**Palestine Polytechnic University**

**Al-Quds University**

**Master Program of Renewable Energy and Sustainability**

# Prediction of Equilibrium Combustion Products of Injecting Additive Urea in Diesel Engine Combustion Chamber

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**April, 2023**

Palestine Polytechnic University

Deanship of Graduate Studies and Scientific Research

Master Program of Renewable Energy and Sustainability

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*Thesis submitted in partial fulfillment of requirements of the degree*

*Master of Science in Renewable Energy & Sustainability*

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April, 2023

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**Prediction of Equilibrium Combustion Products of Injecting Additive Urea in Diesel Engine Combustion Chamber**

Submitted by

**Fadi Younis Alama**

in partial fulfillment of the requirements for the degree of Master in Renewable Energy & Sustainability.

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**Prediction of Equilibrium Combustion Products of Injecting Additive Urea in Diesel Engine Combustion Chamber**

**By: Fadi Younis Alama**

## ABSTRACT

Diesel engines are still the prominent source of pollutant emissions globally, despite efforts to shift to electric motors. In 2020, 28% of vehicles produced utilized diesel engines. However, the automotive industry worldwide is actively pursuing methods to curtail exhaust emissions. Three primary strategies have emerged: optimizing combustion processes, refining after-treatment procedures, and exploring alternative fuels and additives. This thesis focuses on the latter strategy - additives and alternative fuels - with the goal of identifying an additive that is capable of mitigating exhaust pollutants. While electric motors and after-treatment processes like urea solutions show promise, this study delves into the potential of urea solution as a diesel additive. Leveraging theoretical mathematical modeling through chemical atom balancing and equilibrium, emissions predictions are made using various concentrations of urea solution in diesel fuel. The Matlab software is employed to solve the system. Through the model, two scenarios are compared: pure diesel and an 80% diesel with 20% urea solution blend, accounting for factors such as pressure, temperature, and equivalence ratio in the combustion chamber. The findings reveal that introducing urea leads to decreased harmful exhaust emissions. Specifically, CO concentration drops by 0.08% to 0.8%, CO2 concentration decreases within lean mixtures by 0.144% to 0.32%, NO concentration reduces by approximately 0.11% to 0.243%, and NO2 concentration diminishes from 0.18% to 0.387%. Additionally, the lower heating value experiences a 3.67% decrease compared to pure diesel.

**التنبؤ بمنتجات الاحتراق من خلال التوازن الكيميائي عند حقن مضاف اليوريا في غرفة احتراق محرك الديزل**

## ملخص

لا تزال محركات الديزل هي المصدر البارز لانبعاثات الملوثات على مستوى العالم، على الرغم من الجهود المبذولة للتحول إلى المحركات الكهربائية. في عام 2020 كانت نسبة المركبات المنتجة بمحركات ديزل 28٪. ومع ذلك، فإن صناعة السيارات في جميع أنحاء العالم تسعى بنشاط إلى اتباع طرق للحد من انبعاثات العادم. وقد ظهرت ثلاث استراتيجيات أساسية: تحسين عمليات الاحتراق، وتحسين إجراءات ما بعد المعالجة، واستكشاف أنواع الوقود والمواد المضافة البديلة. تركز هذه الأطروحة على الإستراتيجية الأخيرة - المواد المضافة وأنواع الوقود البديلة - بهدف تحديد مادة مضافة قادرة على تخفيف ملوثات العادم. في حين أن المحركات الكهربائية وعمليات المعالجة اللاحقة مثل اليوريا تبدو واعدة، فإن هذه الدراسة تتعمق في إمكانية استخدام محلول اليوريا كمادة مضافة للديزل. سيتم تطوير نموذج رياضي برمجي نظري باستخدام التوزين الذري الكيميائي ومعادلات التوازن الكيميائي للتنبؤ بكميات الانبعاثات باستخدام تركيزات مختلفة من محلول اليوريا في وقود الديزل. تم استخدام برنامج Matlab لحل النظام. من خلال النموذج، تمت مقارنة سيناريوهين: ديزل نقي وديزل بنسبة 80% مع مزيج محلول اليوريا بنسبة 20%، مع الأخذ في الاعتبار عوامل مثل الضغط ودرجة الحرارة ونسبة التكافؤ في غرفة الاحتراق. اظهرت النتائج أن إدخال اليوريا يؤدي إلى انخفاض انبعاثات العادم الضارة. على وجه التحديد، ينخفض تركيز ثاني أكسيد الكربون بنسبة 0.08% إلى 0.8%، وينخفض تركيز ثاني أكسيد الكربون في الخليط الفقير بنسبة 0.144% إلى 0.32%، وينخفض تركيز أكسيد النيتروجين بنسبة 0.11% تقريبًا إلى 0.243%، وينخفض تركيز ثاني أكسيد النيتروجين من 0.18% إلى 0.387%. بالإضافة إلى ذلك، فإن القيمة الحرارية للاحتراق تشهد انخفاضًا بنسبة 3.67% مقارنة بالديزل النقي.

# DECLARATION

I declare that the Master Thesis entitled" **Prediction of Equilibrium Combustion Products of Injecting Additive Urea in Diesel Engine Combustion Chamber**" is my own original work, and herby certify that unless stated, all work contained within this thesis is my own independent research and has not been submitted for the award of any other degree at any institution, except where due acknowledgement is made in the text.

Student Name: **Fadi Younis Alama**

Signature:_____ Date:_____

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# DEDICATION

To our families ……. For their support

To our teachers ……. For help us until the end

To our friends ……. Who give us positive sentiment

To oppressed people throughout the world and their struggle for social justice and egalitarianism

To our great Palestine

To my supervisor Dr. Zuhdi Salhab

To all who made this work is possible

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# INTRODUCTION

# Chapter 1

# Introduction

## 1.1 Overview

From 2000 - 2019, the produced vehicles around the world increased 54% (Demir et al. 2022). 28% of the produced vehicles in 2020 were diesel engine vehicles, this means the world may not dispense with the use of diesel engines (ACEA 2021). Today, the fossil fuels compose about 80% of the total energy needed with about 50% of the needed fuel used in transportation (Escobar et al. 2009).

Diesel engines are widely used especially for commercial vehicles and some of the passenger vehicles. Most of the exhaust emissions produced by these engines are carbon monoxide (CO), carbon dioxide ($CO_2$), unburned hydrocarbon (HC), particulate matter (PM) and nitrogen oxide ($NO_x$) (Heywood 2018, Fayyazbakhsh & Pirouzfar 2017), which all classified as green house gases (GHG) whether direct or indirect GHG. As we know, preserving the environment, reducing environmental pollution and reducing exhaust emissions will decrease the global warming and other phenomena, and these are some of the lofty goals of the search for alternative and renewable energy.

Car manufacturer companies used three methods to reduce the emissions from the combustion process in these engines (Rahman et al. 2021). The first method works on the combustion process itself (Cai & Zhao 2020). The second method is an after treatment processes such as the catalyst converter which convert the CO and the HC into $CO_2$ and water, the selective catalyst converter (SCR) to reduce the $NO_x$, the diesel particulate filter (DPF) is used to reduce the PM and the Adblue system used to

reduce the $NO_x$ (Zhang et al. 2021). The third method is to use alternative fuels and fuel additives like natural gas, methanol and others (Muhssen et al. 2021, Wei et al. 2021).

## 1.2 Problem of Statement

These days the world is racing to find alternatives to environmentally polluting energy sources. Some of diesel applications cannot be dispensed with, even if for a period of time such as diesel engines vehicles. The emissions of these engines are very harmful, such as CO, $CO_2$, NO and $NO_x$. Car manufacturer racing to reduce the emissions as much as possible using one of the three methods that have been explained previously; working on the combustion process, after treatment process and using alternative fuel that reduces the harmful emissions (Muhssen et al. 2021, Wei et al. 2021).

The first method has been studied for many years and reached a dead end, as toxic gases must be produced whatever the improvement on combustion. However the second method is very expensive and add weight to the vehicle which is a bad factor, also these after treatment systems breaks down continuously, especially for vehicles that run within the city at low speed, and the cost of maintenance is high. On the other hand, the last method, which is the search for an alternative fuel or using fuel additives, takes the lead in scientific research because it is the least expensive (Rahman et al. 2021), where this method do not need to add any additional heavy or expensive parts on the vehicle, and do not need maintenance.

Hence, the research problem in this thesis is to find an additive for the diesel fuel to reduce the exhaust emissions without affecting the engine performance.

## 1.3 Project Objectives

Many studies were conducted previously about mixing Alcohols, such as methanol and ethanol, with diesel into the combustion chamber. On the other hand, other studies focused on injecting additives in the exhaust as an after treatment process to treat the $NO_x$. Using urea as a fuel additive was conducted in few studies were only experimental methods were used. Based on that, this thesis aims to:

- Study the effect of mixing urea with diesel as a fuel additive on the concentration of the exhaust harmful emissions for diesel engines by:
  - Investigating whether adding urea to diesel as a fuel additive leads to reducing the concentration of CO and $NO_x$ emissions from the internal combustion process.
  - Investigating whether adding urea to diesel as a fuel additive leads to reducing the lower heating value and the temperature of the combustion.
- Develop a predictive model for combustion products resulting from the mixing of urea with diesel in a diesel engine to compare and validate previous experimental findings.

## 1.4 Research Hypothesis

In this thesis, two research hypotheses were investigated as shown below:

- Adding urea to diesel as a fuel additive leads to reducing the concentration of CO and $NO_x$ emissions from the internal combustion process.
- Adding urea to diesel as a fuel additive leads to reducing the lower heating value and the temperature of the combustion.

## 1.5 Methodology

In this thesis the analytic approach was used to derive the equation of combustion and the equations of chemical equilibrium with thermodynamics for an actual combustion using the diesel fuel with air and urea solution in water as the reactants.

The combustion model atom balancing and the chemical of equilibrium reaction method were used to build the model to predict the concentration of the products of the combustion process.

The Matlab software, version: R2022a was used to solve the equations and plot the needed relations. Also the Chemkin, NASA and JANAF tables were used to derive and calculate the constant of equilibrium at several temperatures for different equilibrium equations.

## 1.6 Thesis Outline

This section will discuss the outline of this thesis, where the first chapter discussed the problem statement, the research hypothesis, the project objectives and the methodology. The second chapter will highlight on relevant literature. The third chapter will discuss the methodology used in this thesis. After that the fourth chapter will show the results and discuss them. Finally, the fifth and last chapter will be the conclusions and future work.

# CHAPTER 2

# LITERATURE REVIEW

# Chapter 2

# Literature Review

## 2.1 Introduction

Diesel engines are used widely in automotive sector, these engines are powered by internal combustion, which produces many harmful gases to the environment. This chapter aims to review the state of the art from previous studies about internal combustion engine technology and the methods used to reduce the exhaust gases in the combustion process or as an after treatment process. Review studies related to combustion process and the prediction and formation of the exhaust gases, the chemical and physical properties of diesel fuel and of urea additive that will be used in this thesis.

## 2.2 Internal Combustion Engine

Diesel engine is a compression ignition engine, also called auto ignition engine, where the mixture of diesel fuel and air mixed in the combustion chamber, the air consists mainly of 21% oxygen and 79 % nitrogen (Reşitoğlu et al. 2015). The air must be compressed in the combustion chamber, which generate high temperature that ignite the fuel when it is injected in the combustion chamber (Heywood 2018). Therefore, heat used to convert the chemical energy of the diesel fuel into a thermal energy, then into a mechanical energy (Bosch 2005).

Internal combustion diesel engines working usually in four strokes system; intake, compression, expansion and exhaust stroke (Heywood 2018). For a complete combustion in an ideal thermodynamic equilibrium, the products of the diesel engine will be $CO_2$ , $H_2O$ and $N_2$ and the lower heating value for diesel fuel is 43.2 MJ/Kg, with air-fuel ratio 14.5 (Prasad & Bella 2010, Heywood 2018).

In actual combustion the engine works under incomplete combustion. Moreover, diesel engines works on a lean mixture where the air-fuel ratio is high ($\lambda$ >1) (Demers & Walters 1999).

Usually the temperature reach 1900 C° in private cars with pressure of 50 atmosphere, where in some commercial trucks the pressure may reach 80 atmosphere (Bosch 2005, Heywood 2018).

## 2.3 Diesel Fuel Properties

According to Pirouzfar et al. (2012) the diesel fuel used in vehicles called diesel #2 or light diesel, contains mainly of alphatic hydrocarbons of $C_{8\text{-}28}$ and it has a boiling temperature between 130 and 370 °C (Song et al. 2007, Escobar et al. 2009).

Diesel fuel mainly consist of carbon and hydrogen, theoretically it has the chemical formula $C_nH_{1.8n}$ for light diesel (Heywood 2018), according to Lapuerta et al. (2014) the practical chemical formula of light diesel is $C_{14.62}H_{26.87}O_{0.08}$ in Spain. Table 2.1 bellow shows some of the properties of light diesel fuel (Global 2019).

**Table 2.1:** Properties of light diesel fuel.

| Property | Value |
|---|---|
| Appearance | Clear or straw-colored liquid. |
| Chemical formula | $C_nH_{1.8n}$ / $C_{14.62}H_{26.87}O_{0.08}$ |
| Molar mass | 202 $g/mole$ |
| Density | 0.849 $g/cm^3$ |
| Melting point | -30 to -18 $C°$ |
| Flammability | Flammable liquid (OSHA defined) |
| Flammable limits | 0.6 % to 6.5% |
| Flash point | $>$ 52 $C°$ |
| Autoignition Temperature | 257 $C°$ |

## 2.4 Exhaust Emissions Formation

For a complete combustion in an ideal thermodynamic equilibrium, the products of the diesel engine will be $CO_2$ , $H_2O$ and $N_2$ as shown in equation 2.1, where $\delta$ is the air-fuel ratio and $\nu_x$ is the number of moles of the combustion products (Prasad & Bella 2010, Heywood 2018).

$$C_nH_{1.8n} + \delta(O_2 + 3.76N_2) \longrightarrow \nu_1CO_2 + \nu_2H_2O + \nu_3N_2 \tag{2.1}$$

In an actual combustion the diesel engine runs on a lean mixture, where the air-fuel ratio is high ($\lambda$ >1) (Demers & Walters 1999). Moreover, due to the changes in the air-fuel ratio, valve and ignition timing, fuel concentration in mixture, combustion temperature and other factors the products in the exhaust emissions increased and became more harmful, where it consist of CO, HC, $NO_x$, $SO_x$ and the PM (Reşitoğlu et al. 2015).

As it was mentioned before many air pollutants come out from the exhaust, the $NO_x$ are one of these emissions and it is responsible of acid rains (Song et al. 2007, Escobar et al. 2009).

Figure 2.1 bellow shows the approximate components of diesel exhaust gases (Khair 2006). The pollutant gases form approximately 1% of the exhaust gases, where the $NO_x$ have the biggest share of about 50% of the pollutant gases. The PM comes after the $NO_x$, besides due to lean combustion in diesel the HC and CO are minimal (Reşitoğlu et al. 2015).

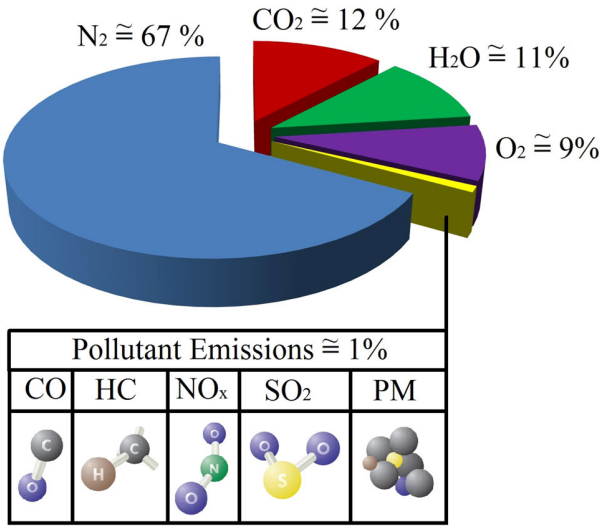



**Figure 2.1:** The components of diesel exhaust gases.

However the sulfur oxide $SO_x$ depending on the quality of the diesel fuel, there are no after treatment for the $SO_x$, but the companies and fuel suppliers prefer to supply a high quality of diesel that contain the minimum amount of sulfur (Reşitoğlu et al. 2015).

On the other hand, many non polluting emissions comes out of the exhaust, such as $O_2$, O, $N_2$, H, $H_2$, OH and others. These gases and the main combustion emissions ( $CO_2$ and $H_2O$ ) are responsible of CO and $NO_x$ formation, due to the chemical of equilibrium reactions (Cengel et al. 2011).

For an actual combustion the equation 2.2 was developed based on Macek (2000), shows the main exhaust emissions that responsible of formation of each other in the chemical of equilibrium reaction (Oppenauer et al. 2011).

$$C_nH_{1.8n} + \frac{\delta}{\phi}(O_2 + 3.76N_2) \longrightarrow$$

$$\nu_1 CO_2 + \nu_2 CO + \nu_3 H_2O + \nu_4 H_2 + \nu_5 O_2 + \nu_6 N_2 + \nu_7 H + \nu_8 O + \nu_9 NO + \nu_{10} OH + \nu_{11} NO_2 \tag{2.2}$$

Where n is the number of carbon atoms in the fuel, $\delta$ is the molar air-fuel ratio, $\phi$ is the equivalence ratio and $\nu_{1-11}$ are number of moles of the combustion products.

In the end, the main exhaust harmful gases formation will be discussed are the carbon monoxide CO, carbon dioxide $CO_2$ and the nitrogen oxides $NO_x$.

### 2.4.1 Carbon Monoxide (CO) Formation

Carbon monoxide forms in the incomplete combustion when the oxidation reaction is not completely finished. The concentration of CO depends on the air-fuel ratio. When the mixture is rich ($\lambda$ <1), the concentration of CO becomes high (Wu et al. 2004). On the other hand, CO is formed in the lean mixture ($\lambda$ >1) due to chemical equilibrium (Faiz et al. 1996).

Also, even if there is a sufficient amount of oxygen, CO will still be formed if the pressure and temperature are high due to the chemical of equilibrium (Ganesan 1996), see equation 2.3.

$$CO + \frac{1}{2}O_2 \rightleftharpoons CO_2 + heat \tag{2.3}$$

The carbon monoxide is colorless and odorless gas, when human inhaled CO it binds with the hemoglobin and reduce oxygen transfer, which leads to asphyxiation (Reşitoğlu et al. 2015).

### 2.4.2 Nitrogen Oxides ($NO_x$) Formation

The formation of $NO_x$ depending on the temperature, when oxygen and nitrogen react at high temperature of 2000 to 3000 K° the chemical of equilibrium forms the $NO_x$ (Heywood 2018). The equations bellow shows the possibilities of NO formation.

$$N + O_2 \longrightarrow NO + O \tag{2.4}$$

$$O + N_2 \longrightarrow NO + N \tag{2.5}$$

$$N + OH \longrightarrow NO + H \tag{2.6}$$

Moreover, at high temperature NO reacts to form $NO_2$, see the equations bellow.

$$NO + H_2O \longrightarrow NO_2 + H_2 \tag{2.7}$$

$$NO + O_2 \longrightarrow NO_2 + O \tag{2.8}$$

Transport sector is one of the most important producers of the $NO_x$, it produce 40-70% of the $NO_x$. Also diesel engines produces 85% of the $NO_x$ from all of the transport sector (Reşitoğlu et al. 2015).

### 2.4.3 Hydrocarbon (HC) Formation

Usually, the temperature near the wall of the cylinder is much lower than the center of the cylinder, this low temperature occur an incomplete combustion that produce an unburned hydrocarbon (Demers & Walters 1999).

Hydrocarbon is toxic, cause cancer and harmful to the environment and cause the ground level ozone, cars engine are responsible of about 50% of the hydrocarbon that cause the ground level ozone (Reşitoğlu et al. 2015).

See figure 2.2 bellow that shows the change of exhaust emissions concentration with varying equivalence ratios (Yildiz & Çeper 2017).

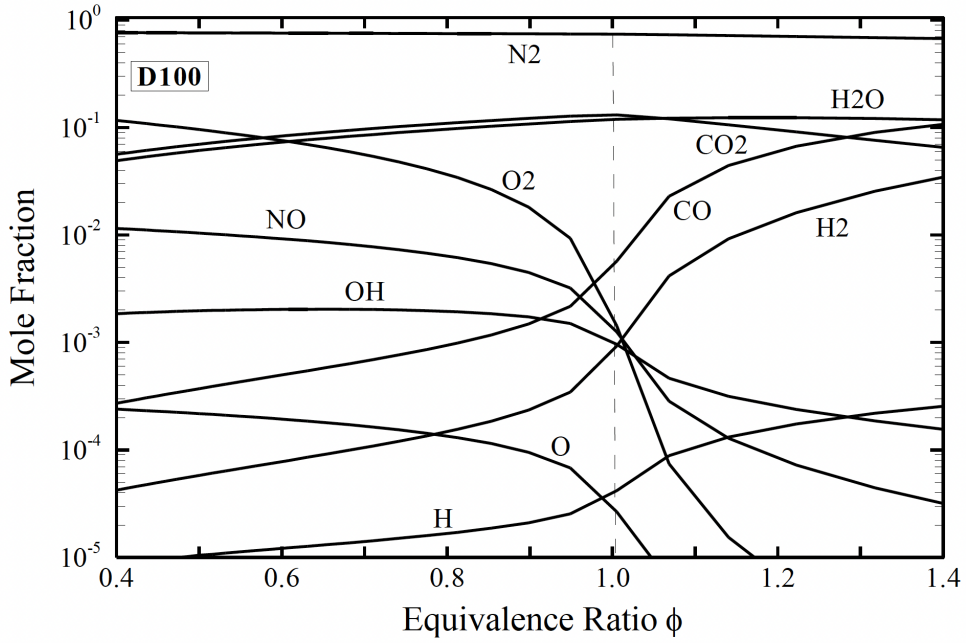



**Figure 2.2:** Diesel exhaust emissions concentration with varying equivalence ratios.

## 2.5 Exhaust Emissions Treatment

Car manufacturer companies racing to reduce exhaust emissions, three methods to reduce the emissions from the combustion process are used in automotive engines (Rahman et al. 2021).

- The first method works on the combustion process itself, such as make changes in the air-fuel ratio, valve and ignition timing, fuel concentration in mixture, combustion temperature and other factors (Cai & Zhao 2020).
- The second method is an after treatment processes such as the catalyst converter which convert the CO and the HC into $CO_2$ and water, the selective catalyst converter (SCR) to reduce the $NO_x$, the diesel particulate filter (DPF) is used to reduce the PM and the Adblue system used to reduce the $NO_x$ (Zhang et al. 2021).
- The third method is to use alternative fuels and fuel additives like natural gas, methanol and others (Muhssen et al. 2021, Wei et al. 2021).

The Adblue system is an after treatment processes which used to reduce the $NO_x$ using the urea solution as a chemical reactor with exhaust gases. The Adblue solution consists of 32.5% urea or it called Carbamide $CO(NH_2)_2$, and about 67.5% of water $H_2O$ (Zhang et al. 2021).

According to Sarsour & Nairoukh (2014) Adblue system injecting urea solution in water into the exhaust pipe, due to high temperature ammonia and carbon dioxide is formed due to the decomposition reaction as shown in equation 2.9. The reaction of ammonia and the nitrogen oxides forms water vapor and $N_2$, see equation 2.10.

$$CO(NH_2)_2 + H_2O \longrightarrow 2NH_3 + CO_2 \tag{2.9}$$

$$4NH_3 + 4NO + O_2 \longrightarrow 4N_2 + 6H_2O \tag{2.10}$$

Figure 2.3 bellow shows the block diagram of the traditional after treatment Adblue system (Reşitoğlu et al. 2015).

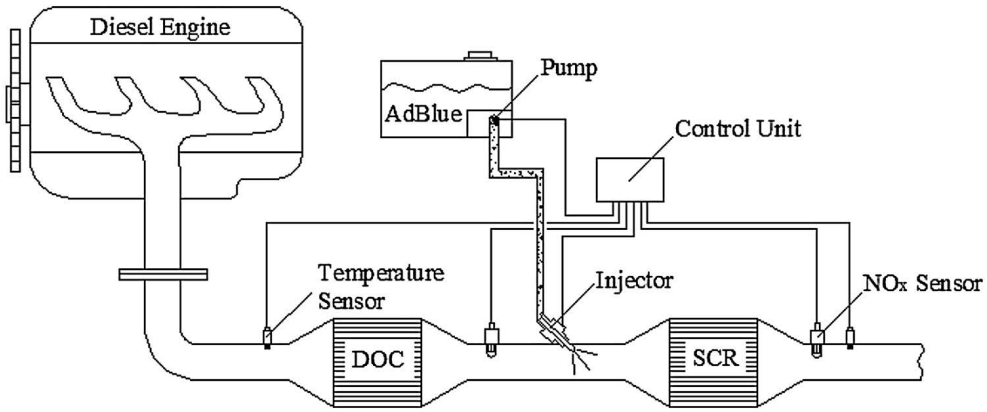



**Figure 2.3:** Adblue system diagram.

Unfortunately, the Adblue system can not reach to 100% $NO_x$ reduction due to the decrease of temperature in the exhaust pipe, were it drops from around 450 $C°$ to 200 $C°$. Moreover, the dynamics of the catalyst is much slower than the reaction inside the engine, were the catalyst need several minutes to reach the chemical equilibrium were just a few seconds are enough to reach the equilibrium inside the engine (Sarsour & Nairoukh 2014).

According to Sarsour & Nairoukh (2014), injecting urea in the exhaust line as an after treatment process increased the efficiency of the catalyzer to reduce $NO_x$ and CO in average of (25 - 35 %).

Demir et al. (2022) tested the effect of injecting urea solution in the combustion chamber on the exhaust emissions, it was only an experimental test, $NO_x$ emissions was decreased about 12 %, $CO_2$ emissions was increased by 38 % and the CO was decreased by 233 %.

## 2.6 Urea Additive Properties

Table 2.2 bellow shows some of the properties of urea, some values are not available because it was not studied before as an alternative fuel (Capuci et al. 2016, Fertiglob 2010).

**Table 2.2:** Properties of Urea.

| **Property** | **Value** |
|---|---|
| Appearance | White solid |
| Chemical formula | $CO(NH_2)_2$ or $CH_4N_2O$ |
| Molar mass | 60.06 $g/mole$ |
| Density | 1.32 $g/cm^3$ |
| Melting point | 133 - 135 $C°$ |
| Solubility in water | 545 $g/l$ @ 25 $C°$ |
| Flammability | Non flammable |
| Flash point | Non available |
| Enthalpy $\Delta_f h°$ for solid | -333.39 KJ/mole |

Also urea has some physical properties such as it known as colorless crystalline solid material, it has a high solubility in water as less in alcohols. From a chemical point of view it behaves as a mono acid base, and it reacts with acid to form salts, it reacts with nitrous acid to form nitrogen, carbon dixoide and water (Capuci et al. 2016).

According to Demir et al. (2022) urea was never used as an additive fuel before. Demir et al. (2022) used the urea as an additive to the diesel fuel and tested its effects on engine performance and exhaust emissions practically only, but they didn't make any analytic model for using the urea in combustion.

## 2.7 Heating Value

Internal combustion engines convert the chemical energy of the diesel fuel into a thermal energy, then into a mechanical energy (Bosch 2005). Thus, the amount of heat produced by the combustion process is directly proportional to the resulting mechanical energy. This heat related directly to the nature of fuel used in the combustion and the combustion reaction, and can be expressed as the heating value.

Heating value or as other references called it calorific value of a fuel, is the amount of heat produced of a reaction at constant pressure or constant volume at constant temperature, 1 atmosphere and 25 $c^{\circ}$, for a complete combustion of the unit of mass of the fuel, see equation 2.11 (Heywood 2018, Cengel et al. 2011).

$$\begin{aligned} Heating\ value &= |h_c| \\ &= H_{prod} - H_{react} \\ &= \sum N_p h^{\circ}_{f,p} - \sum N_r h^{\circ}_{f,r} \end{aligned} \tag{2.11}$$

Where $h_c$ is the enthalpy of combustion, $H_{prod}$ and $H_{react}$ are the enthalpy of the products and the enthalpy of reactants, $N_p$ and $N_r$ are the number of moles of the products and the reactants, finally the $h^{\circ}_{f,p}$ and $h^{\circ}_{f,r}$ are the standard enthalpy of formation of the products and reactants. The heating value expressed in joules per kilogram or joules per kilomole of fuel (Heywood 2018).

According to Cengel et al. (2011), the complete combustion means that in the combustion reaction all of the carbon atoms converted into $CO_2$, and all of the hydrogen atoms converted into $H_2O$, and sulfur atoms converted into $SO_2$, see equation 2.1.

Heating value could be lower or higher heating value, based on the phase of $H_2O$ in the products, when the $H_2O$ in products in vapor phase lower heating value (LHV) is used, and when it liquid higher heating value (HHV) is used.

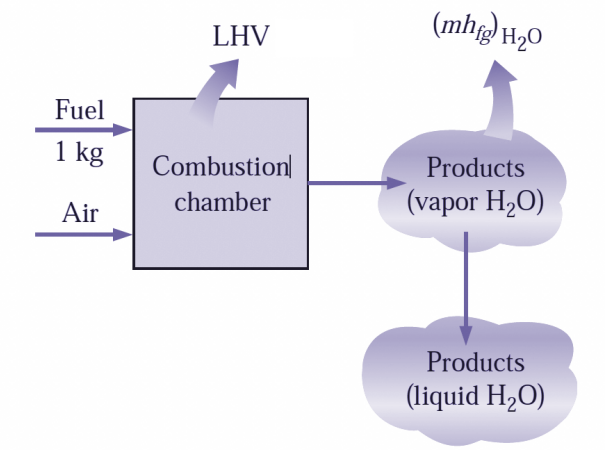



**Figure 2.4:** Lower-Higher heating value block diagram.

Where the higher heating value equals the sum of lower heating value and the latent heat of vaporization of the $H_2O$ in the products, see figure 2.4 (Cengel et al. 2011).

$$HHV = LHV + (mh_{fg})_{H_2O} \tag{2.12}$$

Where m is the mass of $H_2O$ in products per unit mass of fuel, $h_{fg}$ is the enthalpy of vaporization of water at specified temperature.

**Table 2.3:** Enthalpy of formation at standard conditions 1 atmosphere, $25C^{\circ}$.

| Substance | Formula | $h_f^{\circ}$ KJ/Kmole |
|---|---|---|
| Hydrogen | $H_{2(g)}$ | 0 |
| Nitrogen | $N_{2(g)}$ | 0 |
| Oxygen | $O_{2(g)}$ | 0 |
| Carbon dioxide | $CO_{2(g)}$ | -393,520 |
| Water vapor | $H_2O_{(g)}$ | -241,820 |
| Water | $H_2O_{(l)}$ | -285,830 |
| n-Dodecane | $C_{12}H_{26(g)}$ | -291,010 |
| Urea* | $CO(NH_2)_{2(Solid)}$ | -333,390 |

* Value from table 2.2.

Table 2.3 shows that the hydrogen, nitrogen and oxygen has a zero enthalpy of formation, the n-Dodecane value was choosed to replace the light diesel because it is the nearest value to the real diesel enthalpy of formation (Cengel et al. 2011).

# CHAPTER 3

# MODELING AND EVALUATION

**3.1 Model Assumptions**
**3.2 Equilibrium Combustion Model**
**3.3 Code Verification**
**3.4 Matlab Programming**

# Chapter 3

# Modeling and Evaluation

## 3.1 Model Assumptions

In this chapter the analytical methodology will be discussed to derive the equation of combustion and the equations of chemical equilibrium with thermodynamics for an actual combustion using the diesel fuel with air and urea solution in water as the reactants. The model will be able to estimate the concentration of each exhaust emissions gases with varying temperature, pressure, urea concentration in diesel and different equivalence ratio. Finally, the heating value will be calculated after adding the urea additive and will be compared with pure diesel. In this thesis, the model will be built based on the following assumptions, see table 3.1.

**Table 3.1:** Model assumptions.

| **Property** | **Value** |
|---|---|
| Diesel formula | $C_{14.62}H_{26.87}$ |
| Intake air components | 21% Oxygen and 79% Nitrogen |
| Urea concentration in diesel | up to 20 % urea solution in diesel |
| Urea solution | 32.5 % urea and 67.5 % water |
| Combustion temperature | 1200 to 2000 $K^{\circ}$<br>and fixed on 1900 $K^{\circ}$ |
| Combustion pressure | 50 Atm. |
| Equivalence ratio | 0.4 to 1.2 |

For the urea concentration in diesel, combustion temperature and the equivalence ratio two are chosen to be installed at a time.

## 3.2 Equilibrium Combustion Model

The analytical model for a complete combustion of diesel fuel, assumed a light diesel $C_nH_{1.8n}$, mixed with air consists of 21% oxygen and 79% nitrogen, the products will be $CO_2$, $H_2O$ and $N_2$, as shown in equation 3.1, where $\delta$ is the air-fuel ratio and $\nu_x$ is the number of moles of the combustion products (Prasad & Bella 2010, Heywood 2018).

$$C_nH_{1.8n} + \delta(O_2 + 3.76N_2) \longrightarrow \nu_1CO_2 + \nu_2H_2O + \nu_3N_2 \tag{3.1}$$

Rashidi (1998) and Macek (2000) developed the previous model to solve an incomplete combustion, see equation 3.2, where $\phi$ is the equivalence ratio.

$$C_nH_{1.8n} + \frac{\delta}{\phi}(O_2 + 3.76N_2) \longrightarrow$$
$$\nu_1CO_2 + \nu_2CO + \nu_3H_2O + \nu_4H_2 + \nu_5O_2 + \nu_6N_2 + \nu_7H + \nu_8O + \nu_9NO + \nu_{10}OH + \nu_{11}NO_2 \tag{3.2}$$

The analytical model was developed to handle adding urea solution in water with diesel at different concentrations, this model prepared to handle 11 combustion products; $CO_2$, CO, $H_2O$, $H_2$, $O_2$, $N_2$, H, O, NO, OH and $NO_2$, see equation 3.3 bellow.

$$x_dC_nH_{1.8n} + x_uCO(NH_2)_2 + x_wH_2O + \frac{\delta}{\phi}(O_2 + 3.76N_2) \longrightarrow$$
$$\nu_1CO_2 + \nu_2CO + \nu_3H_2O + \nu_4H_2 + \nu_5O_2 + \nu_6N_2 + \nu_7H + \nu_8O + \nu_9NO + \nu_{10}OH + \nu_{11}NO_2 \tag{3.3}$$

Where n is the number of carbon atoms in the fuel, $\delta$ is the molar air-fuel ratio, $\phi$ is the equivalence ratio and $\nu_{1-11}$ are number of moles of the combustion products, and $x_d, x_u, x_w$ are the number of moles of diesel, urea and water respectively. Also it is necessary to derive the stoichiometric air-fuel ratio for the combustion equation for the new fuel for different concentration as given in equation 3.4.

$$\delta = x_d(1.45n) + 1.5x_u \tag{3.4}$$

By using the chemical atom balancing for C-H-O-N on equation 3.3, four equations will be obtained as shown below.

C balance:

$$x_d(n) + x_u - (\nu_1 + \nu_2) = 0 \tag{3.5}$$

H balance:

$$x_d(1.8n) + 4x_u + 2x_w - (2\nu_3 + 2\nu_4 + \nu_7 + \nu_{10}) = 0 \tag{3.6}$$

O balance:

$$x_u + x_w + 2\left(\frac{\delta}{\phi}\right) - (2\nu_1 + \nu_2 + \nu_3 + 2\nu_5 + \nu_8 + \nu_9 + \nu_{10} + 2\nu_{11}) = 0 \tag{3.7}$$

N balance:

$$2x_u + (2)(3.76)\left(\frac{\delta}{\phi}\right) - (2\nu_6 + \nu_9 + \nu_{11}) = 0 \tag{3.8}$$

So by using the combustion model atom balancing for carbon, hydrogen, oxygen and nitrogen, equations 3.5 to 3.8 were derived. However, the model consists of 11 unknown, so another 7 equations must be used to have a system of 11 unknowns with 11 variables.

According to Cengel et al. (2011), if a reaction in the combustion chamber assumed at a pressure and temperature that leads to an equilibrium, the mixture component will react between each other in a certain way to achieve the equilibrium state, as shown in equation 3.9, where A, B, C and D are the component of the mixture, $dN_s$ are the differential changes of the number of moles of each component.

$$dN_{\mathrm{A}} + dN_{\mathrm{B}} \longrightarrow dN_{\mathrm{C}} + dN_{\mathrm{D}} \tag{3.9}$$

For an equilibrium the relation between the number of moles shown in equation 3.9 is needed, the corresponding stoichiometric (theoretical) reaction will be used to rewrite the equation, see equation 3.10.

$$\nu_{\mathrm{A}} A + \nu_{\mathrm{B}} B \rightleftharpoons \nu_{\mathrm{C}} C + \nu_{\mathrm{D}} D \tag{3.10}$$

Where $\nu$'s are the stoichiometric coefficients. Another constant needed to calculate the equilibrium which is the equilibrium constant $\mathrm{K_p}$, see equation 3.11, bellow.

$$K_{\mathrm{p}} = \frac{{N_C}^{\nu_C} {N_D}^{\nu_D}}{{N_A}^{\nu_A} {N_B}^{\nu_B}} \left(\frac{P}{N_{total}}\right)^{\Delta\nu} \tag{3.11}$$

Where P is the pressure in atmosphere, and $\Delta\nu$ is the summation of the products coefficients minus the summation of the reactants coefficients.

Finally to find the constant of equilibrium $\mathrm{K_p}$, see equation 3.12 bellow, where T is the temperature in Kelvin, $\mathrm{a_{1\text{-}7}}$ are the curve fit coefficients found in The Chemkin thermodynamic data base (Kee et al. 1990).

$$lnK_{\mathrm{p}} = a_1(1 - lnT) - a_2\left(\frac{T}{2}\right) - a_3\left(\frac{T^2}{6}\right) - a_4\left(\frac{T^3}{12}\right) - a_5\left(\frac{T^4}{20}\right) + a_6\left(\frac{1}{T}\right) - a_7 \tag{3.12}$$

Using the chemical of equilibrium reaction method that was mentioned before could give us the needed 7 equations, calculate the constant of equilibrium at different temperatures using NASA and the Chemkin thermodynamics data base and applying this model on matlab software using the Newton's Raphson method with Creamer rule can solve the 11 nonlinear system we have, see equation 3.13 used for the chemical

of equilibrium was derived using equations (3.10, 3.11 and 3.12) (Heywood 2018). According to Kayadelen & Ust (2013), the choosed methodology to build the model in this thesis was guaranteed with a maximum deviation of -1.452 % compared with the Chemkin software results.

$$\frac{1}{2}H_2 \rightleftharpoons H \qquad K_{p1} = y_7\sqrt{P}/\sqrt{y_4} \tag{3.13a}$$

$$\frac{1}{2}O_2 \rightleftharpoons O \qquad K_{p2} = y_8\sqrt{P}/\sqrt{y_5} \tag{3.13b}$$

$$\frac{1}{2}H_2 + \frac{1}{2}O_2 \rightleftharpoons OH \qquad K_{p3} = y_{10}/(\sqrt{y_5}\sqrt{y_4}) \tag{3.13c}$$

$$\frac{1}{2}N_2 + \frac{1}{2}O_2 \rightleftharpoons NO \qquad K_{p4} = y_9/(\sqrt{y_6}\sqrt{y_5}) \tag{3.13d}$$

$$H_2 + \frac{1}{2}O_2 \rightleftharpoons H_2O \qquad K_{p5} = y_3/(y_4\sqrt{P}\sqrt{y_5}) \tag{3.13e}$$

$$CO + \frac{1}{2}O_2 \rightleftharpoons CO_2 \qquad K_{p6} = y_1/(y_2\sqrt{P}\sqrt{y_5}) \tag{3.13f}$$

$$NO + \frac{1}{2}O_2 \rightleftharpoons NO_2 \qquad K_{p7} = y_{11}/(y_9\sqrt{P}\sqrt{y_5}) \tag{3.13g}$$

Where P is the pressure in atmosphere, $y_{1-11}$ are the mole fraction of the exhaust emissions and N are the number of moles.

$$y_i = \frac{\nu_i}{N} \qquad N = \sum_{i=1}^{11} \nu_i \qquad \sum_{i=1}^{11} y_i - 1 = 0 \tag{3.14}$$

The final model contains 11 nonlinear equations with 11 unknowns, these equations found from the 4 linear equations (3.5 - 3.8) and the 7 nonlinear equations in 3.13. Using Newton's Raphson method is the way used to solve this model by writing the

11 equations in the form for 11 unknowns respectively as shown below;
i=1:11;

$$\begin{aligned} f_1(\nu_1, \nu_2, ...,\nu_i) &= 0 \\ f_2(\nu_1, \nu_2, ...,\nu_i) &= 0 \\ &. \\ &. \\ &. \\ f_i(\nu_1, \nu_2, ...,\nu_i) &= 0 \end{aligned} \tag{3.15}$$

The vector for unknowns,

$$\nu = [\nu_1, \nu_2, ..., \nu_i]^T \tag{3.16}$$

The initial guess for $\nu$,

$$\nu_0 = [\nu_1^0, \nu_2^0, ..., \nu_i^0]^T \tag{3.17}$$

The following expressions yields for the approximations to $\Delta\nu_i$,

$$\begin{bmatrix} f_1\left(\nu_1^{(0)}, \nu_2^{(0)}, ..., \nu_i^{(0)}\right) \\ f_2\left(\nu_1^{(0)}, \nu_2^{(0)}, ..., \nu_i^{(0)}\right) \\ . \\ . \\ f_i\left(\nu_1^{(0)}, \nu_2^{(0)}, ..., \nu_i^{(0)}\right) \end{bmatrix} + \begin{bmatrix} \frac{\partial f_1}{\partial \nu_1} \frac{\partial f_1}{\partial \nu_2} ... \frac{\partial f_1}{\partial \nu_i} \\ \frac{\partial f_2}{\partial \nu_1} \frac{\partial f_2}{\partial \nu_2} ... \frac{\partial f_2}{\partial \nu_i} \\ . \\ \frac{\partial f_i}{\partial \nu_1} \frac{\partial f_i}{\partial \nu_2} ... \frac{\partial f_i}{\partial \nu_i} \end{bmatrix} . \begin{bmatrix} d\nu_1 \\ d\nu_2 \\ . \\ . \\ d\nu_i \end{bmatrix} = 0 \tag{3.18}$$

The first fraction of the second term in equation 3.18 is a Jacobian matrix and was calculated using finite differences; K = 1 to 11

$$\frac{\partial f_i}{\partial \nu_k} \approx \frac{f_i(\nu + \Gamma) - f_i(\nu)}{\Gamma} \tag{3.19}$$

The value of $\Gamma$ is very close to zero to estimate any truncation error. So to solve for $d\nu_i$ , the next iteration was calculated as follows;

$$x_i^{iter} = x_i^{iter-1} + d\nu_i \tag{3.20}$$

The iteration process ended when the solving process reached the desired converge criteria t1 and t2 as follows;

$$|x_i^{iter} - x_i^{iter+1}| < t_1 \tag{3.21}$$

or

$$|f_i^{iter} - f_i^{iter+1}| < t_2 \tag{3.22}$$

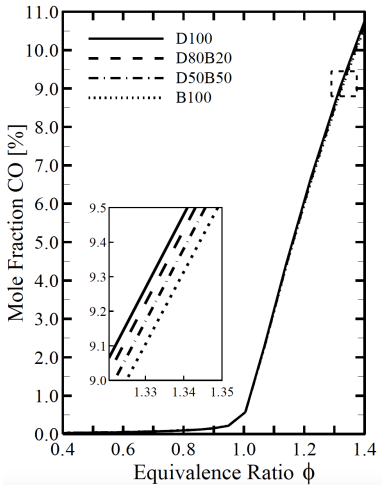
The iterations used in this model for Newton's Raphson method was a tolerance to be less than $1 \times 10^{-8}$ with maximum iterations of 20 loops.

## 3.3 Code Verification

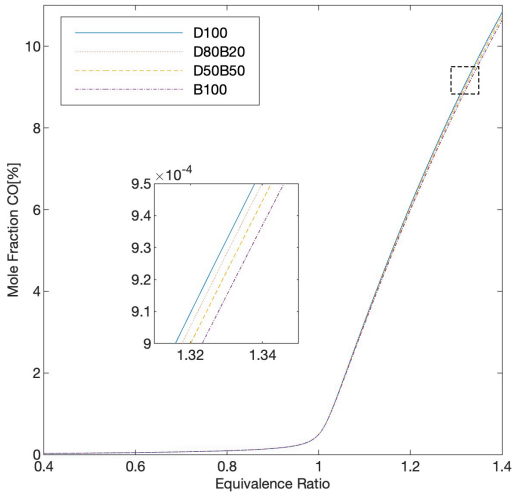
Before starting to apply the model and finding the results, it is necessary to verify the validity of the model's work. Therefore, a previous study with known results was chosen to be applied to the model to compare the results. The study was chosen is "Estimation of equilibrium combustion products of diesel-biodiesel fuel blends using the developed solving process for $C_nH_m$ and $C_\alpha H_\beta O_\gamma$ fuel types" (Yildiz & Çeper 2017), this study was published in 2017 to estimate the concentration of the exhaust gases emissions due to mix bio-diesel with diesel in different blends ratios.

The urea in this model was replaced by bio-diesel to find the needed results for the validation, the results was found as shown in figure 3.1 (Yildiz & Çeper 2017).

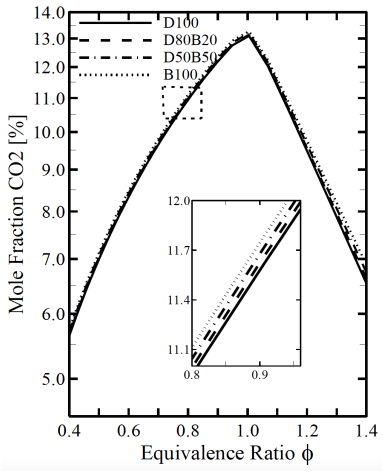
The results shows a maximum deviation of 0.57 % for the CO concentration in exhaust emissions between the selected study and the built model, and around 2.2 % for the $CO_2$ and 0.32 % for the NO concentration. These results are satisfactory to complete the application of the model of urea blends.



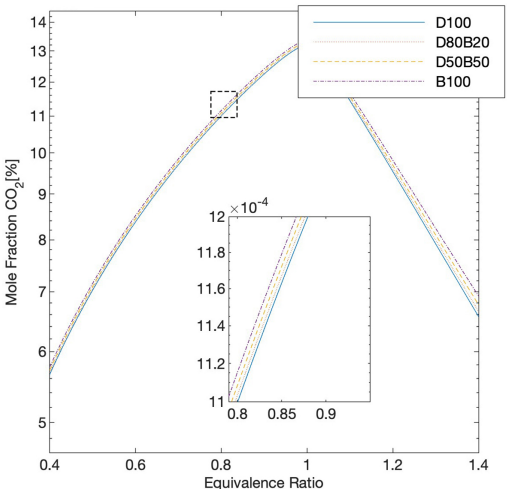

**(a)** CO reference results



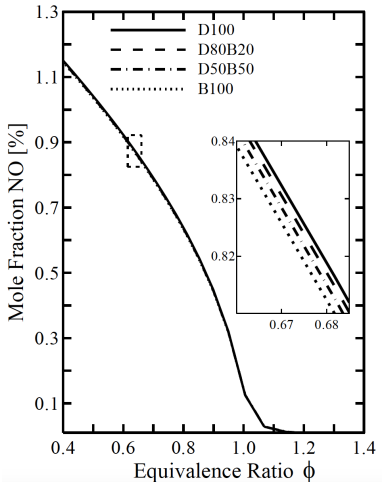

**(b)** CO model results



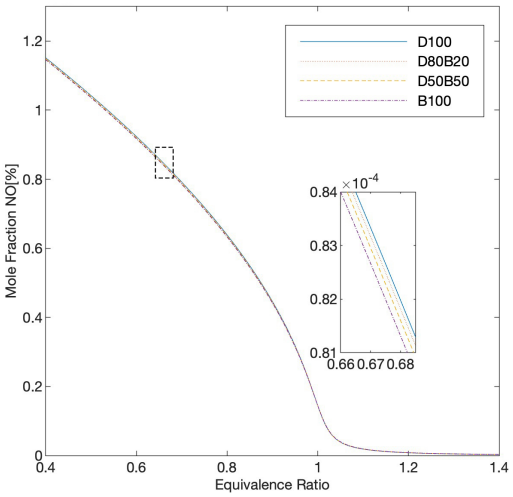

**(c)** $CO_2$ reference results




**(d)** $CO_2$ model results




**(e)** NO reference results




**(f)** NO model results

**Figure 3.1:** Comparison results for exhaust emissions concentration between the selected study and the built model.

## 3.4 Matlab Programming

Matlab R2022a software used to solve the developed model. The model consists of 11 non-linear equations with 11 unknowns. Newton's Raphson method were used to solve the mathematics.

The model in this thesis will investigate the effect of injecting Adblue solution (32.5 % urea and 67.5 % water) with light diesel, the diesel ratio was tested between 80 and 100 %, were the Adblue between 0 and 20 %. The pressure used was 50 atmosphere, with temperature between 1200 and 2000 kelvin, and the equivalence ratio between 0.4 and 1.2.

Moreover, for Newton's Raphson method the tolerance was programmed to be less than $1 \times 10^{-8}$ with maximum iterations of 20 loops, that for minimizing the error and get more accurate results, and the values of gases mole fraction were calculated for equivalence ratios between 0.4 to 1.2 in 0.005 each step for smoother results. See figure 3.2 below, which illustrates the Matlab code algorithm for the model.

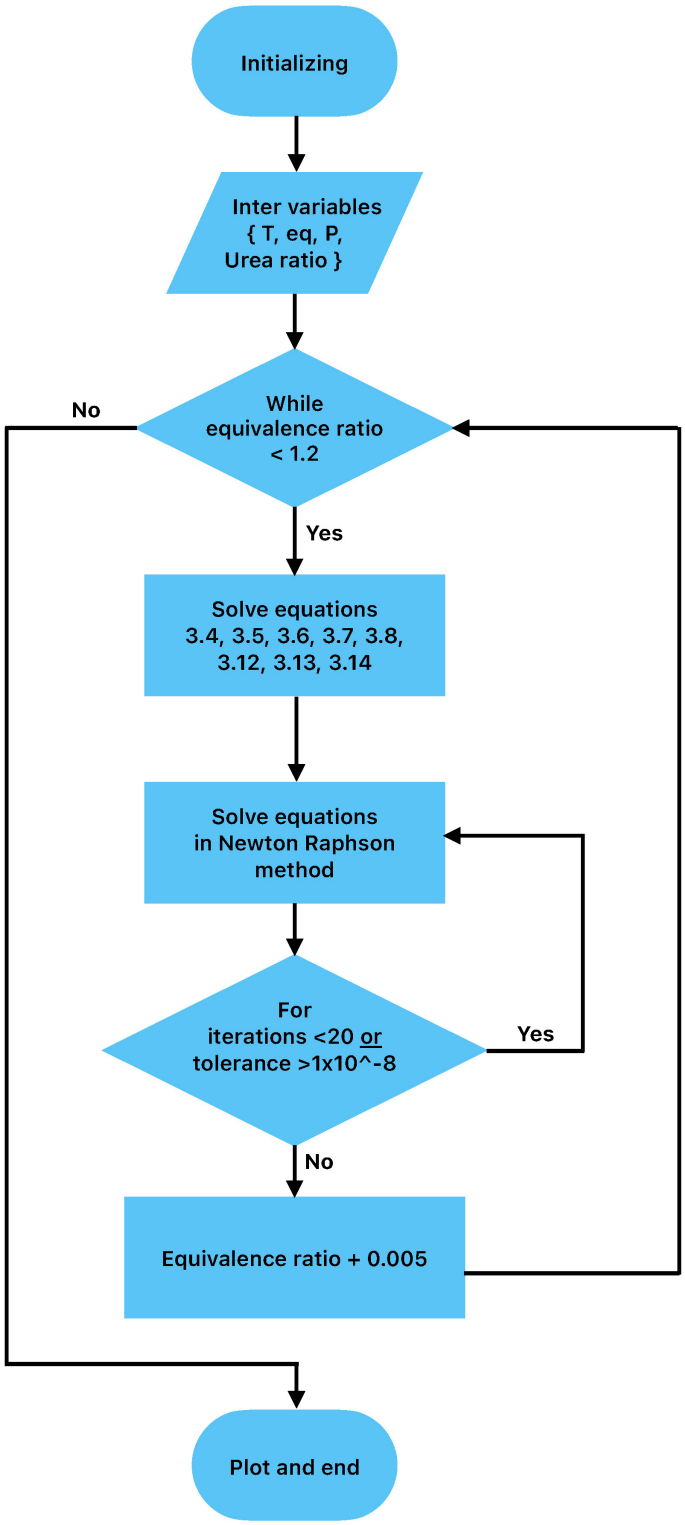



**Figure 3.2:** Matlab code algorithm.

# CHAPTER 4

# RESULTS AND DISCUSSION

# Chapter 4

# Results and Discussion

## 4.1 Introduction

In this chapter the results of the developed model after applying it on Matlab R2022a software will be discussed. Using the Chemkin tables with equation 3.10 on equation 3.13, the curve-fit coefficients for the chemical equilibrium constants $a_1$ to $a_7$ were calculated for $K_{p1}$ to $K_{p7}$ in the same order of equation 3.13 as shown in table 4.1 bellow.

**Table 4.1:** Curve-fit coefficients for chemical equilibrium constants.

| | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ | $a_6$ | $a_7$ |
|---|---|---|---|---|---|---|---|
| $K_{p1}$ | -1.034E+0 | 4.133E-4 | -7.320E-8 | 7.705E-12 | -3.444E-16 | -2.588E+4 | -6.548E-2 |
| $K_{p2}$ | -7.132E-1 | 3.555E-4 | -6.638E-8 | 5.335E-12 | -1.700E-16 | -2.983E+4 | -3.215E+0 |
| $K_{p3}$ | 4.584E-1 | -3.659E-4 | 1.502E-7 | -2.408E-11 | 1.429E-15 | -4.712E+3 | -4.649E+0 |
| $K_{p4}$ | 4.606E-2 | -1.644E-4 | 1.122E-7 | -1.986E-11 | 1.080E-15 | -1.099E+4 | -1.725E+0 |
| $K_{p5}$ | 2.086E+0 | -1.818E-3 | 5.568E-7 | -6.873E-11 | 2.931E-15 | 2.846E+4 | -6.199E+0 |
| $K_{p6}$ | 2.425E-1 | -1.062E-3 | 4.395E-7 | -7.124E-11 | 3.814E-15 | 3.415E+4 | 9.660E+0 |
| $K_{p7}$ | 2.312E+0 | -6.022E-3 | 4.473E-6 | -2.87E-10 | -5.645E-13 | 6.419E+3 | -2.765E+0 |

Using equations 3.11 and 3.12, the constant of equilibrium of each equilibrium reaction from $K_{p1}$ to $K_{p7}$ were calculated with varying temperature from 1400 to 3000 $K^{\circ}$, see figure 4.1.

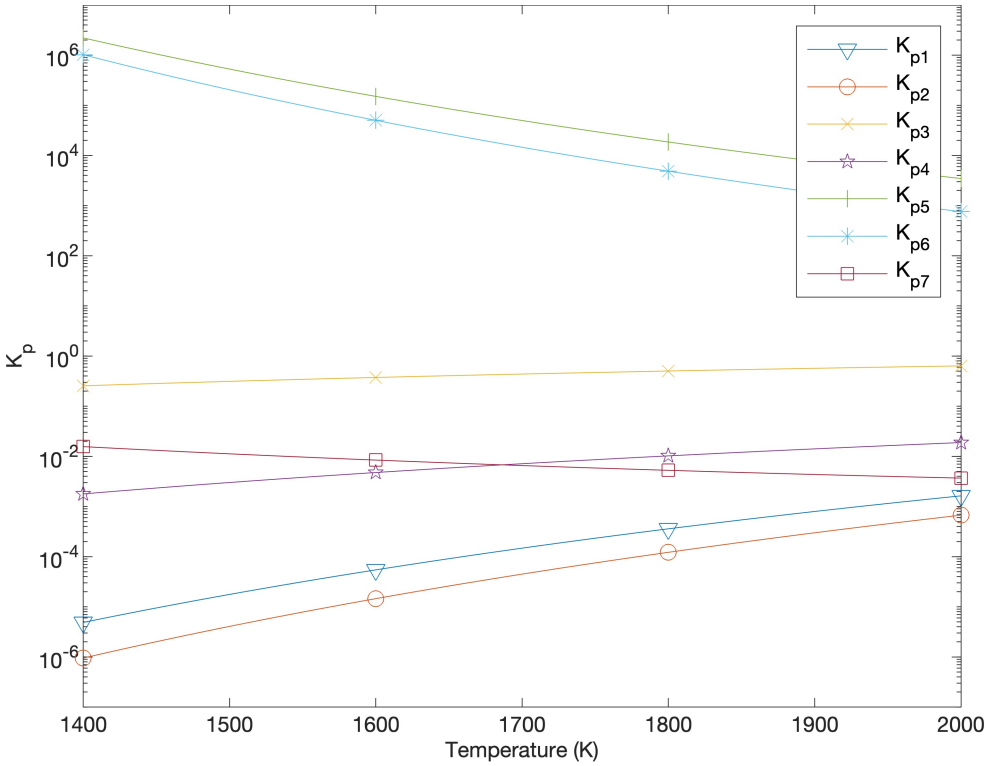


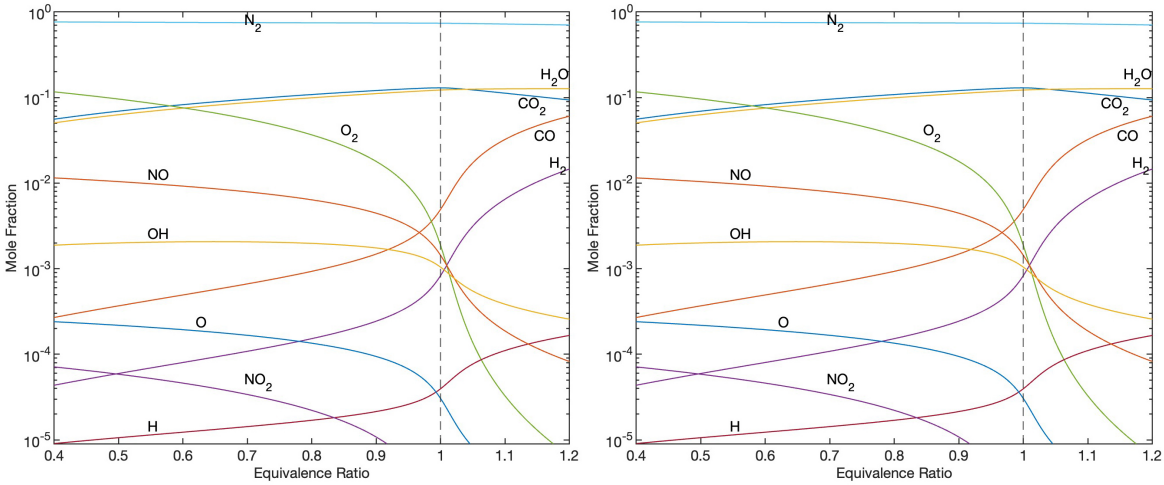

**Figure 4.1:** The relation between constant of equilibrium $K_p$ and temperature.

## 4.2 Results and Discussion

Using the previously built model equation for the actual combustion of urea solution in water as an additive to diesel fuel from equation 3.3 with chemical atom balancing produced 4 equations with 11 unknowns of 11 numbers of moles of the products. On the other hand, using the chemical equilibrium from equation 3.13 with the constant of equilibrium found in figure 4.1 produced more 7 equations.

After applying the model on matlab R2022a software, a specific operating conditions were choosed, the simulation worked on 1900 $K°$ combustion temperature, 50 atmosphere combustion chamber pressure. Two cases were tested, pure diesel fuel compared with 80D20U fuel that consists of 80% pure diesel fuel ($C_{14.62}H_{26.87}$) and 20% of Adblue solution which consists of 32.5% urea and 67.5% water. Figure 4.2 bellow shows the mole fraction of each exhaust emissions gases change with the equivalence

ratio varying between 0.4 to 1.6 for pure diesel compared with 80D20U fuel at specified conditions of temperature and pressure.




**(a)** Pure Diesel **(b)** 80D20U

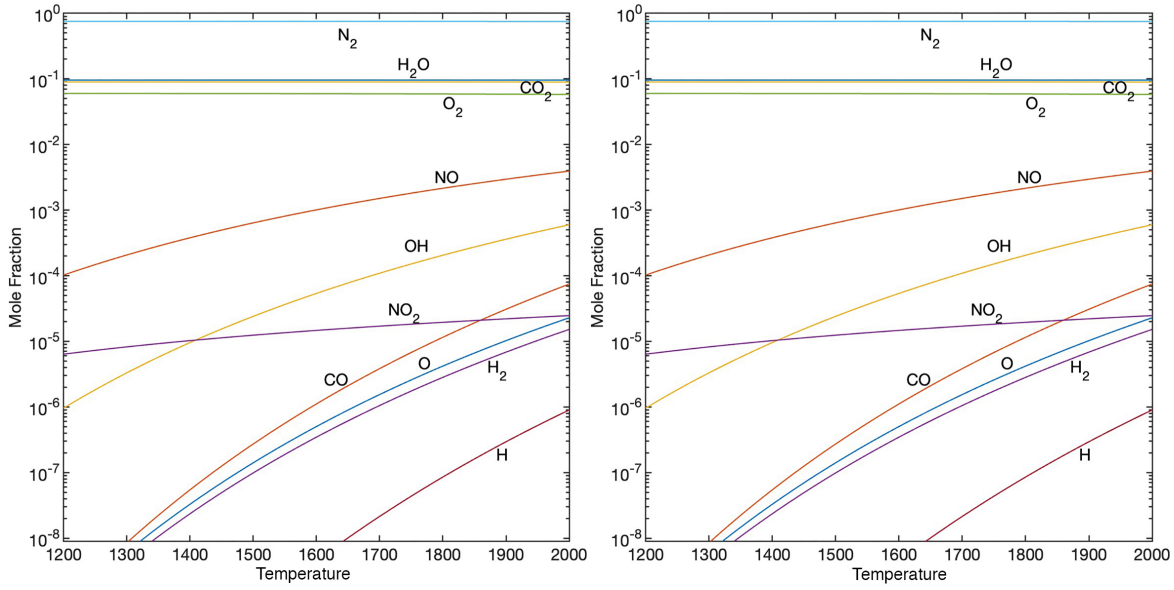
**Figure 4.2:** The relation between mole fraction of exhaust emissions with varying equivalence ratios at 1900 K° and 50 Atm.

Figure 4.2 shows that adding the urea additive to diesel fuel will not make radical change to the overall look of the concentration of the emissions. The highest mole fraction is for nitrogen. At lean mixture the least mole fraction is for hydrogen then for $NO_2$. Moreover, it was found that the relation between the urea solution fraction to diesel is perpendicular with decreasing if the harmful exhaust gases. Because of that, all the results shown were between pure diesel versus 80D20U.

The mixture called lean when the equivalence ration is less than 1, in this case there is excess of oxygen for a complete combustion. So, the $CO_2$ concentration is high. On a stoichiometric and lean mixture where $\phi \leq 1$, the $CO_2$ concentration decreases, but the CO concentration will increase because of the lack of oxygen. As a result of decreasing CO in lean mixture, the NO, OH, O and $NO_2$ will increase due to chemical equilibrium of formation. On the other hand, decreasing of OH formation will increase the formation of H and $H_2$.

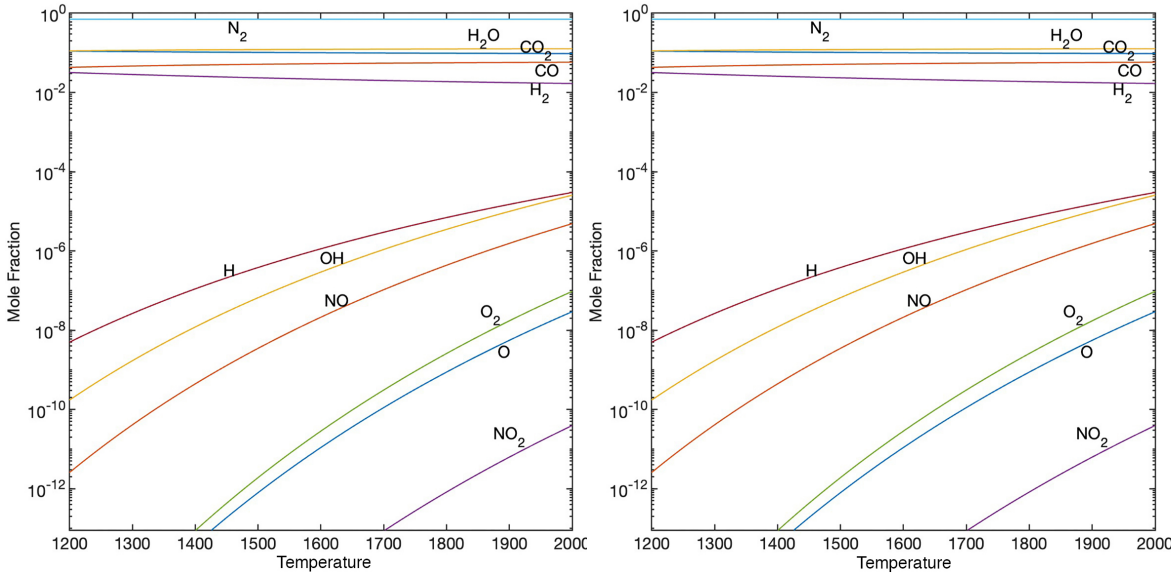
Figure 4.3 and 4.4 shows the relation between mole fraction of exhaust emissions with varying temperatures at lean and rich mixtures respectively, at a constant pressure of 50 atmosphere for pure diesel versus 80D20U fuel. For lean mixture the concentration of $H_2O$ and $CO_2$ slightly decreases with temperature increasing, that because in this case the activity of reactants 3.13e and 3.13f increases due to the decreasing of their constant of equilibrium as shown in figure 4.1 for $K_{p5}$ and $K_{p6}$.

Figure 4.3 shows that in lean mixture which is the most working condition in the engine, the $NO_2$ concentration is much higher than in rich mixture, that because the increasing concentration of $O_2$ in lean mixture will increase the formation of $NO_2$ reaction, see equation 3.13g.




**(a)** Pure Diesel **(b)** 80D20U

**Figure 4.3:** The relation between mole fraction of exhaust emissions with varying temperatures at $\phi = 0.7$ and 50 Atm.

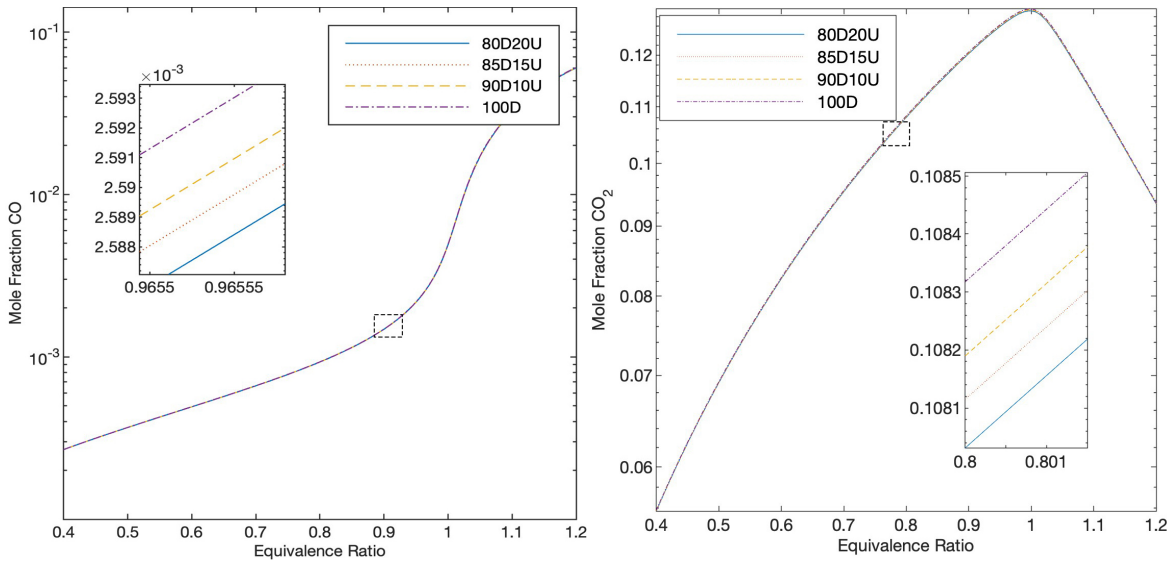



**(a)** Pure Diesel **(b)** 80D20U

**Figure 4.4:** The relation between mole fraction of exhaust emissions with varying temperatures at $\phi = 1.2$ and 50 Atm.

The developed model was able to make a comparison between pure diesel and urea solution blends, to compare the concentration of the exhaust emissions gases. The results were shown in figure 4.5 compared the concentration of the main harmful gases, which are the CO, $CO_2$, NO and $NO_2$ at pure diesel (100D), 90% pure diesel with 10% urea solution (90D10U), (85D15U) and (80D20U).

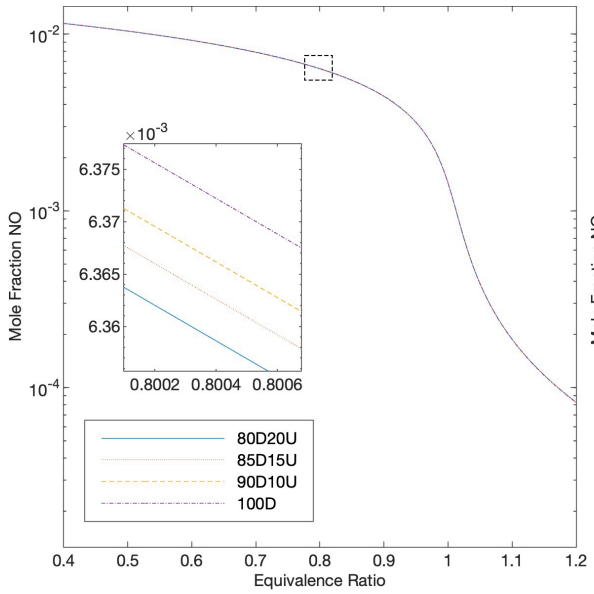
Adding Urea solution will increase the reactant carbon atoms but in a very small amount, while the urea solution will increase the nitrogen and hydrogen much more. All of that will result a very small varying in the concentration of the exhaust gases at different fuel blends. However, as it shown in figure 4.5 the concentration of emissions decreases with the increasing of concentration of the urea solution in the fuel blends.



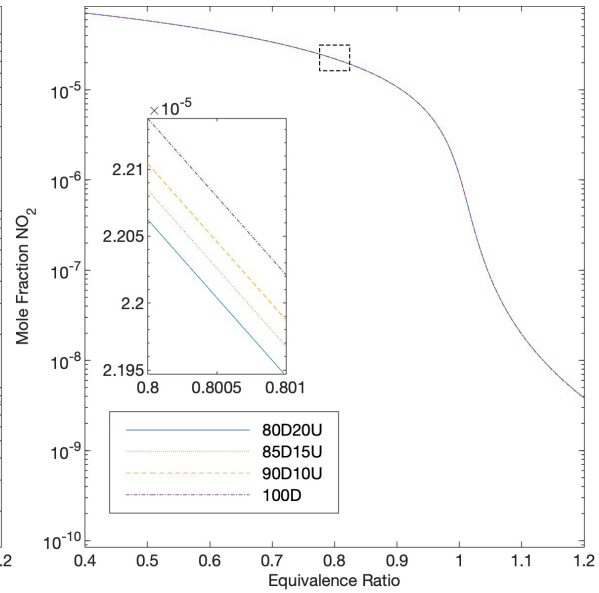

**(a)** CO




**(b)** $CO_2$



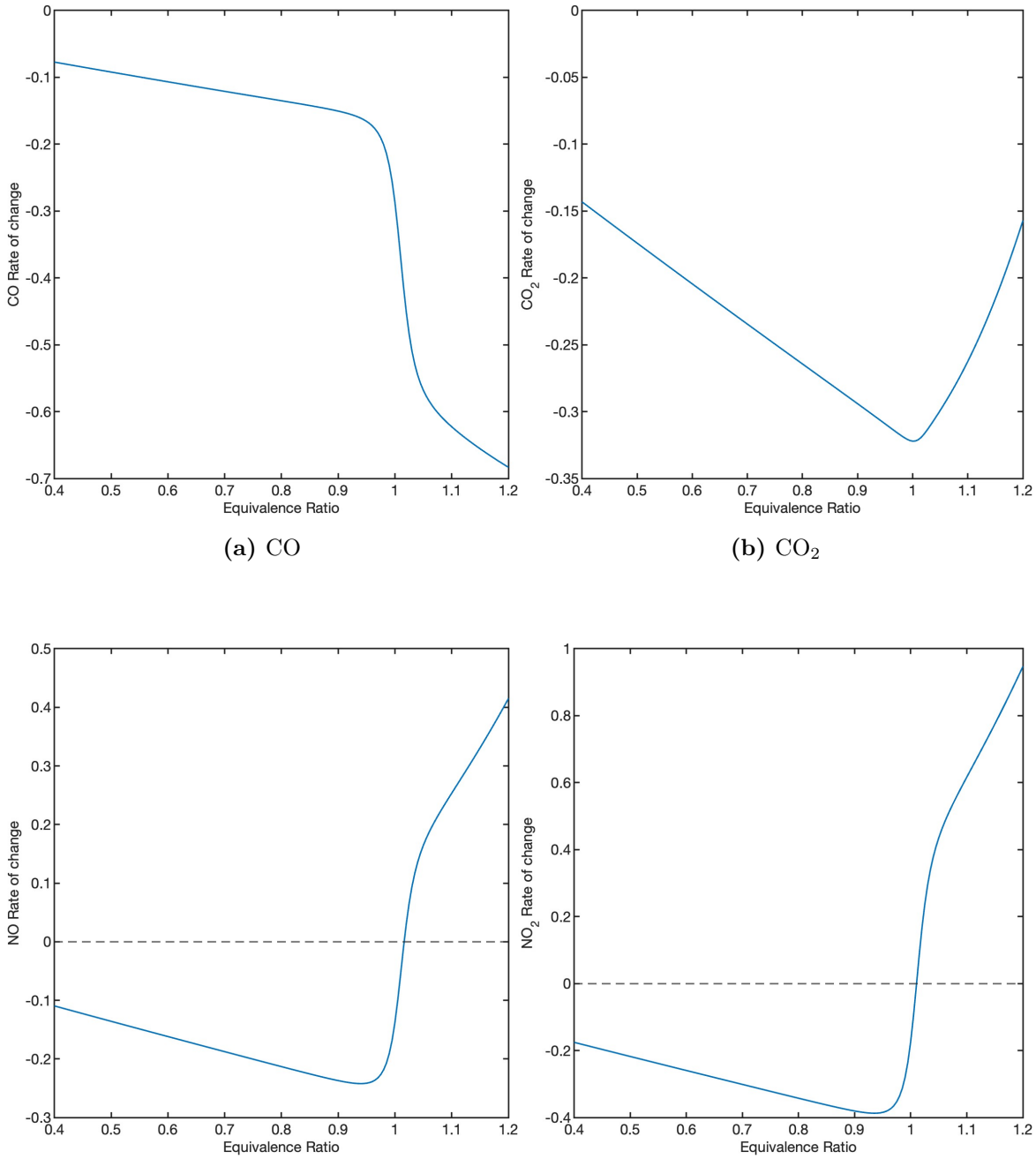

**(c)** NO




**(d)** $NO_2$

**Figure 4.5:** The relation between mole fraction of exhaust emissions with varying equivalence ratios at 1900 K° and 50 Atm.

Finally, the developed model shows the rate of change of the exhaust emissions with varying equivalence ratios at constant pressure and temperature of 1900 K° and 50 atmosphere, as shown in figure 4.6 bellow. The results were shown for the main harmful emissions at a fuel blend 80D20U for CO, $CO_2$, NO and $NO_2$.




**(a)** CO **(b)** $CO_2$

**(c)** NO **(d)** $NO_2$

**Figure 4.6:** The relation between the rate of change [%] of exhaust emissions with varying equivalence ratios for 80D20U fuel blend at 1900 K° and 50 Atm.

The results shows that CO concentration decreased by 0.08 to 0.8 %, the $CO_2$ concentration decreased on lean mixture from 0.144 to 0.32 %, NO concentration also decreased around 0.11 to 0.243 % and finally, $NO_2$ concentration decreased from 0.18 to 0.387 %. Compared to the huge number of diesel engine vehicles all around the

world, these tiny decrease of emissions will be tons of harmful emission gases.

After applying data from table 2.3 in equation 2.11 on the combustion reaction of pure diesel and 80D20U fuel blend, the results gave a decrease in the lower heating value by 3.67 % than pure diesel, that means less heat which will cause less $NO_x$ formation, as shown in table 4.2 bellow.

**Table 4.2:** Lower heating value of fuels at standard conditions of complete combustion.

| Fuel | Molar Mass Kg/Kmole | Lower heating value KJ/Kg |
|---|---|---|
| Light Diesel | 202 | 43,200 |
| Urea solution in water (32.5% Urea - 67.5 % water) | 31.66 | 4,642 |
| 80D20U | 168.18 | 41,611 |

According to Palestinian Central Bureau of Statistics (2019), there were 130287 registered diesel cars in West Bank in the beginning of 2019, which constitutes 51.2% of the total number of the registered cars. O'Driscoll et al. (2018) said that in average the diesel cars produce 170 g $CO_2$/km and about 0.44 g $NO_x$/km. In average each car may travel a distance of 15000 km/year for normal use. Using all of the above data and the rate of change that was discussed in the model results, using the urea with diesel in west bank may decrease the $CO_2$ around 1063 tons in the year, and around 2.579 tons of $NO_x$. Comparing these numbers to the total number of cars all around the world, a huge numbers will be achieved.

As a result, using urea as an additive with diesel will decrease the harmful exhaust emissions form the combustion process. On the other hand, some factors were the reason for not using it in the cars, such as this solution will increase the cost of the fuel. Also urea is a solid substance needs to be dissolved in water, were water makes some damage to the engine. Finally, the urea substance is forbidden to use in many countries due to security reasons, were it used in explosives industry.

# CHAPTER 5

# CONCLUSIONS AND FUTURE WORK

# Chapter 5

# Conclusions and Future Work

## 5.1 Conclusion

In this thesis, the effect of injecting additive urea in diesel engine combustion chamber on exhaust emissions were investigated using a model that have been developed based on the chemical atom balancing with the chemical of equilibrium equations. The fuel blends applied on the model were pure diesel (100D), 90% pure diesel with 10% urea solution (90D10U), (85D15U) and (80D20U). Those fuel blends applied on varying temperature, pressure and equivalence ratios. Matlab R2022a software used to solve the developed model that used the Newton's Raphson method. The following conclusion can be stated:

- Increasing the urea solution fraction in diesel fuel will not make radical change to the overall look of the concentration of the emissions.
- Urea additive decreases the concentration of the CO up to 0.8 %, $CO_2$ up to 0.32 %, NO up to 0.243 % and $NO_2$ up to 0.387 %.
- The amount of CO, $CO_2$, NO and $NO_2$ decreases when the fraction of urea additive increased in diesel fuel.
- The lower heating value for 80D20U fuel blend decreases by 3.67 % than pure diesel.

## 5.2 Future Work

In this work, the developed model is independent of the engine mechanical design, so it can be easily developed again to investigate another fuel additive. Unfortunately, no diesel car was found in the university's laboratories or in the police facilities to apply the practical experiment on it. Therefore, the theoretical results were satisfied. I suggest that students in future may do the experimental test to make a comparison between the real results with the developed model. Moreover, it may be developed to handle the calculation of the soot particles results.

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