DEVELOPMENT OF IGNITION MECHANISM THROUGH TRANSIENT SPECIES ANALYSIS

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ACKNOWLEDGEMENTS

Special thanks to internal grant RDU 1703144 from Universiti Malaysia Pahang for granting this fund for my research development. It was my first time to apply and utilize the fund given. I hope UMP may continue to support my current and future support.

ABSTRAK

Projek ini adalah untuk mengkaji mekanisme pencucuhan nombor oktana yang rendah dan tinggi daripada campuran bahan api melalui simulasi yang komprehensif. Pencucuhan mampatan caj seragam (HCCI) adalah untuk pembakaran alternatif konsep dalam enjin reciprocating yang menawarkan manfaat yang ketara dari segi kecekapan tinggi dan rendah pelepasan. HCCI adalah yang paling biasa digunakan nama untuk pencucuhan auto pelbagai bahan api dan salah satu alternatif yang paling menjanjikan untuk SI pembakaran dan pembakaran CI. Objektif projek ini adalah untuk mengkaji mekanisme tindak balas pencucuhan mampatan pada pengoksidaan suhu rendah (LTO) dan reka bentuk model ringkas mekanisme tindak balas bagi n-heptane + toluene (NTF). Pengoksidaan suhu rendah (LTO) mentakrifkan sebagai pengoksidaan pada suhu yang berhampiran atau di bawah 25 °C. Mekanisma heptane telah dikaji secara meluas dalam kesusasteraan hari dan yang lepas kerana kepentingannya sebagai rujukan utama minyak. Dalam kajian ini, n-heptane sebagai minyak asas dan toluene sebagai bahan api kecil, akan menggunakan sebagai bahan api campuran simulasi ini. Selain itu, bagi angka analisis, model Reka bentuk yang ringkas mekanisme tindak balas bagi n-heptane yang disokong oleh perisian MATLAB. Model ringkas yang telah dibincangkan dalam projek ini. Hasil yang ketara daripada projek ini, ia boleh dilihat bahawa peningkatan toluene kandungan boleh menyebabkan reaksi Kumpulan aldehyde dan pembiakan OH. Akhirnya, tesis menyimpulkan bahawa model mudah dibina dengan balasan harta tindak balas berlaku pada n-heptane (bahan api asas) ditambah dengan toluene (api kecil) di mana OH pembiakan dan bahan api + OH reaksi memainkan peranan penting.

ABSTRACT

This project is to study the ignition mechanism of low and high octane number of fuel blends through comprehensive simulation. Homogenous Charge Compression Ignition (HCCI) is an alternative combustion concept for in reciprocating engines which offers significant benefits in terms of its high efficiency and low emissions. HCCI is the most commonly used name for the auto-ignition of various fuels and one of the most promising alternatives to SI combustion and CI combustion. The objectives of this project is to study reaction mechanism of compression ignition at Low Temperature Oxidation (LTO) and design the simplified model of reaction mechanism for n-heptane + toluene (NTF). Low Temperature Oxidation (LTO) define as oxidation at temperatures near or below 25°C. The low temperature oxidation mechanisms of n-heptane have been extensively studied in recent and past literature because of its importance as a primary reference fuel. In this study, n-heptane as a base fuel and toluene as a sub fuel, will use as a fuel mixture in this simulation. Moreover, for numerical analysis, to design simplified model of reaction mechanism for n-heptane supported by MATLAB software. The simplified model has been discussed in this project. The significant result of this project, it can observed that the increasing of toluene content can caused the reaction of aldehyde group and OH reproduction. Finally, thesis conclude that the simplified model constructed with a consideration of the property of reaction happen in n-heptane (base fuel) added with toluene (sub fuel) in which OH reproduction and fuel + OH reaction plays important role.

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k_b	Rate constant of base fuel
k_s	Rate constant of sub fuel

LIST OF ABBREVIATIONS

LTO	Low Temperature Oxidation
pHIAS	Pre-Heated Intake Air System
NTF	n-heptane and toluene mixture
HCCI	Homogeneous Charge Compression Ignition
NO_x	Nitrogen oxide

CHAPTER 1

INTRODUCTION

1.1 Project Background

In general, a heat engine is known as a mechanical system that converts chemical energy to thermal energy and then to mechanical energy or to electrical energy. A heat engine can be defined as external combustion engines and internal combustion engines by the method of heating the working fluid. An internal combustion engine gets the energy directly using heat energy generated by the combustion in the interior of the working fluid [1]. Typical example of internal combustion engine is an engine used in automobile, in which the high temperature is achieved by burning the gasoline-air mixture in the cylinder itself. On the other hand, an external heat engine is a heat engine where an internal working fluid is heated by combustion through the engine wall or a heat exchanger and also known as Stirling engines [2]. For example, steam engines are external combustion engines, where the working fluid is separate from the combustion products.

Homogeneous Charge Compression Ignition (HCCI) engine is a promising alternative with high thermal efficiency and ultra-low emission characteristics to the existing internal combustion engines. Ideal HCCI combustion is characterized by the lean and low temperature reactions because it can initiated at multiple sites simultaneously without any flame propagation. HCCI combustion is the process in which a homogeneous mixture is auto-ignited through compression. HCCI has the potential to reduce both particulate matter and NO_x emissions while maintaining the fuel efficiency [3].

Chemical kinetic reaction mechanisms in combustion play an important role in the study of hydrocarbon fuels. Today, we see that hydrocarbon fuels are an essential source of energy used for transportation in our daily life. The combustion models for these fuels are used to predict the performance of internal combustion engines. With these combustion models, engines can be designed to improved efficiency and reduced emissions in system. This project is to study the ignition mechanism of compression ignition at Low Temperature Oxidation (LTO) by develop the simplified model of reaction mechanism of fuel mixture, and numerical simulation by using MATLAB software where the ignition behaviour of n-heptane changing with the fuel mixing ratio. Low Temperature Oxidation is a reaction which occur at or below room temperature (usually 500K-1000K).

1.2 Problem Statement

The oxidation of normal n-heptane (nC_7H_{16}) already has been subject of many experiment and model of the studies. But still most of the studies were carried out under High Temperature Oxidation (HTO) and very few to the Low Temperature Oxidation (LTO) of the n-heptane especially regarding the characterization reaction products. Low temperature oxidation (LTO) of hydrocarbons is of importance for the development of diesel and homogenous charge compression ignition (HCCI) engines, as this particular chemistry triggers auto-ignition phenomena. Low Temperature Oxidation (LTO) regions is highly depending on complicated chemical reaction mechanism as well as ignition delay and also for reaction pathway of both base fuel and sub fuel. In this project, by developing a simplified model of the reaction mechanism of fuel mixture (base fuel and sub fuel), the analysis of the reaction mechanism of the fuel mixture in low temperature oxidation becomes easier in term of time effective because it can minimize the time by doing this concept of analysis. Moreover, it also benefit in term of cost saving and friendly environment because no need to do the experimental process.

1.3 Objectives

The purpose of this project is to study reaction mechanism of low and high octane number of fuel and develop a simplified model of ignition behaviour for n-heptane by numerical simulation. The main objectives of this project are listed below:

- To study reaction mechanism of compression ignition at Low Temperature Oxidation (LTO).
- To develop of simplified model of reaction mechanism for n-heptane fuel at Low Temperature Oxidation (LTO).

1.4 Scope of Study

This project research is about to analyse the ignition behaviour of n-heptane changing with the fuel mixing ratio. The main scopes of this project are listed below:

- To identify the n-heptane + toluene (NTF) fuel at various percentage.
- To analyse the reaction mechanism of compression at small heat generation as known as Cool Ignition (600-800K).
- To develop the simplified model of reaction mechanism for fuel mixture supported by MATLAB software.
- To develop a GUI for simplified model of reaction mechanism for fuel mixture at Low Temperature Oxidation.

CHAPTER 2

LITERATURE REVIEW

2.1 Internal Combustion Engine

Combustion, also known as burning, is the basic chemical process of releasing energy from a fuel and air mixture. In an internal combustion engine, the ignition and combustion of the fuel occurs within the engine itself. The internal combustion engine is an engine that uses the explosive combustion of fuel to push or move a piston within the cylinder engine [1, 4, 5]. There are basically two types of internal combustion ignition engines which are ignite by using spark plug and rely on the compression of a fluid [1, 4]. Spark ignition engines take a mixture of fuel and air then compress it and burn it by using spark plug [1, 4, 5]. The piston cylinder engine is basically a crank-slider mechanism. The piston is moved up and down by the rotary motion of the two arms or link, where the crankshaft rotates which make the links also rotate [1, 4, 5]. The piston encapsulated within a combustion chamber. The bore is the diameter of the chamber. The valves on the top represent of induction and exhaust valves where the induction is the intake of air-fuel mixture and the exhaust valves for exhaust of chamber residuals [4-6]. In a spark ignition system, a spark plug required electrical discharge to ignite the mixture of air-fuel. In compression ignition system, at high temperature and pressure will ignite the mixture [4-6]. The highest point where the piston reaches is called Top Dead Centre and the lowest point where the piston reaches is called Bottom Dead Centre. The ratio of the bottom dead centre and top dead centre is called compression ratio. The compression ratio is very important aspect in both compression and spark ignition system which defining as the efficiency of engines [7].

2.2 History of Internal Combustion Engine

The well-known Otto engine was invented by Dr. Nicholas Otto, of Germany, and was patented in this country in 1877. It follows the cycle that has been described by Beau de Rochas, now known as the four-cycle, or sometimes as the Otto cycle. The engine was first known as the Otto-Silent, to distinguish it from the free-piston engine, which was rather noisy. It immediately established the internal-combustion engine on a firm footing, and the engines of the four-cycle type sold today show merely minor improvements. Research on Internal Combustion Engine has been improved up until 1970's [1, 4, 7]. However, as oil shock happens and pollutions problems came ahead, the research has moved on mainly towards engines efficiency and environment friendly. This trend is not stop until now and rule on exhaust gas has been more strict years by year. More than that, CO_2 has caused the global warming problem and depletion of petroleum throughout the world has been critically until now.

These days gasoline engines and diesel engine has been widely used as an internal combustion engine. However, these two engines have disadvantages and one of the solutions is Homogeneous Charge Compression Ignition engine known as HCCI engine. Most of researchers tend to develop a gasoline and diesel engine that can be operated in HCCI mode. The table 2.1 below shows the classification of internal combustion engine with fuel injection system and ignition system.

Table 2.1 Classification of Reciprocated Engine [8].

	Fuel Injection system	**Ignition system**
Gasoline Engine	Pre-injection	Spark ignition
Diesel Engine	Direct injection	Charge Compression
HCCI Mode Engine	Pre-injection	Charge Compression

The four-stroke engine was first demonstrated by Nikolaus Otto in 1876, hence it is also known as the Otto cycle [1, 4, 5, 7]. The technically correct term is actually four stroke cycles. Engines based on the four-stroke cycle or Otto cycle have one power stroke for every four strokes (up-down-up-down) and are used in cars, larger boats and many light aircraft. They are generally quieter, more efficient and larger than their two-stroke counterparts. The four strokes of the cycle are intake, compression, power, and exhaust. Each corresponds to one full stroke of the piston. Therefore, the complete cycle requires two revolutions of the crankshaft to complete.

The steps involved here are:

1. Intake stroke: the piston moves downward, drawing a fresh charge of vaporized fuel/air mixture.
2. Compression: Fuel vapor and air are compressed and ignited
3. Ignition: Fuel combusts and piston is pushed downward
4. Exhaust stroke: At the bottom of the power stroke, the exhaust valve is opened by the cam/lifter mechanism. The upward stroke of the piston drives the exhausted fuel out of the cylinder [1, 4, 5, 7].

2.3 Homogenous Charge Compression Ignition (HCCI) engine

HCCI has characteristics of the two combinations of combustion used in SI (spark ignition) engines- homogeneous charge spark ignition (gasoline engine) and CI engine: stratified charge compression ignition (diesel engine) [9]. As in homogeneous discharge spark ignition, the fuel and oxidizer are mixed together. However, rather than using an electric discharge to ignite a portion of the mixture, the density and temperature of the mixture are raised by compression until the entire mixture reacts spontaneously [9]. Stratified charge compression ignition also relies on temperature and density increase resulting from compression, but combustion occurs at the boundary of fuel-air mixing, caused by an injection event, to initiate combustion [9, 10].

The definition characteristic of HCCI is that the ignition occurs at several places at a time which makes the fuel/air mixture burn nearly simultaneously [11]. There is no direct initiator of combustion. This makes the process inherently challenging to control. However, with advances in microprocessors and a physical understanding of the ignition process, HCCI can be controlled to achieve gasoline engine-like emissions along the diesel engine-like efficiency [11]. In fact, HCCI engines have been shown to achieve extremely low levels of Nitrogen oxide emissions (NOx) without an after-treatment catalytic converter [12]. The unburned hydrocarbon and carbon monoxide emissions are still high (due to lower peak temperatures), as in gasoline engines, and must still be treated to meet automotive emission regulations.

Recent research has shown that the use of two fuels with different reactivity (such as gasoline and diesel) can help solve some of the difficulties of controlling HCCI ignition and burn rates [13]. RCCI or Reactivity Controlled Compression Ignition has been demonstrated to provide highly efficient, low emissions operation over wide load and speed ranges [14, 15].

2.3.1 Advantages

- HCCI provides up to a 30% fuel savings, while meeting current emissions standards.
- Since HCCI engines are fuel-lean, they can operate at a Diesel-like compression ratio (>15), thus achieving higher efficiency than conventional spark-ignited gasoline engines.
- Homogeneous mixing of the fuel and air leads to cleaner combustion and lower emissions. Actually, because peak temperatures are significantly lower than in typical spark ignited engines, NO_x levels are almost negligible. Additionally, the premixed lean mixture does not produce soot.
- In regards to gasoline engines, the emission of throttle losses improve HCCI efficiency [16, 17].

2.3.2 Disadvantages

- High in-cylinder peak pressure may cause damage to the engine.
- High heat release and pressure rise rates contribute to engine wear.
- The auto ignition event is difficult to control, unlike the ignition event in spark ignition (SI) and diesel engine which are controlled by spark plug and in-cylinder fuel injection.
- HCCI engines have a small power range, constrained at low loads by lean flammability limits and high loads by in-cylinder pressure restrictions.
- Carbon monoxide (CO) and hydrocarbon (HC) pre-catalyst emissions are higher than a typical spark ignition engine, caused by incomplete oxidation (due to the rapid combustion event and low in-cylinder temperatures) and trapped crevice gases [16, 18]

2.4 Process of Compression Ignition in Hydrocarbon Fuels

2.4.1 Reaction mechanism of Compression Ignition

From the figure below, there are two-stage of heat generation from ignition mechanism of hydrocarbons. Relatively, around 700K there is small heat generation called "Cool Ignition" while around 1000K, there is a large heat generation as main combustion flame called "Hot Ignition". This Hot ignition is dominated and influenced by the Cool Ignition. Figure 2.1 below shows in-cylinder pressure institutions, heat generation and temperature profiles for HCCI engine with n-heptane (nC_7H_{16}) as a fuel.

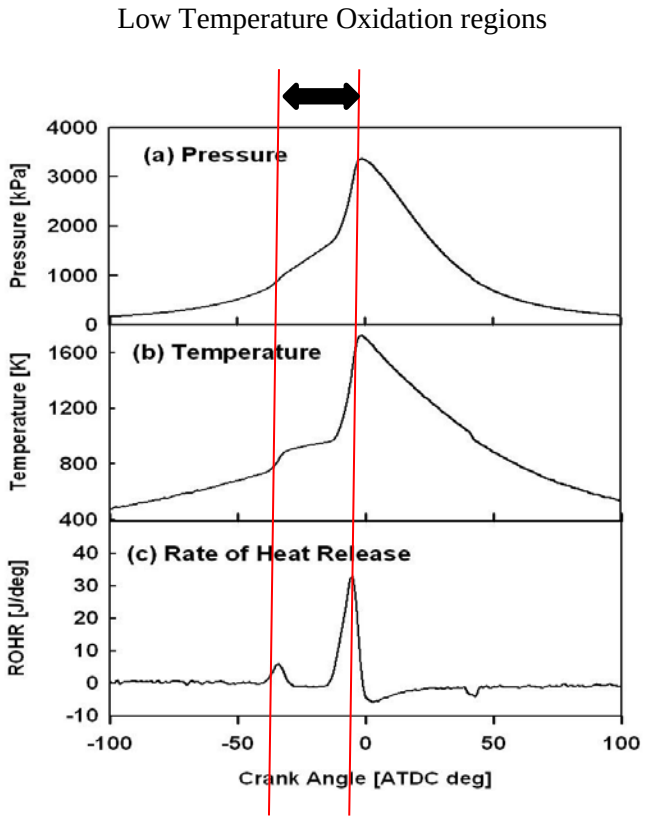


Figure 2.1: Observed pressure (a), temperature (b) and rate of heat release (c) in n-heptane fueled HCCI engine.(φ= 0.43, intake gas temperature = 413K) [8].

According to Westbrook, hydrogen peroxide reaction has significant impact in a hot flame oxidation reaction that shown below [19].

$$H_2O_2 + M = 2OH + M \quad (2.1)$$

Moreover, there is H_2O_2 loop reaction that dominates hot ignition in the region between hot and cool ignition called "Region for Heat ignition preparation reaction" that suggested from Ando et al [20]. This H_2O_2 loop reaction helps the heat generation as shown in Fig. 2.2.

The overall reaction of H_2O_2 loop reaction is,

$$2HCHO + O_2 \rightarrow H_2O + 2CO + 473KJ \quad (2.2)$$

Not H_2O_2, $HCHO$ acts as the consumer and all of the reactions in the entire loop has a large heat and has an important role in the ignition preparation region.

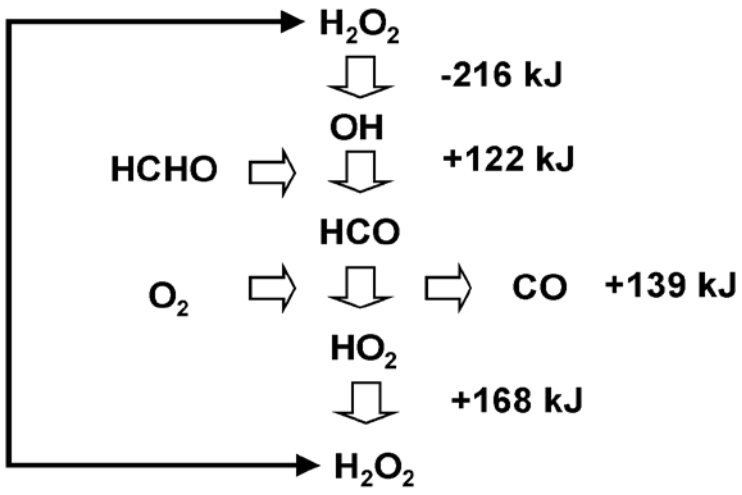


Figure 2.2: H_2O_2 loop reaction effective in the hot ignition preparation period [8, 21].

Below indicates the reaction pathways for hot flame oxidation.

$$RH + OH \rightarrow C + H_2O \tag{2.3}$$

$$R(+M) \rightarrow H, CH_3 + Q(olefine\ etc.) \tag{2.4}$$

$$H + O_2 \rightarrow OH + O \tag{2.5}$$

$$O + RH \rightarrow OH + R \tag{2.6}$$

$$H + O_2(+M) \rightarrow HO_2(+M) \tag{2.7}$$

From loop (2.3) until (2.6) is a proliferative reaction of OH, reaction rate for chain branching reaction is rate-limited by (2.5), and stops at reaction (2.7). Here, k_5 as the reaction rate constant for reaction (2.5) must win reaction rate constant k_5 [M] as the prerequisite to achieve hot ignition. Although k_5 has significance temperature dependence, while not in k_7, k_7[M] is dependent on the total pressure. Therefore, conditions to achieve heat hot flame are determined by temperature and pressure [8, 22].

Heat generation for low temperature oxidation and thermal ignition preparation period has significant influence to the time when the temperature reached for the occurrence of hot flame. In addition, by supplying OH reactant into H_2O_2 presence reaction can accelerate the generation of hot flame [21]. Therefore, to understand and control low temperature oxidation reaction that has dominated cool flame that cause the hot flame as the main combustion becoming important task in realizing HCC1 engine [23]. Fig. 2.3 shows schematic diagram of the low temperature oxidation reaction in hydrocarbon fuel.

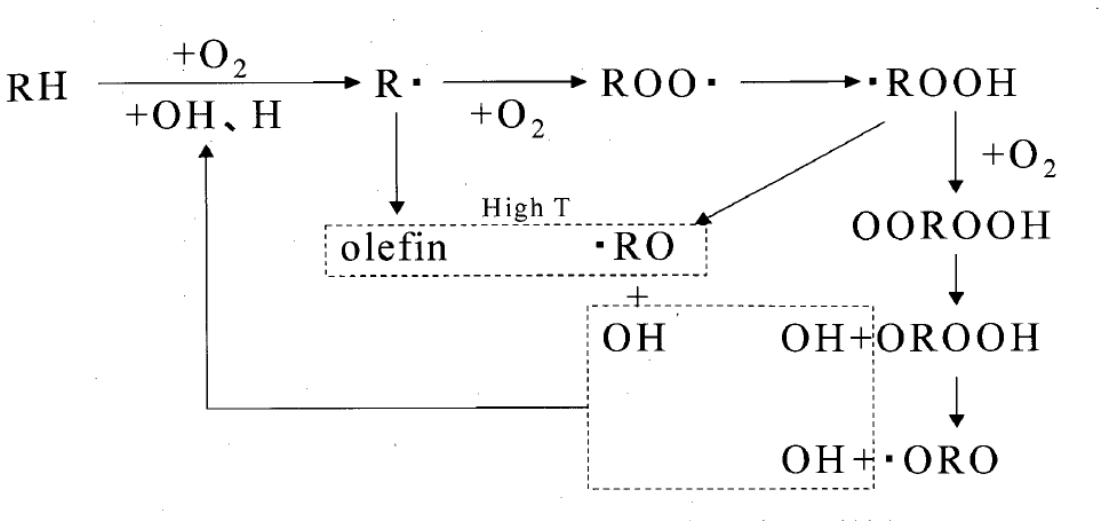


Figure 2.3: General Oxidation Scheme for hydrocarbon at low and high [8].

Apparently, Hydrogen Oxide produced by thermal decomposition. This reaction generates 2 *OH* radicals in low temperature oxidation that leads to fuel consumption through acceleration of hot flame. On the other hand, the fuel follows a complex reaction pathways is highly dependent on the fuel structure in the low temperature oxidation. In general, Hydrocarbon fuel (RH) in the low temperature range (R) of cool flame firstly reacted with oxygen molecules O_2 and H atom are withdrawn to generates Alkyl radicals (R) [8, 24, 25].

$$RH + O_2, H, OH \rightarrow R + HO_2, H_2, H_2O \qquad (2.8)$$

Then, O_2 is added to one of the following reaction of R which is generated in the process of generating Alkyl Peroxyl Radical (ROO).

$$R + O_2(+M) \leftrightarrow ROO(+M) \qquad (2.9)$$

Also, R is causing β-scission by carbon atom coupled (C-C) being thermally decomposited resulting Alkyl radical R_S that C atoms fewer than alkenes (R1=R2) and R being generated [8, 25].

$$R \rightarrow R1 = R2 + R_s \quad (2.10)$$

However, hydrocarbon must be equal or greater than 850K to achieve reaction (2.12), energy is not enough to get this reaction if less than that and because of that (2.11) is mainly occurs in the early period of low temperature oxidation. There are many reactions that responsible in generating ROO but the most important reaction in radical chain reaction in the stage before ignition is the reaction of hydroperoxyl alkyl radical that generates an internal isomerization reaction. In this reaction O atom as a radical center pulled out H atom in the molecule [8, 25-27].

$$ROO \leftrightarrow ROOH \quad (2.11)$$

At this time, the H atom abstraction occurs through the structure ring members. Hydrocarbon structure in which the reactions take place via 6-membered ring structure is most likely to occur with followed by 7-membered ring and also 5-memebered ring structure [8, 25-27].

4 reactions below are the main reactions that produce ROOH.

$$ROOH \rightarrow RO + OH \quad (2.12)$$

$$ROOH \rightarrow olefine + HO_2 \quad (2.13)$$

$$ROOH \rightarrow olefine + Carbonyl + OH \quad (2.14)$$

$$ROOH + O_2 \leftrightarrow OOROOH \quad (2.15)$$

In the atmosphere of excess oxygen, O_2 second addition is most likely to occur ROOH molecule. Thereafter, reactions that generated Hydroperoxyl Alkyl Peroxyl Radical OOROOH are;

$$OOROOH \rightarrow OROOH + OH \quad (2.16)$$

$$OROOH \rightarrow ORO + OH \quad (2.17)$$

From the reactions, 2 or more active OH has been generated. Generated OH causes a series of low temperature oxidation reaction by reacting with the fuel again. In this way, reaction that produces plurality of reactive molecules from the reaction of one molecule is called "Chain Branching Reaction" and Low Temperature Oxidation became active because of this reaction. From this chain reaction, temperature risen, as been expressed by reaction (2.12) and (2.14), one active molecule being consume while another being reproduce as called chain propagation reaction gradually become dominant. Moreover, reverse reaction in (2.9), by means ROO being decomposed and R being reproduce again as in (2.11). This kind of reaction mostly to occur, so-called chain termination reaction that does not produce reactive molecules leads to higher branching ratio. From this, temperature has risen up and negative reaction is suppressed and called negative temperature coefficient (NTC). Moreover, when the temperature risen, makes the change in composition in low temperature oxidation that leads to high temperature oxidation [8, 25-27].

Because of the problems in operating range and controlling ignition timing in HCCI engine, researchers lately began to pursue their studies from the chemical reaction inside this kind of engine. Although certain level of results has been acquired, results on low temperature oxidation is hardly known.

2.5 Modelling Low Temperature Oxidation (LTO)

The first modelling studies of the oxidation of n-heptane were carried out in the late of 1970s and in the 1980s by Coats and Williams where only for high temperature oxidation [8, 28]. In 1989, Westbrook has proposed the first detailed kinetic accounting for the low and high temperature oxidation of n-heptane [29, 30]. Since then, several of low and high temperature of this species has been introduced.

2.6 Model Calculation Hydrocarbon in LTO

The low temperature oxidation mechanism of hydrocarbons consists of complicated reactions such as H-abstraction, O_2-addition, isomerization, second O_2-addition, decomposition and branching passes [26]. The oxidation mechanism of mixture of n-heptane (base fuel) and iso-octane or toluene (sub fuel) is expressed in a summarized manner as below [8];

$$nC_7H_{16} + OH \rightarrow \alpha_b OH + \beta_b HCHO + other\ products \quad (2.17)$$

$$iC_8H_{18}\left(or\ C_6H_5CH_3\right) + OH \rightarrow \alpha_s OH + \beta_s HCHO + other\ products \quad (2.18)$$

Where $\alpha_{b,s}$ can be expressed as the reproduction index of OH from base or sub fuel, and $\beta_{b,s}$, the reproduction yield of chain terminating intermediate represented by HCHO from base or sub fuel. Other products are represented as an unreactive during the course of low temperature reaction. Differential equations time evolution of relevant species can be described as [8];

$$\frac{d[nC_7H_{16}]}{dt} = -k_b[C_7H_{16}][OH] \quad (2.19)$$

$$\frac{d[subfuel]}{dt} = -k_s[subfuel][OH] \quad (2.20)$$

$$\frac{d[OH]}{dt} = \left\{(\alpha_b - 1)k_b[C_7H_{16}] + (\alpha_s - 1)k_s[subfuel] - k_a[HCHO]\right\}[OH] \quad (2.21)$$

$$\frac{d[HCHO]}{dt} = \left\{\beta_b k_b[C_7H_{16}] + \beta_s k_s[subfuel] - k_a[HCHO]\right\}[OH] \quad (2.22)$$

From the equation (2.19) until (2.22), where $k_{b,s}$ is the rate constant of base or sub fuel with OH product, and α expressed as an aldehyde. From the equation, it can be translated into a form in which the independent variable which is percentage consumption of base fuel, known as *x*, which are below [8];

$$dy_s = -\left(\frac{g_1 y_s}{1-x}\right) dx \tag{2.23}$$

$$dy_{ald} = \left(\beta_b - \frac{\beta_s y_s}{1-x} - \frac{g_2}{1-x}\right) dx \tag{2.24}$$

$$dy_{OH} = \left((\alpha_b - 1) + \frac{(\alpha_s - 1) g_1 y_s}{1-x} - \frac{g_2 y_{ald}}{1-x}\right) dx \tag{2.25}$$

From the equation (2.23) until (2.25), y_s is the remaining amount of sub fuel (relative to initial amount of base fuel and so forth), y_{ald} is the accumulated amount of aldehyde, and y_{OH} is the amount of OH product, $g_1 = k_s/k_b$ and $g_2 = k_a/k_b$, where g_1 is the ratio of rate constant between sub fuel with OH and base fuel with OH, and g_2 is the ration of rate constant between aldehyde with OH and base fuel with OH. The α_b of low octane number of fuel is necessarily exceeding unity, but α_s may differ. The OH concentration increases with repetition of the reaction chain when initial overall OH reproduction index is over unity. The slope of OH increase gradually reduces and finally the chain system is terminated that according to decrease in fuel and increase in the OH consuming aldehyde. The point of termination is represented by the overall OH reproduction index = 1 [8]. The parameters used for NTF (n-heptane and toluene mixture) are $\frac{k_b}{k_s} = 5,\ \alpha_b = 2,\ \alpha_s = 0,\ \beta_b = 1.6,$ and $\beta_s = 0$. It is a part of which was assumed by overlooking the toluene oxidation mechanism [31].

CHAPTER 3

METHODOLOGY

3.1 Introduction

This study was conducted in order to analyse the ignition behaviour of n-heptane changing with the fuel mixing ratio. The focus of the study was to identify the reaction mechanism for n-heptane and toluene mixture (NTF) at various percentage. Toluene and iso-octane are typical high octane number fuels that reduce ignition activity of n-heptane when mixed, but some different behaviours between these fuels on the ignition control [32]. Finally, the method of this study is using numerical analysis for numerical simulation to analyse the ignition behaviour changing with the fuel mixing ratio.

3.2 Software

For the numerical simulation, it use the MATLAB software version R2013a for the numerical analysis which by creating the Graphical User Interface (GUI) using this software.

3.3 Numerical Simulation Flow Chart

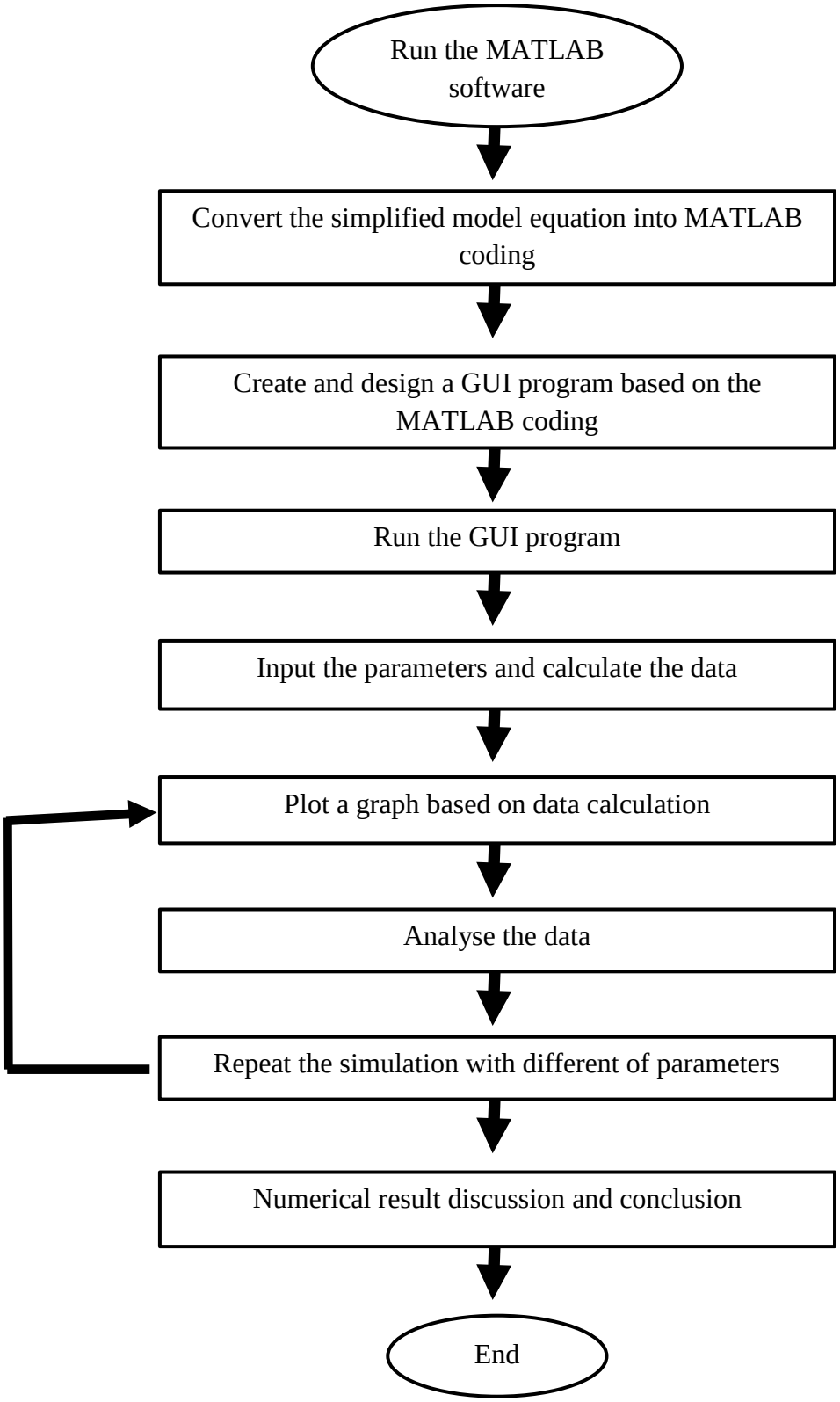


Figure 3.1: Flow chart of the simulation project

3.4 Theoretical of Simplified Model

The theoretical formula of the simulation is based on the equation (2.23) until (2.25) which taken from the literature research that have been reviewed. The purpose of the calculation is to determine the ignition behaviour of n-heptane and toluene mixture with various percentages. The design GUI simulation program consist of assumed parameters input, calculation output and data calculation. The table 3.1 shows the assumed parameter input for simulation program.

Table 3.1 Assumed parameters

Parameters	Symbol
The ratio of rate constant of toluene with OH and n-heptane with OH	g_1
The ratio of rate constant of aldehyde with OH and n-heptane with OH	g_2
The index of aldehyde reproduction from n-heptane	β_h
The index of aldehyde reproduction from toluene	β_t
The index of OH reproduction from n-heptane	α_h
The index of OH reproduction from toluene	α_t

Firstly, before the simplified model translate into MATLAB code, the reaction mechanism of n-heptane (base fuel) and toluene (sub fuel) mixture is expressed in a summarize manner as below:

$$n-Heptane: nC_7H_{16} + OH \rightarrow \alpha_h OH + \beta_h HCHO + other\ products \quad (3.1)$$

$$toluene: C_6H_5CH_3 + OH \rightarrow \alpha_t OH + \beta_t HCHO + other\ products \quad (3.2)$$

Where α is expressed as the production index, meanwhile β is expressed as the production yield and other product are unreactive product during the course of low temperature oxidation. There are product absorbs OH other than HCHO but they are still considered as a “HCHO” group.

From the previous reaction mechanism (3.1 & 3,2), it will convert into differential equations of time revolution which can be described as below:

$$\frac{d[nC_7H_{16}]}{dt} = -k_b[C_7H_{16}][OH] \quad (3.3)$$

$$\frac{d[C_3H_5CH_3]}{dt} = -k_s[C_3H_5CH_3][OH] \quad (3.4)$$

$$\frac{d[OH]}{dt} = \{(\alpha_b - 1)k_b[C_7H_{16}] + (\alpha_s - 1)k_s[C_3H_5CH_3] - k_a[HCHO]\}[OH] \quad (3.5)$$

$$\frac{d[HCHO]}{dt} = \{\beta_b k_b[C_7H_{16}] + \beta_s k_s[C_3H_5CH_3] - k_a[HCHO]\}[OH] \quad (3.6)$$

From the equation above (3.2 until 3.6), k_b is the rate of constant for base fuel with OH product, k_s is the rate of constant for sub fuel with OH product and k_a is the rate of constant for aldehyde product. But, for this equation, base fuel will be n-heptane and sub fuel will be toluene. After that, this equation will be translated into a form in which independent variable where it is known as *x*, which are below:

$$dy_t = -\left(\frac{g_1 y_t}{1-x}\right)dx \quad (3.7)$$

$$dy_{ald} = \left(\beta_h - \frac{\beta_t y_t}{1-x} - \frac{g_2}{1-x}\right)dx \quad (3.8)$$

$$dy_{OH} = \left((\alpha_h - 1) + \frac{(\alpha_t - 1)g_1 y_t}{1-x} - \frac{g_2 y_{ald}}{1-x}\right)dx \quad (3.9)$$

From the equation (3.7) until (3.9), where the variable x can be described as a percentage consumption of n-heptane fuel, y_t is the remaining amount of toluene fuel (which relative to initial amount of n-heptane and so forth), y_{ald} is the accumulated amount of aldehyde product, y_{OH} is the amount of OH product, g_1 is the ratio of rate constant between toluene with OH product and n-heptane with OH product, meanwhile g_2 is the ratio of rate constant between aldehyde with OH product and n-heptane with OH product. So it can be simplified as $g_1 = k_s/k_b$ and $g_2 = k_a/k_b$. From the equation (3.7) until (3.9), it will translated into Microsoft Excel and then from the Microsoft Excel, it will convert into MATLAB codes. This is the part of simulation codes where the equation (3.7) until (3.9) have been translated into MATLAB codes which shown as below:

```
g1 = get(handles.g1_edittext, 'String');
yh = get(handles.yh_edittext, 'String');
dx = 0.01;
yt = get(handles.yti_edittext, 'String');
for i =2:length(str2num(get(handles.x_edittext, 'String')))
total2 = str2num(yt) - (str2num(g1)*str2num(yt)./str2num(yh)).*dx;
end
yt = num2str(total2);
set(handles.yt_edittext, 'String', yt);

yh = get(handles.yh_edittext, 'String');
g2 = get(handles.g2_edittext, 'String');
bh = get(handles.bh_edittext, 'String');
bt = get(handles.bt_edittext, 'String');
dx = 0.01;
yt = get(handles.yt_edittext, 'String');
yald = get(handles.yaldi_edittext, 'String');
for i = 2:length(str2num(get(handles.x_edittext, 'String')))
    total1 = str2num(yald) + (str2num(bh) +
str2num(bt)*str2num(yt)./str2num(yh) -
str2num(g2)*str2num(yald)./str2num(yh)).*dx;
end
yald = num2str(total1);
set(handles.yald_edittext, 'String',yald);

yh = get(handles.yh_edittext, 'String');
g1 = get(handles.g1_edittext, 'String');
g2 = get(handles.g2_edittext, 'String');
yt = get(handles.yt_edittext, 'String');
ah = get(handles.ah_edittext, 'String');
at = get(handles.at_edittext, 'String');
dx = 0.01;
yaldi = get(handles.yaldi_edittext, 'String');
yoh = get(handles.yohi_edittext, 'String');
for i = 2:length(str2num(get(handles.x_edittext, 'String')))
total3 = str2num(yoh) + ((str2num(ah)-1) + (str2num(at)-
1)*str2num(g1)*str2num(yt)./str2num(yh) -
str2num(g2)*str2num(yaldi)./str2num(yh)).*dx;
end
```

```
yoh = num2str(total3);
set(handles.yoh_edittext, 'String',yoh);
```

3.5 Numerical Procedure

1) Start the GUI program.

2) Set up the parameters on the GUI program according to assumed parameters on table 3.1.

3) Click on ‘Calculate’ button on the GUI program to start the calculation.

4) Click on ‘Plot Graph’ button to analyse the data plot graph.

5) Lastly, click on ‘Extract Data’ to extract the data calculation and the data will save in format of Excel file.

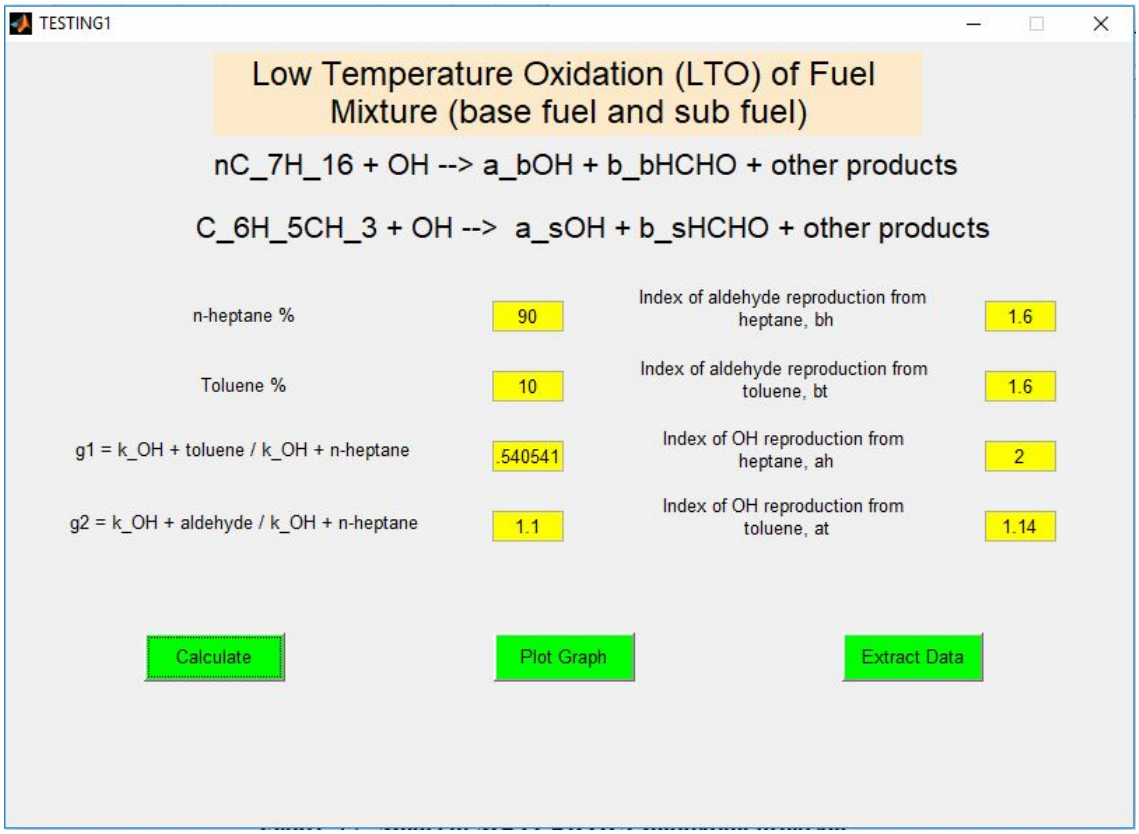


Figure 3.2: Model of MATLAB GUI simulation program

3.6 Project System Workflow

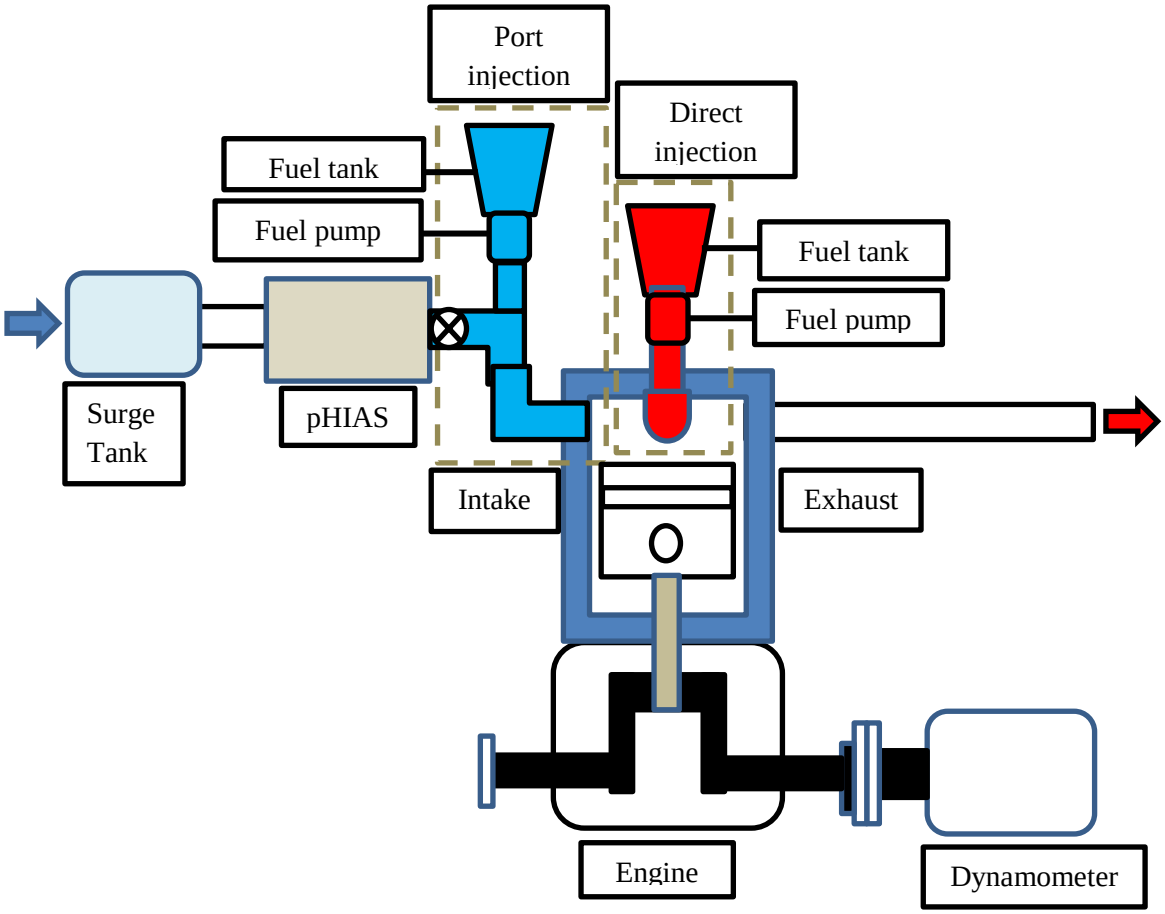


Figure 3.3: Workflow for pre-Heated air and fuel System in CI Engine

- The atmospheric air will enter from the intake pipe into pre-Heated Intake Air System (PHIAS).
- The air is heated using heating element inside the PHIAS with desired temperature.
- The limitation of the temperature is in-between 0 °C to 400 °C can be controlled at the PID controller.
- The preheated air will mix with fuel with the air of fuel injector at the throttle valve.

- The air fuel mixture will draw into the Compression ignition engine and compressed.
- At the power stroke, diesel is injected.
- Thus, auto ignition occurs and combustion happens.
- Finally the product of combustion is flow thru the exhaust system.

3.7 pHIAS Heating System

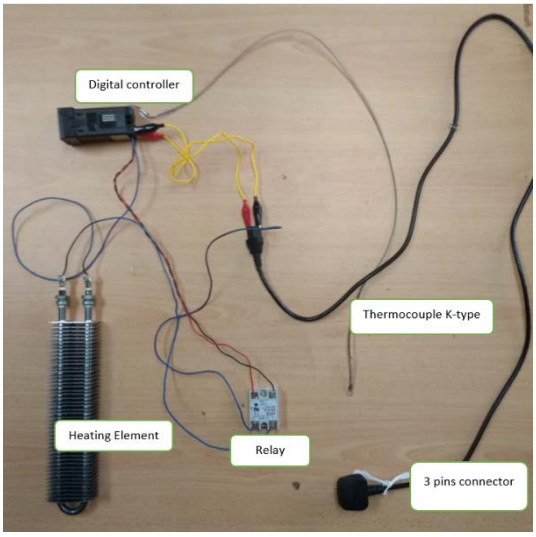


Figure 3.4: PHIAS circuit

The heating system was setup according to diagram above. Digital controller REX-C100FK02 will be connected with thermocouple K-type, Heating Element, relay and wire connector. The function of wire connector is to connect the system with AC power supply. The digital controller C100FK02 was used to controlled and set the desired temperature and send the input to the heating element. Thermocouple K-type was used to measure the temperature of heating element and the relay helps to control the voltage flow from digital controller to the heating element. The heating system was simply using the schematic diagram as shown in figure.

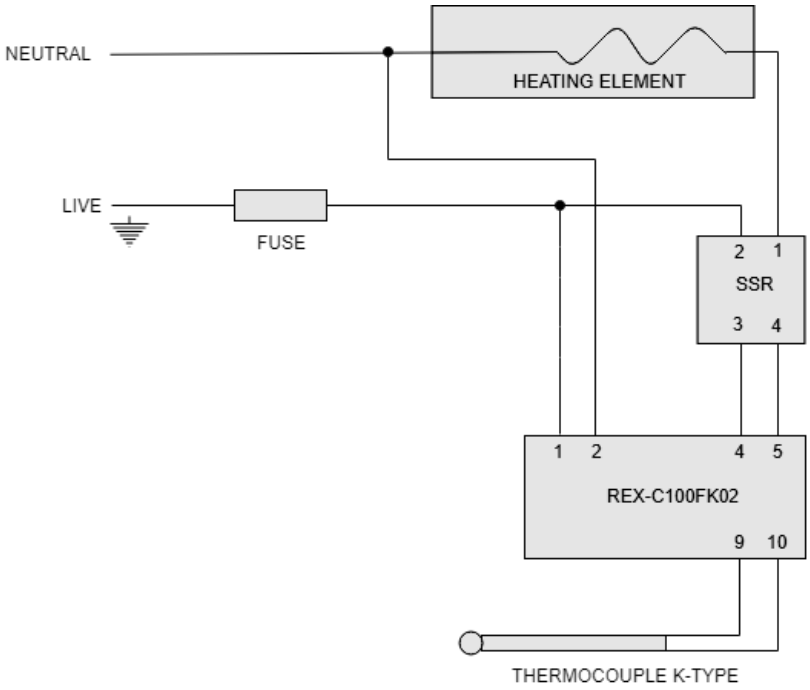


Figure 3.5: Schematic diagram for pHIAS heating system

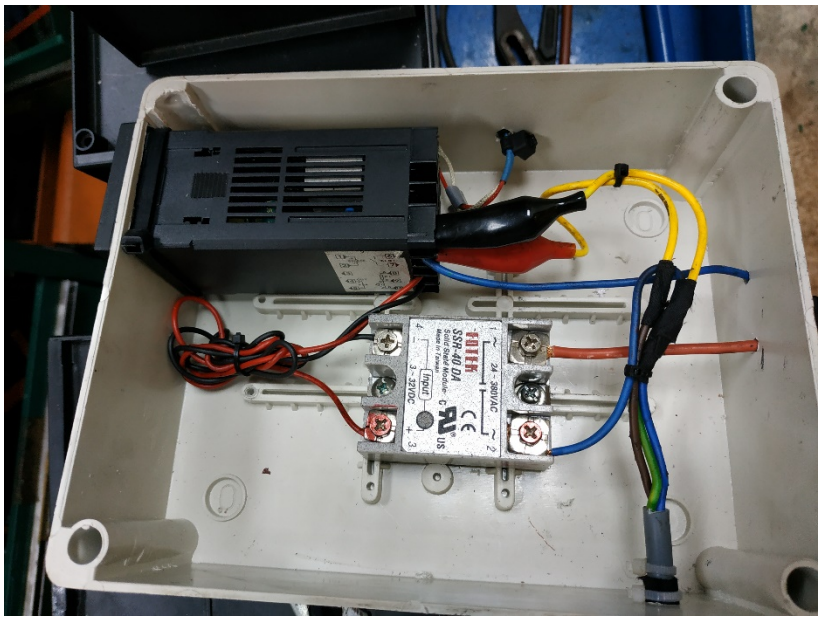


Figure 3.6: Wiring diagram for pHIAS heating system

3.8 List of Hardware

List of Components	Name of Components	Specifications
Heating Element	Ribbed Heating Element	**Power:** 200W to 10kW **Product length:** 350mm **Product Height:** 40mm **Product Width:** 70mm
Inner wall	Stainless steel	**Surface Area:** 400 x 200 mm **Thickness:** 1.5"
		Surface Area: 280 x 200 mm **Thickness:** 1.5"
		Surface Area: 400 x 280 mm **Thickness:** 1.5"
Outer body	Mild Steel	**Surface Area:** 500 x 260 mm **Thickness:** 1.5"
		Surface Area: 350 x 260 mm **Thickness:** 1.5"

		Surface Area: 500 x 350 mm **Thickness:** 1.5"
Thermocouple sensor	K Type Thermocouple Wire Digital Thermometer Temperature Sensor Probe	**Measurement range:** -50°C to 750°C **Resolution:** 1°C **Accuracy:** 0°C to 500°C:± (0.75%+1°C) 500°C to 750°C:±(1%+1°C) 0°C to 20°C:±2°C -20°C to -40°C:±3°C -40°C to -50°C:±4°C **Working temperature:** 0 to 50°C **Storage temperature:** -30°C to 60°C **Humidity:** ≤80%RH **Power supply**: one 9V battery (included) **Dimension:** 24 x 72 x 108 mm
Pipe	Stainless Steel	**Diameter:** 50 mm **Length:** 200 mm **Thickness:** 1.5
Insulator	Glass fibre	**Surface Area:** 250 x 150 mm **Thickness:** 4.5"
Controller	Digital controller REX-C100FK02	**Voltage**: 0 to 5 V DC, 1 to 5 V DC **Input impedance:** 250 kW or more **Current:** 0 to 20 mA DC, 4 to 20 mA DC **Input impedance:** Approx. 250 Ω

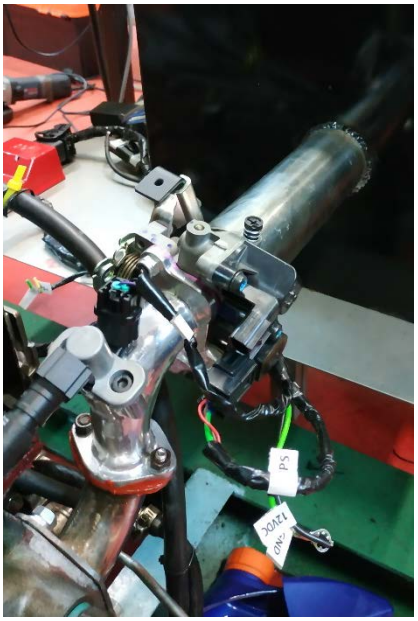
Relay	SSR 40da	**Load:** 24 – 380 V

3.9 Port Injection System

The port injection system on the compression ignition engine is something very new. Since this is a conversion of CI engine to HCCI it is compulsory to supply air fuel mixture on the intake stroke of the CI engine.

The fuel injection system consist of 38.1mm, mechanically operated throttle valve with a Throttle Position Sensor (TPS), fuel injector, Electronic Control Unit (ECU). The TPS sensor measures the throttle opening and sends the input to ECU. The ECU will trigger the fuel injector to spray the metered amount of fuel which will draw into the engine on the intake stroke.

The duty cycle of the injector and the air fuel ratio can be controlled in this system since the ECU can be tune to our preferences. This helps to enhance the engine performance by giving adequate amount of air fuel mixture into the engine.



Port injection system

CHAPTER 4

RESULTS AND DISCUSSION

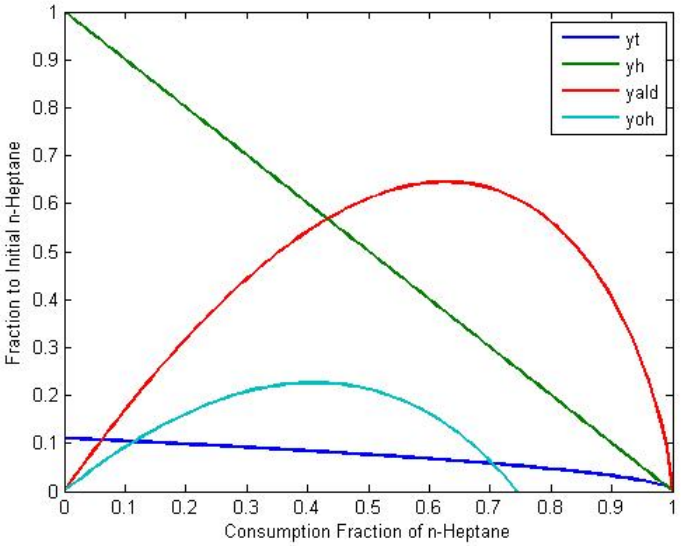
4.1 Introduction

Numerical analysis using MATLAB software version R2013a. The simplified model has been translated in the MATLAB software by using Graphical User Interface (GUI) methods. Then, the GUI will be converted into a program or application so that it can run without MATLAB software but must have a MATLAB Compiler. The aim of this GUI program is to generate the calculation results of a simplified model of the reaction mechanism of n-heptane and toluene mixture (NTF) at the Low Temperature

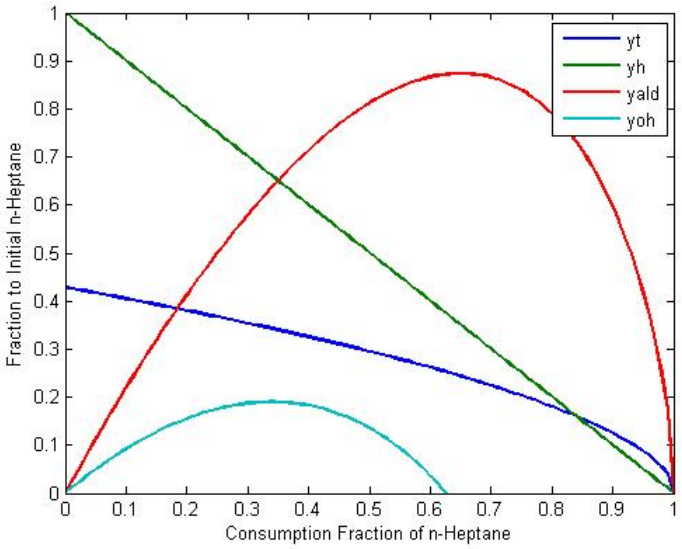
Oxidation (LTO) by plotting the graph. The result of this simplified model is plotted into “Fraction to Initial n-heptane” versus “n-heptane Consumption x” and also all results will be summarised in one graph. The result are obtained from the simulation on MATLAB GUI that have been created. The program also can extract the data from the graph and save the data in excel file.

4.2 MATLAB GUI Simulation Results

The simulation is run by different percentage of NTF. NTF is the fuel with a mixture of toluene and n-heptane. Toluene has a high octane fuel and n-number of heptane has a low octane number of fuel. While the octane number is a value indicating knock resistance of the fuel engine which is the higher octane number, the less to occur knocking. Firstly, to start the simulation, run the program and setup the parameters by input the value of initial condition of each parameter. Then, the program will stimulate the calculation of the modelled evolution of chemical composition in Low Temperature Oxidation (LTO) and the result will be displayed in a graph. The assumed parameters used for NTF (n-heptane and toluene mixture) are g_1 = 0.540541, g_2 = 1.1, $\alpha_{h,n-heptane} = 2$, $\alpha_{t,toluene} = 1.14, \beta_{h,n-heptane} = 1.6$ and $\beta_{t,toluene} = 1.6$.

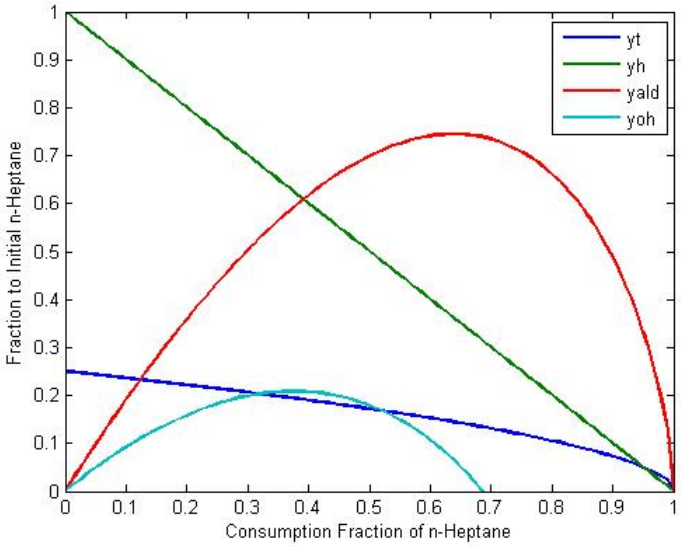


1) NTF 10 (mixture of n-heptane with toluene 10%)

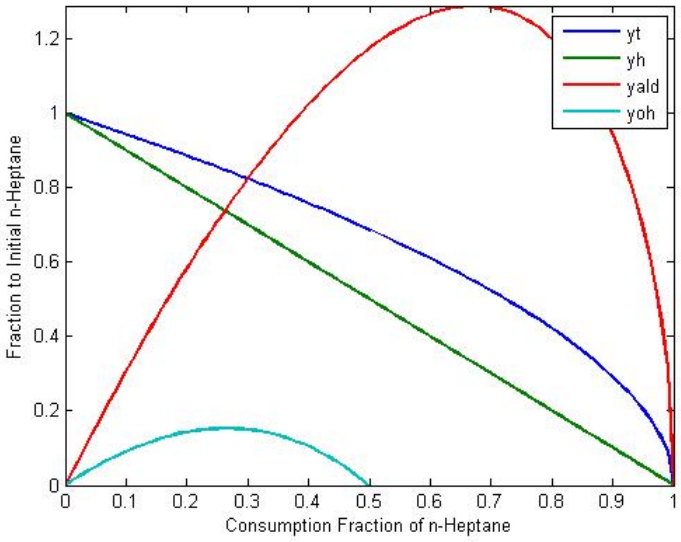
Figu  of NTF 10.

2) N

TF 20 (mixture of n- heptane with toluene 20%)

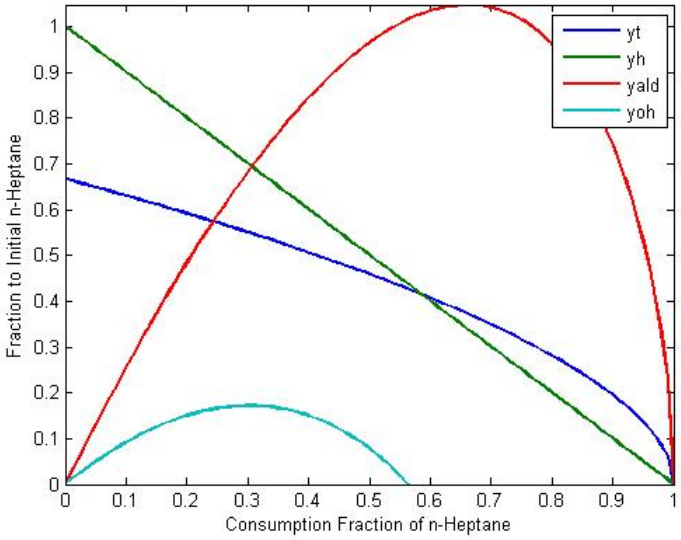
Figu  of NTF 20.

3) NTF 30 (mixture of n-heptane with toluene 30%)

Figure 4 

NTF 30.

4) NTF 40 (mixture of n-heptane with toluene 40%)

Figure 4 

NTF 40.

5) NTF 50 (mixture of n-heptane with toluene 50%)

Figure 4.5: Modelled evolution of chemical composition in LTO of NTF 50.

6) NTF 60 (mixture of n-heptane with toluene 60%)

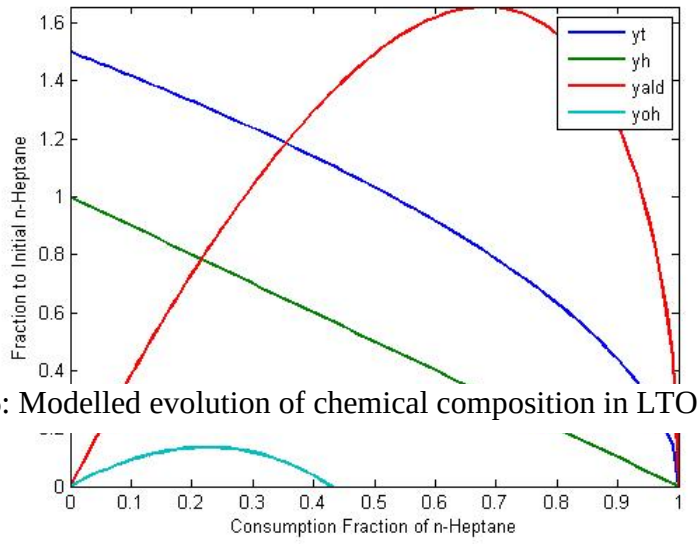


Figure 4.6: Modelled evolution of chemical composition in LTO of NTF 60.

7) NTF 70 (mixture of n-heptane with toluene 70%)

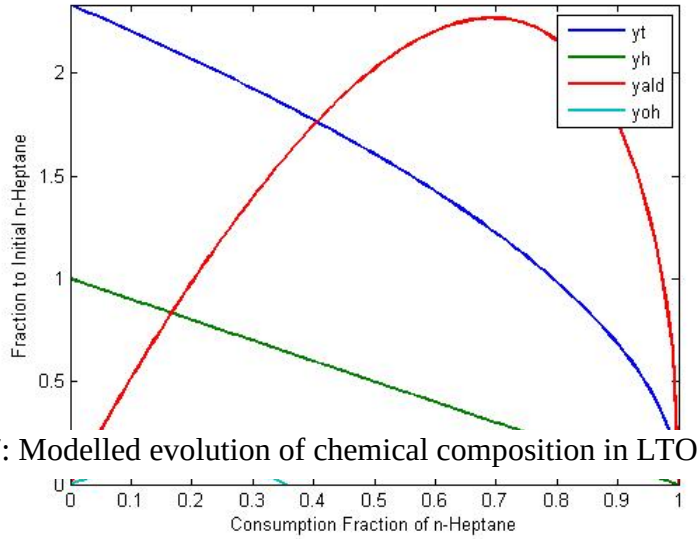


Figure 4.7: Modelled evolution of chemical composition in LTO of NTF 70.

8) NTF 80 (mixture of n-heptane with toluene 80%)

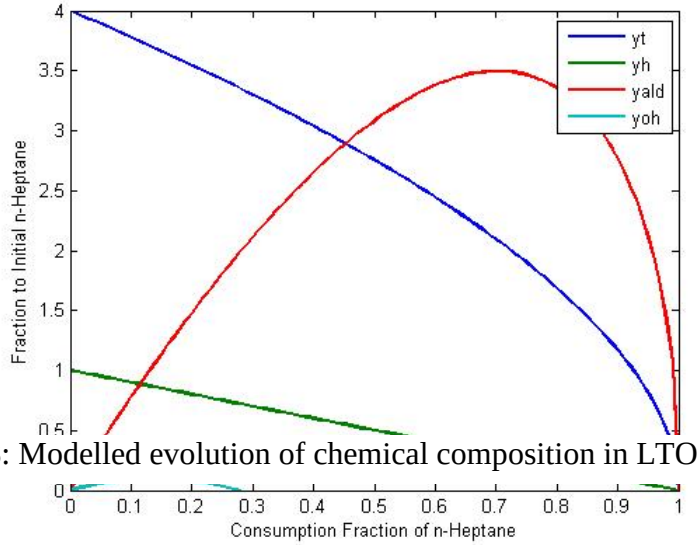


Figure 4.8: Modelled evolution of chemical composition in LTO of NTF 80.

9) NTF 80 (mixture of n-heptane with toluene 90%)

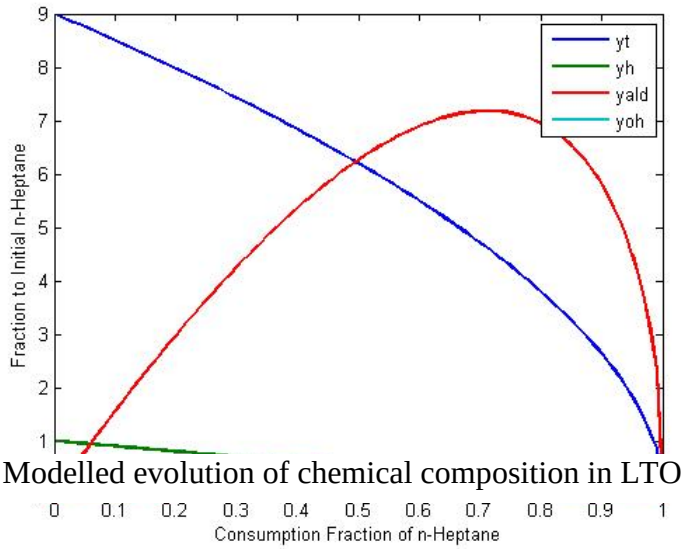


Figure 4.9: Modelled evolution of chemical composition in LTO of NTF 90.

Starting figure 4.1 until 4.9, show the modelled evolution of the chemical composition for NTF 10, 20, 30, 40, 50, 60, 70, 80, 90 in Low Temperature Oxidation (LTO). These calculations show that the toluene consumption (*yt)* is less than n-heptane consumption, the effect of reducing n-heptane consumption is less than in toluene, and aldehyde production (*yald*) increases with decreasing toluene content. Also, from figure 4.1 until 4.9, the results show the differences of the final composition of OH (*yoh*) approaching to 0. Interaction between the mixture of fuel components (n-heptane + toluene) will be resulting decrease in n-heptane consumption because of competition between n-heptane with OH and toluene with OH reaction rate. Toluene is typical high octane number fuels that reduce the ignition activity of n-heptane when mixed.

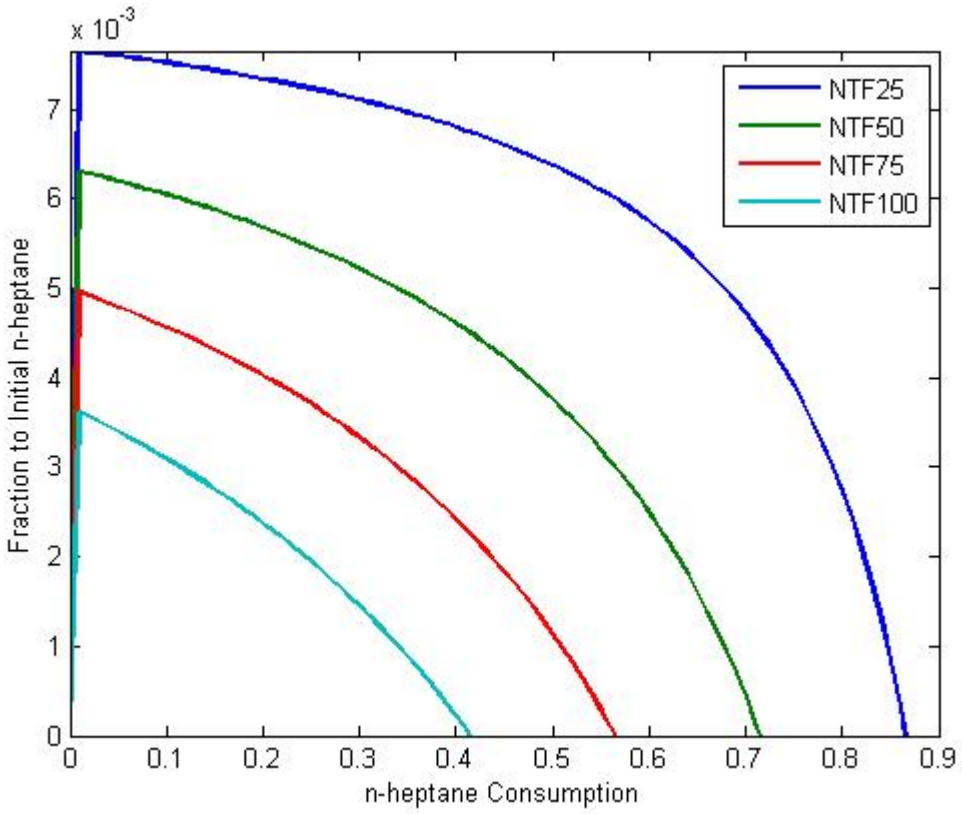


Figure 4.10: Comparison in final composition of OH in LTO from various percentages of NTF.

Figure 4.6 shows a comparison of OH production graph for NTF fuels from a different percentage of toluene. From the graph, it can be observed that by increasing toluene percentage, OH production become decrease as predicted by toluene character. OH as the middle product that propagates high temperature oxidation decrease by increasing toluene percentage.

However, the simplified model could not match experimental result from other studies by just manipulated the value of mole in the simplified model represented as α and β. Many parameters such as temperature and pressure did not being considered in the model calculation while it can be influenced to the whole reaction.

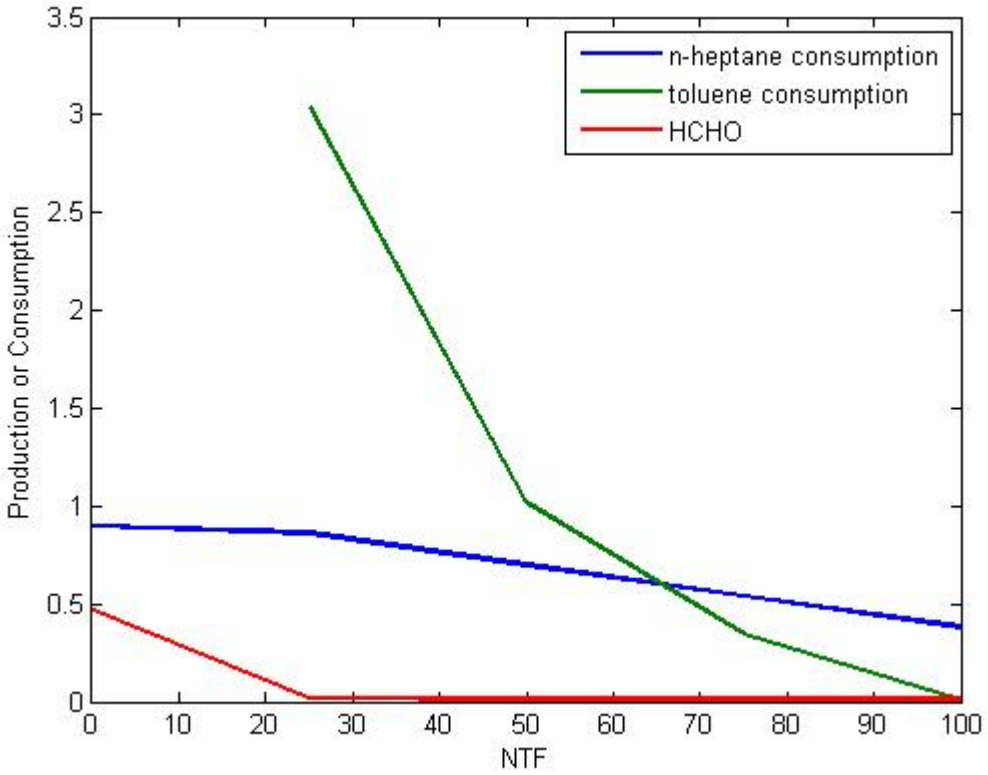


Figure 4.11: Fuel consumption and formaldehyde production at the end of low temperature chain reaction in NTF.

Here, fuel consumption means the consume amount relative to the initial fuel charge. From figure 4.7, it shows that the high percentage of toluene, the chain reaction does not start from the beginning, so that low temperature oxidation (LTO) heat release does not occur. To summarize the mixing effect of high octane number of fuel to n-heptane ignition property, toluene acts as a simple dilution agent, since the toluene-OH reaction rate is slow and OH production index is very low. Fuel consumption decreases with increasing of toluene/n-heptane ratio although it is weak. It is because toluene has lower rate constant with OH, so that toluene barely interrupts the OH reproducing chain reaction of n-heptane. The reaction mechanism is quietly complicated but already been approved through many research. In the previous study, there are a 26 reactions and 25 species mechanism for n-heptane which has been derived from two detailed mechanisms for developed by Lawrence Livermore National Laboratory (LLNL).

CHAPTER 5

CONCLUSION

5.1 Conclusion

In this study, the numerical simulation was done by developed a simplified model that has been translated into MATLAB software by creating Graphical User Interface (GUI) program. The objective of this program is to study the ignition mechanism of low and high octane number of fuel in low temperature oxidation and this program also is one of the objectives of this project.

From the result simulation, based on the calculation of the equation (3.7), (3.8) and (3.9), it can be concluded that the amount of toluene content becomes decreasing with the increasing of n-heptane consumption, and the aldehyde production also increases with the decreasing of toluene content. Moreover, the increasing of toluene percentage has big influence in OH production. It is because OH production become decrease as predicted by toluene character and OH as the middle product that propagates high temperature oxidation decrease by increasing toluene percentage.

Nevertheless, to compare the experimental result from other studies, this simplified model could not match quantitatively as it just manipulated the value of mole in the simplified model represented as α and β. Some parameters such as temperature and pressure has not been considered in the simulation. In addition, the simulation also

requires some improvement in term of data calculation, so that the model calculation data can shows trend with other experimental results in the future.

5.2 Recommendations

In the future works, there are some improvements need to be considered in order to ensure the success of this project with less errors during simulation. During setup the parameters of this program simulation, there is some calculation errors that have been shown in the graph. In order to solve this problem, to learn more about MATLAB software such as loop calculation, MATLAB Simulink or other software which can calculate based on the simplified model equations. Other than that, for further research, we can consider other parameters such as temperature and pressure in the model calculation to improve the data calculation. Also, it can be referenced for comparison between fuel combustion simulation and fuel combustion experiment.

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APPENDIX