

**MATHEMATICAL MODELLING ON THE EFFECT OF EQUIVALENCE RATIO
IN EMISSION CHARACTERISTIC OF COMPRESSION IGNITION ENGINE
WITH BIODIESEL FUEL**

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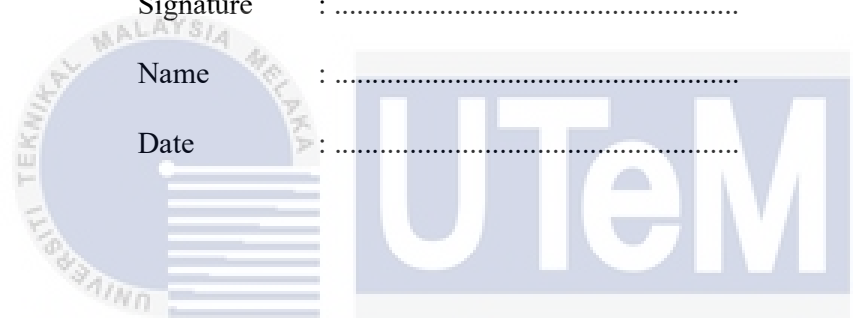
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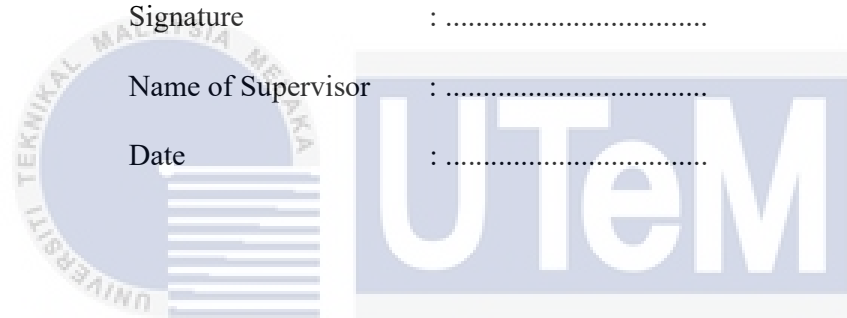
APPROVAL

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.

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DEDICATION

To my beloved mother and father



ABSTRACT

In this study, the mathematical modelling on the effect of equivalence ratio in emission characteristic of compression ignition engine with biodiesel fuel is discussed in the methodology section. The increasing needs for fuel in everyday life, as well as the dangers associated with it, pose a severe threat to the world. Attention must be paid to this issue in order to recognise it. This study is performed to prove that the biodiesel fuel has many advantages compare to the diesel fuel. In the literature review section, the general knowledge about the biodiesel are explain including the production of biodiesel, the technique used to produce the biodiesel and all the costing need to produce the biodiesel fuel. There will be a simulation using a MATLAB and Microsoft Excel software to calculate the mole fractions of the product in the chemical reaction of the biodiesel fuel. Then, every graph of the mole fraction of every product will be explained briefly in Chapter 4. The emission of combustion product like carbon dioxide, carbon monoxide and nitrogen oxide that may affect the environment will be discussed.

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ABSTRAK

Dalam projek ini, pemodelan matematik mengenai kesan nisbah kesetaraan dalam pelepasan ciri-ciri enjin penyalaan mampatan dengan biodiesel terdapat dalam bahagian metodologi. Keperluan bahan api yang semakin meningkat dalam kehidupan seharian serta bahaya yang berkaitannya telah menimbulkan ancaman yang teruk kepada dunia. Perhatian mesti diberikan kepada isu ini untuk mengenalinya. Kajian ini dilakukan untuk membuktikan bahawa bahan api biodiesel mempunyai banyak kelebihan berbanding dengan bahan api diesel. Dalam bahagian kajian literatur, pengetahuan am tentang biodiesel diterangkan termasuk penghasilan biodiesel, teknik yang digunakan untuk menghasilkan biodiesel dan semua keperluan kos untuk menghasilkan bahan api biodiesel. Akan ada simulasi menggunakan perisian MATLAB dan 'Microsoft Excel' untuk mengira pecahan mol produk dalam tindak balas kimia bahan api biodiesel. Kemudian, setiap graf pecahan mol setiap produk akan diterangkan secara ringkas dalam bab 4. Pembebasan produk pembakaran seperti karbon dioksida, karbon monoksida dan nitrogen dioksida yang boleh menjejaskan alam sekitar akan dibincangkan.

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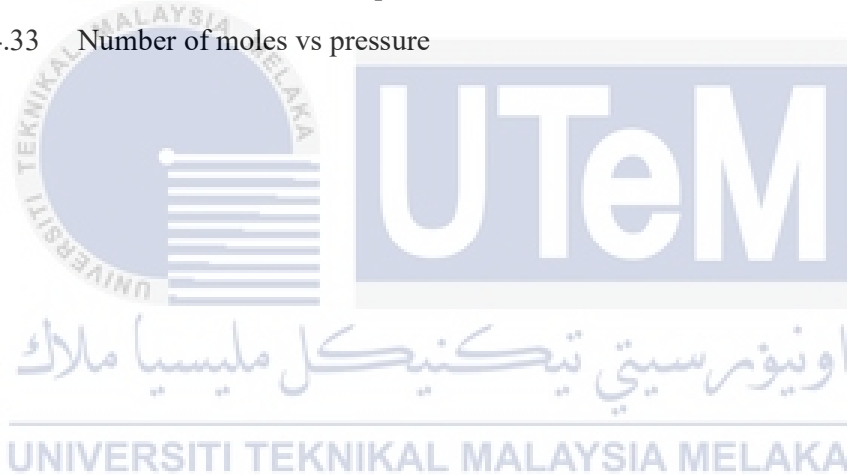
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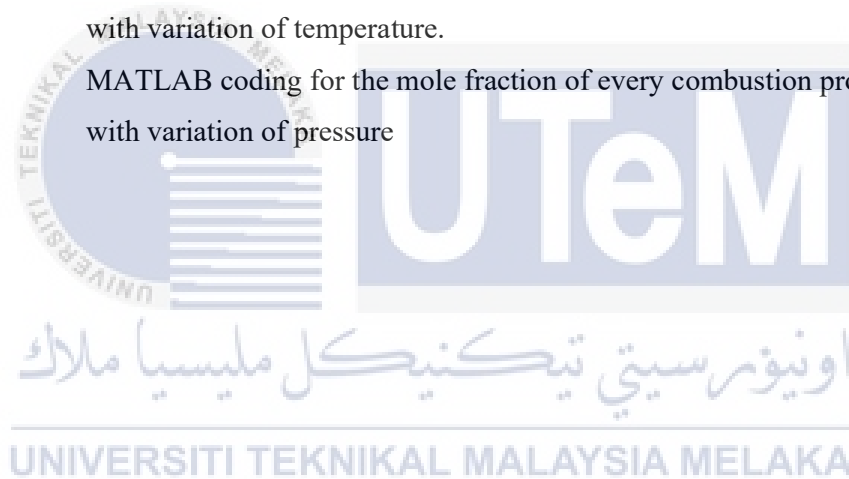


LIST OF ABBREVIATIONS

PM	-	Particulate Matter
KOH	-	Potassium Hydroxide
SO ₂	-	Sulphur Dioxide
CO	-	Carbon Monoxide
CO ₂	-	Carbon Dioxide
NO ₂	-	Nitrogen Oxide
N ₂	-	Nitrogen gas
OH	-	Hydroxide
H ₂ O	-	Water
O ₂	-	Oxygen
GHG	-	Greenhouse Gas
FAME	-	Fatty Acid Methyl Ester
CI	-	Compression Ignition
FFA	-	Free Fatty Acid
GCFID	-	Gas Chromatography-Flame Ionisation Detector
GCMS	-	Gas Chromatography-Mass Spectroscopy Detector
ASTM	-	American Society for Testing and Materials
EN	-	European Union

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CHAPTER 1

INTRODUCTION

1.1 Background

Nowadays, people are really taking care the importance of the used of energy and technology that are not harmful to the environment. There is some renewable energy that has been identified as a good resource that can replaced the old source that has been used for a long time. Biodiesel can be said as the alternative fuel that can be used to replace the used of the diesel that are not eco-friendly to this world. Biodiesel can be made by some methods of production, and it will be discussed and explained briefly in the next chapter. The process to make this biodiesel is also quite expensive for some methods because of their operating costs and the processing time that are longer. Those method are known as biocatalyst and supercritical fluid processes and this method has rarely been used in the industrial. The other factor is because of the enzymes use has higher cost besides it also has slow rate of reaction. The developments of the catalysts in the biodiesel production are still investigated by the researcher around the world.

In the transportation sector, diesel is the most used as the source of energy and this scenario has led to the pollution of air and water. Thus, the researchers are now focused on to how to make a biodiesel fuel that are appropriate to the engine that are used in the most automobiles. A various resource of feedstock which has edible or non-edible along the methyl esters are investigated in order to find the most suitable for biodiesel fuel. There are some advantages of using biodiesel instead of other types of petroleum that has been researched such as it has better lubricity, has low sulphur content and it also a biodegradable which helps in improve the aquatic ecosystem. Biodiesel also helps to clean the engine of

the automobiles and it can reduce the greenhouse gas (GHG) emission. The most important thing if we want a biodiesel to be widely used is every country need to have their own biodiesel production in their industrial and make sure every resource is sufficient to be used in a long term or else these alternative fuels cannot be used in future.

The combustion process in the engine will be much early when biodiesel is used as the major source of energy because it has higher number of cetane number. Biodiesel can be compared with diesel that are now has been widely used in term of the cetane number and it can reduce the ignition delay period and it will make the pressure inside the cylinder engine higher.

Most of the article that has been used as references are discussing more about the biodiesel and the effects of using biodiesel in the compression ignition engine. Due to the difficulties involved in the experiment that are conducted by the researcher, they are also used a predictions and suggestions methods although it is not preferred but it is also helps to give a better data and results of their researched. Most of the analysis of the project are using a software such as Microsoft Excel and MATLAB and more data can be obtained by using different input to get various results to be compared with each other. MATLAB program also assist in giving the graphs that are needed for this research and from the graph, the difference of mole fractions of the substances or components with variation of equivalence ratio will be seen.

1.2 Problem Statement

People nowadays are preferred to use automobiles in their daily life as it can make their daily affairs easier and there are about 550 million of automobiles used by people around the world and this scenario will be continuously used from time to time. This scenario has led to some other major problems where the source of energy in this world are decreasing and it also has led to environmental pollution like air and water pollution. All the professional people around the world that are related to this problem are now thinking to reduce greenhouse gas emissions and proactive steps have to be taken so that it can be stopped before it is too late to handle the problems. The other solution that can help to reduce the problems is by finding a new source of energy that is cleaner and does not give any pollution to the environment.

Most of the researchers around the world are now preferred to use biodiesel as the new source of energy to replace old diesel fuel that has been proved are not eco-friendly to this world. This biodiesel fuel is actually has been used nowadays and there are some advantages that can be obtained by using this fuel such as it helps to increase the water quality and the aquatic ecosystem. All the sources that are used to make biodiesel such as corn oil, palm oil and rapeseed oil has been proved that all of it can give a high biodegradation rate in the water ecosystem. The biodegradation level also can be increased through the co-metabolism with the presence of biodiesel. There is also a researcher that did an experiment and it showed the primary molecules in the biodiesel which is the fatty acid methyl ester has been degraded so much faster than the diesel in sea water.

1.3 Objective

There are some objectives that has been targeted for this project like:

1. To solve all the equation from the chemical equation of biodiesel by using mathematical modelling method assist by MATLAB program.
2. To study the other alternative of renewable fuel that can be used in the future.
3. To illustrate the engine performance, fuel properties and the emission characteristics of biodiesel fuel at different conditions.
4. To study the number of moles of every combustion product at variation of equivalence ratio, temperature and pressure.
5. To analyse the emission of the combustion products that cause the environmental pollution of the air.

1.4 Scope of the Project

The scope of the project that will be discussed are:

1. This research has been specific to use the biodiesel as a main substance that is used in the compression ignition engine.
2. This research is only required to solve the unknown in the chemical equation based on the substances in the biodiesel product.
3. All the calculation can be calculated manually by using every step that needed in a curtain formula that is used to solve the unknown.
4. MATLAB program is another platform that can be used to solve all the calculation and some graph can be obtained from it that may be help in the research purpose.

1.5 General Methodology

For this semester, there are some methods that are chosen to be used and the other will be continued on the next semester. To accomplish the objective of this project, the actions are listed below.

1. Literature review

There is about 50 journals and articles that have been used as the guidelines and references in order to complete these researched. Most of the articles were discussed related to the title of the project.

2. Calculation

All the governing equations need to be calculated by following all the steps in the article or any other references. There will be some other formula that needed to solve the equation like Newton Raphson method.

3. Simulation

Simulation of the compression ignition engine will be made based on the chemical equation of biodiesel components and products.

4. Analysis and proposed solution

Analysis will be presented on how the effect of equivalence ratio in emission characteristic of compression ignition engine with biodiesel fuel. Solutions will be proposed based on the data that has been collected and analysed.

5. Report writing

A full report will be written and all the calculation and data that has been achieved will be discussed briefly in this report.

CHAPTER 2

LITERATURE REVIEW

2.1 What is biodiesel

As previously stated, biodiesel can be defined as alkyl fatty acid esters such as ethyl fatty acid esters, methyl ester of fatty acid esters, and propyl esters of fatty acid esters that can be obtained through the reactions of the transesterification process of animal fats or plant oils using short chain fatty acids such as methanol and ethanol. The use of alternate solution or renewable fuels can play a significant role in lowering fossil fuel usage and, thus, in reducing carbon dioxide emissions.

An example of a renewable element that may be added to gasoline and result in a reduction in fossil fuel usage is ethanol, which is created from biomass from food crops that is commonly thrown away. Similarities exist for compression ignition engines, where fatty acid methyl ester, also known as FAME, is created from vegetable oil, generally generated from seeds, and has been added to diesel fuel for a long period of time to prolong the life of crude oil-derived fuels. Because it offers engine efficiency that is equivalent to regular diesel, biodiesel is expected to be employed in diesel engines in the future. When utilised in conjunction with diesel, biodiesel may be utilised in both blended and pure form.

In addition to its non-explosive, non-flammable, non-toxic, and recyclable qualities, biodiesel also has the ability to reduce a variety of harmful exhaust emissions. With no sulphur oxide pollutants, no particle or soot emissions are produced, and heavy hydrocarbons emissions can be reduced. However, there are some downsides to using biodiesel, such as the fact that it can enhance nitrogen oxide emissions, has poor low temperature flow

qualities, and is subject to more stringent environmental laws when compared to traditional diesel fuel (Rashedul et al., 2014). Because it includes double bond bonds in the free fatty acid, biodiesel fuel has a low chemical stability, which is another drawback of the fuel.

With the presence of bio-based fuels, there is an additional hurdle in the usage of these fuels, for which a variety of additives can bring significant advantages. All of the aspects, including the reduction of the possibility for enhanced injector deposit development, oxidation stability, bad influence on cold flow characteristics, corrosion during long-term storage, and enhanced microbiological contamination, are taken into account. This is an example of where additives serve a valuable and extremely expensive function in reducing the likelihood of operating difficulties and achieving fuel specification standards, which can be difficult or impossible to do without the use of additives.

Additional chemicals should be used to enhance the characteristics of fuel, which are then mixed with fuel such as biodiesel, diesel, aviation oil, natural gas as well as other fuels to optimize the effectiveness of the fuel and the economy as a whole. Additives are used to promote the properties of fuel and are used in a variety of fuels, including biodiesel and diesel. In addition, additives increase the fuel's ability to fulfil environmental pollution control standards as well as the performance of the vehicle's engine. The economic feasibility, blending property, toxicity, additive solubility, viscosity of the fuel blend, solubility of water in the blend, flash point of the fuel blend, and water partitioning of the addition are all factors to consider when selecting additives for biodiesel fuel on gasoline. The usage of biodiesel in the modern world has provided us with a promising option. Not only does it have the potential to minimise reliance on traditional diesel fuel, but it is also a clean energy source that may be utilised for an extended length of time if handled properly.

2.2 The production of biodiesel

There are many various manufacturing procedures used in the production of biodiesel as CI diesel engines across the world today, and each one should be recognized and made accessible to those who are just starting out in their careers in the industry (Datta & Mandal, 2016). Each country's raw resources requirements differ from one another in a manufacturing environment. Researchers are working hard to develop new ways to make biodiesel from a variety of feedstock, including vegetable oil (neither edible nor non-edible), excess cooking oil, animal tallow, and algae, among other things.

There is much increased in number of viscosities in the oils and fats that have been formed from the material that has been acquired, and they are thus unsuitable for use in conventional CI engines. In order to lower the viscosity number, the first and most crucial step is to use a chemical process known as transesterification to accomplish this. During this reaction, the triglyceride contained in the oil or fat combines with an alcohol like as methanol and ethanol, while also there are the catalysts that is alkaline in nature is available to accelerate the reaction. This method requires the use of a catalyst, such as sodium or potassium hydroxide, as the examples. Glycerol, commonly known as glycerin, is formed as a byproduct of the production of other substances. The equation below depicts the total response of the transesterification reaction.

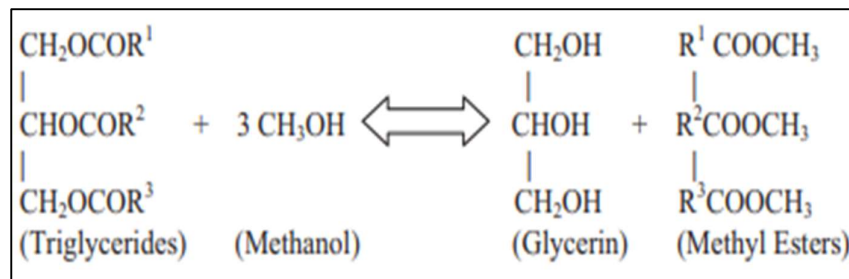


Figure 2.3 Transesterification Process

Methanol is typically employed in the production of biodiesel due to its shorter response time and ease of accessibility. The finished biodiesel fuel is referred to as the methyl ester of the extracted oil that was utilised in its production. Ethyl alcohol is occasionally used in the synthesis of biodiesel however it is not always necessary. The ethyl esters of the relevant oil are referred to as such. As previously stated, transesterification has the potential to be a more cost-effective method of converting the huge and branched chemical composition of bio-oils into the thinner and linear chain molecules necessary for use in conventional diesel engines. Transesterification reactions with 100kgs of oil and 10kgs of methanol generate 100kgs of biodiesel and 10kgs of glycerol, as examples of approximate difference between these two reactants and products. It is possible to create a biodiesel blend by combining pure biodiesel with petro-diesel in the proper amounts. Biodiesel blends are denoted by the letters Bxx, where the 'xx' refers to the percentage of biodiesel in the total volume of biodiesel and petroleum. B85, in contrast, is a combination of 85 percent biodiesel and 15 percent petroleum by volume, which is the most common.

For more than 30 years, biodiesel manufacturing methods have advanced from batch types to semi-continuous flow arrangements and, finally, to full continuous flow arrangements, which are now the standard. Batch type is the most widely used approach, and it continues to be quite popular, particularly in smaller operations. In general, batch types require more people per hour of production for every gallon of product produced when compared to other techniques, although there are certain advantages to adopting batch types. The batch system's advantages include being inexpensive in cost, versatile, and simple to set up and stop down as necessary.

2.3 Techniques to produce biodiesel

The methodologies for producing biodiesel from a variety of raw feedstocks, as described by various authors, are provided in the following section of this chapter. There are many other approaches that may be described, but three of them will be featured in this chapter.

2.3.1 Rapeseed oil as the main source

Two researchers developed a technique for producing biodiesel through all the transesterification process of rapeseed oil, which does not require the use of a catalyst. The reaction step is performed out without the need of a catalyst (Saka & Kusdiana, 2001). An experimental investigation was carried out in a batch-type reaction vessel that has been warmed at 350°C and 400°C and at a pressure of 4565 MPa, with a molar ratio of 1:42 of rapeseed oil to methanol used in the experiment. As a result, it was discovered that at a preheating temperature of 350°C, 240 s of supercritical treatment of methanol was sufficient to transform rapeseed oil to biodiesel, despite the fact that the properties of the biodiesel produced were the same as those obtained using the conventional method with a basic catalyst. Compared to the latter, the former produced significantly greater yields of methyl esters. Furthermore, it was discovered that this novel supercritical methanol approach necessitates a shorter purifying technique as well as a quicker response time due to the absence of a catalyst in the procedure.

2.3.2 Production of biodiesel from plant oils that are both edible and non-edible

Non-edible plant oils which including *Pongamia glabra* (karanja) and *Jatropha curcas*, as well as edible plant oils which including canola and corn, were discovered to be

great resources for the production of biodiesel in laboratory tests (Patil & Deng, 2009). For the purpose of optimising the biodiesel manufacturing process, the production of biodiesel from several types of edible and non-edible plant oils were tested against one another. In the course of the examination of the experiment, the researcher examines the differences between the different fuel qualities, oil characteristics, and process parameter improvement of non-edible and edible plant oils in great detail. The manufacture of biodiesel from rich FFA edible plant oils and non-edible oils was accomplished by a single-step transesterification method and a multiple transesterification method, respectively. Using KOH as a catalyst in the reactions, this technique produces yields of around 80–85 percent for *Pongamia glabra*, 90–95 percent for *Jatropha curcas*, 80–95 percent for canola, and 85–96 percent for maize. The fuel qualities of biodiesel that had been created at the time were compared to those specified by the American Society for Testing and Materials (ASTM).

2.3.3 Biodiesel with used of palm oil

This researcher has taken palm oil that has been obtained from several place at some district at southern India, and then converted it into methyl esters, which are then converted into biodiesel by the transesterification method, as described above (Sharon et al., 2012). The biodiesel, which is made from the palm oil that was utilised at the time, was mixed with the diesel in various volume proportions, with 25 percent, 50 percent, and 75 percent being the most common. After that, the biodiesel and its mixes were studied in a DI diesel engine at steady velocity with varied loads ranging from 20 percent to 100 percent in order to study their emissions, performance, and combustion profile. The findings that were achieved were compared to those obtained with diesel fuel. At full load, the performance of B25 and B50 was comparable to that of diesel, while the smoke density of B75 and B100 was lower than that of diesel by 19 percent and 10 percent, respectively. The observed CO emissions for

B100 and B75 at full load were 52.9 percent and 35.2 percent lower than those for diesel, respectively. B100 and B75 had HC emissions that were 38.09 percent and 19.05 percent lower than diesel, respectively. The amount of NOX emitted by all biodiesel mixes was greater. B75 also produced much less emissions during the course of the test.

It has been demonstrated in the preceding study that biodiesel may be created from a variety of substrates through the transesterification process under a variety of circumstances and with a variety of catalysts, depending on the acidity of the raw feedstocks. The production of biodiesel is not only dependent on the type of feedstocks utilised, but also on the kind and amount of catalyst employed, the molar ratio of alcohol to oil, and the reaction parameters, which include time, temperature, and pressure. Some other important thought to mention is that the yield might not be the same as a particular oil; instead, it is dependent on the fatty acid composition and distribution of the fatty acids, as an acid esterification process may be required prior to the alkaline esterification process in order to lower the acid value of the oil. If just alkaline esterification is utilised in the case of oil containing a high concentration of free fatty acids, this procedure can yield a greater yield of biodiesel.

Table 2.2 The differences between all the techniques

Researchers	Feedstock	Alcohol type	Molar ratio of alcohol to oil	Catalyst	Biodiesel yield
Saka and Kusdiana	Rapeseed oil	Methanol	42:1	NaOH	95%
Patil and Deng	Karanja, jatropa, canola and corn oil	Methanol	9:1	H2SO4 KOH	80%
Sharon	Palm oil	Methanol	6:1	NaOH	87%

2.4 Biodiesel yield

Biodiesel yield is described as the quantity of biodiesel produced from raw oil that includes a certain proportion of fatty acid methyl esters. Methods such as chromatography or spectroscopy are used to characterise biodiesel. Thin-layer chromatography (TLC) is used to tabulated and presented biodiesel (Singh et al., 2020). For the evaluation of monoglycerides, diglycerides and tryglycerides, as well as fatty acids, this approach was selected as the principal approach. It has certain drawbacks, including a high sensitivity to moisture and a limited degree of accuracy. GCFID or GCMS detectors are used in the categorization of biodiesel. Gas chromatography is used in combination with these detectors for biodiesel classification. The precise amounts of main and secondary elements in biodiesel may be determined using gas chromatography. Every component in the data is assigned to a distribution zone using this systematic approach. Analytical methods are used to estimate the approximate quantity of fatty acid methyl esters used in biodiesel manufacture. These may be discovered by the outcomes of a gas chromatography examination performed in the distribution area. It is the percentage of fatty acid methyl esters in a feedstock that is the most essential parameter for determining biodiesel production and it can be determined using equation 1.

$$\text{Production of biodiesel yield} = \text{FAME \%} \times \text{Volume yield} \quad (2.1)$$

The following equation may be used to calculate the percentage yield of biodiesel produced from oil feedstock:

$$\text{Volume yield \%} = \frac{\text{Volume of product}}{\text{Volume of feed}} \times 100 \quad (2.2)$$

It is possible to use infrared spectroscopy to investigate the intricate details of biodiesel and triglycerides in greater detail. Standards such as ASTM D6751 (United States), EN 14213 (European Union), and IS 15607 (India) are used to enhance the integrity of biodiesel produced. These requirements implement to pure biodiesel (B100), not biodiesel blends, and are not applicable to other fuels. The American Society for Testing and Materials (ASTM) is the only organization that develops benchmarks for biodiesel blends.

2.5 Operating Cost

It is also included in the net profit of the production of biofuels the costs associated with raw materials, infrastructure, renovations, workers, servicing, and depreciation (Gebremariam & Marchetti, 2018). These are the most often encountered raw materials: crude oil feedstock, ethanol, washing water, catalyst, and other raw materials. In all biodiesel production systems, the cost of production contributed for the entire cost of operation. This is exacerbated if pure vegetable oil is utilised as a feedstock in the operation at any stage of production. The value of the vegetable oil feedstock, where it contributes for 77 percent of the total operational cost in a simple biodiesel manufacturing process plant, is the most key factor affecting the production expenses of the facility. The market performance of producing biodiesel conducted by the researcher reported that natural resources and utility costs together contributed for 86 percent of operating expenses, while labour force and servicing, depreciation, as well as other spending accounted for 5 percent, 5 percent, and 4 percent of total operating expenses, respectively.

A process plant's ability to produce biodiesel determines the amount of resources required. The material balance of producing biodiesel is also used as a reference to calculate the quantity of raw materials necessary to attain the desired manufacturing capability. Utility

consumption is thus determined by a multitude of variables, including the process routes utilised, as well as the kind and amount of equipment used. On the basis of the energy balance of the process, it's commonly computed for the purpose of calculating the total operating cost, the values for manufacturing costs and infrastructure are typically based on the latest market prices. Depending on the plant's capacity, it is possible to compute the quantity of labour necessary. Maintenance, repair, and other types of operating expenses are usually presented as percent of the overall operating expenses in other subcategories like maintenance and repair. However, depreciation prices are typically expressed as a percentage of the equipment's original cost.

Many researchers claim that biodiesel's high cost is a factor. The cost of the feedstock plays a big role in the manufacturing operations and this feedstock contribution to cost can be significant in some circumstances. As the production scale grows larger, the cost per unit of output will rise and making it more expensive. Hence, the production of biodiesel is likely to increase. When production capabilities are limited, the feedstock cost portion of overall production costs can be as high as 75 percent, and as production capabilities improve, the feedstock cost share can rise to 90 percent (Apostolakou et al., 2009). The other researcher said that the cost of oil feedstock contributes the most to the total cost of biodiesel manufacturing, accounting for around 88 percent of the total. According to this study, the overall expenses in producing biodiesel directly connected with the soy oil price (Haas et al., 2006). The overall purchase price for producing biodiesel is projected to vary depending on the technological option taken. This is mainly due to differences in the amount and kind of raw materials utilised in the operations, as well as the equipment used. As a result, determining and comparing the overall expenses of the innovations to decide the most cost-effective technical solution appears logical.

CHAPTER 3

METHODOLOGY

3.1 Introduction

In this chapter, the derivation of governing equations for the reaction combustion equation that are used for the mathematical modelling will be shown. For the first semester of this project, the topic that will be discussed is more towards to find the value of every unknown in the equation. There are about 10 product species that has been assumed and there is also about 11 nonlinear equations that appear from the reaction combustion equation and it can be solved by using Newton Raphson methods or any other methods that are suitable to be used. But in the next topic, the solutions for the reaction combustion equation using Newton Raphson method will be discussed and every step will be explained briefly. The simulation for this project will be conducted in the next semester.

This project starts by revising all the article journals and the past research thesis that are related to this study. Then, the derivation of governing equation to calculate the mole fraction of combustion product for biodiesel using Equilibrium Constant Method (ECM). Then, the use of MATLAB or Microsoft Excel is applied in order to solve the governing equation. In other hand, the main objective of this study will be achieved by performing an analysis on the emission characteristic of biodiesel at different equivalence ratio.

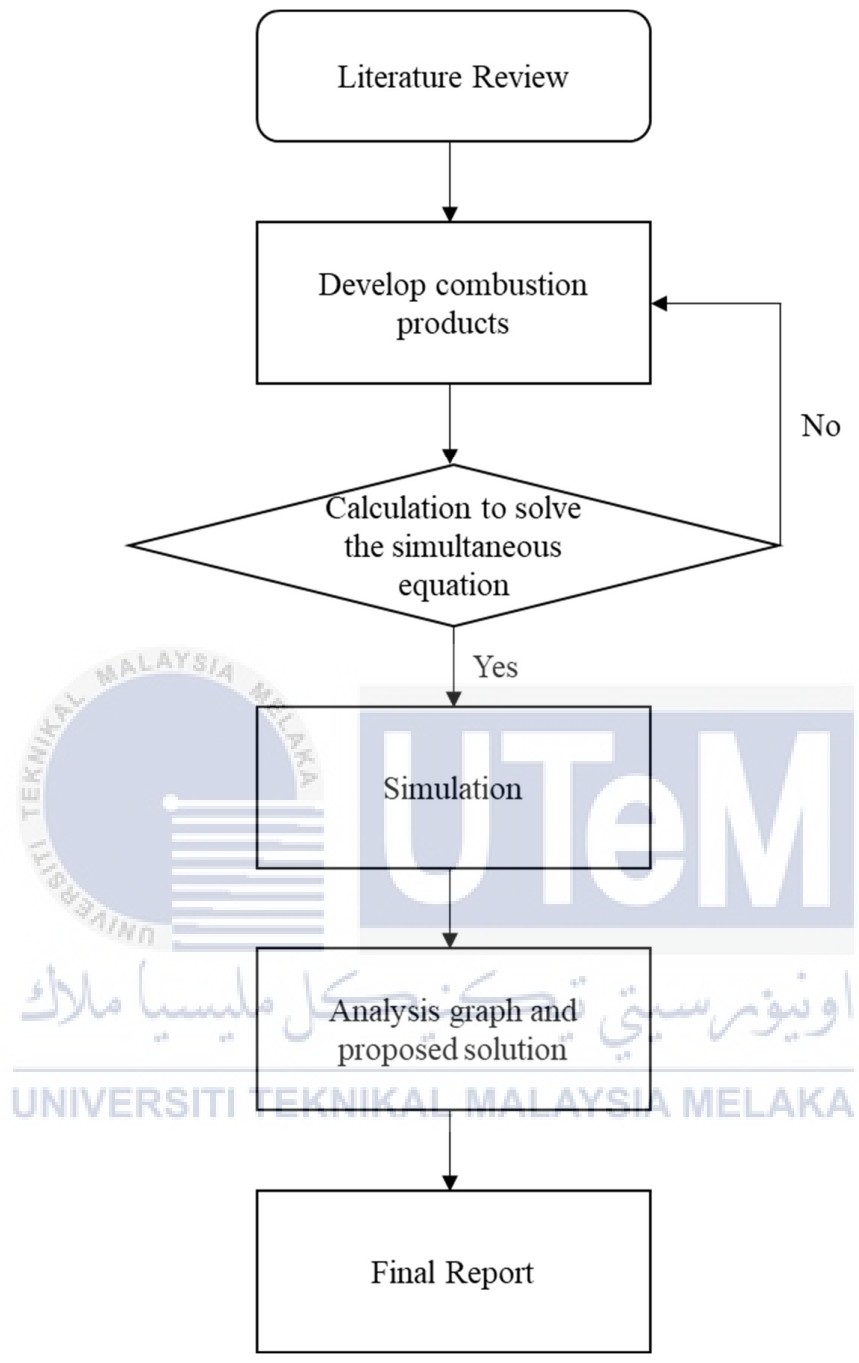


Figure 3.1 Flow chart of the methodology

3.2 Combustion Modelling Approach

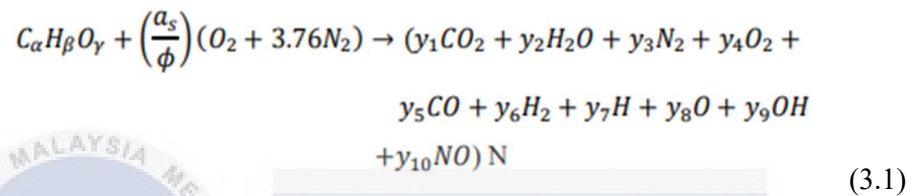
The main objective of this study is to analyse the emission characteristic of compression ignition engine with biodiesel using the computational simulation program which is MATLAB. In order to achieve the main objective, the mole fraction of combustion product for biodiesel need to be calculated manually using Equilibrium Constants Method (ECM). (Lei Han et al 2020) used an Equilibrium Constants Method (ECM) in their study to investigated the influences of biodiesel blending ratio on the equilibrium concentrations of the combustion products and thermodynamic properties of burned gas mixture, by using Equilibrium Constants Methods. The researcher used the equilibrium constant from the JANAF database and then the equation was solved using the Newton-Raphson method.

(Adnan et al., 2011) carried out a study on the effect of equivalence ratio in emission characteristics of diesel engine with hydrogen substitution. In other to solve a nonlinear system consist 18 of combustion product, they used MATLAB program. Thus, as mentioned above in this study the Equilibrium Constants Method will be used in order to determine the mole fraction of each species of combustion product. In the next section, the derivation of governing equations for the reaction combustion equation that used in this study which is biodiesel will be presented.

In this study, 10 product of combustion emission has been assumed and a system of 11-nonlinear equations appear from the derivation of the reaction combustion. In other to solve the 11-nonlinear equations Newton-Raphson method will be used. Therefore, the solution for 11-nonlinear equation by using Newton-Raphson methods will be explained and discussed as well as the input that needed when implemented the Newton-Raphson method in MATLAB program.

3.2 Governing Equation

In combustion products of biodiesel fuels, the major species present at low temperature are N_2 , H_2O , CO_2 and O_2 for lean mixtures and N_2 , H_2O , CO_2 , CO and H_2 for rich mixtures. The temperature which are higher than 1600 K will dissociate and react to form additional species in significant amounts. By consideration these phenomena and assumes for 10 product species of the combustion reaction in this project, then the reaction combustion equation of the biodiesel fuel with the air can be written as:



For diesel fuel used in this project the subscripts α is 14 while β is 25 respectively. A stoichiometric reaction can be defined as the fuel that burns completely and water and carbon dioxide are the only. The stoichiometric molar air--fuel ratio (a_s) can be determined by using the equation below:

$$a_s = \alpha + \frac{\beta}{4} - \frac{\gamma}{2} \quad (3.2)$$

In other to solve the mole fraction, y_i (for $i=1,2,3,\dots,10$) of the product species (product emission combustion) and the total mole number, N in Eq. 1 , the following condition might be employ:

- a) Concentration of combustion product condition are at equilibrium which is in these conditions the summation of mole fraction, $\sum y_i$ each species is equal to unity. These conditions are written as shown below in:

$$\sum_{i=1}^{10} y_i = 1$$

$$y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7 + y_8 + y_9 + y_{10} = 1 \quad (3.3)$$

b) The balance of atoms on both sides in Eq. 3.3. So, from this condition four (4) equation can be obtained from these conditions as shown below:

$$\text{Atom C: } \alpha = (y_1 + y_5)N \quad (3.4)$$

$$\text{Atom H: } \beta = (2y_2 + 2y_6 + y_7 + y_9)N \quad (3.5)$$

$$\text{Atom O: } \gamma + \frac{2as}{\phi} = (2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10})N \quad (3.6)$$

$$\text{Atom N: } \delta + \frac{7.52as}{\phi} = (2y_3 + y_{10})N \quad (3.7)$$

c) The chemical equilibrium equations. So, from these conditions six (6) equations that related to the equilibrium constant, K can be obtained from these equations as shown below:

$$\frac{1}{2} H_2 \rightleftharpoons H, \quad K_1 = \frac{y_7 P^{1/2}}{y_6^{1/2}} \quad (3.8)$$

$$\frac{1}{2} O_2 \rightleftharpoons O, \quad K_2 = \frac{y_8 P^{1/2}}{y_4^{1/2}} \quad (3.9)$$

$$\frac{1}{2} H_2 + \frac{1}{2} O_2 \rightleftharpoons OH, \quad K_3 = \frac{y_9}{y_4^{1/2} y_6^{1/2}} \quad (3.10)$$

$$\frac{1}{2} O_2 + \frac{1}{2} N_2 \rightleftharpoons NO, \quad K_4 = \frac{y_{10}}{y_4^{1/2} y_3^{1/2}} \quad (3.11)$$

$$H_2 + \frac{1}{2} O_2 \rightleftharpoons H_2O, \quad K_5 = \frac{y_2}{y_4^{1/2} y_6^{1/2}} \quad (3.12)$$

$$CO + \frac{1}{2} O_2 \rightleftharpoons CO_2, \quad K_6 = \frac{y_1}{y_4^{1/2} y_5^{1/2}} \quad (3.13)$$

By assuming the temperature is sufficiently high, these dissociation reactions will always be in a state of chemical equilibrium, i.e. the forward and reverse reaction rates are equal, so the concentration of each combustion product remains in state of equilibrium. The equilibrium constant, K is used to define the equilibrium state of a chemical reaction. K is defined as:

$$K = \prod_i \left(\frac{p_i}{p_0}\right)^{v_i} \times (y_i)^{v_i} \quad (3.14)$$

Based on the formula in Eq., p is defined as the total pressure of the gas mixture and is equal to the sum of partial pressure of the components multiply the mole fraction, y_i of the component i while p_0 is defined as reference pressure which is can be assumed as $1 \times 10^5 \text{ pa}$ and v_i in this formula represents the stoichiometric coefficient of the i component. In combustion modelling, the value of equilibrium constant, K , from polynomial equations must be calculated. For the temperature data range 600 K to 4000 K, the equilibrium constant, K can be obtained by using the table Equilibrium Constant, K_i which is have been curve fit from JANAF data table by the least square method (Olikara & Borman, 1975). It can be written as shown below:

$$\text{Log}K_i(T) = A_i \ln \left(\frac{T}{1000}\right) + \frac{B_i}{T} + C_i + D_i + E_i T^2 \quad (3.15)$$

Next, the Eq. 3.8 to Eq. 3.13 can be rearranged to express mole fractions of all products species in terms of y_3 , y_4 , y_5 , and y_6 which are namely mole fractions of N_2 , O_2 , CO and H_2 , respectively.

$$y_7 = c_1 y_6^{1/2} \quad (3.16)$$

$$y_8 = c_2 y_4^{1/2} \quad (3.17)$$

$$y_9 = c_3 y_4^{1/2} y_6^{1/2} \quad (3.18)$$

$$y_{10} = c_4 y_4^{1/2} y_3^{1/2} \quad (3.19)$$

$$y_1 = c_5 y_4^{1/2} y_6 \quad (3.20)$$

$$y_2 = c_5 y_4^{1/2} y_5 \quad (3.21)$$

Where,

$$c_1 = \frac{k_1}{P^{1/2}} \quad (3.22)$$

$$c_2 = \frac{k_2}{P^{1/2}} \quad (3.23)$$

$$c_3 = k_3 \quad (3.24)$$

$$c_4 = k_4 \quad (3.25)$$

$$c_5 = \frac{k_5}{P^{1/2}} \quad (3.26)$$

$$c_6 = \frac{k_6}{P^{1/2}} \quad (3.27)$$

Then, to lessen the difficulty of solving the equations from atom balance, the total number of mole fraction, N need to be eliminated by dividing Eq. 3.5 to the Eq. 3.4 and obtained:

$$2y_2 + 2y_6 + y_7 + y_9 + \frac{\beta}{\alpha} y_1 - \frac{\beta}{\alpha} y_5 = 0 \quad (3.28)$$

After that, Eq. 3.29 and Eq. 3.30 can be obtained by divided Eq. 3.6 and Eq. 3.7 by Eq. 3.4 as shown below:

$$2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 - \left(\frac{\gamma}{\alpha} + \frac{2a_s}{\phi\alpha}\right)y_1 - \left(\frac{\gamma}{\alpha} + \frac{2a_s}{\phi\alpha}\right)y_5 = 0 \quad (3.29)$$

$$2y_3 + y_{10} - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right)y_1 - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right)y_5 = 0 \quad (3.30)$$

Then, by substituting Eq. 3.16 until Eq. 3.21 into Eq. 3.28 until Eq. 3.30 and Eq. 3.2 four (4) equation with four (4) unknowns $y_3, y_4, y_5,$ and y_6 are obtained. From the equation obtained it can be seen as a nonlinear equation. In order to solve the equation, most of the

researcher suggest that Newton-Raphson iteration method is the best method to solve that nonlinear equation. This method will be discussed in detail at section 3.3. The four nonlinear equation are written as shown below:

$$2(c_5y_4^{1/2}y_5) + 2y_6 + c_1y_6^{1/2} + c_3y_4^{1/2}y_6^{1/2} + \frac{\beta}{\alpha} (c_5y_4^{1/2}y_6) - \frac{\beta}{\alpha} y_5 = 0 \quad (3.31)$$

$$2(c_5y_4^{1/2}y_5) + c_5y_4^{1/2}y_5 + 2y_4 + y_5 + c_2y_4^{1/2} + c_3y_4^{1/2}y_6^{1/2} - \left(\frac{\gamma}{\alpha} + \frac{2a_s}{\phi\alpha}\right)(c_5y_4^{1/2}y_6) - \left(\frac{\gamma}{\alpha} + \frac{2a_s}{\phi\alpha}\right)y_5 = 0 \quad (3.32)$$

$$2y_3 + c_4y_4^{1/2}y_3^{1/2} - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right)(c_5y_4^{1/2}y_6) - \left(\frac{\delta}{\alpha} + \frac{7.52a_s}{\phi\alpha}\right)y_5 = 0 \quad (3.33)$$

$$c_5y_4^{1/2}y_6 + c_5y_4^{1/2}y_5 + y_3 + y_4 + y_5 + y_6 + c_1y_6^{1/2} + c_2y_4^{1/2} + c_3y_4^{1/2}y_6^{1/2} + c_4y_4^{1/2}y_3^{1/2} - 1 = 0 \quad (3.34)$$

3.3 Newton Raphson Method

As mentioned in section 3.2, the Newton- Raphson iteration method will be used to solve the four non-linear equations in order to obtain the mole fraction of emission combustion product at the equilibrium constant and it can be written as shown below:

$$f_1 (y_3, y_4, y_5, y_6) = 0 \quad (3.35)$$

$$f_2 (y_3, y_4, y_5, y_6) = 0 \quad (3.36)$$

$$f_3 (y_3, y_4, y_5, y_6) = 0 \quad (3.37)$$

$$f_4 (y_3, y_4, y_5, y_6) = 0 \quad (3.38)$$

The system can be written in more compact vector form as $F(y)=0$, where:

$$f (y_3, y_4, y_5, y_6) = 0 \quad (3.39)$$

$$F(y) = \begin{bmatrix} f_1(y) \\ f_2(y) \\ f_3(y) \\ f_4(y) \end{bmatrix} \quad (3.40)$$

$$0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (3.41)$$

Then, for solving of nonlinear equations by a Newton-Raphson method the evaluation of a matrix which is known a Jacobian Matrix method are required and it is defined as:

$$J = \frac{\partial(f_1, f_2, f_3, f_4)}{\partial(y_3, y_4, y_5, y_6)} = \begin{bmatrix} \frac{\partial f_1}{\partial y_3} & \frac{\partial f_1}{\partial y_4} & \frac{\partial f_1}{\partial y_5} & \frac{\partial f_1}{\partial y_6} \\ \frac{\partial f_2}{\partial y_3} & \frac{\partial f_2}{\partial y_4} & \frac{\partial f_2}{\partial y_5} & \frac{\partial f_2}{\partial y_6} \\ \frac{\partial f_3}{\partial y_3} & \frac{\partial f_3}{\partial y_4} & \frac{\partial f_3}{\partial y_5} & \frac{\partial f_3}{\partial y_6} \\ \frac{\partial f_4}{\partial y_3} & \frac{\partial f_4}{\partial y_4} & \frac{\partial f_4}{\partial y_5} & \frac{\partial f_4}{\partial y_6} \end{bmatrix} \quad (3.42)$$

From the equation 3.35 until 3.38, the elements of Jacobian matrix, J for the combustion emission equations derives previously are:

$$J(1,3) = \frac{\partial f_1}{\partial y_3} = 0 \quad (3.43)$$

$$J(1,4) = \frac{\partial f_1}{\partial y_4} = 2 \left(\frac{C_5 y_6}{2 y_4^{1/2}} \right) - \left(\frac{\beta}{\alpha} \right) \left(\frac{C_6 y_5}{2 y_4^{1/2}} \right) \quad (3.44)$$

$$J(1,5) = \frac{\partial f_1}{\partial y_5} = - \left(\frac{\beta}{\alpha} \right) (C_6 y_4^{1/2}) - \left(\frac{\beta}{\alpha} \right) \quad (3.45)$$

$$J(1,6) = \frac{\partial f_1}{\partial y_6} = 2 (C_5 y_4^{1/2}) + 2 + \frac{C_1}{2 y_6^{1/2}} + \left(\frac{C_3 y_4^{1/2}}{2 y_6^{1/2}} \right) \quad (3.46)$$

$$J(2,3) = \frac{\partial f_2}{\partial y_3} = \frac{C_4 y_4^{1/2}}{2 y_3^{1/2}} \quad (3.47)$$

$$J(2,4) = \frac{\partial f_2}{\partial y_4} = 2 (C_5 y_4^{1/2}) + \left(\frac{C_5 y_6}{2 y_4^{1/2}} \right) + 2 + \frac{C_2}{2 y_4^{1/2}} + \frac{C_3 y_6^{1/2}}{2 y_4^{1/2}} + \frac{C_4 y_3^{1/2}}{2 y_4^{1/2}} - \left(\frac{\gamma}{\alpha} + \frac{2 a_s}{\phi \alpha} \right) \left(\frac{C_6 y_5}{2 y_4^{1/2}} \right) \quad (3.48)$$

$$J(2,5) = \frac{\partial f_2}{\partial y_5} = 2 (C_6 y_4^{1/2}) + 1 - \left(\frac{\gamma}{\alpha} + \frac{2 a_s}{\phi \alpha} \right) (C_6 y_4^{1/2}) - \left(\frac{\gamma}{\alpha} + \frac{2 a_s}{\phi \alpha} \right) \quad (3.49)$$

$$J(2,6) = \frac{\partial f_2}{\partial y_6} = C_5 y_4^{1/2} + \frac{C_3 y_4^{1/2}}{2 y_6^{1/2}} \quad (3.50)$$

$$J(3,3) = \frac{\partial f_3}{\partial y_3} = 2 + \frac{C_4 y_4^{1/2}}{2 y_3^{1/2}} \quad (3.51)$$

$$J(3,4) = \frac{\partial f_3}{\partial y_4} = \frac{C_4 y_3^{1/2}}{2 y_4^{1/2}} - \left(\frac{\delta}{\alpha} + \frac{7.52 a_s}{\phi \alpha} \right) \left(\frac{C_6 y_5}{2 y_4^{1/2}} \right) \quad (3.52)$$

$$J(3,5) = \frac{\partial f_3}{\partial y_5} = - \left(\frac{\delta}{\alpha} + \frac{7.52 a_s}{\phi \alpha} \right) (C_6 y_4^{1/2}) - \left(\frac{\delta}{\alpha} + \frac{7.52 a_s}{\phi \alpha} \right) \quad (3.53)$$

$$J(3,6) = \frac{\partial f_3}{\partial y_6} = 0 \quad (3.54)$$

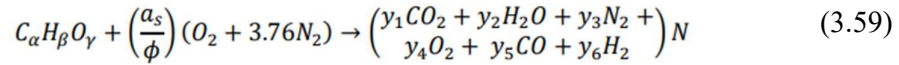
$$J(4,3) = \frac{\partial f_4}{\partial y_3} = 1 + \frac{C_4 y_4^{1/2}}{2 y_3^{1/2}} \quad (3.55)$$

$$J(4,4) = \frac{\partial f_4}{\partial y_4} = \frac{C_6 y_5}{2 y_4^{1/2}} + \frac{C_5 y_6}{2 y_4^{1/2}} + 1 + \frac{C_2}{2 y_4^{1/2}} + \frac{C_4 y_3^{1/2}}{2 y_4^{1/2}} + \frac{C_3 y_6^{1/2}}{2 y_4^{1/2}} \quad (3.56)$$

$$J(4,5) = \frac{\partial f_4}{\partial y_5} = C_6 y_4^{1/2} + 1 \quad (3.57)$$

$$J(4,6) = \frac{\partial f_4}{\partial y_6} = C_5 y_4^{1/2} + 1 + \frac{C_1}{2 y_6^{1/2}} + \frac{C_3 y_4^{1/2}}{2 y_6^{1/2}} \quad (3.58)$$

After that, to solve this nonlinear equation by using Newton-Raphson iteration method the initial guess value for four (4) unknown mole fraction which is y_3, y_4, y_5, y_6 must be obtained first, so low-temperature combustion modelling are being used to obtained the initial guess for mole fraction (y_3, y_4, y_5, y_6) as shown in chemical equation below:



By assuming the temperature is at room temperature and for the stoichiometric combustion is assumed either lean combustion, $\phi < 1$ or rich combustion, $\phi > 1$, If lean combustion is assumed the emission combustion for CO and H₂ is assumed zero while if rich combustion is assumed the emission combustion for O₂ is assumed zero. Then, by using this assumption the approximate initial value for mole fraction y_3, y_4, y_5, y_6 are obtained. Next if $y=y_0$ represents the initial guess for the solution, successive approximations to the solution are obtained from

$$y_{n+1} = y_n - J^{-1} F(y_n) = y_n - \Delta y_n \quad (3.60)$$

Where J^{-1} , is from the solution of Jacobian Matrix method as mentioned above and Δy_n , is from $\Delta y_n = y_n - y_{n+1}$.

3.4 MATLAB input

There is many software that can be used to calculate the mole fraction of combustion products, such as GASEQ, CHEMKIN, MATLAB, and CEA. In this study, MATLAB computer programming will be developed in other to validate the value of mole fraction that obtained from Newton-Raphson Method and analyse the emission characteristic of biodiesel at the difference value of equivalence ratio. In MATLAB, the input that user need to Key-in into the MATLAB program are:

- a. Temperature, T in Kelvin,
- b. Equivalence ratio, ϕ
- c. Pressure, P in atm

CHAPTER 4

RESULT AND ANALYSIS

In this study, MATLAB code for the combustion simulation has been developed. In this study for the mole fraction of every combustion product with variation of equivalence ratio, the temperature and combustion pressure were fixed to constant values of 3000 K and 30 bar respectively and the equivalence ratio has been set at the range of 0.4-2.8 with increment of 0.4.

Next, for the study of the mole fraction of every combustion product with variation of temperature, the equivalence ratio and combustion pressure were fixed to constant values of 1.2 and 30 bar, respectively and the temperature has been set at the range of 1000 K to 3000 K with increment of 400 K.

For the third study of this project which is the mole fraction of every combustion product with variation of combustion pressure, the equivalence ratio and temperature were fixed to constant values of 1.2 and 3000 K, respectively and the combustion pressure has been set at the range of 30 bar to 90 bar with increment of 10 bar.

It is noted that this project only focused to used 100% of biodiesel fuel to completely replaced diesel fuel that has been used nowadays. Thus, all the advantages and disadvantages when use this fuel will be explained in the discussion part. Area of improvement also will be discussed to make sure the research regarding to this project will be continued in future.

4.1 The mole fraction of every combustion product with variation of equivalence ratio

4.1.1 Carbon Dioxide (CO₂)

Table 4.1 Mole fraction of CO₂ with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Mole fraction	0.055809	0.091712	0.084805	0.040416	0.018605	0.00776	0.001191

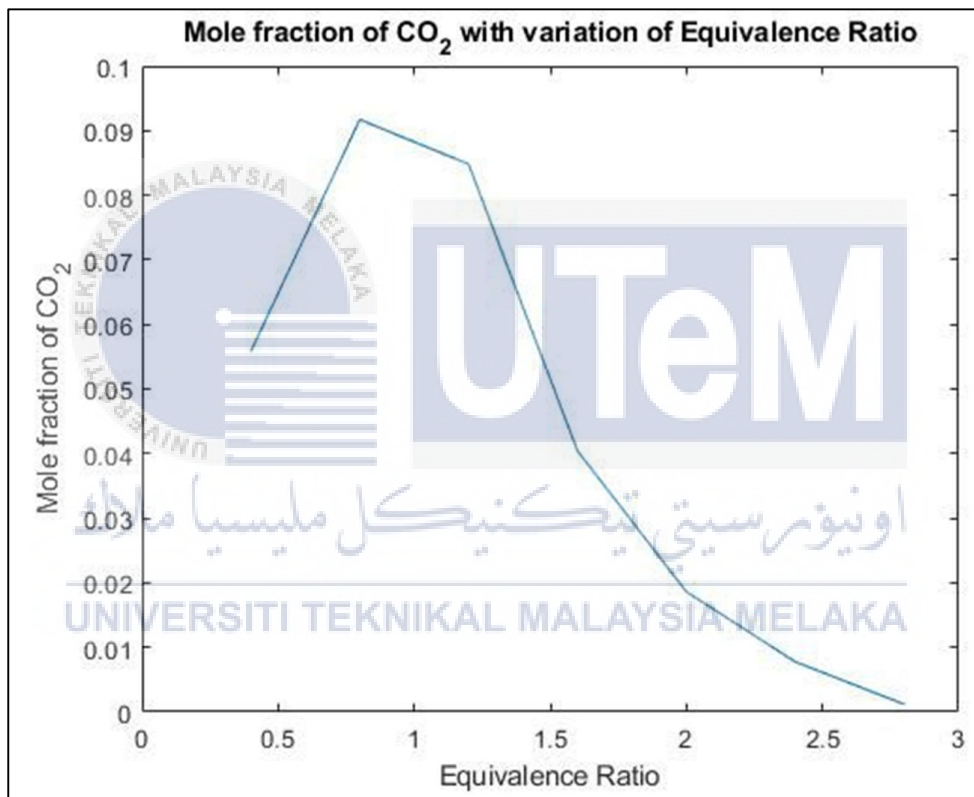


Figure 4.1 Mole fraction of CO₂ with variation of equivalence ratio

The graph in figure 4.1 shows the trends is starting to decrease after reach the stoichiometric combustion. The mole fraction is increasing rapidly during the lean combustion before it is rapidly decreasing during the rich combustion. The mole fraction of CO₂ is depending on the combustion process that occur inside the combustion chamber. The higher quantity of oxygen and the lesser quantity of carbon are the reason why the mole fraction of carbon dioxide is higher during stoichiometric combustion.

4.1.2 Water (H₂O)

Table 4.2 Mole fraction of H₂O with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.056416	0.099228	0.124536	0.111747	0.078127	0.04161	0.007456

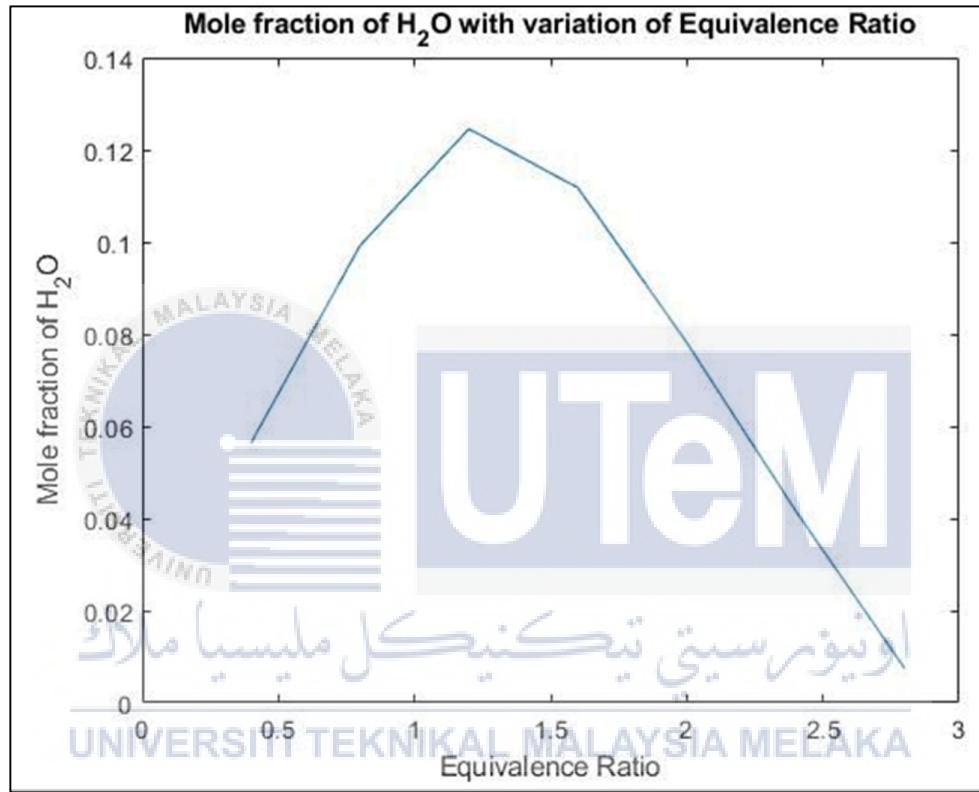


Figure 4.2 Mole fraction of H₂O with variation of equivalence ratio

The graph in figure 4.2 shows the mole fractions of water with variation of equivalence ratio from 0.4 to 2.8 the trends is starting to decrease after reach the highest point at equivalence ratio 1.2. The mole fraction is increasing rapidly from equivalence ratio of 0.4 to 1.2 before it is decreasing rapidly after the highest point until the equivalence ratio at 2.8 which has 0.007456 number of moles. It can be seen that biodiesel fuel will emit higher content of H₂O during the stoichiometric combustion process before it decreasing during rich combustion.

4.1.3 Nitrogen gas (N₂)

Table 3.3 Mole fraction of N₂ with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.877796	0.782207	0.705392	0.642315	0.589593	0.544869	0.506452

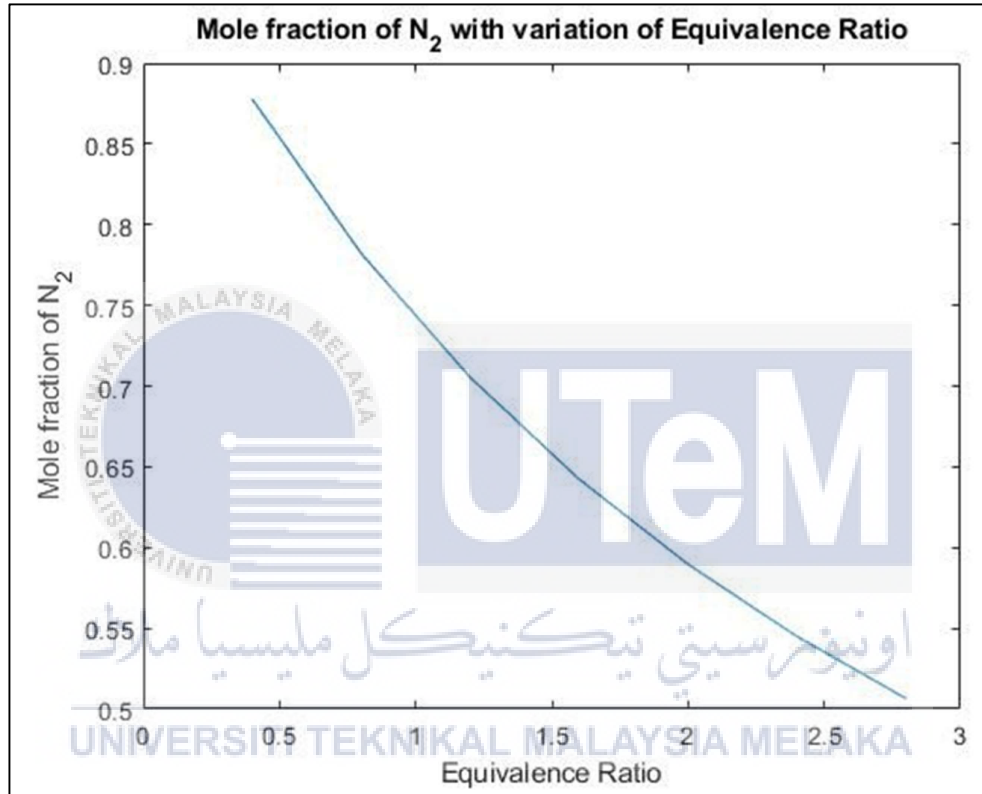


Figure 4.3 Mole fraction of N₂ with variation of equivalence ratio

The graph in figure 4.3 shows the mole fractions of nitrogen gas with variation equivalence ratio from 0.4 to 2.8 and the graph trends is decreasing since lean combustion. The mole fraction is decreasing rapidly starting from the lean combustion at equivalence ratio 0.4 which has 0.877796 number of moles and it keep drop during the stoichiometric and rich combustion until the equivalence ratio is at 2.8 that has 0.506452 number of moles. The supplied air is not enough for the combustion process resulting in the decreasing mole fraction of N₂ from the combustion product.

4.1.4 Oxygen gas (O₂)

Table 4.4 Mole fraction of O₂ with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.145063	0.055033	0.005112	0.000264	3.14E-05	3.97E-06	7.51E-08

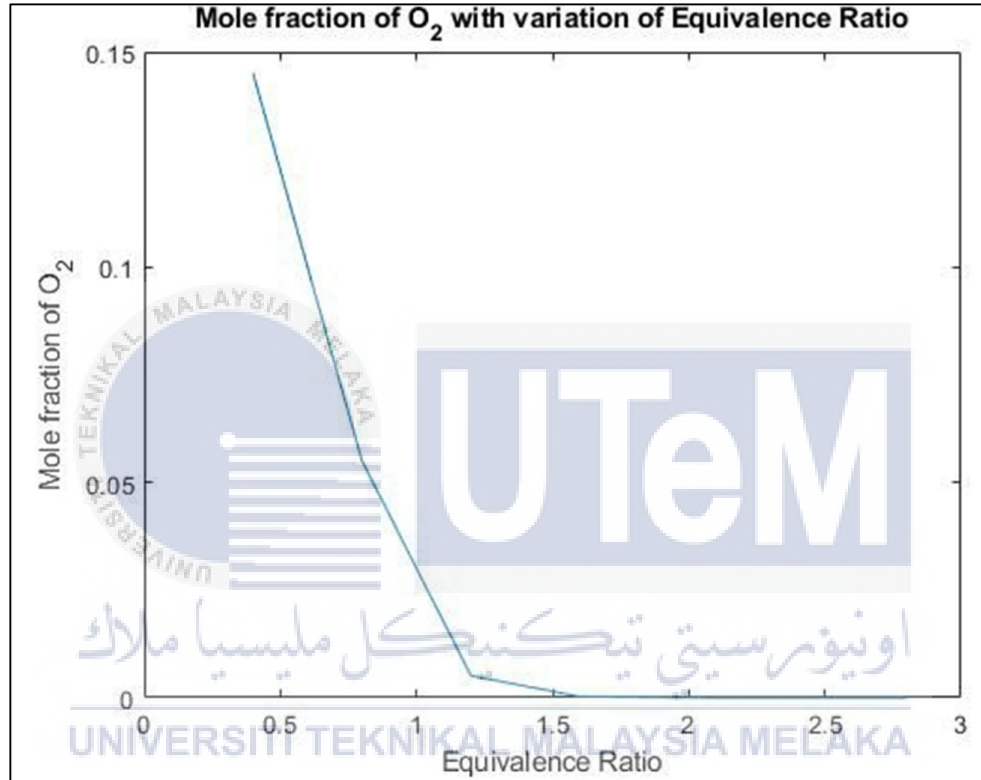


Figure 4.4 Mole fraction of O₂ with variation of equivalence ratio

The graph in figure 4.4 shows the mole fractions of oxygen gas with variation equivalence ratio from 0.4 to 2.8 and the graph trends is decreasing since lean combustion. The mole fraction is decreasing rapidly at lean combustion throughout all the equivalence ratio before it is slightly decreasing at rich combustion until the equivalence ratio reach 2.8 that has 7.51E-08 number of moles. As the equivalence ratio increase, the oxygen is also increase because more fuel is used during the combustion process and all the oxygen gas will be used during the process resulting the decreasing of mole fraction of oxygen gas.

4.1.5 Carbon Monoxide (CO)

Table 4.5 Mole fraction of CO with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.008751	0.023349	0.070837	0.148549	0.198214	0.232687	0.259551

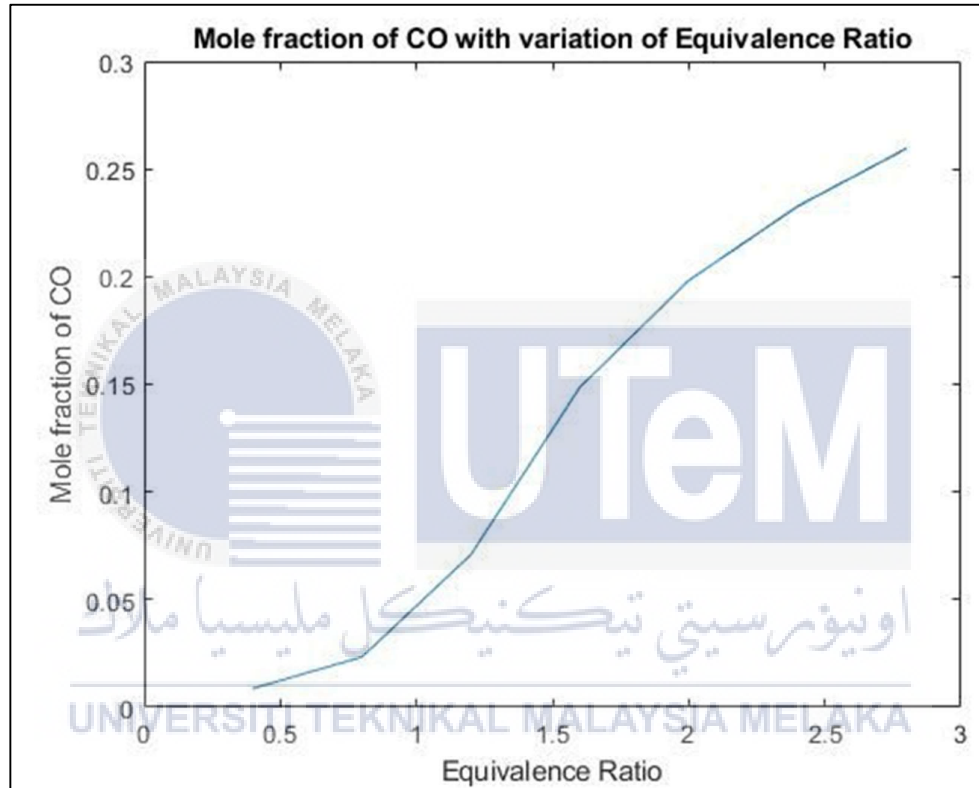


Figure 4.5 Mole fraction of CO with variation of equivalence ratio

The graph in figure 4.5 shows the trends is increasing from the start. The mole fraction is increasing rapidly during lean combustion from equivalence ratio 0.4 which and it keep rise through the stoichiometric and rich combustion until the equivalence ratio is at 2.8. This is because, during rich combustion, lack of oxygen provided for the combustion process, resulting in the incomplete of combustion reaction where carbon monoxide CO is formed. The low excess of oxygen will increase the formation of CO.

4.1.6 Hydrogen gas (H₂)

Table 4.6 Mole fraction of H₂ with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.001227	0.003504	0.01443	0.056973	0.115462	0.173075	0.22535

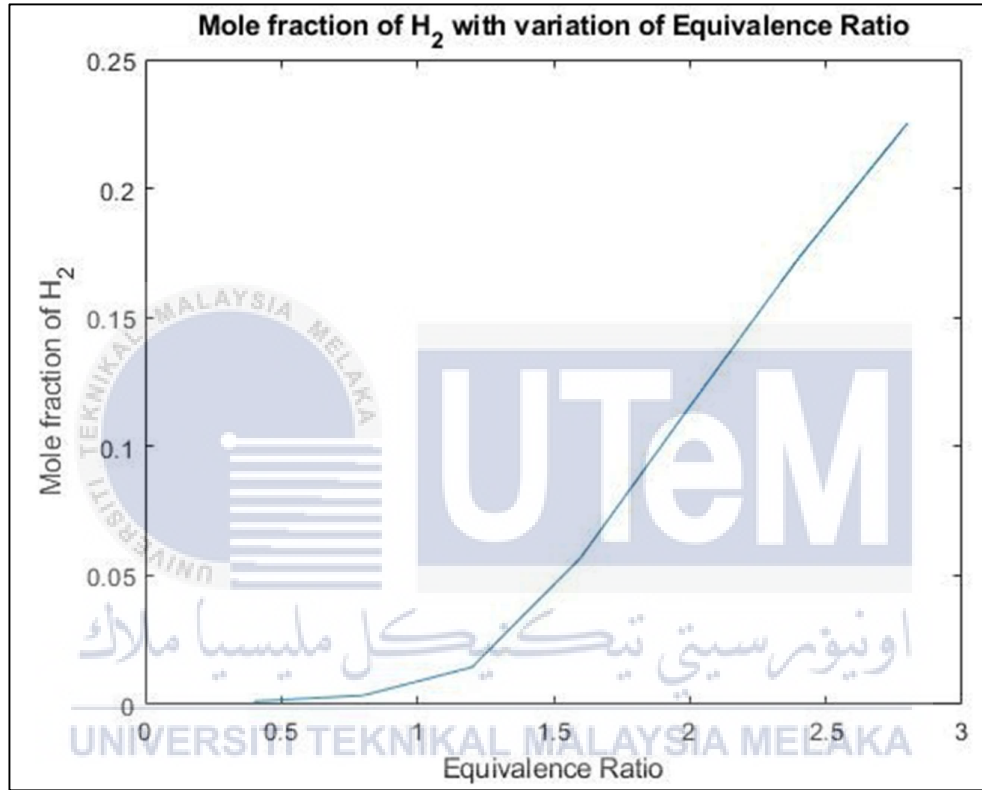


Figure 4.6 Mole fraction of H₂ with variation of equivalence ratio

The graph in figure 4.6 shows the trends is increasing from the start. The mole fraction is slightly increasing during lean combustion from equivalence ratio 0.4 to 0.8 which rise from 0.001227 to 0.003504 number of moles. Then it is increasing rapidly starting from stoichiometric combustion until the equivalence ratio at 2.8 that has 0.22535 number of moles. Due to the lack of oxygen supplied by the air inside of the combustion chamber when the equivalence ratio is increasing, the formation of H₂O does not complete resulting in the formation of H₂.

4.1.7 Hydrogen atom (H)

Table 4.7 Mole fraction of H with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.001006	0.0017	0.00345	0.006856	0.00976	0.011949	0.013635

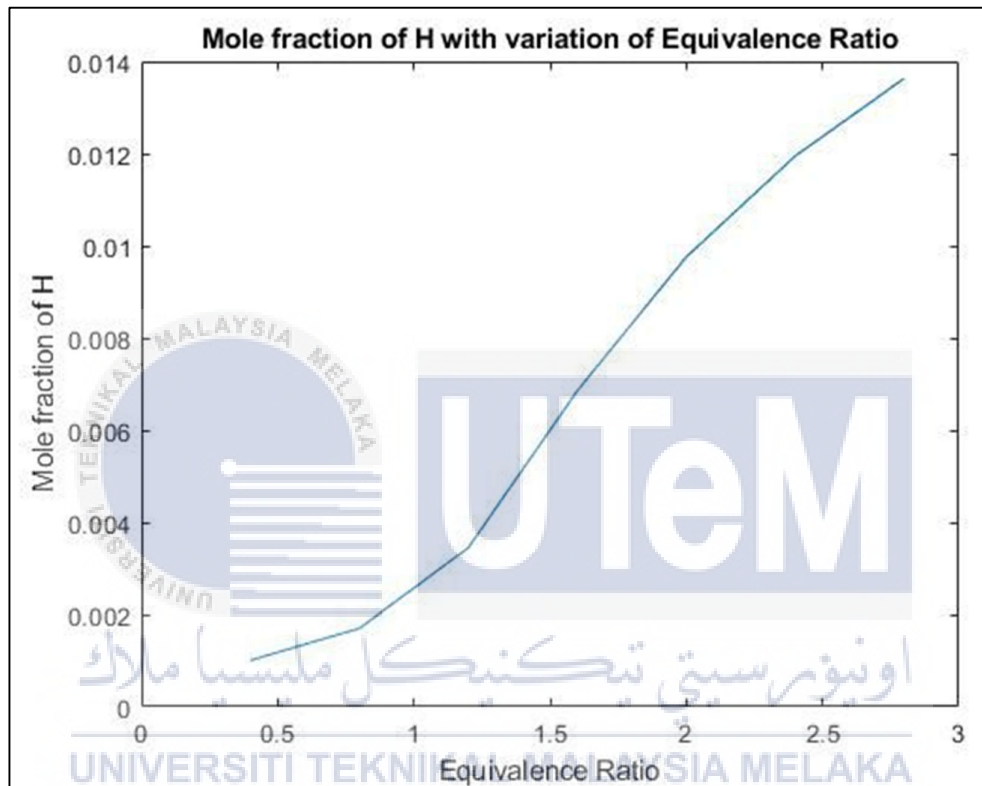


Figure 4.7 Mole fraction of H with variation of equivalence ratio

The graph in figure 4.7 shows the trends is increasing throughout all equivalence ratio. The mole fraction is increasing rapidly starting from the lean combustion from equivalence ratio 0.4 which has 0.001006 number of moles and it keep rise until the rich combustion where the equivalence ratio is at 2.8 that has 0.013635 number of moles. As the equivalence ratio increase, the amount of oxygen supplied by the available air inside of the combustion chamber is decreasing until it is not enough for the formation of H_2O , leaving hydrogen atom alone emitted from the combustion process.

4.1.8 Oxygen atom (O)

Table 4.8 Mole fraction of O with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.007816	0.004814	0.001467	0.000333	0.000115	4.09E-05	5.62E-06

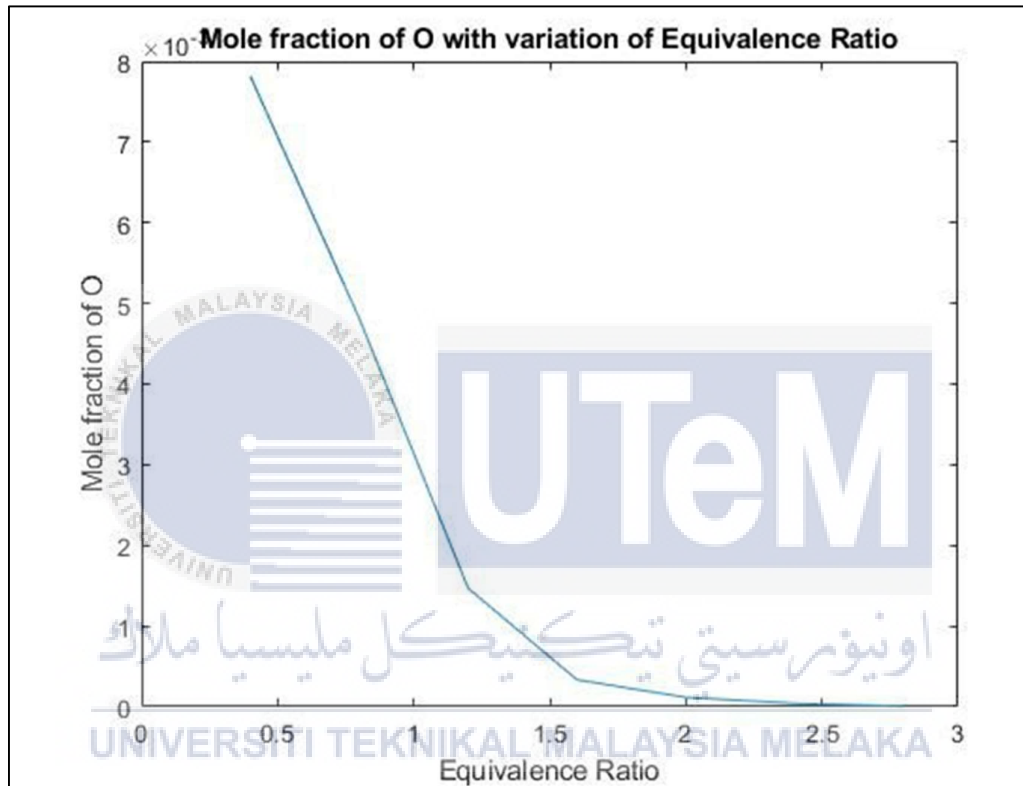


Figure 4.8 Mole fraction of O with variation of equivalence ratio

The graph in figure 4.8 shows the trends is decreasing from the start. The mole fraction is decreasing rapidly during lean combustion from equivalence ratio 0.4 to 1.6 which drop from 0.007816 to 0.004814 number of moles. Then it is slightly decreasing during rich combustion until the equivalence ratio reach 2.8 that has 5.62E-06 number of moles. Along with the decreasing volume of air supplied for the combustion process, the oxygen atom that is one of the important factors for combustion is also decreasing and it cause the amount of oxygen getting decrease.

4.1.9 Hydroxide (OH)

Table 4.9 Mole fraction of OH with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.414694	0.241116	0.069788	0.015134	0.005002	0.001709	0.000227

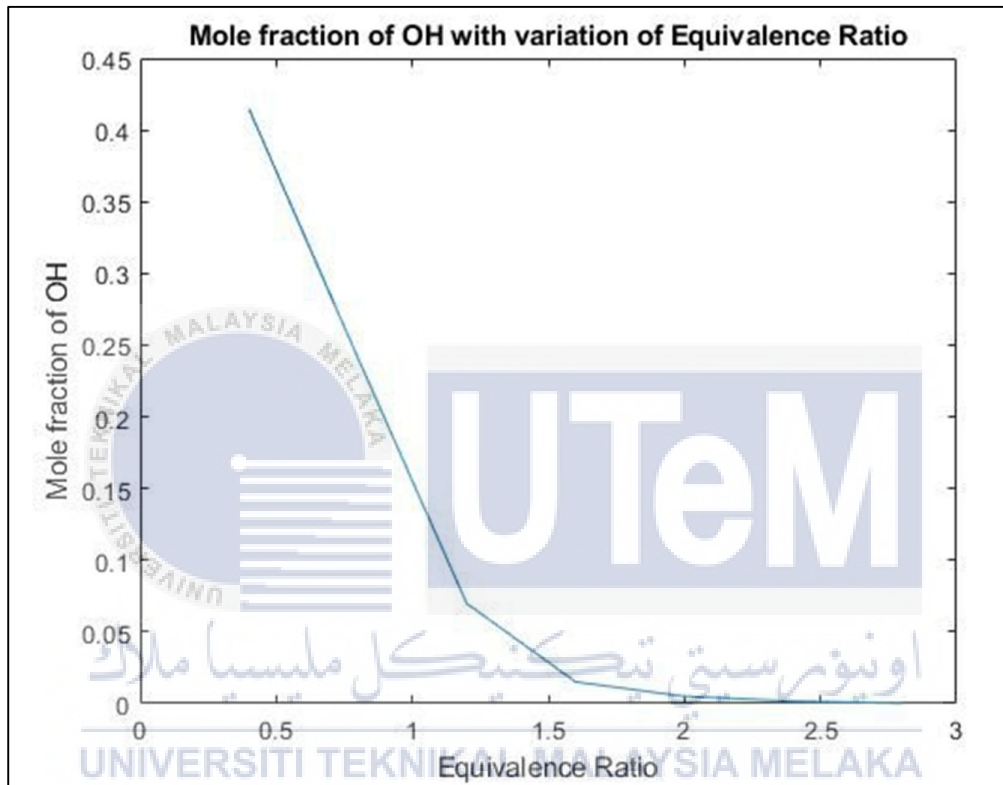


Figure 4.9 Mole fraction of OH with variation of equivalence ratio

The graph in figure 4.9 shows the trends is decreasing from the start. The mole fraction is decreasing rapidly during lean combustion from equivalence ratio 0.4 to 1.6 which drop from 0.414694 to 0.241116 number of moles. Then it is slightly decreasing during rich combustion until the equivalence ratio reach 2.8 that has 0.000227 number of moles.

4.1.10 Nitrogen Oxide (NO)

Table 4.10 Mole fraction of NO with variation of equivalence ratio

Equivalence Ratio	0.4	0.8	1.2	1.6	2.0	2.4	2.8
Number of Mole	0.043608	0.025355	0.007339	0.001591	0.000526	0.00018	2.38E-05

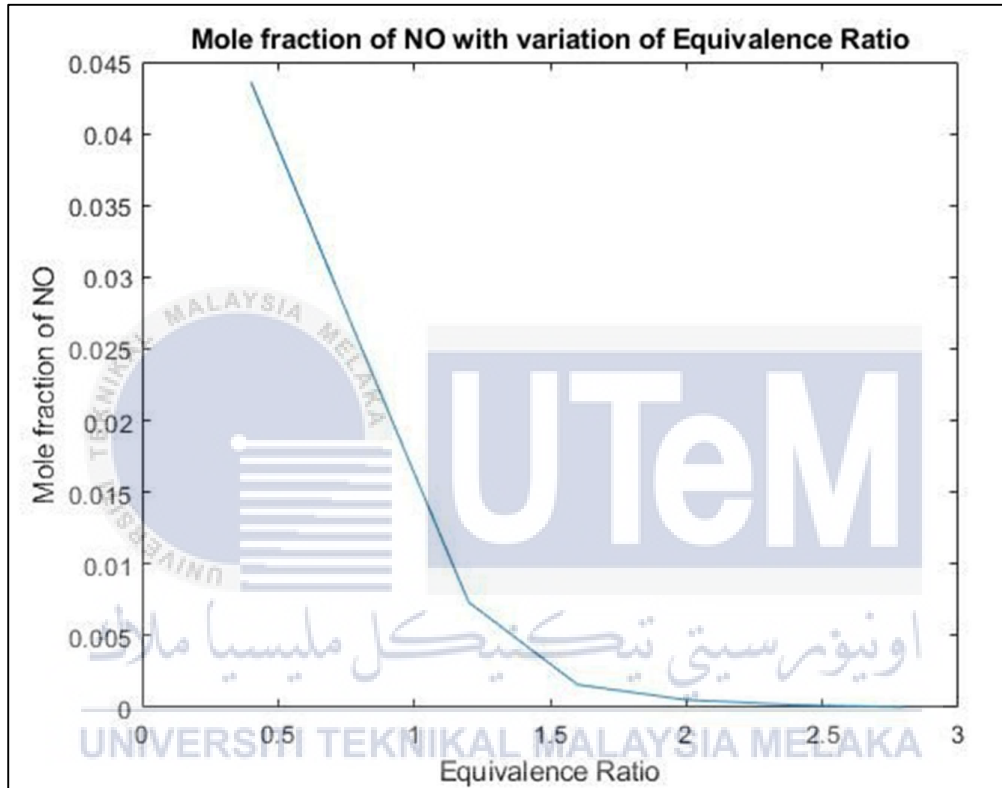


Figure 4.10 Mole fraction of NO with variation of equivalence ratio

The graph in figure 4.10 shows the trends is decreasing from the start. The mole fraction is decreasing rapidly during lean combustion from equivalence ratio 0.4 to 1.6 which drop from 0.043608 to 0.025355 number of moles. Then it is slightly decreasing during rich combustion until the equivalence ratio reach 2.8 that has 2.38E-05 number of moles. As the equivalence ratio is increase, the quantity of oxygen is decrease and it cause the mole fraction of nitrogen oxide is decreasing towards higher equivalence ratio.

4.2 The mole fraction of every combustion product with variation of temperature

4.2.1 Carbon Dioxide (CO₂)

Table 4.11 Mole fraction of CO₂ with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	0.121118	0.105635	0.098909	0.095571	0.093303	0.084805

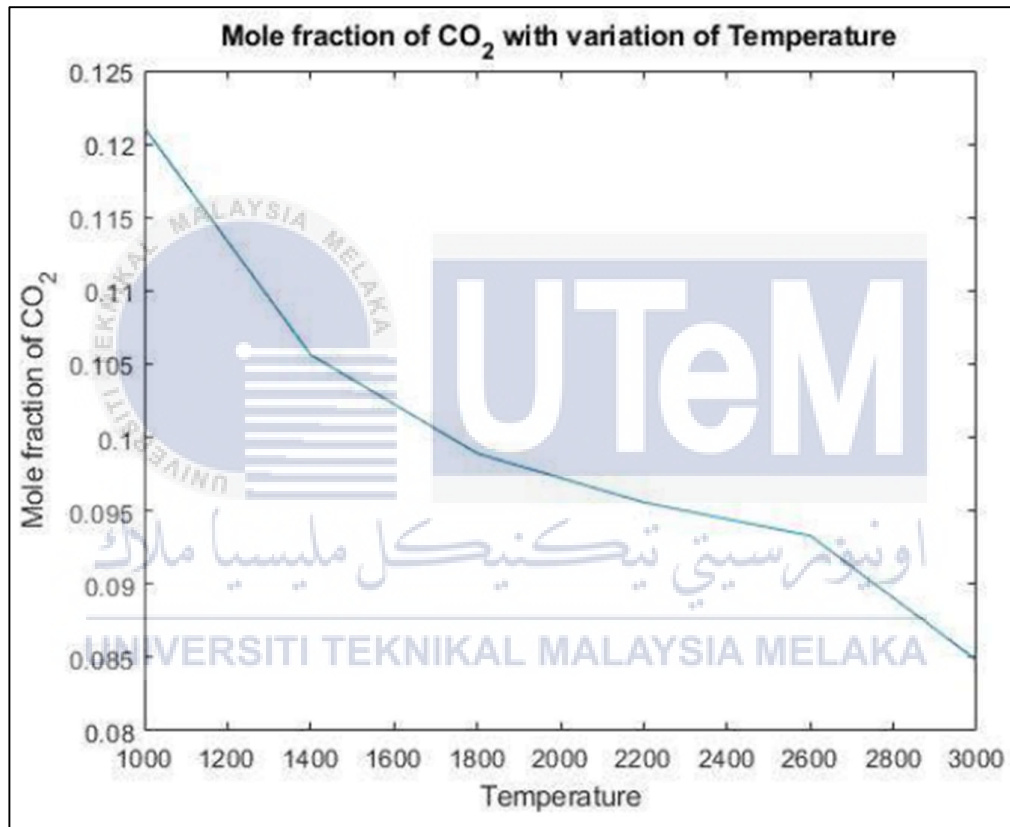


Figure 4.11 Mole fraction of CO₂ with variation of temperature

The graph in figure 4.11 shows the mole fractions of carbon dioxide with variation temperature from 1000 K to 3000 K and the graph trends is decreasing from the start. It can be mentioned that when the equivalence ratio is set to be constant at rich combustion ($\phi > 1$) which is 1.2, the emission of CO₂ is decrease as the temperature of combustion is increases. The decreasing number of moles of carbon dioxide is a proof that biodiesel fuel can reduce the emission of carbon dioxide to the air.

4.2.2 Water (H₂O)

Table 4.12 Mole fraction of H₂O with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	0.098449	0.113932	0.120658	0.12399	0.125717	0.124536

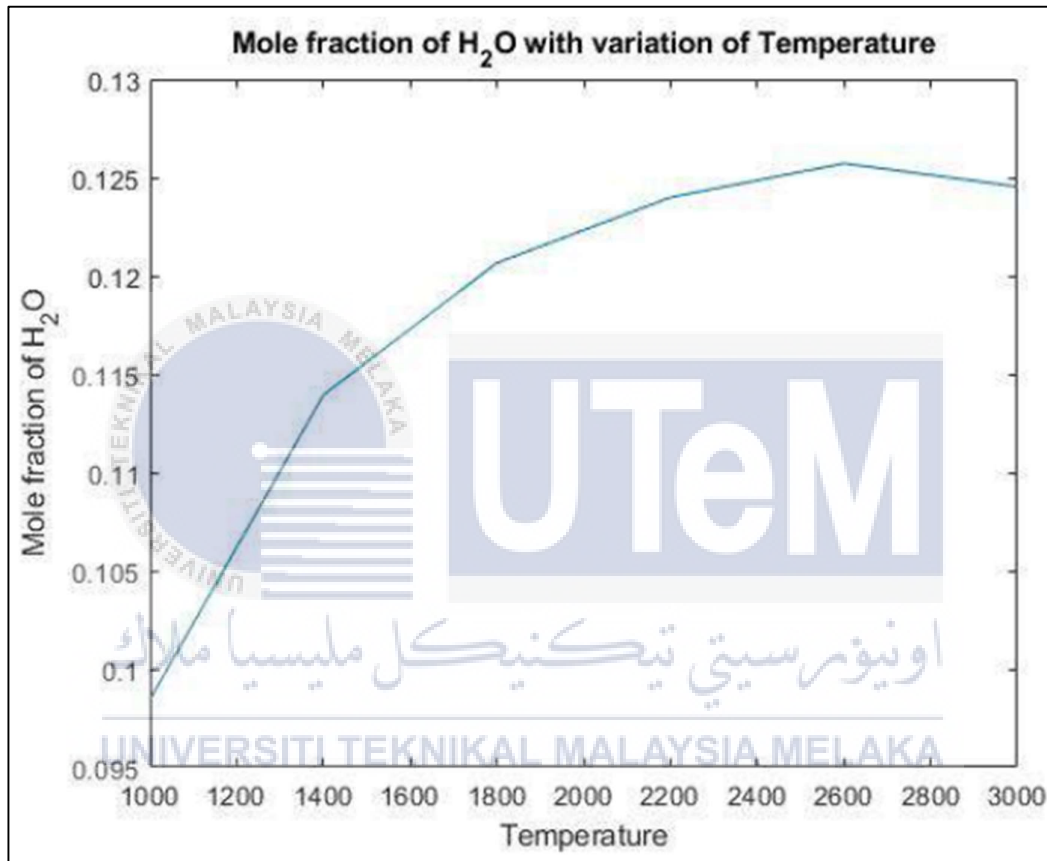


Figure 4.12 Mole fraction of H₂O with variation of temperature

The graph in figure 4.12 shows the mole fractions of water with variation of temperature from 1000 K to 3000 K the trends is starting to decrease after reach the highest point at 2600 K. The mole fraction is rapidly increasing from 1000 K to 2600 K which rise from 0.098449 to 0.125717 number of moles before it is decreasing at temperature 3000 K that has 0.124536 number of moles. The increasing number of moles is about 22 % from 1000 K to 2600 K before it decreases about 1 % at 3000 K.

4.2.3 Nitrogen gas (N₂)

Table 4.13 Mole fraction of N₂ with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	0.705392	0.705392	0.705392	0.705392	0.705392	0.705392

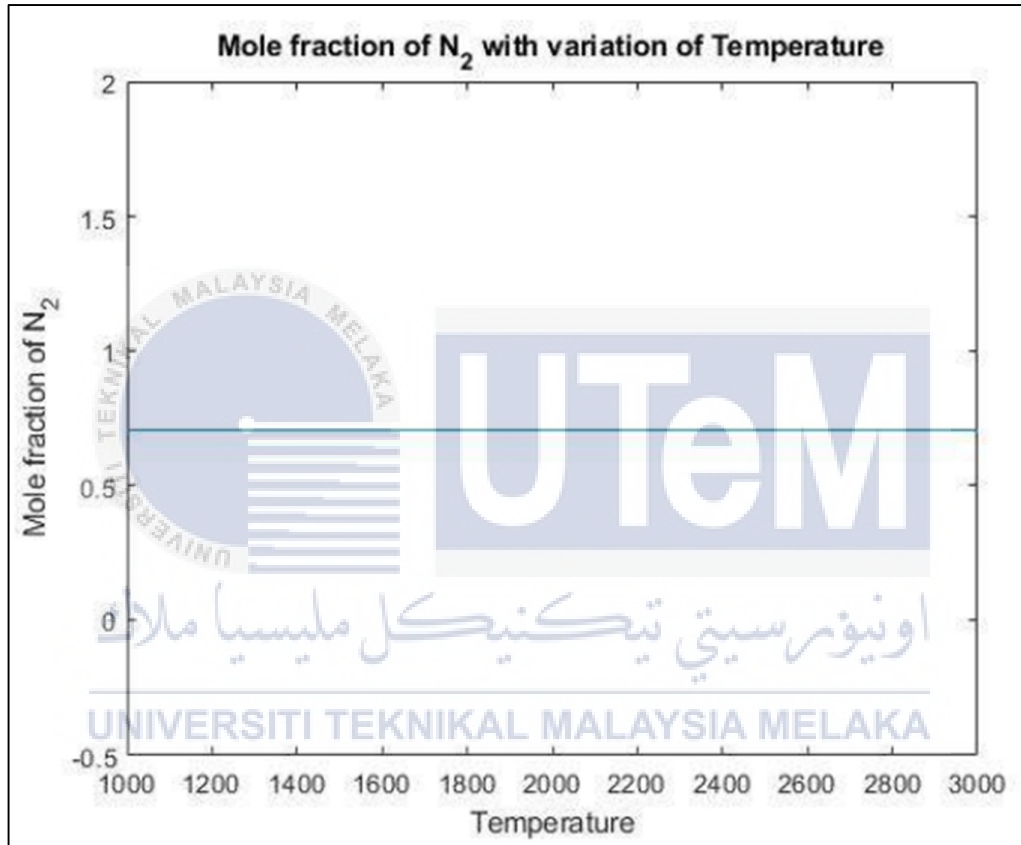


Figure 4.13 Mole fraction of N₂ with variation of temperature

The graph in figure 4.13 shows the mole fractions of nitrogen gas with variation of temperature from 1000 K to 3000 K and the trends is consistent from the start until the end. The number of moles is static at 0.705392 from 1000 K until 3000 K. This shown that the emission of Nitrogen gas, N₂ is decomposed completely when the temperature of combustion reach 1000 K. There is no percentage difference between the range of temperature from 1000 K to 3000 K.

4.2.4 Oxygen gas (O₂)

Table 4.14 Mole fraction of O₂ with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	1.48E-21	1.39E-13	4.18E-09	2.98E-06	0.000273	0.005112

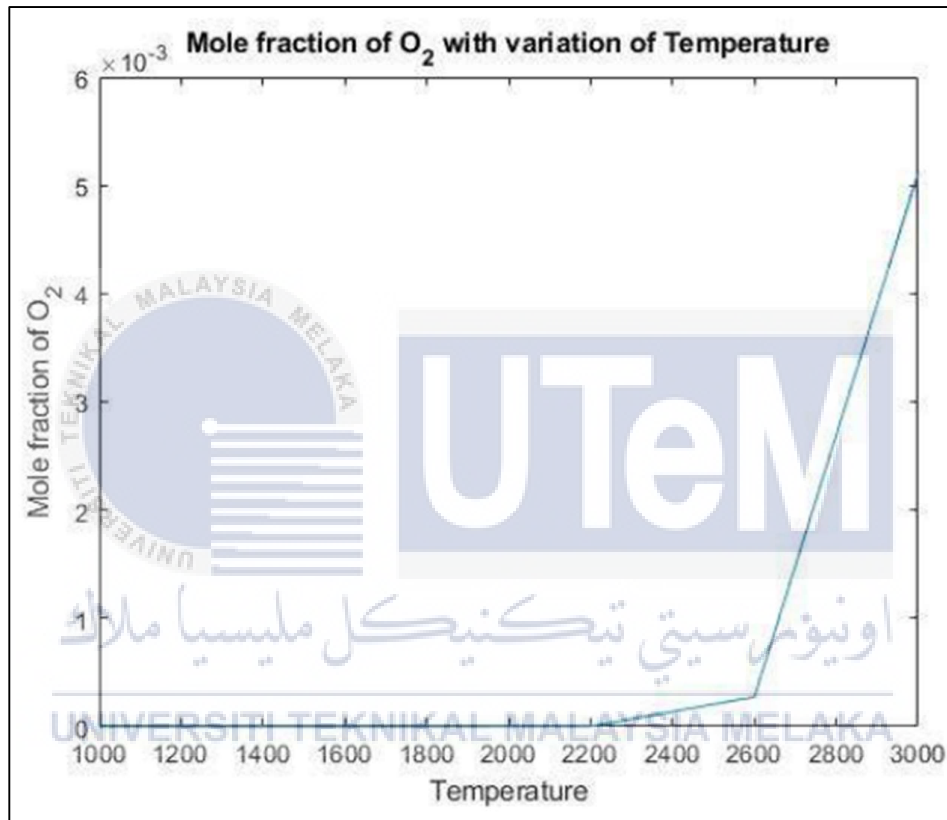


Figure 4.14 Mole fraction of O₂ with variation of temperature

The graph in figure 4.14 shows the mole fractions of oxygen gas with variation of temperature from 1000 K to 3000 K and the trends is increasing slowly before it is increasing rapidly at 2600 K. The mole fraction is increasing slowly from 1000 K to 2600 K which rise from 1.48E-21 to 0.000273 number of moles. Then it is increasing rapidly until the temperature reach 3000 K that has 0.005112 number of moles. The increasing number of moles is about 100 % from 1000 K to 3000 K.

4.2.5 Carbon Monoxide (CO)

Table 4.15 Mole fraction of CO with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	0.034524	0.050007	0.056733	0.060071	0.062339	0.070837

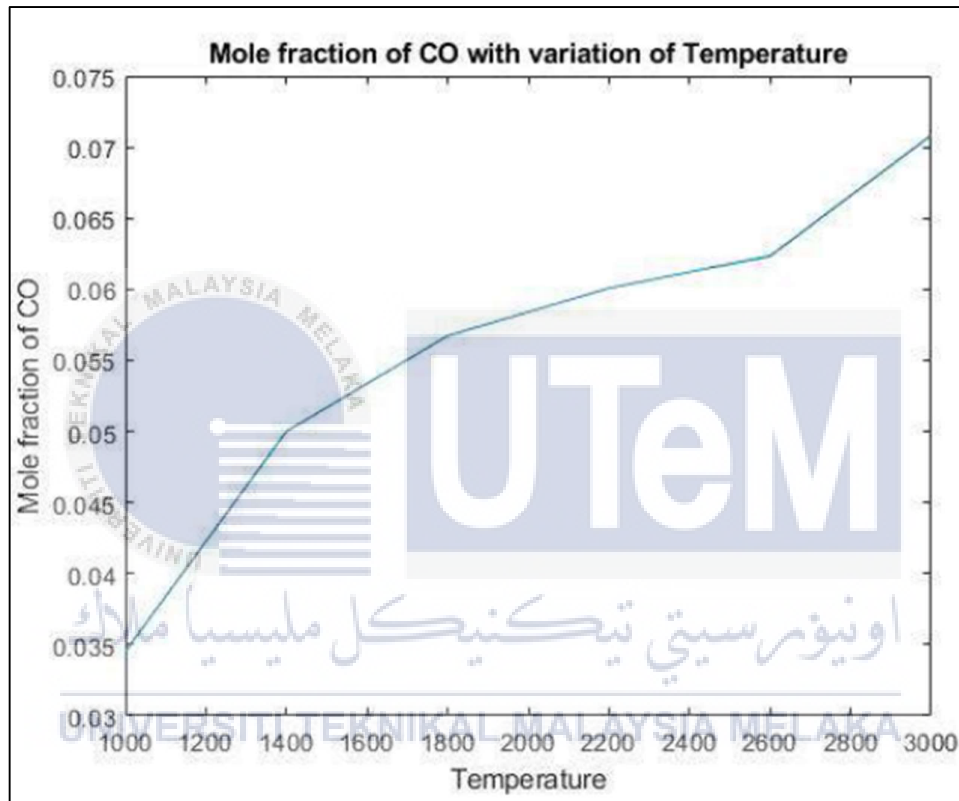


Figure 4.15 Mole fraction of CO with variation of temperature

The graph in figure 4.15 shows the mole fractions of carbon monoxide with variation of temperature from 1000 K to 3000 K and the trends is increasing from the start. It can be noted that as the equivalence ratio is at 1.2, the mole fraction of O_2 is increases throughout all the range temperature that has been set. The number of moles at 1000 K is 0.034524 and it ended at 3000 K with 0.070837 number of moles. The increasing number of moles is about 51 % from 1000 K to 3000 K.

4.2.6 Hydrogen gas (H₂)

Table 4.16 Mole fraction of H₂ with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	0.040517	0.025034	0.018308	0.014976	0.013249	0.01443

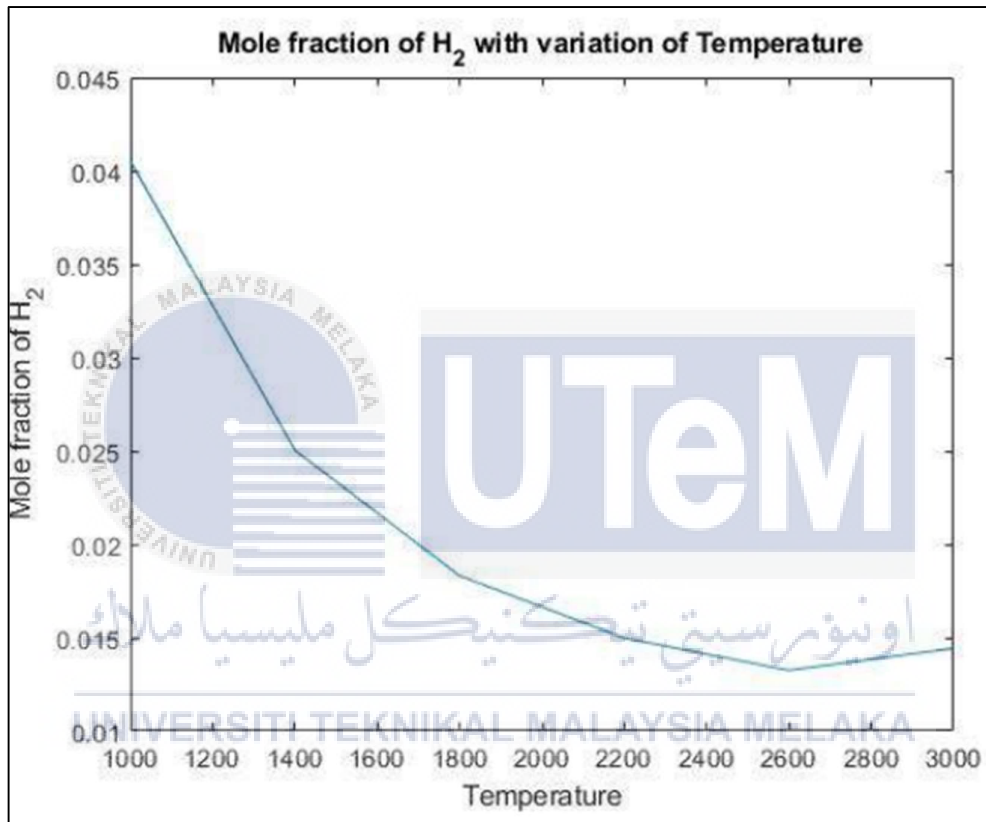


Figure 4.16 Mole fraction of H₂ with variation of temperature

The graph in figure 4.16 shows the mole fractions of hydrogen gas with variation of temperature from 1000 K to 3000 K and the trends is decreasing until it reaches the lowest point. The mole fraction is decreasing until it reaches 2600 K which drop from 0.040517 to 0.013249 number of moles. Then the number of moles is slightly increasing where the number of moles is at 0.01443 when the temperature enters 3000 K. The decreasing number of moles is about 67 % from 1000 K to 2600 K before it increases about 8 % at 3000 K.

4.2.7 Hydrogen atom (H)

Table 4.17 Mole fraction of H with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	8.31E-11	1.4E-07	8.81E-06	0.000125	0.000804	0.00345

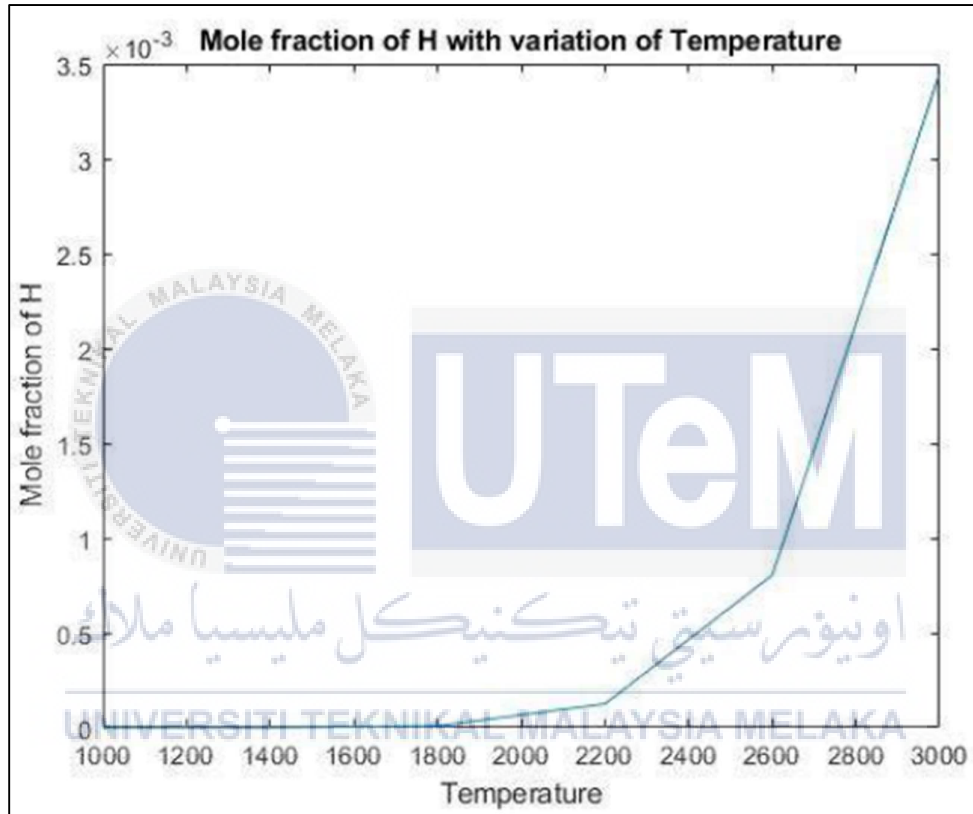


Figure 4.17 Mole fraction of H with variation of temperature

The graph in figure 4.17 shows the mole fractions of hydrogen atom with variation of temperature from 1000 K to 3000 K and the trends is increasing from the start. The mole fraction is slightly increasing from 1000 K to 2200 K which rise from 8.31E-11 to 0.000125 number of moles. Then it is increasing rapidly until the temperature reach 3000 K that has 0.00345 number of moles. The increasing number of moles is about 100 % from 1000 K to 3000 K.

4.2.8 Oxygen atom (O)

Table 4.18 Mole fraction of O with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	1.1E-21	6.4E-14	1.43E-09	8.47E-07	6.97E-05	0.001467

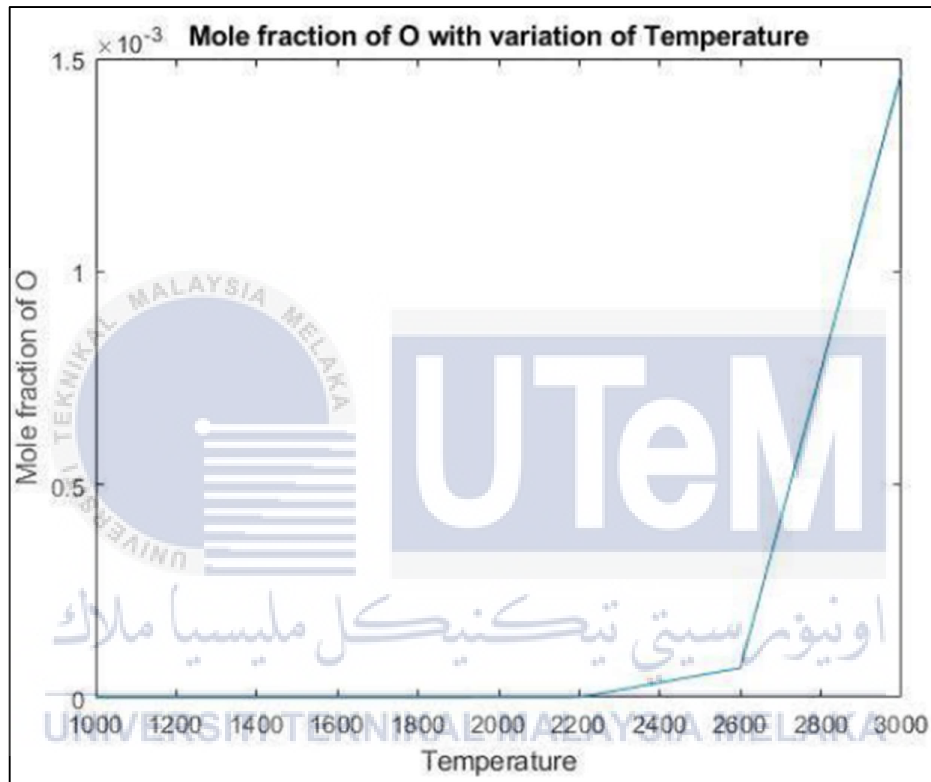


Figure 4.18 Mole fraction of O with variation of temperature

The graph in figure 4.18 shows the mole fractions of oxygen gas with variation of temperature from 1000 K to 3000 K and the trends is increasing slowly before it is increasing rapidly at 2600 K. The mole fraction is increasing slowly from 1000 K to 2600 K which rise from 1.1E-21 to 6.97E-05 number of moles. Then it is increasing rapidly until the temperature reach 3000 K that has 0.001467 number of moles. The increasing number of moles is about 100 % from 1000 K to 3000 K.

4.2.9 Hydroxide (OH)

Table 4.19 Mole fraction of OH with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	1.83E-12	6.64E-08	2.36E-05	0.000992	0.012922	0.069788

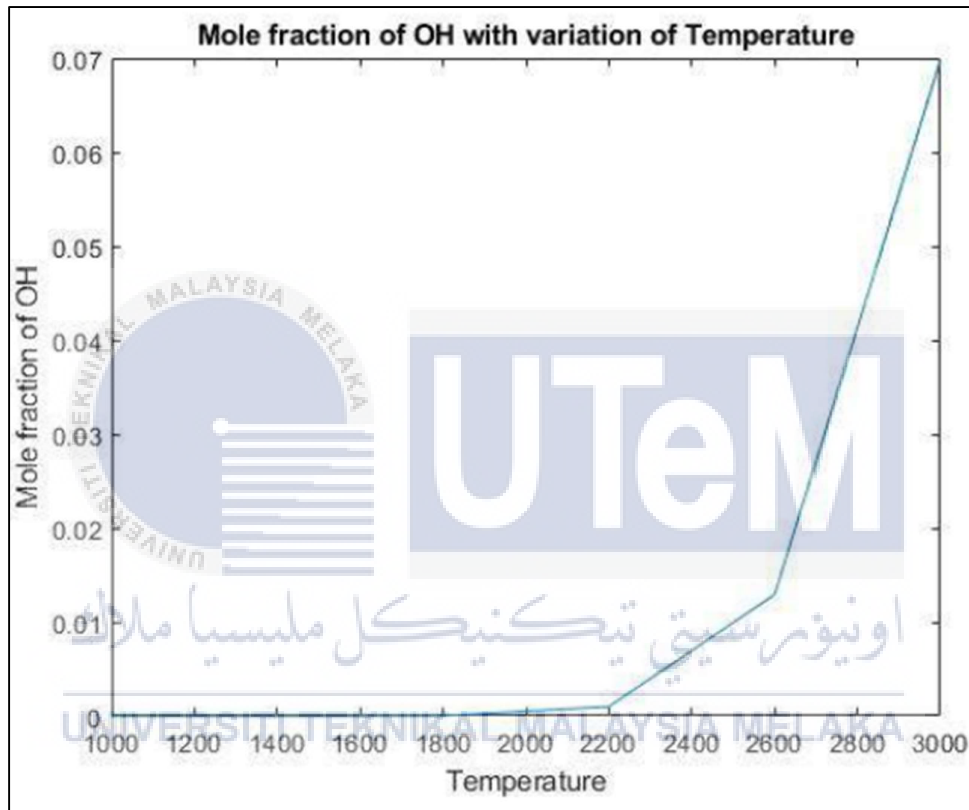


Figure 4.19 Mole fraction of OH with variation of temperature

The graph in figure 4.19 shows the mole fractions of hydroxide with variation of temperature from 1000 K to 3000 K and the trends is increasing from the start. The mole fraction is slightly increasing from 1000 K to 2200 K which rise from 1.83E-12 to 0.000992 number of moles. Then it is increasing rapidly until the temperature reach 3000 K that has 0.069788 number of moles. The increasing number of moles is about 100 % from 1000 K to 3000 K.

4.2.10 Nitrogen Oxide (NO)

Table 4.20 Mole fraction of NO with variation of temperature

Temperature (K)	1000	1400	1800	2200	2600	3000
Number of Mole	2.8E-15	6.08E-10	5.93E-07	4.76E-05	0.000973	0.007339

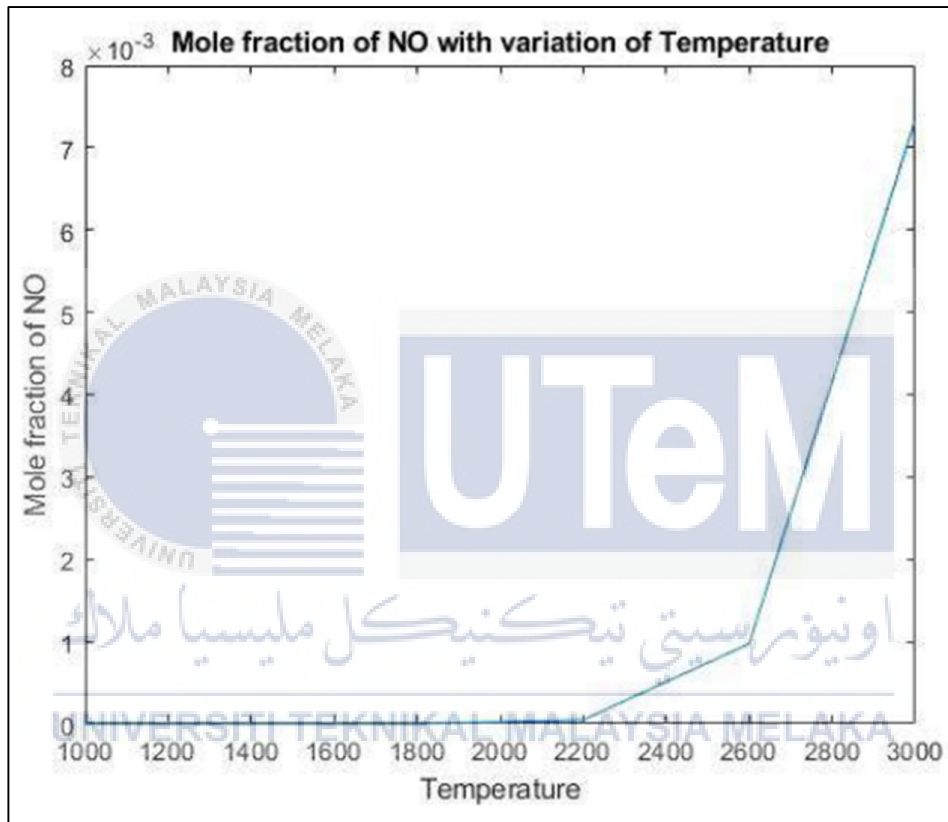


Figure 4.20 Mole fraction of NO with variation of temperature

The graph in figure 4.20 shows the mole fractions of nitrogen oxide with variation of temperature from 1000 K to 3000 K and the trends is increasing from the start. The mole fraction is slightly increasing from 1000 K to 2200 K which rise from 2.8E-15 to 4.76E-05 number of moles. Then it is increasing rapidly until the temperature reach 3000 K that has 0.007339 number of moles. The increasing number of moles is about 100 % from 1000 K to 3000 K.

4.3 The mole fraction of every combustion product with variation of pressure

4.3.1 Carbon Dioxide (CO₂)

Table 4.21 Mole fraction of CO₂ with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.084805	0.086271	0.087257	0.087971	0.088513	0.088939	0.089283

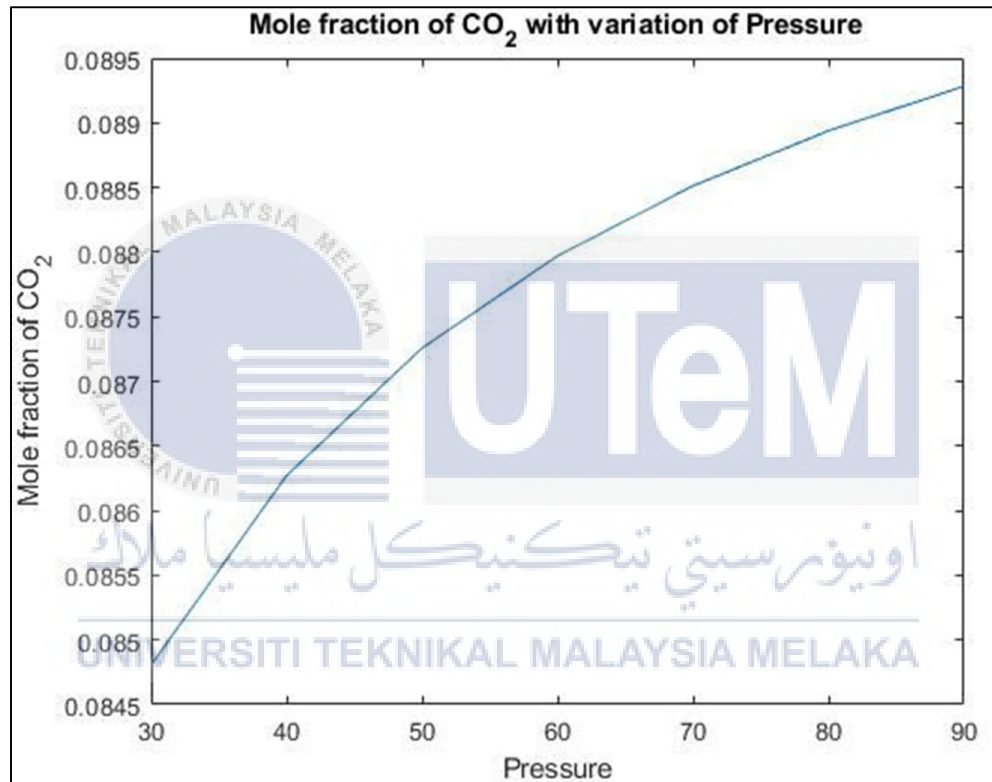


Figure 4.21 Mole fraction of CO₂ with variation of pressure

The graph in figure 4.21 shows the mole fractions of carbon dioxide with variation of pressure from 30 bar to 90 bar and the trends is increasing from the start. The mole fraction is increasing consistently from 30 bar which has 0.084805 number of moles and it keep rising until the pressure at 90 bar that has 0.089283 number of moles. The increasing number of moles is about 5 % from 30 bar to 90 bar.

4.3.2 Water (H₂O)

Table 4.22 Mole fraction of H₂O with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.124536	0.125021	0.12534	0.125567	0.125738	0.125871	0.125978

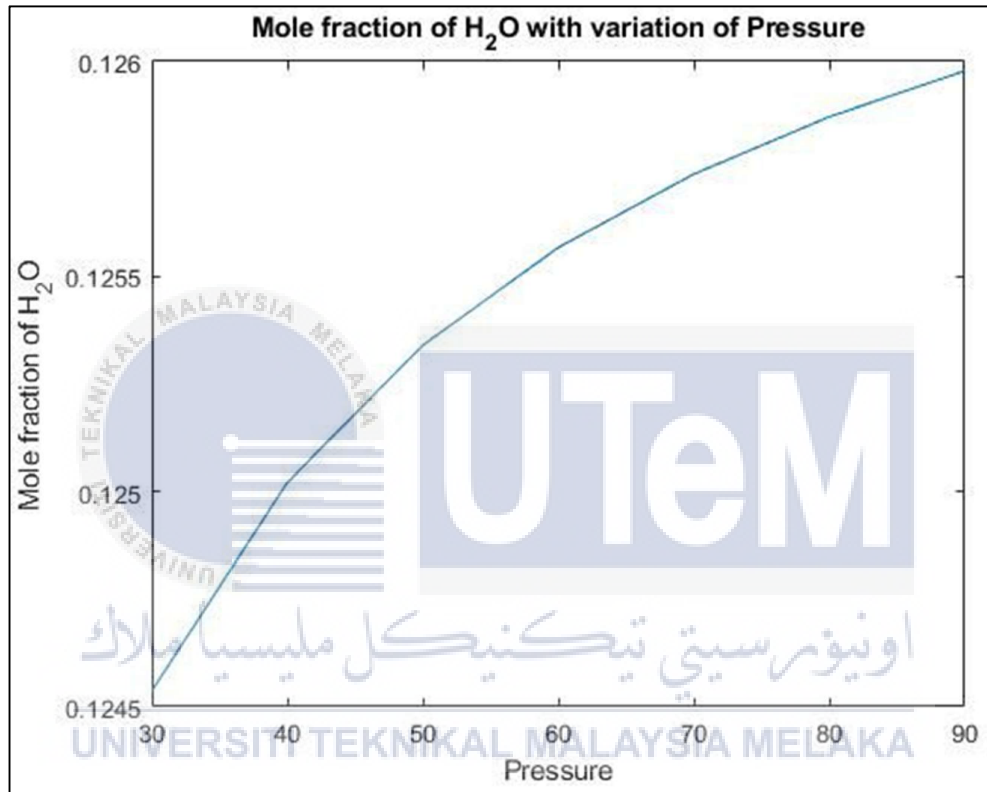


Figure 4.22 Mole fraction of H₂O with variation of pressure

The graph in figure 4.22 shows the mole fractions of water with variation of pressure from 30 bar to 90 bar and the trends is increasing from the start. The mole fraction is increasing consistently from 30 bar which has 0.124536 number of moles and it keep rising until the pressure at 90 bar that has 0.125978 number of moles. The increasing number of moles is about only 1 % from 30 bar to 90 bar.

4.3.3 Nitrogen gas (N₂)

Table 4.23 Mole fraction of N₂ with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.705392	0.705392	0.705392	0.705392	0.705392	0.705392	0.705392

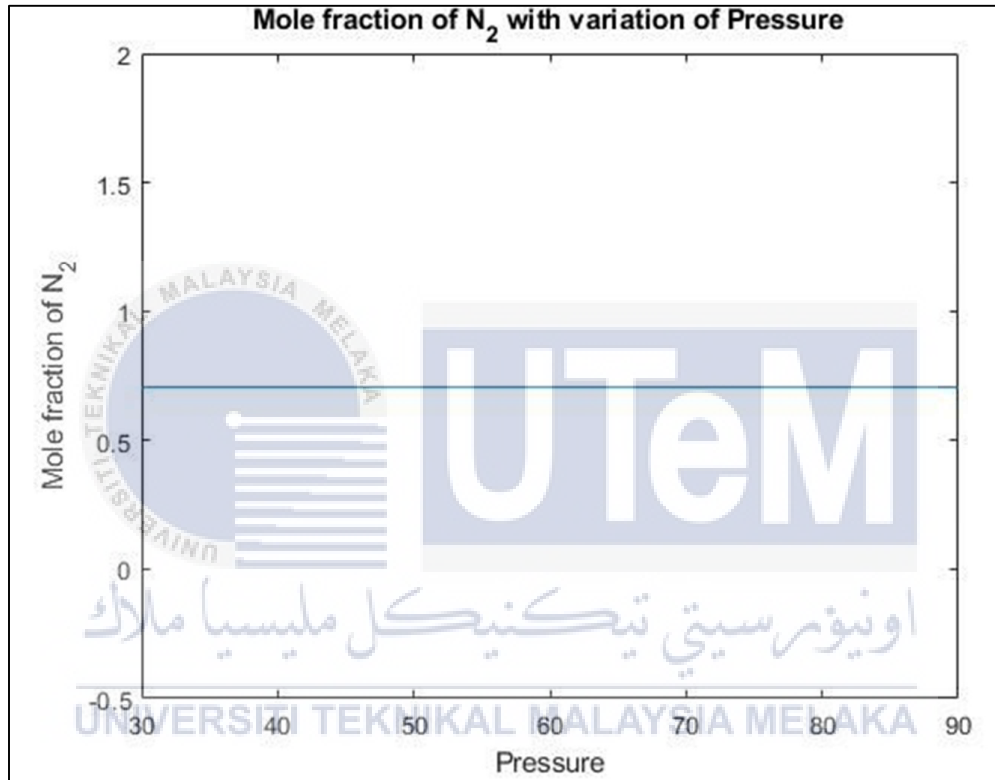


Figure 4.23 Mole fraction of N₂ with variation of pressure

The graph in figure 4.23 shows the mole fractions of nitrogen gas with variation of pressure from 30 bar to 90 bar and the trends is consistent from the start until the end. The number of moles is static at 0.705392 from 30 bar to 90 bar. This shown that the emission of Nitrogen gas, N₂ is decomposed completely when the temperature of combustion reaches 30 bar. There is no percentage difference between the range of temperature from 30 bar to 90 bar.

4.3.4 Oxygen gas (O₂)

Table 4.24 Mole fraction of O₂ with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.005112	0.004137	0.003485	0.003014	0.002658	0.002378	0.002152

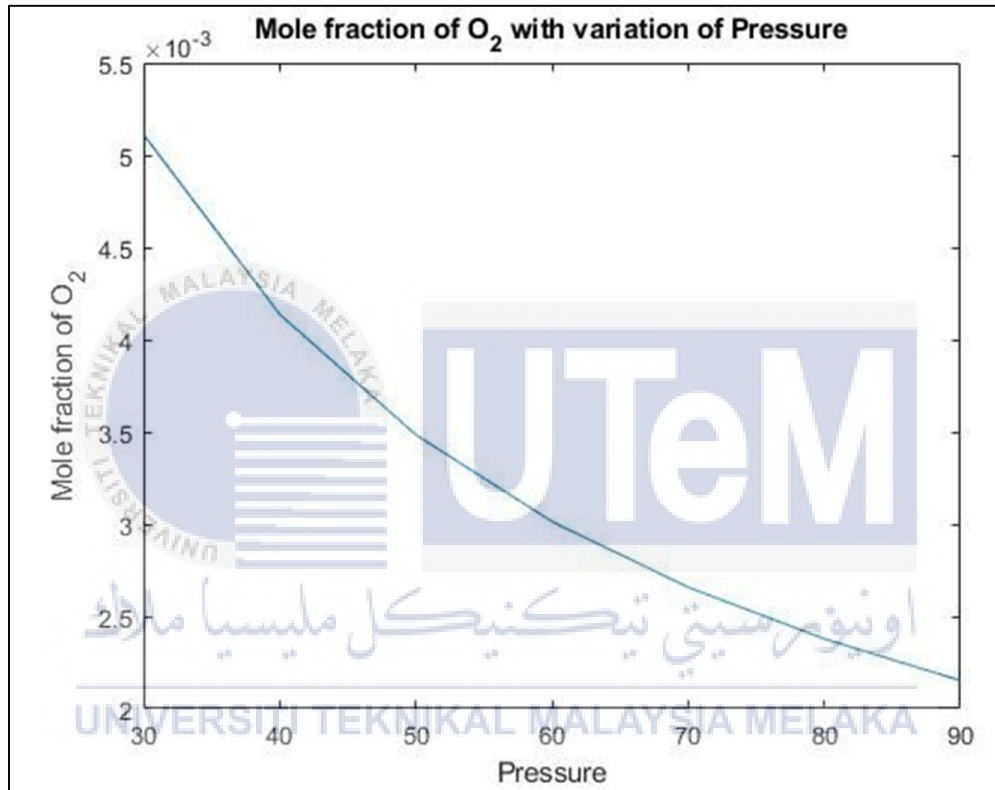


Figure 4.24 Mole fraction of O₂ with variation of pressure

The graph in figure 4.24 shows the mole fractions of oxygen gas with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting at the pressure of 30 bar which has 0.005112 number of moles and it keep decreasing until the pressure at 90 bar that has 0.002152 number of moles. The decreasing number of moles is about 58 % from 30 bar to 90 bar.

4.3.5 Carbon Monoxide (CO)

Table 4.25 Mole fraction of CO with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.070837	0.069371	0.068385	0.067671	0.067129	0.066703	0.066359

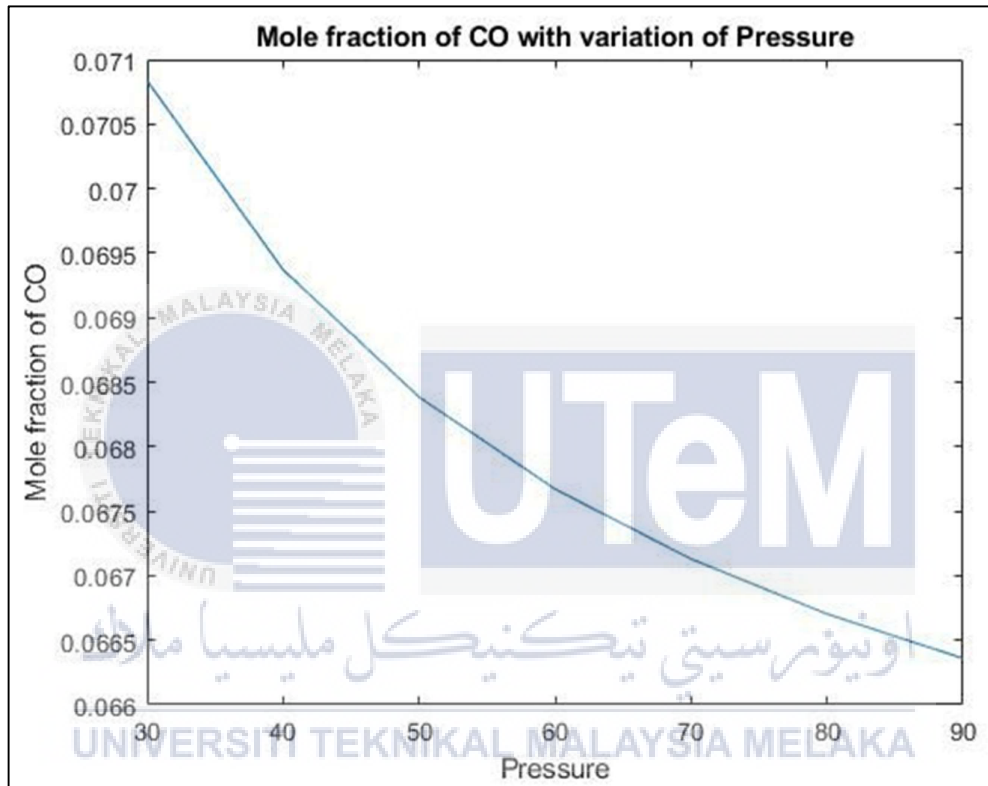


Figure 4.25 Mole fraction of CO with variation of pressure

The graph in figure 4.25 shows the mole fractions of carbon monoxide with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting t the pressure of 30 bar which has 0.070837 number of moles and it keep decreasing until the pressure at 90 bar that has 0.066359 number of moles. The decreasing number of moles is about 6 % from 30 bar to 90 bar.

4.3.6 Hydrogen gas (H₂)

Table 4.26 Mole fraction of H₂ with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.01443	0.013945	0.013626	0.013399	0.013228	0.013095	0.012988

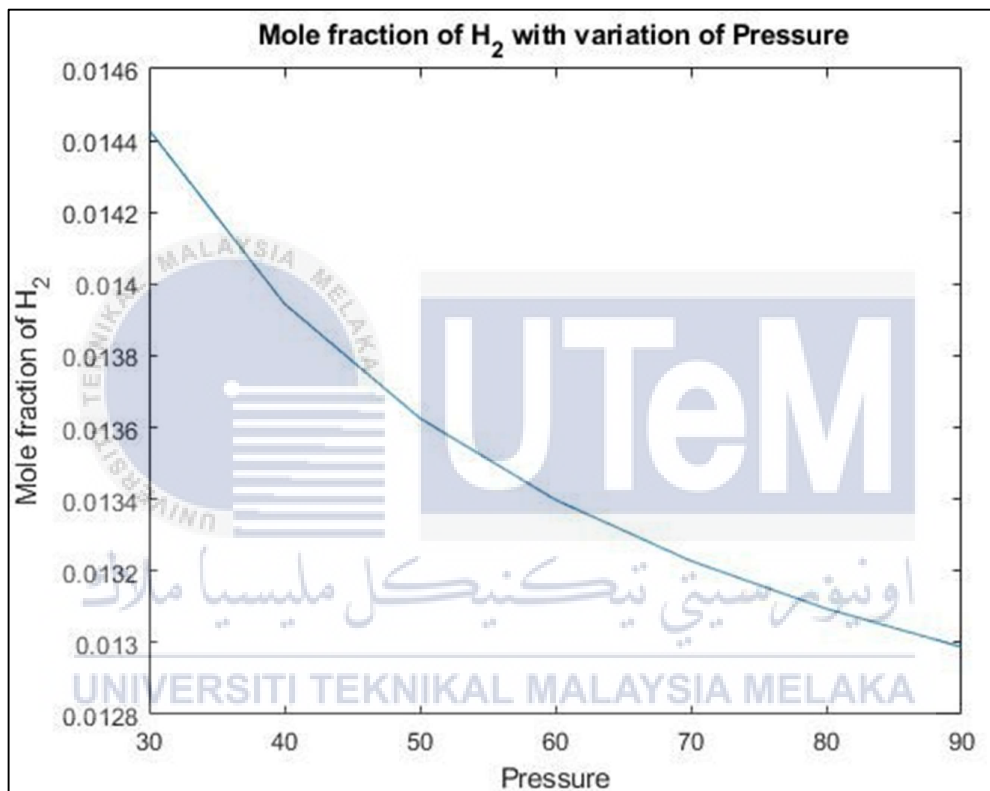


Figure 4.26 Mole fraction of H₂ with variation of pressure

The graph in figure 4.26 shows the mole fractions of hydrogen gas with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting pressure of 30 bar which has 0.01443 number of moles and it keep decreasing until the pressure at 90 bar that has 0.012988 number of moles. The decreasing number of moles is about 10 % from 30 bar to 90 bar.

4.3.7 Hydrogen atom (H)

Table 4.27 Mole fraction of H with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.00345	0.002937	0.002597	0.002351	0.002163	0.002013	0.00189

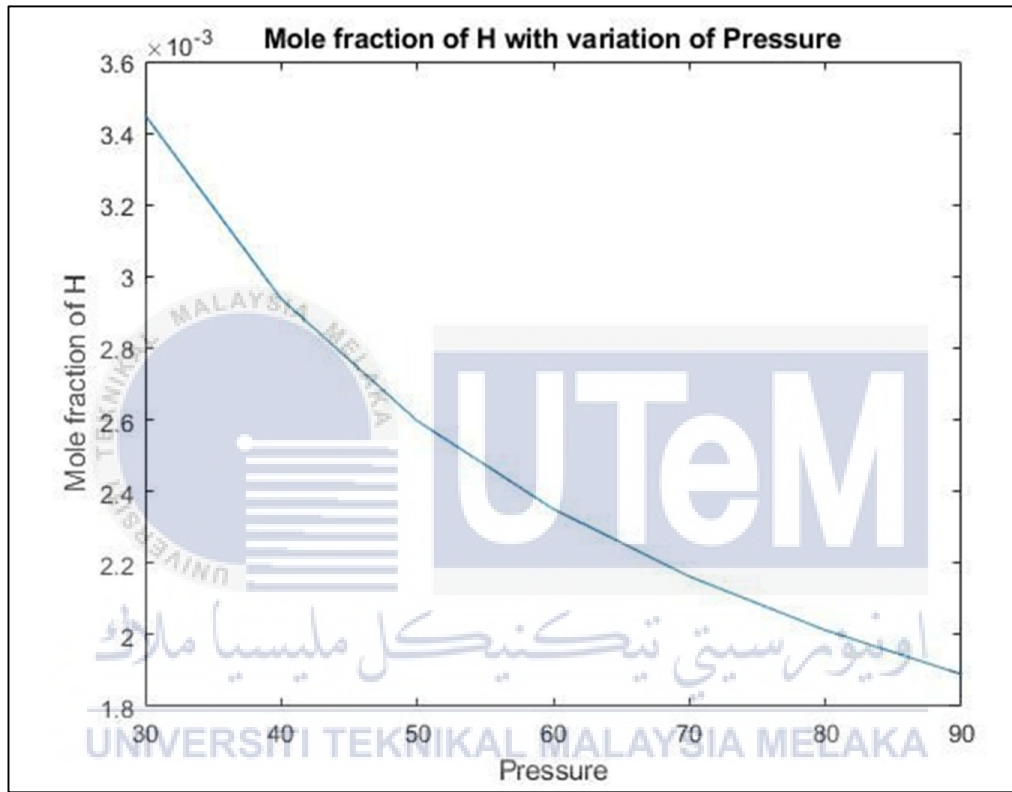


Figure 4.27 Mole fraction of H with variation of pressure

The graph in figure 4.27 shows the mole fractions of hydrogen atom with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting pressure of 30 bar which has 0.00345 number of moles and it keep decreasing until the pressure at 90 bar that has 0.00189 number of moles. The decreasing number of moles is about 45 % from 30 bar to 90 bar.

4.3.8 Oxygen atom (O)

Table 4.28 Mole fraction of O with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.001467	0.001143	0.000938	0.000797	0.000693	0.000613	0.00055

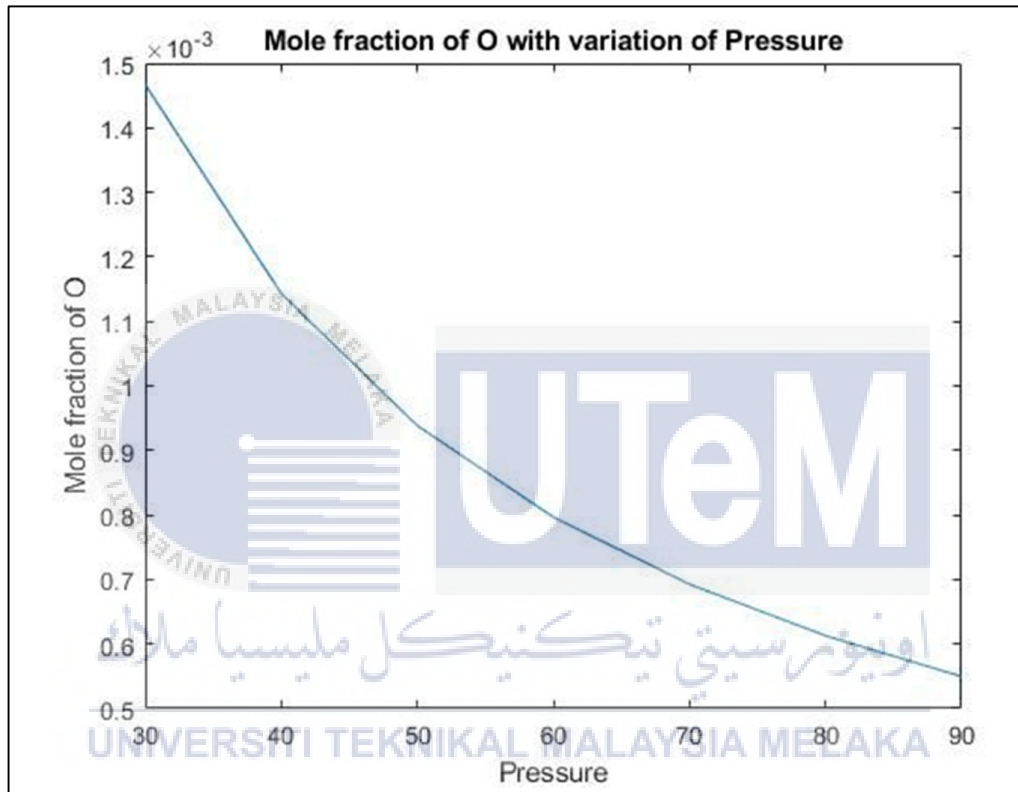


Figure 4.28 Mole fraction of O with variation of pressure

The graph in figure 4.28 shows the mole fractions of oxygen atom with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting pressure of 30 bar which has 0.001467 number of moles and it keep decreasing until the pressure at 90 bar that has 0.00055 number of moles. The decreasing number of moles is about 63 % from 30 bar to 90 bar.

4.3.9 Hydroxide (OH)

Table 4.29 Mole fraction of OH with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.069788	0.062782	0.057615	0.053585	0.050318	0.047597	0.045283

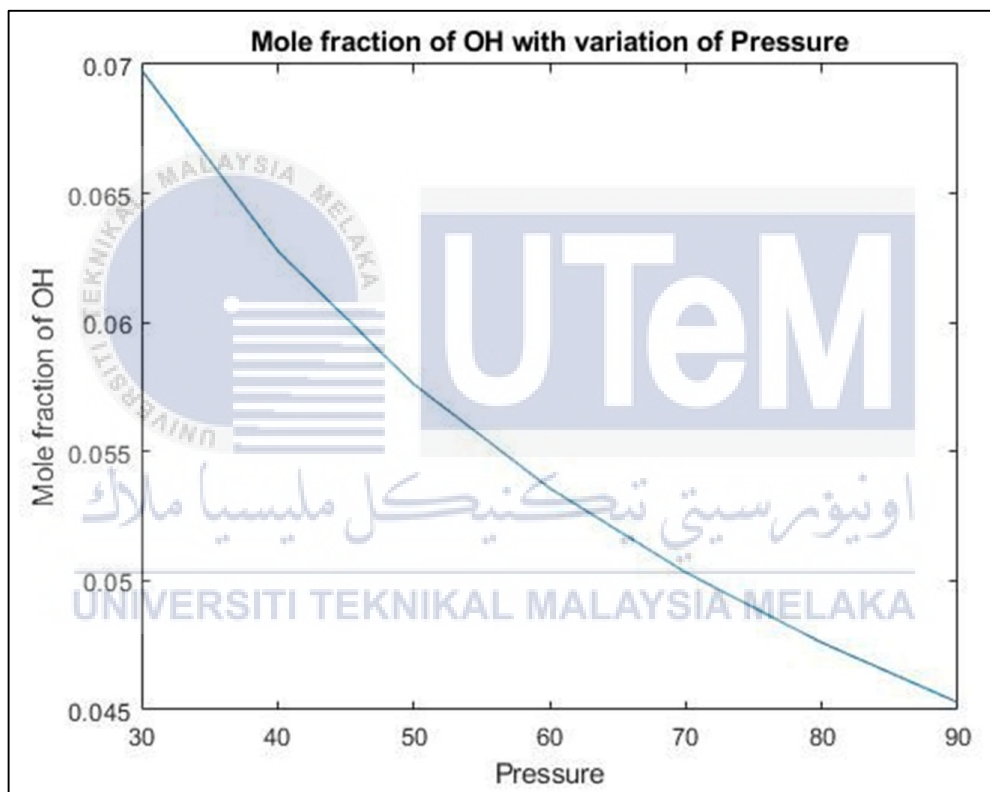


Figure 4.29 Mole fraction of OH with variation of pressure

The graph in figure 4.29 shows the mole fractions of hydroxide with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting pressure of 30 bar which has 0.069788 number of moles and it keep decreasing until the pressure at 90 bar that has 0.045283 number of moles. The decreasing number of moles is about 35 % from 30 bar to 90 bar.

4.3.10 Nitrogen Oxide (NO)

Table 4.30 Mole fraction of NO with variation of pressure

Pressure (bar)	30	40	50	60	70	80	90
Number of Mole	0.007339	0.006602	0.006059	0.005635	0.005291	0.005005	0.004762

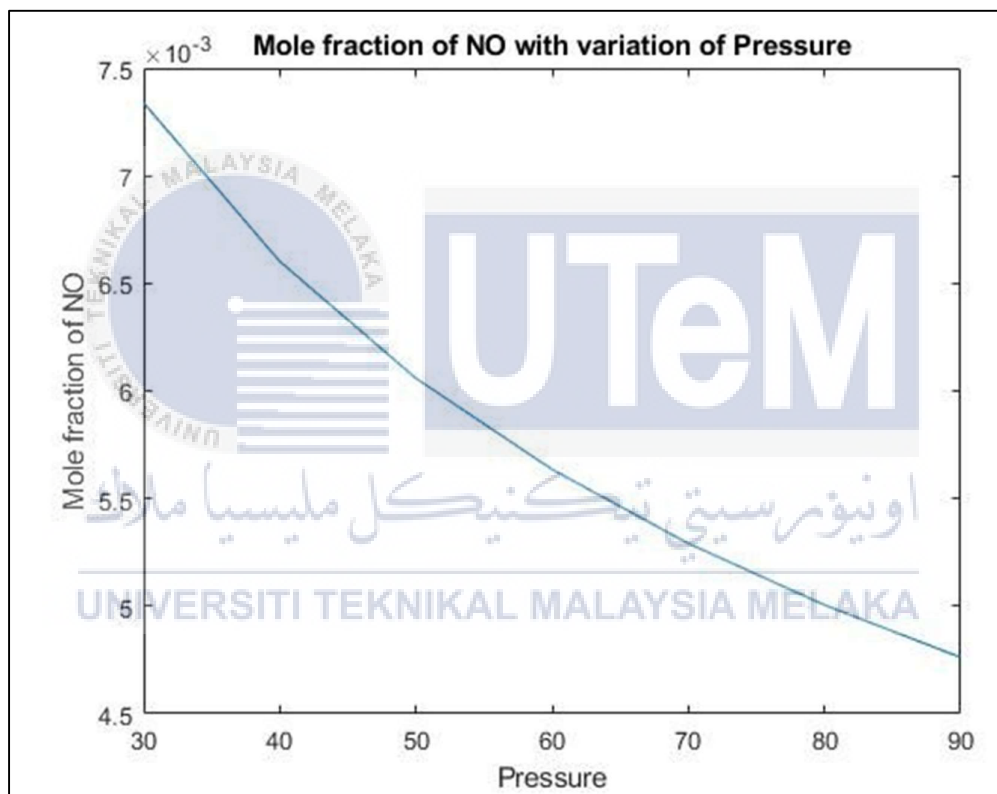


Figure 4.30 Mole fraction of NO with variation of pressure

The graph in figure 4.30 shows the mole fractions of nitrogen oxide with variation temperature from 30 bar to 90 bar and the graph trends is decreasing from the start. The mole fraction is drop starting pressure of 30 bar which has 0.007339 number of moles and it keep decreasing until the pressure at 90 bar that has 0.004762 number of moles. The decreasing number of moles is about 35 % from 30 bar to 90 bar.

4.4 Discussion

4.4.1 Emission of combustion product

The emission of the combustion product of the biodiesel fuel will be discussed in this part. The combustion product like CO, NO and CO₂ are the most critical emission that can give bad effect to the environment. Thus, biodiesel fuel as a clean energy source has the potential to be a realistic alternative to fossil fuels. This fuel may help to reduce the greenhouse gases by lowering the amount of this kind of combustion products released into the atmosphere.

4.4.1.1 Carbon dioxide emission

The emission of the carbon dioxide can be seen in the data and graph where the number of moles is slowly decreased as the equivalence ratio and the temperature is increase. When comparing biodiesel blends to diesel oil, it was discovered that biodiesel fuel will produce lower number of carbon dioxide emissions. In order to explain the decrease in carbon dioxide emissions, it was determined that biodiesel blends had a greater oxygen concentration than conventional diesel oil. The greater amount of carbon dioxide levels is caused by the larger amount of oxygen contained in biodiesel fuel and the lower amount of carbon.

4.4.1.2 Carbon monoxide emission

Colourless and odourless, carbon monoxide is a by-product of hydrocarbon combustion that is regarded an intermediate product. Low oxygen that are reacts with the carbon in fuel to form carbon dioxide gas, which results in the generation of carbon monoxide. Incomplete combustion fuel is the source of the carbon monoxide produced by the incomplete combustion of fuels. Most of the researcher are agreed that a large proportion of biofuel in blends has the potential to reduce the quantity of carbon dioxide emitted. This

is since biofuels include naturally occurring oxygen, which makes it simpler for them to be burned at greater temperatures in the chambers. In this way, the data demonstrate that a greater proportion of biofuel in the blends resulted in lower carbon monoxide emissions.

4.4.1.3 Nitrogen oxide emission

The creation of nitrogen oxide (NO) emissions is directly proportional to the temperature of the combustion chamber, the lower enthalpy of vaporisation, and the concentration of oxygen in the combustion chamber. All biodiesel fuel mixes with additives normally create increasing of the nitrogen oxide emissions when the engine load is increased, and this is true for all of them. When compared to base diesel and biodiesel blends, the increase in NO_x emissions is mostly based on the concentration of oxygen in biodiesel and biodiesel blends that are utilised. The cetane number is a significant factor in the generation of nitrogen oxides. It demonstrates that increasing the proportion of biodiesel in gasoline results in an increase in NO_x emissions.

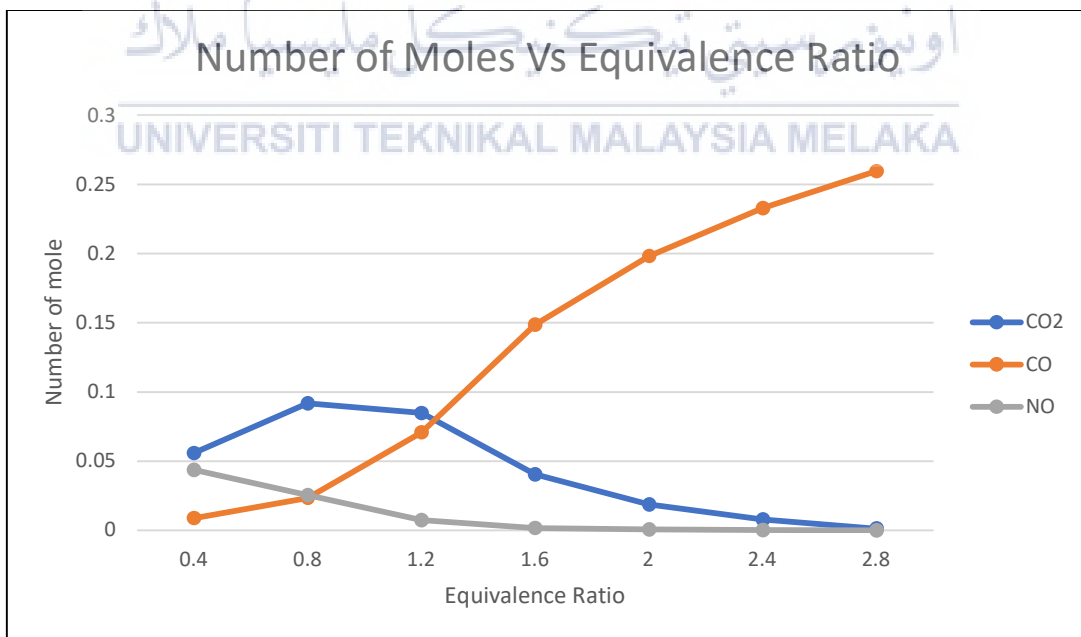


Figure 4.31 Number of moles vs equivalence ratio

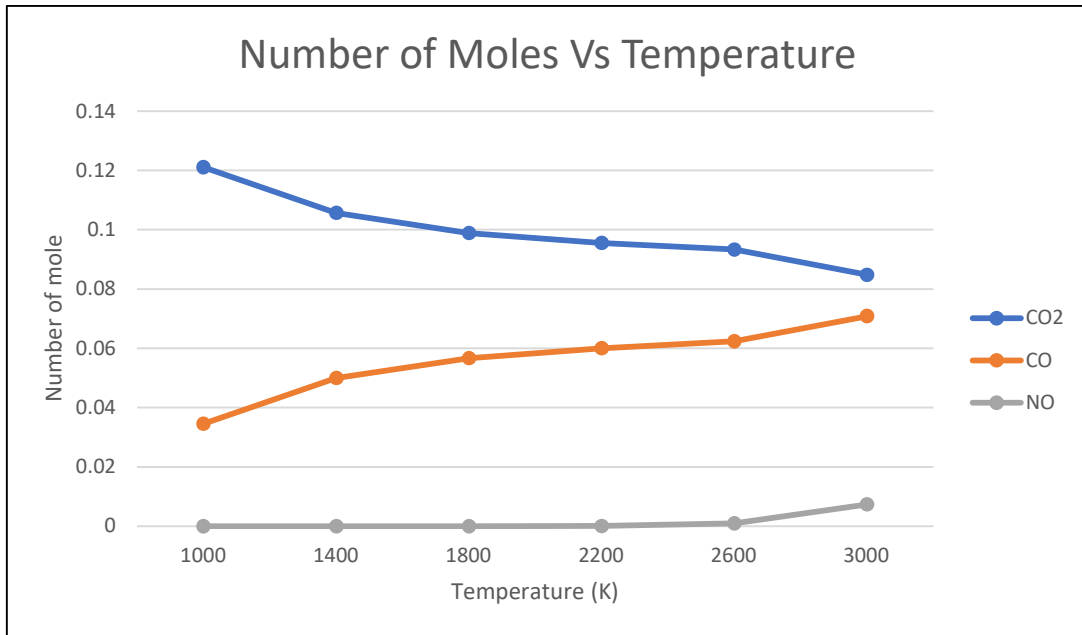


Figure 4.32 Number of moles vs temperature

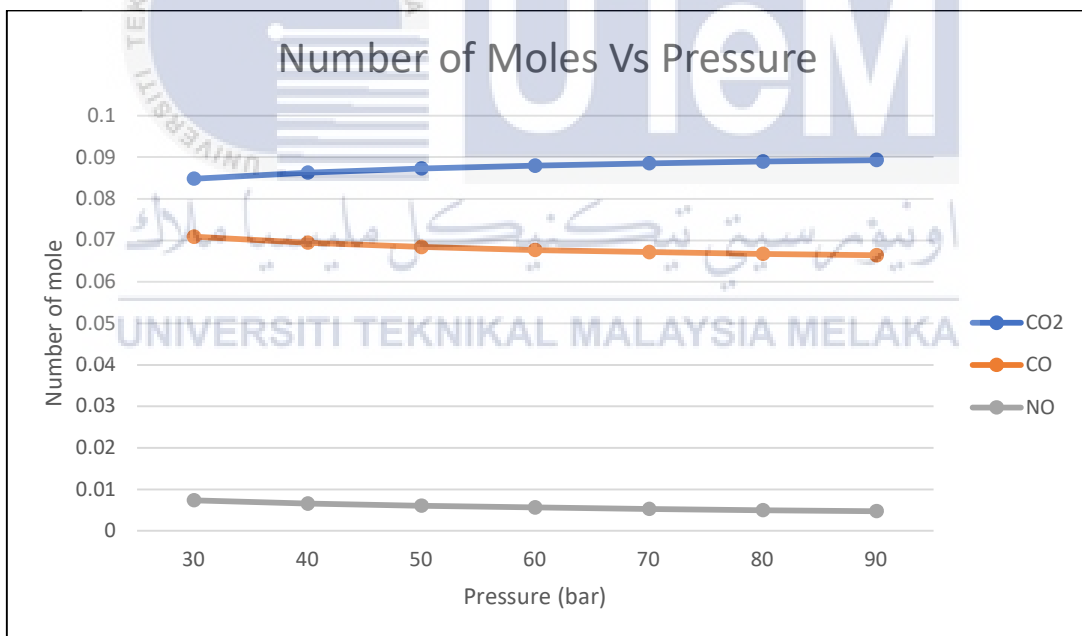


Figure 4.33 Number of moles vs pressure

CHAPTER 5

CONCLUSION AND RECOMMENDATION

5.1 Project Conclusion

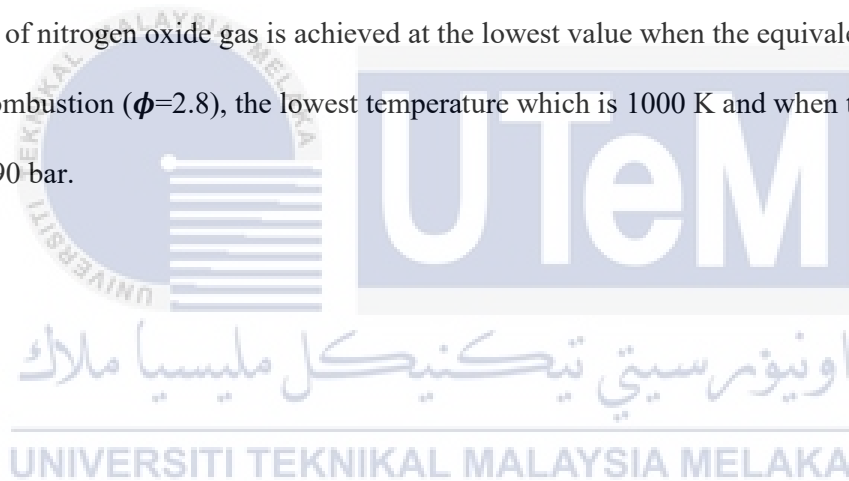
In this study, the characteristic and the number of moles of 10 combustion products were analysed by using some methods that have been discussed in the methodology part. The effects of equivalence ratio which set at the range (0.4 – 2.8), temperature (1000 K - 3000 K), and pressure (30 bar- 90 bar) on premixed combustion species mole fraction are studied using extensive parametric analysis. The equivalence ratio is the mass of air divided by the stoichiometric air fuel ratio and it can be either lean combustion, stoichiometric combustion or rich combustion. From the analysis and the discussion in chapter 4, there are some conclusions that can be made from the study.

First, the mole fraction of H_2O , CO , H_2 and atom H is at their minimum during the lean combustion where the equivalence ratio is lower than 1. The lower the value of the equivalence ratio, the lower the number of moles of these species throughout the combustion process. In comparison, the mole fraction of CO_2 , N_2 , O_2 , O , OH and NO is at their minimum during the rich combustion where the equivalence ratio is higher than 1. The higher the value of the equivalence ratio, the lower the number of moles of these species throughout the combustion process.

Next, the mole fraction of combustion product H_2O , O_2 , CO , atom H, atom O, OH and NO is increased when the temperature is increased while the mole fraction of combustion product CO_2 and H_2 is decreased as the temperature is increased. N_2 is the only species that shown same number of moles through all temperature. For the mole fraction with variation

pressure, it can be seen where the number of moles of the combustion products H_2O and CO_2 is increase as the pressure is increase while the mole fraction of O_2 , H_2 , CO , atom H, atom O, OH and NO is decreased when the pressure is increased. N_2 once again become the only species that has same mole fraction through all the pressure.

To conclude, the emission of carbon dioxide gas is at the lowest when the equivalence ratio is at rich combustion ($\phi=2.8$), the temperature reached the highest point which is 3000 K and during the 30 bar of pressure. Then, the emission of carbon monoxide gas is achieved at the lowest value when the equivalence ratio is at lean combustion ($\phi=0.4$), the lowest temperature which is 1000 K and when the pressure reached 90 bar. Lastly, the emission of nitrogen oxide gas is achieved at the lowest value when the equivalence ratio is at rich combustion ($\phi=2.8$), the lowest temperature which is 1000 K and when the pressure reached 90 bar.



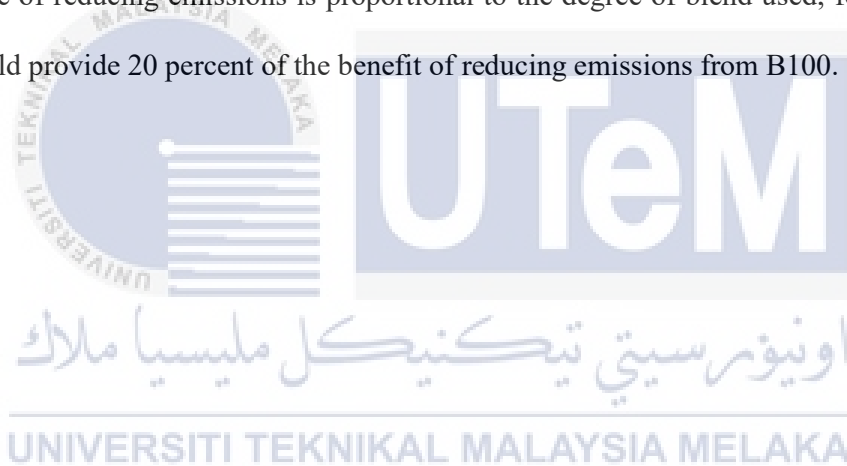
5.2 Area of Improvement

From my personal point of view, the title of this study which the mathematical modelling on the effect of equivalence ratio, temperature and pressure in emission characteristic of compression ignition engine with biodiesel fuel can be improved if more data can be collected during the simulation. In general, this study is focused on using 100 % value of biodiesel to be used in the ignition compression engine. So, it is better if this study can also focus on using the variation blends of biodiesel like B20, B40, B60 and B80. A comparison also can be done if the number of moles of pure diesel is calculated in this study. It is important so that the number of moles of the combustion product in the diesel can be compared easily to the blends of biodiesel. Thus, a clear explanation on every graph can be proved that biodiesel fuel has produce less emission that using the diesel fuel.

Next, the variation blends of biodiesel fuel are also important because the existing ignition compression engine cannot use B100 as there will be some problems that might be occur to the engine itself. Some of the most serious drawbacks of biodiesel are related to its impact on the engine functioning, including the blockage of fuel lines and injectors. As biodiesel is a liquid, it may leave deposits in the fuel system, clog the fuel filter, and cause deposits to build up in the fuel tank, among other things. The replacement of the gasoline filter is generally sufficient to resolve the issue.

B20 is a typical blend because it provides an excellent combination of cost, emissions and cold-weather performance, while also being compatible with a variety of materials and capable of acting as a solvent. A large proportion (B20 or lower blends) of biodiesel consumers get their product through their regular gasoline distributors or from biodiesel marketers. In general, B20 and lower-level blends may be utilised in contemporary engines without requiring any changes. a large number of diesel engine original equipment manufacturers (OEMs) support the usage of B20.

Compared to engine running on diesel fuel, engines running on B20 use less fuel, produce more horsepower, and have more torque. In comparison to petroleum diesel, B20 with 20 percent biodiesel content will have 1 to 2 percent less energy per gallon of fuel. However, many B20 users have reported no perceptible differences in performance or fuel efficiency. Some of the environmental advantages of biodiesel are also applicable to engines built before 2010. Engines fitted with selective catalytic reduction (SCR) systems provide the same advantages in terms of environmental impacts whether they are powered by biodiesel or petroleum diesel. Although biodiesel emits less greenhouse gas than traditional pure diesel, it nevertheless has a bigger impact on global warming. Generally speaking, the advantage of reducing emissions is proportional to the degree of blend used; for example, B20 would provide 20 percent of the benefit of reducing emissions from B100.



APPENDICES

A1 MATLAB coding for the mole fraction of every combustion product with variation of equivalence ratio.

```

clear all
clc
close all

% Mathematical modelling on the effect of equivalence ratio in emission
% characteristic of compression ignition engine with biodiesel fuel.

T = 3000; % Temperature
t = T/10000;
P = 30; % Total Pressure
eqratio = 0.4:0.4:2.8; % 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 = 14; % Carbon
    beta = 25; % Hydrogen
    gamma = 0;
    delta = 0;
    as = alpha+(beta/4)-0;
    gamma = gamma + (2*as/eqratio(i)); % Oxygen
    delta = delta + (7.52*as/eqratio(i)); % Nitrogen

```

*It is noted that only 50% of the coding were shown in the appendices part

A2 MATLAB coding for the mole fraction of every combustion product with variation of temperature.

```

clear all
clc
close all

% Mathematical modelling on the effect of temperature in emission
% characteristic of compression ignition engine with biodiesel fuel.

% 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 = 1000:400:3000; % Temperature
P = 30; % Total Pressure
eqratio = 1.2; % Equivalence Ratio

alpha = 14; % Carbon
beta = 25; % Hydrogen
gamma = 0;
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(5,10);

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;
        K(j) = 10^log10K(j);
    end
end

```

*It is noted that only 50% of the coding were shown in the appendices part

A3 MATLAB coding for the mole fraction of every combustion product with variation of pressure.

```

clear all
clc
close all

% Mathematical modelling on the effect of equivalence ratio in emission
% characteristic of compression ignition engine with biodiesel fuel.

% 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 = 30:10:90; % Total Pressure
eqratio = 1.2; % Equivalence Ratio
matY = zeros(7,10);

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

alpha = 14; % Carbon
beta = 25; % Hydrogen
gamma = 0;
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;

```

*It is noted that only 50% of the coding were shown in the appendices part

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