure

Based on figure 4.3.1, the mole fraction for CO_2 increases along with the increase of the pressure. The reason behind this increase pattern is because the combustion rate increase with the increase of pressure, causing faster combustion and higher emission of CO_2. Highest mole fraction of CO_2 can be seen at pressure 50 bar where percentage increase of 8% from the starting value obtained at 20 bar.

4.3.2 Water (H_2O)

Table 4.3.2: Mole fraction of H_2O with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.1641	0.1655	0.1664	0.1669

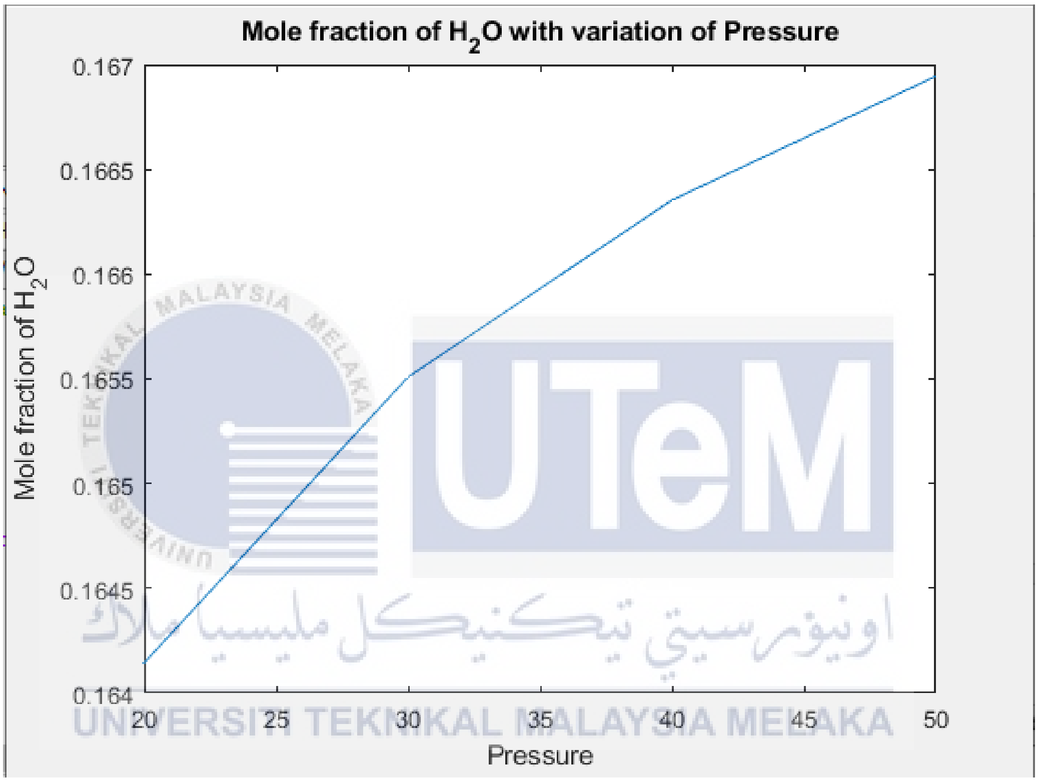


Figure 4.3.2: Mole fraction of H_2O with variation of Pressure

Similar pattern recorded for figure 4.3.2 with figure 4.3.1 that is the responding mole fraction increases as the pressure of combustion increase. The highest mole fraction recorded is at 50 bar with the value of 0.1669. This shows that emission for both CO_2 and H_2O increase with the increase of pressure. Complete combustion occurs frequently at high pressure.

4.3.3 Nitrogen gas(N_2)

Table 4.3.3: Mole fraction of N_2 with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.6905	0.6905	0.6905	0.6905

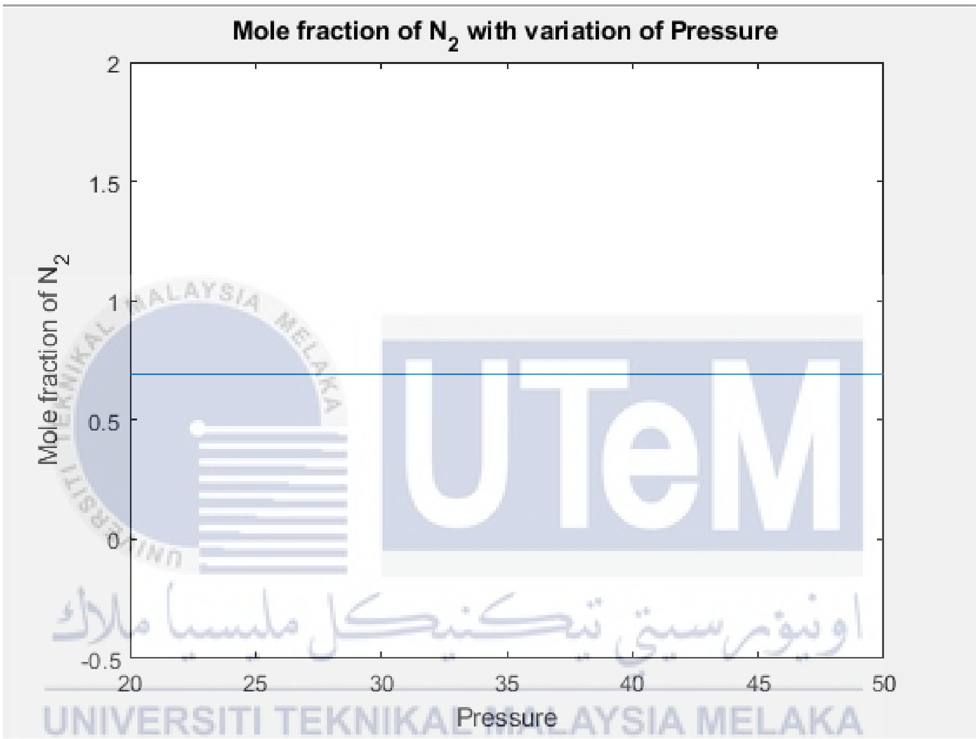


Figure 4.3.3: Mole fraction of N_2 with variation of Pressure

Although different pressure applied in the combustion chamber, the emission product of N_2 is not affected by it. As shown on the figure 4.3.3, the mole fraction of N_2 remain on the same values that is 0.6905 throughout the study. Since there are no changes occur to mole fraction of N_2 when the pressure increases, we can conclude that the pressure does not affect the emission of N_2.

4.3.4 Oxygen gas(O_2)

Table 4.3.4: Mole fraction of O_2 with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.0141	0.0117	0.0102	0.0091

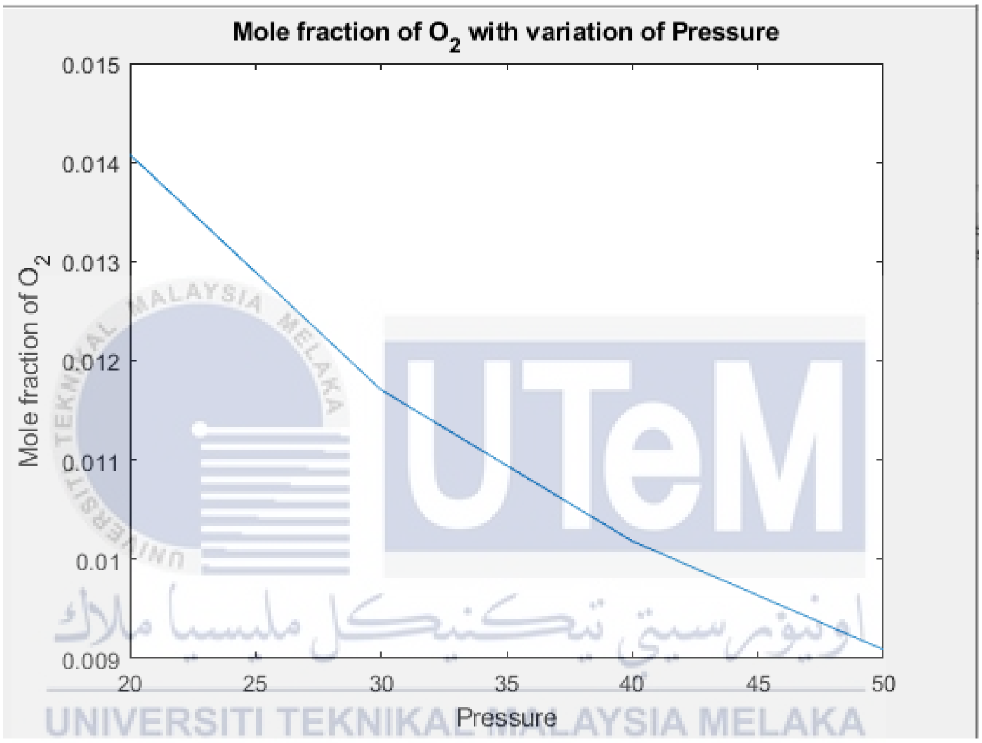


Figure 4.3.4: Mole fraction of O_2 with variation of Pressure

The emission of O_2 is affected by the changes of pressure applied during the combustion. From Figure 4.3.4, it can be stated that the larger the pressure applied, the lower the emission of O_2. The lowest mole fraction of O_2 emission recorded is during the highest pressure given that is at 50 bar at only 0.0091.

4.3.5 Carbon Monoxide (CO)

Table 4.3.5: Mole fraction of CO with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.0501	0.0467	0.0445	0.0429

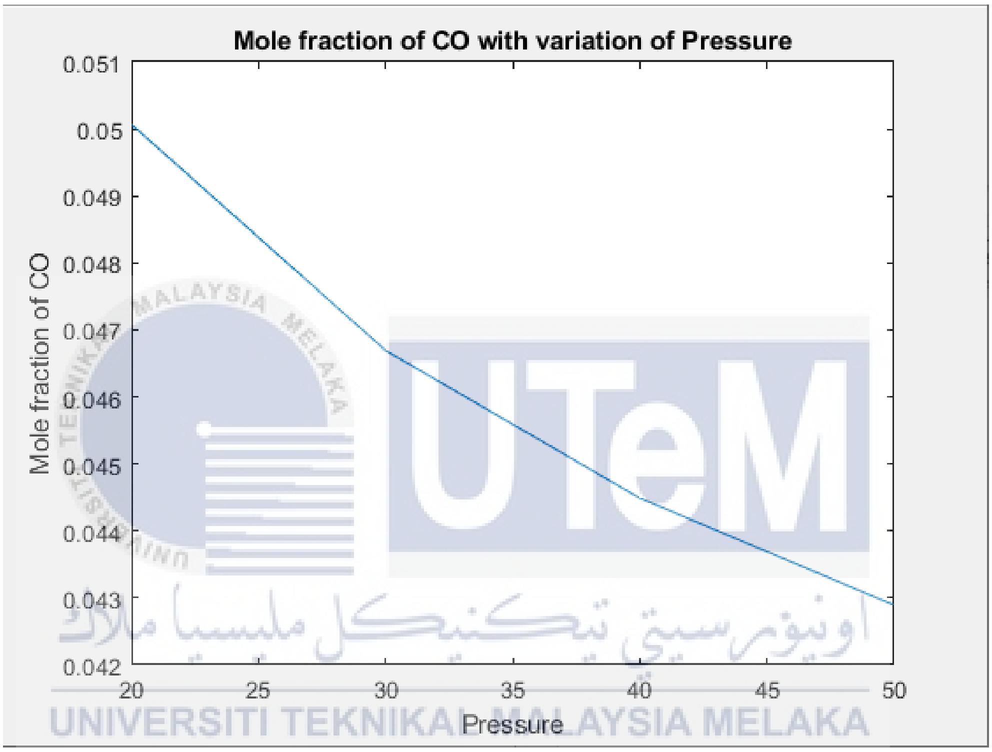


Figure 4.3.5: Mole fraction of CO with variation of Pressure

Mole fraction of CO decreases as the pressure increase as shown in figure 4.3.5. The decreasing pattern shows that the decrease percentage decreases for every increment of 10 bars. For pressure between 20 bar to 30 bar, the decrease percentage is 7% while for pressure between 30 bar to 40 bar, the decrease percentage is 5% and for pressure between 40 bar to 50 bar, the decrease percentage is only 4%. Lowest emission of CO is at 50 bar with the value of 0.0429.

4.3.6 Hydrogen gas (H_2)

Table 4.3.6: Mole fraction of H_2 with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	00140	0.0127	0.0118	0.0112

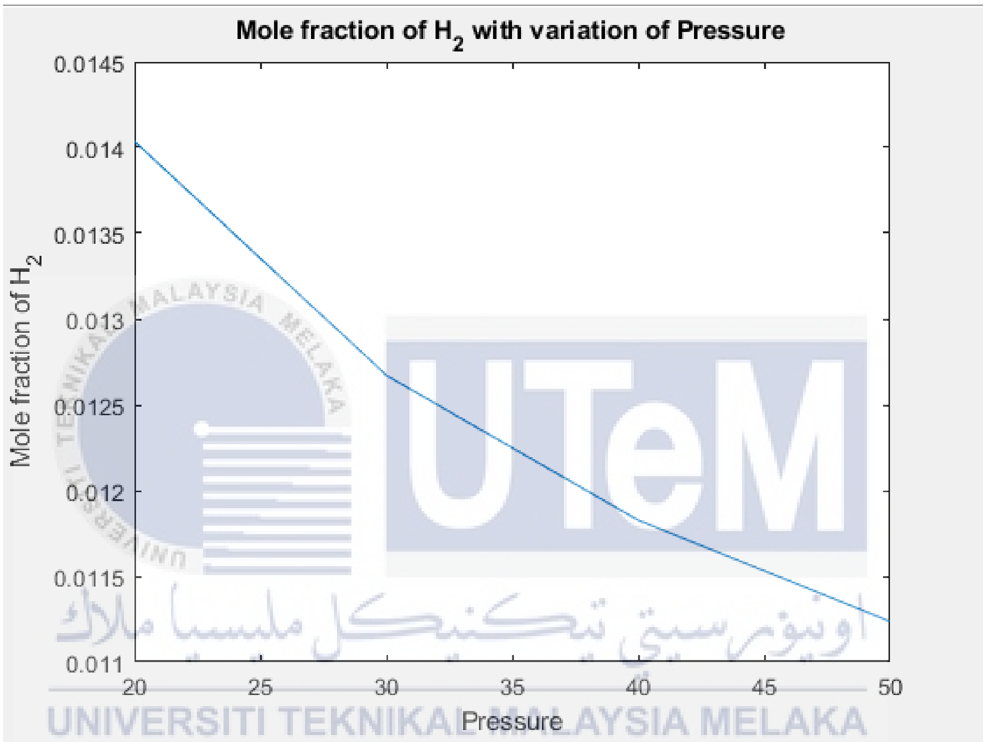


Figure 4.3.6: Mole fraction of H_2 with variation of Pressure

Figure 4.3.6 has the same decrease pattern just like figure 4.3.5. The mole fraction of H_2 decreases when the pressure is increase. Lowest mole fraction obtained is at pressure of 50 bar, with value of 0.0112.

4.3.7 Hydrogen atom (H)

Table 4.3.7: Mole fraction of H with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.0042	0.0032	0.0027	0.0024

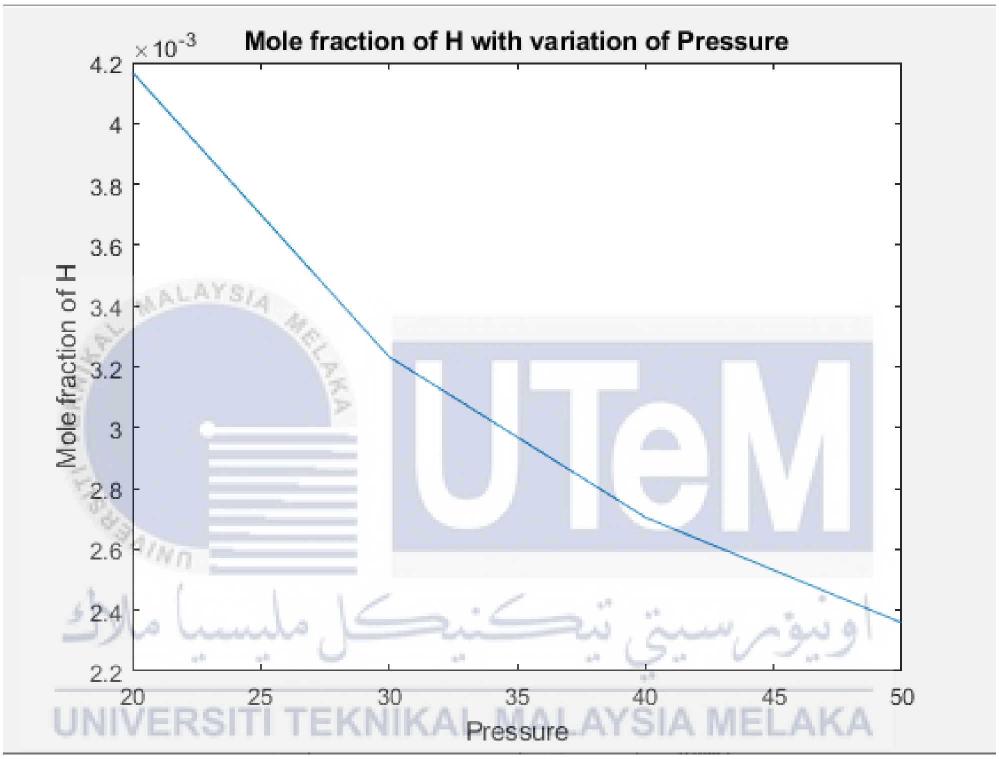


Figure 4.3.7: Mole fraction of H with variation of Pressure

From figure 4.3.7, the pattern that can be observed from the graph is decreasing with different percentage of decrease for increment of 10 bar of pressure. The higher the pressure, the lower the emission of H for the combustion of gasoline with H_2O_2 addition.

4.3.8 Oxygen atom (O)

Table 4.3.8: Mole fraction of O with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.0030	0.0022	0.0018	0.0015

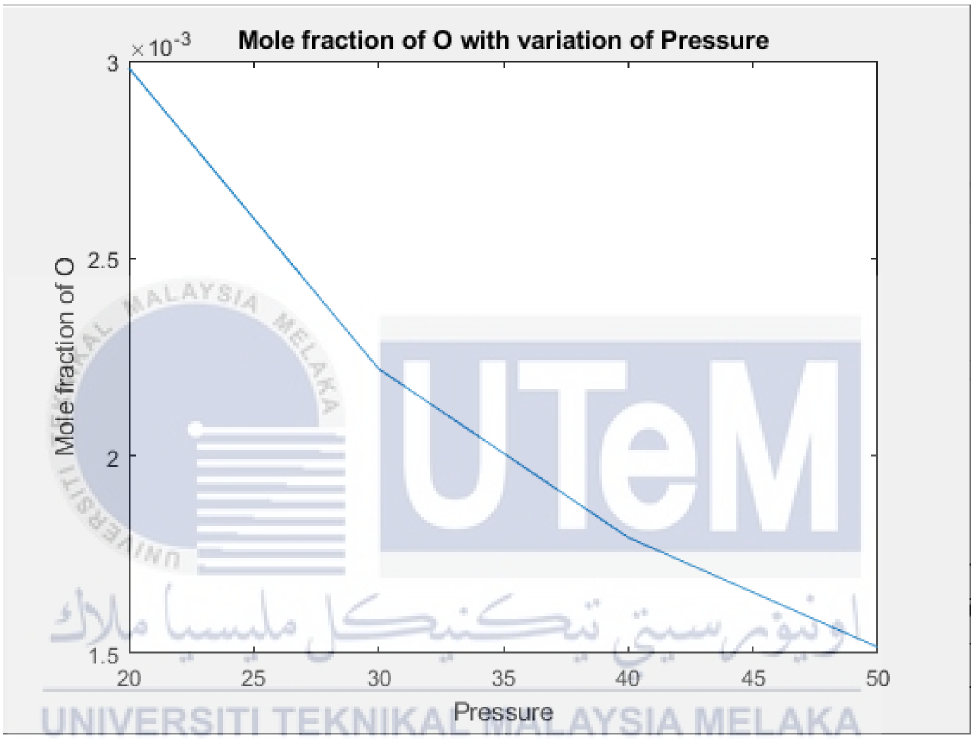


Figure 4.3.8: Mole fraction of O with variation of Pressure

The fraction of mole for O obtained in the combustion product is very small during low pressure of combustion that is at 20 bar. Although the pressure increase, the emission of O is decreasing as shown in the figure 4.3.8, that is only 0.0015 at pressure of 50 bar. Complete combustion occurs frequently, causing formation of incomplete compound is little. Thus, emission of O also decreasing with the increasing of pressure.

4.3.9 Hydroxide (OH)

Table 4.3.9: Mole fraction of OH with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.1146	0.1045	0.0975	0.0921

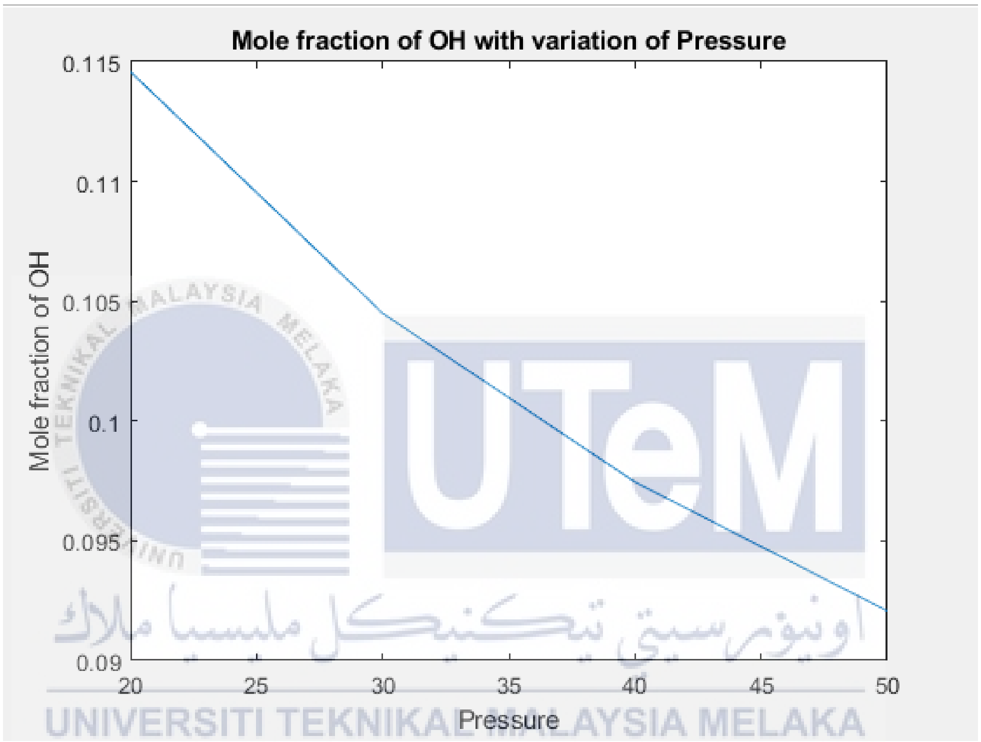


Figure 4.3.9: Mole fraction of OH with variation of Pressure

Emission of OH decreases as the pressure increase. The percentage of decrease for the mole fraction is about 21% throughout the process. This is because of the complete combustion that occur more often compared to incomplete combustion, causing the emission of OH decreases.

4.3.10 Nitrogen Oxide (NO)

Table 4.3.10: Mole fraction of NO with variation of Pressure

Pressure (bar)	20	30	40	50
Mole Fraction	0.0120	0.0110	0.0102	0.0097

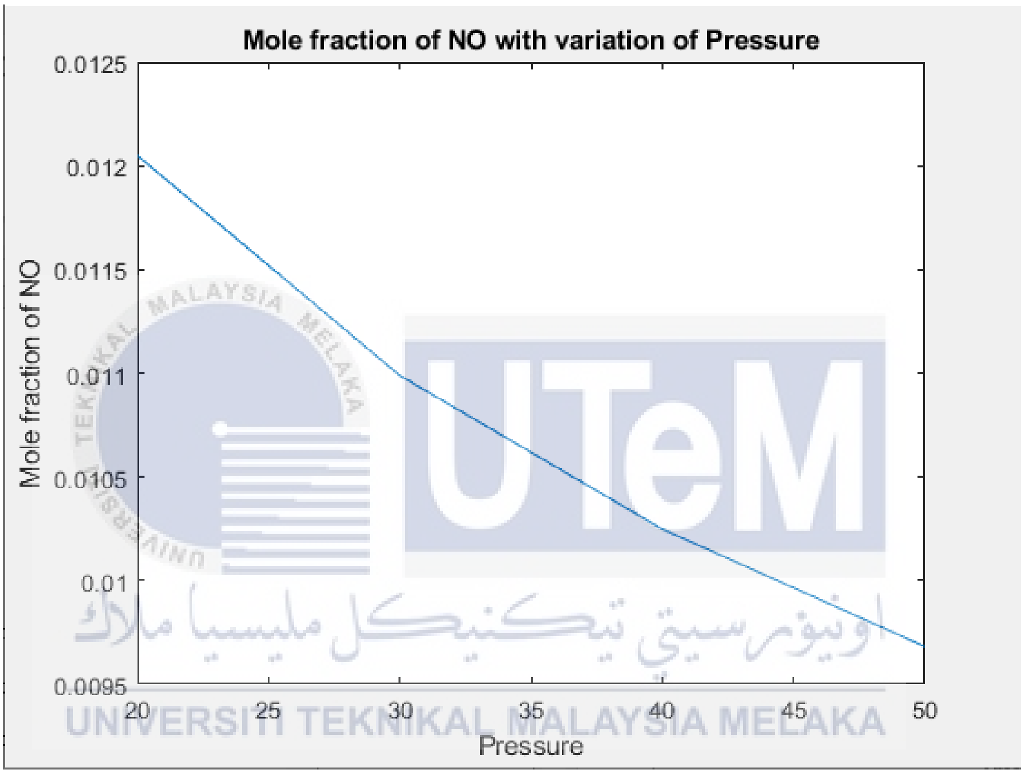


Figure 4.3.10: Mole fraction of NO with variation of Pressure

As observed, we can see similar pattern for mole fraction of emission product from Figure 4.3.4 to Figure 4.3.10 that is combustion products of O_2, CO, H_2, H, O, OH and NO decreases as the value of pressure increase. The lowest emission of NO can is recorded at pressure of 50 bars, that is 0.0097.

CHAPTER 5

CONCLUSION AND RECOMMENDATION FOR FUTURE WORK

5.1 Conclusion

Mathematical modelling has been successfully used to calculate the mole fraction for the combustion products of spark ignition engine with hydrogen peroxide addition. There are total of 10 combustion products that are observed to study the effect of variables equivalence ratio (0.4 - 1.4), temperature (1500 – 3000 K) and pressure (20 – 50 bars) on the emission characteristics of the combustion products. Equivalence ratio can be obtained by dividing the mass of air by the mass of fuel. The fuel used is gasoline with hydrogen peroxide addition.

For the first study, equivalence ratio is manipulated with values range from 0.4 to 1.4 while temperature and pressure are kept constant. First, as observed from graph of CO_2, mole fraction of CO_2 increase during lean combustion (ϕ<1) and peak value is recorded at stoichiometric combustion (ϕ=1). As it enters rich combustion (ϕ>1), the mole fraction of CO_2 decreases as the equivalence ratio increase. Next, mole fraction of H_2O, CO, H_2 and H has the same pattern where lowest mole fraction are obtained at lowest equivalence ratio and since then the value increases as the equivalence ratio increase. Then, for mole fraction of N_2, O_2, O, OH and NO, the higher the equivalence ratio, the smaller the mole fraction of the species obtained during the combustion.

Second study is focusing on effect of temperature of combustion to the combustion products with constant equivalence ratio and pressure. From the result, most of the combustion products have significant changes when the temperature exceeds 2500K except for N_2 where the temperature does not affect the emission of N_2. For CO_2, the mole fraction slightly decreases with the increase of temperature. As the temperature exceed 2500K, drastic decrease occurs to the emission of CO_2. Next, the increase of temperature has a positive impact to H_2O where the graph has increase pattern and significant increase in H_2O emission recorded when temperature exceed 2500K. Similar pattern observed for the emission of mole fraction of O_2, CO, H, O, OH and NO where the emission decreases as the temperature of combustion increase. Significant decrease recorded for the species at temperature exceed 2500K. For H_2, the mole fraction decrease as the temperature getting higher but as it reaches 2500K, the emission of H_2 increase significantly.

Third study is about the effect of pressure to the emission of combustion product. From the observation, the increase of combustion pressure has a positive impact on CO_2 and H_2O where the mole fraction of both product increase along with the pressure. The opposite result is recorded for O_2, CO, H_2, H, O, OH and NO where the increase in pressure causing the mole fraction of the products decrease. Nothing changes for N_2 where the mole fraction is the same although the pressure is changed.

The simulation works successfully and accurate that the most ideal condition for combustion of spark ignition engine with hydrogen peroxide addition can be obtain. From the result, the most ideal condition for combustion is during lean combustion($\boldsymbol{\phi}$>1), lower temperature (1500K) and higher pressure (50 bar) respectively to obtain stable and efficient combustion with lower emission of toxic combustion product such as Nitrogen Oxide (NO) and Carbon Monoxide (CO).

5.2 Recommendation for Future Work

For the recommendation for future work, a spark ignition engine does not emit exactly 10 type of emission products as used during this study. It may be lesser or more types of compounds emitted during the combustion, depending on the situation such as type of fuel used, technologies used by the engine or other related event that effecting the combustion products of the SI engine. Thus, mathematical modelling covering on more larger types of emission product can be conducted for future works.

Then, the advantage of hydrogen peroxide for being a good oxidizing agent helps gasoline fuel to perform efficient and complete combustion in the combustion chamber. However, CO_2 emission must still be taken into account. For future work, hydrogen peroxide can be mixed with other compound as fuel additive, so the hydrocarbon fuel-based technology can reduce CO_2 emission that has been a serious threat for the environment, thus creating a safer world for the mankind and other living creatures.

Lastly, to determine the efficiency or accuracy of the simulation programme used, experiments can be performed based on the simulations programme done. This can strengthen the theoretical data obtain for the use of future works.

APPENDICES

A. MATLAB coding for Mole fraction of every combustion product with variation of Equivalence Ratio, ϕ. (Only part of the coding is presented to avoid code stealing)

```
clear all
clc
close all

% Mathematical modelling on the effect of equivalence ratio in emission
% Characteristic of spark ignition engine with hydrogen peroxide
addition.

T = 3000;               % Temperature
t = T/10000;
P = 30;                 % Total Pressure
eqratio = 0.4:0.2:1.4;  % Equivalence Ratio

% Curve fit Coefficient
A = [+0.432168e+00 +0.310805e+00 -0.141784e+00 +0.150879e-01 -
0.752364e+00 -0.415302e-02];
B = [-0.112464e+05 -0.129540e+05 -0.213308e+04 -0.470959e+04
+0.124210e+05 +0.148627e+05];
C = [+0.267269e+01 +0.321779e+01 +0.853461e+00 +0.646096e+00 -
0.260286e+01 -0.475746e+01];
D = [-0.745744e-04 -0.738336e-04 +0.355015e-04 +0.272805e-05 +0.259556e-
03 +0.124699e-03];
E = [+0.242484e-08 +0.344645e-08 -0.310227e-08 -0.154444e-08 -0.162687e-
07 -0.900227e-08];

for j=1:6
    log10K(j) = A(j)*log(T/1000) + B(j)/T + C(j) + D(j)*T + E(j)*T*T;
    K(j) = 10^log10K(j);
end

partialY1 = K(6)*sqrt(P);
partialY2 = K(5)*sqrt(P);
partialY7 = K(1)/sqrt(P);
partialY8 = K(2)/sqrt(P);
partialY9 = K(3);
partialY10 = K(4);

lnk = 2.743 - (1.761/t) - (1.611/t^2) + (0.2803/t^3);
k = exp(lnk);
matY = zeros(6,10);
for i=1:size(eqratio,2)

    alpha = 7;                             % Carbon
    beta = 19;                              % Hydrogen
    gamma = 2;
    delta = 0;
    as = alpha+(beta/4)-0;
    gamma = gamma + (2*as/eqratio(i));      % Oxygen
```

B. MATLAB coding for Mole fraction of every combustion product with variation of Temperature, T (Only part of the coding is presented to avoid code stealing)

```
clear all
clc
close all

% Mathematical modelling on the effect of temperature in emission
% characteristic of spark iginition engine with hydrogen peroxide
addition.

% Curve fit Coefficient
A = [+0.432168e+00 +0.310805e+00 -0.141784e+00 +0.150879e-01 -
0.752364e+00 -0.415302e-02];
B = [-0.112464e+05 -0.129540e+05 -0.213308e+04 -0.470959e+04
+0.124210e+05 +0.148627e+05];
C = [+0.267269e+01 +0.321779e+01 +0.853461e+00 +0.646096e+00 -
0.260286e+01 -0.475746e+01];
D = [-0.745744e-04 -0.738336e-04 +0.355015e-04 +0.272805e-05 +0.259556e-
03 +0.124699e-03];
E = [+0.242484e-08 +0.344645e-08 -0.310227e-08 -0.154444e-08 -0.162687e-
07 -0.900227e-08];


Temp = 1500:500:3000;    % Temperature
P = 30;                  % Total Pressure
eqratio = 1.2;           % Equivalence Ratio

alpha = 7;              % Carbon
beta = 19;               % Hydrogen
gamma = 2;
delta = 0;
as = alpha+(beta/4)-0;
gamma = gamma + (2*as/eqratio);       % Oxygen
delta = delta + (7.52*as/eqratio);    % Nitrogen

d1 = beta/alpha;
d2 = gamma/alpha + (2*as/(eqratio*alpha));
d3 = delta/alpha + (7.52*as/(eqratio*alpha));

d = 2*as*(1-(1/eqratio));

matY = zeros(4,10);


for i=1:size(Temp,2)
    t = Temp(i)/10000;
    T = Temp(i);

    for j=1:6
        log10K(j) = A(j)*log(T/1000) + B(j)/T + C(j) + D(j)*T + E(j)*T*T;
```

C. MATLAB coding for Mole fraction of every combustion product with variation of Pressure, P. (Only part of the coding is presented to avoid code stealing)

```
clear all
clc
close all

% Mathematical modelling on the effect of equivalence ratio in emission
% characteristic of spark ignition engine with hydrogen peroxide
addition.

% Curve fit Coefficient
A = [+0.432168e+00 +0.310805e+00 -0.141784e+00 +0.150879e-01 -
0.752364e+00 -0.415302e-02];
B = [-0.112464e+05 -0.129540e+05 -0.213308e+04 -0.470959e+04
+0.124210e+05 +0.148627e+05];
C = [+0.267269e+01 +0.321779e+01 +0.853461e+00 +0.646096e+00 -
0.260286e+01 -0.475746e+01];
D = [-0.745744e-04 -0.738336e-04 +0.355015e-04 +0.272805e-05 +0.259556e-
03 +0.124699e-03];
E = [+0.242484e-08 +0.344645e-08 -0.310227e-08 -0.154444e-08 -0.162687e-
07 -0.900227e-08];


T = 3000;          % Temperature
t = T/10000;
P = 20:10:50;      % Total Pressure
eqratio = 1.2;     % Equivalence Ratio
matY = zeros(4,10);

lnk = 2.743 - (1.761/t) - (1.611/t^2) + (0.2803/t^3);
k = exp(lnk);

alpha = 7;        % Carbon
beta = 19;         % Hydrogen
gamma = 2;
delta = 0;
as = alpha+(beta/4)-0;
gamma = gamma + (2*as/eqratio);       % Oxygen
delta = delta + (7.52*as/eqratio);    % Nitrogen

d1 = beta/alpha;
d2 = gamma/alpha + (2*as/(eqratio*alpha));
d3 = delta/alpha + (7.52*as/(eqratio*alpha));

d = 2*as*(1-(1/eqratio));

a1 = 1-k;
b1 = (beta/2) + k*alpha - d*(1-k);
c1 = -alpha*d*k;

n5 = (-b1 + sqrt(b1^2-4*a1*c1))/(2*a1);
n1 = alpha - n5;
n2 = beta/2 - d + n5;
n3 = 3.76*as/eqratio;
```

REFERENCES

Abdollahi, M., & Hosseini, A. (2014). Hydrogen Peroxide. In *Encyclopedia of Toxicology: Third Edition* (Third Edit, Vol. 2). Elsevier. https://doi.org/10.1016/B978-0-12-386454-3.00736-3

Adlan, Z. S., Adnan, R., Munir, F. A., Thazaly, M. Z., & Najib, M. A. W. (2018) *Performance and emission characteristics for petrol engine with H 2 O 2 addition*. 2–5.

Adnan, R., Masjuki, H. H., & Mahlia, T. M. I. (2011). Mathematical modeling on the effect of equivalence ratio in emission characteristics of compression ignition engine with hydrogen substitution. *Applied Mathematics and Computation*, *217*(13), 6144–6158. https://doi.org/10.1016/j.amc.2010.12.096

Adnan, R., Sabri Adlan, Z., Munir, F. A., & Asnawi, M. O. (2018). Experimental study on the effect of intake air temperature on the performance of spark ignition engine fueled with hydrogen peroxide. *ARPN Journal of Engineering and Applied Sciences*, *13*(10), 3388–3394.

Born, C., & Peters, N. (1998). Reduction of soot emission at a di diesel engine by additional injection of hydrogen peroxide during combustion. *SAE Technical Papers*, *724*. https://doi.org/10.4271/982676

Chaichan, M. T. (2015). *CYLINDER S . I . ENGINE FUELED WITH DIFFERENT KINDS OF HYDROCARBON EXPERIMENTAL COMPARISON OF CO EMISSIONS EMITTED FROM SINGLE CYLINDER S . I . ENGINE FUELED WITH DIFFERENT KINDS OF□□□ CO □□□□ □□□□□□ □□□□□□ □□□□□ □□□□□□□*

□□□□□□□□□. *February*.

Damyanov, A., & Hofmann, P. (2019). Operation of a diesel engine with intake manifold alcohol injection. *Automotive and Engine Technology*, *4*(1–2), 17–28. https://doi.org/10.1007/s41104-019-00040-2

El Morabet, R. (2019). Effects of outdoor air pollution on human health. In *Encyclopedia of Environmental Health* (2nd ed.). Elsevier Inc. https://doi.org/10.1016/B978-0-12-409548-9.11509-X

Encyclopedia, B. O. (2021). *6/9/2021 Gasoline -- Britannica Online Encyclopedia*. 1–2.

Ferguson, C. R., & Kirkpatrick, A. T. (2016). *Internal Combustion Engine* (Third Edit).

Francqueville, L., Michel, J., & Nouvelles, I. F. P. E. (2014). *On the Effects of EGR on Spark-Ignited Gasoline Combustion at High Load*. https://doi.org/10.4271/2014-01-2628

Guo, H., Liko, B., Luque, L., & Littlejohns, J. (2018). *ICEF2017-3585 COMBUSTION PERFORMANCE AND UNBURNED HYDROCARBON EMISSIONS OF A NATURAL GAS – DIESEL DUAL FUEL ENGINE AT A LOW LOAD CONDITION*. 1–9.

HE, L. Y., & QIU, L. Y. (2016). Transport demand, harmful emissions, environment and health co-benefits in China. *Energy Policy*, *97*(15), 267–275. https://doi.org/10.1016/j.enpol.2016.07.037

Jiang, X., Mei, X., & Feng, D. (2016). *Air pollution and chronic airway diseases : what should people know and do ? 2012*(1), 31–40. https://doi.org/10.3978/j.issn.2072-1439.2015.11.50

Kayadelen, H. K., & Ust, Y. (2013). Prediction of equilibrium products and thermodynamic properties in H 2O injected combustion for CαH βOγNδ type fuels. *Fuel*, *113*(x), 389–401. https://doi.org/10.1016/j.fuel.2013.05.095

Kumar, S., Gupta, S. K., & Rawat, M. (2019). Resources and utilization of geothermal energy in India: An Eco - friendly approach towards sustainability. *Materials Today: Proceedings*, *26*(xxxx), 1660–1665. https://doi.org/10.1016/j.matpr.2020.02.347

Lee, L. C. W. (2001). An investigation of a cause of backfire and its control due to crevice volumes in hydrogen fueled engine. *Journal of Engineering for Gas Turbines and Power*, *123*(1), 204–210. https://doi.org/10.1115/1.1339985

Liu, G., Yan, B., & Chen, G. (2013). Technical review on jet fuel production. *Renewable and Sustainable Energy Reviews*, *25*, 59–70. https://doi.org/10.1016/j.rser.2013.03.025

Manias, D. M., Tingas, E. Al, Frouzakis, C. E., Boulouchos, K., & Goussis, D. A. (2016). The mechanism by which CH2O and H2O2 additives affect the autoignition of CH4/air mixtures. *Combustion and Flame*, *164*, 111–125. https://doi.org/10.1016/j.combustflame.2015.11.008

Muhammad Saad Khan, Hassan, Z. Bin, & Iqbal, A. (2009). Influence of Hydrogen Peroxide on Liquefied Petroleum Gas (Lpg) Performance. *National Conference on Postgraduate Research (NCON-PGR) 2009*, *October*, 107–113

Olikara, C., & Borman, G. L. (1975). A computer program for calculating properties of equilibrium combustion products with some applications to I.C. engines. *SAE Technical Papers*. https://doi.org/10.4271/750468

Oor, G. U. G., Ag, D., Lenneberg, R. G., & Ag, D. (2000). *Hydrogen Peroxide*.

https://doi.org/10.1002/14356007.a13

Pourkhesalian, A. M., Shamekhi, A. H., & Salimi, F. (2010). Alternative fuel and gasoline in an SI engine : A comparative study of performance and emissions characteristics. *Fuel*, *89*(5), 1056–1063. https://doi.org/10.1016/j.fuel.2009.11.025

Schultze, M., & Mantzaras, J. (2013). Hetero-/homogeneous combustion of hydrogen/air mixtures over platinum: Fuel-lean versus fuel-rich combustion modes. *International Journal of Hydrogen Energy*, *38*(25), 10654–10670. https://doi.org/10.1016/j.ijhydene.2013.06.069

Srivastava, S.P., Hancsok, J. (2014). *Fuels and fueladditives*.

Tajudin, M. A. B. A., Khan, M. F., Mahiyuddin, W. R. W., Hod, R., Latif, M. T., Hamid, A. H., Rahman, S. A., & Sahani, M. (2019). Risk of concentrations of major air pollutants on the prevalence of cardiovascular and respiratory diseases in urbanized area of Kuala Lumpur, Malaysia. *Ecotoxicology and Environmental Safety*, *171*(December 2018), 290–300. https://doi.org/10.1016/j.ecoenv.2018.12.057

Xu, H., & Yang, D. (2020). LNG-fuelled container ship sailing on the Arctic Sea : Economic and emission assessment. *Transportation Research Part D*, *87*(September), 102556. https://doi.org/10.1016/j.trd.2020.102556

Yusof, Z. A. M., Ahmed, I., Khan, M. S., Hussain, S. A., Hussain, A., Mutalib, I. bin A., Balkhair, K. S., & Albeirutty, M. H. (2015). Thermal Evaluation of Diesel/Hydrogen Peroxide Fuel Blend. *Chemical Engineering and Technology*, *38*(12), 2170–2180. https://doi.org/10.1002/ceat.201400039

Zhou, A., Zhang, C., Li, Y., Li, S., & Yin, P. (2019). Effect of hydrogen peroxide additive on the combustion and emission characteristics of an n-butanol homogeneous charge compression ignition engine. *Energy*, *169*, 572–579. https://doi.org/10.1016/j.energy.2018.12.076