COMBUSTION AND EMISSIONS OF DIESEL FUEL AND DIESEL-HYDROGEN MIXTURE USING 1D SOFTOWER

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Abstract : Due to fast depletion of fossil fuels and their detrimental effect on the environment, considerable efforts have been made to find out the viable alternative fuels for meeting sustainable energy demand with minimum environmental impact.

This work describes a simple model for calculating the combustion process, it was written in MATLAB code. The simulation was carried out at pure diesel with different equivalence ratios. Carbon dioxide, carbon monoxide, water vapor and oxygen in the exhaust were determined.

A simulation for numerical analysis of hydrogen-diesel mixture combustion was presented in this work. Hydrogen was substituted for diesel fuel on a percent energy basis of 0 %, 20 %, 40 %, 60 % and 80% at different constant equivalence ratios.

This work involves the simulation program for determining the mole fraction of each of the exhaust species when the hydrogen is burnt along with diesel and the results are presented. The proportion of hydrogen in the hydrogen–diesel blend affecting the mole fraction of the exhaust species is also simulated. The code developed gave reasonably good results which are in good agreement with the experimental values.

Keywords: hydrogen-diesel mixture, combustion, equivalence ratios, mole fraction.

1. Introduction

During the past several decades, a number of researchers have investigated the advantages and disadvantages associated with addition of hydrogen to conventional hydrocarbon fuels engines. Numerous studies have reported on the performance of (SI) spark ignition engines with hydrogen - natural gas fuel [1,2] and hydrogen –gasoline fuel [3].

Also, several researchers have investigated the replacement of diesel fuel by hydrogen as a technique to improve the performance and emissions of diesel engines. Saravanan et al. [4,5] have reported studies using a DI diesel engine with hydrogen in the dual fuel mode. In general, they observed that a significant improvement in thermal efficiency and reduction in hydrocarbon (HC), CO and CO2 emissions could be obtained under certain operating conditions by running a diesel engine in the dual fuel mode using hydrogen. However, as reported by McWlliam et al. [6], the addition of large amount of H2 can significantly increase the emissions of NOx. H. An et al. [7] studied the performance and emission characteristics of a dual fuel (hydrogene/diesel) engine. They concluded that the CO and soot emissions were shown to be reduced under most of the engine operating conditions due to the “carbon free” nature of hydrogen, while NOx emissions increased.

Zhou et al [8] have been investigated experimentally the performance, regulated and unregulated emissions of a diesel engine with hydrogen addition. They concluded that hydrogen addition also has the potential to reduce unregulated emissions, such as olefins (C2H4 and C3H6), BTX (C6H6, C7H8 and C8H10) and acetaldehyde (CH3CHO). H. An et al. [9] numerically investigated the influence of hydrogen substitution on performance, combustion and emission characteristics in a diesel engine fueled by biodiesel, three-dimensional CFD model has been used. Numerical results indicated that with the hydrogen addition, CO and soot emissions at all the engine speeds and loads decreased. However, NOx emission was increased due to higher combustion temperature associated with hydrogen addition. Satbir Singh [10] carried out a numerical analysis to investigate the impact of H2 addition on NO2 emissions from a H2-diesel dual-fuel engine using a CFD model integrated with a reduced chemistry model and a NOx formation model. They have shown that the addition of H2 up to 4% by volume lead to an increase in NO2, and then start to decrease beyond of 4 % by volume. Nguyen et al. [11] investigated the characteristics of combustion noise from a dual fuel (hydrogen/diesel) engine. They showed that the diesel engine noise with hydrogen addition was lower than that with diesel fuel alone at late diesel-fuel injection timings.

1.1 Properties of hydrogen in comparison with diesel

The main advantage of burning hydrogen in internal combustion engines is its lack of carbon content, leading locally to no exhaust emissions of particulate matter, unburned hydro-carbons, CO and CO_2. Some of hydrogen's properties, particularly relevant to in-cylinder mixture formation and combustion, are summarized in Table 1 in comparison to diesel fuel.

Table (1) Properties of hydrogen in comparison with diesel

Properties	**Hydrogen**	**Diesel**
Auto-ignition temperature (K)	858	530
Minimum ignition energy (mJ)	0.02	-
Flammability limits in air (Vol. %)	4-75	-
Flame speed (m/s)		
Net heating value (mJ\Kg)	120	42.2
Stoichiometric air\fuel (mass)	34.3	14.5
Density at ambient temperature (Kg\m^3) @ 1.01 bar	0.083	824

Auto-ignition temperature of hydrogen is very high (858 K).This means that hydrogen is most suitable as a fuel for spark ignition engine. Hydrogen's minimum ignition energy is about one order of magnitude less than that of common fuels which means that it can autoignite easily. Hydrogen has a wide flammability range in comparison with all other fuels. As a result, hydrogen can be used in running an engine on a lean mixture that allows for greater fuel economy due to a more complete combustion of the fuel. Additionally, it allows for lower combustion temperature and hence, decreases the amount of NOx. The flame speed of hydrogen is higher and hydrogen allows operation at significantly higher excess air ratios than conventional hydrocarbon fuels. Hydrogen's heating value on a mass basis is very high in comparison to diesel fuel (120 MJ/kg for hydrogen, 42.2 MJ/kg for diesel).

Emissions of carbon monoxide and unburnt hydrocarbons are practically eliminated with a hydrogen-fuelled engine, as the only source of carbon will be the lubricating oil. For the same reason the engine does not emit carbon dioxide. The only non-trivial exhaust gas emissions will be nitrogen oxides, which result from the oxidation of atmospheric nitrogen under high temperatures.

Hydrogen has very low density. This results in a problem when used in an internal combustion engine. A very large volume is necessary to store enough hydrogen to give a vehicle an adequate driving range.

1.2 Advantages of hydrogen as fuel for IC engines

The merits of hydrogen as a fuel are given below;

- Hydrogen – air mixture burns early 10 times faster compared to diesel air mixture.

- Being burning rate considerably high it is more preferred in high speed engine. As the burning rate are very high, working approaches to instantaneous combustion of an ideal Otto cycle performance.
- Hydrogen ignition limits are much wider. So it can burn easily and give considerably higher efficiency.
- Its clean exhaust is the most attractive feature of all. As it does not produce carbon dioxide, there is no greenhouse effect.
- The exhaust heat can be used to extract hydrogen from the hydride reducing the load on engine.

Less cyclic variations are encountered with hydrogen than with other fuels even for very lean mixture operation. This leads to a reduction in emissions, improved efficiency, and quieter and smoother operation.

1.3 Disadvantages of hydrogen as fuel for IC engines

The demerits of hydrogen as a fuel are given below;

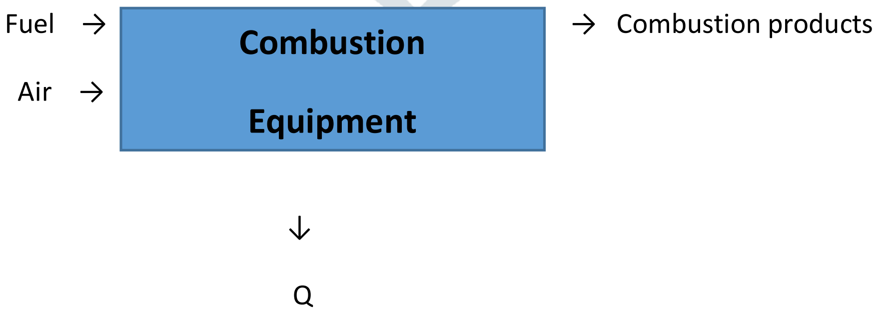
- Hydrogen engines have been in the danger of back fire during combustion. Therefore flame trappers are necessary in hydrogen fueled engines.
- Hydrogen fueled engine are having low pollution level but produce toxic emission of NOx.
- The handling of hydrogen is more difficult and storage requires high capital and running cost particularly for liquid H2 It can detonate.

2. Combustion Processes

Combustion is chemical reaction between a fuel and oxygen (or air) which produces heat and combustion products such as

$CO_2\ ,\ H_2O\ ,\ N_2\ ,\ CO\ ,\ NO_x\ ,\ HC$

$[Fuel + Air\ \rightarrow Heat + Combustion\ products]$



There are certain condition required for combustion:

1- Presence of fuel

2- Air or oxygen

3- Ignition temperature

Combustion stoichiometry

Complete oxidation of simple hydrocarbon fuels forms carbon dioxide (CO_2) from as of the carbon and water (H_2O) from all hydrogen that is for hydrocarbon fuel with the general composition $C_x\,H_y$

$$C_x\,H_y + a\,O_2 \rightarrow n_1\,CO_2 + H_2O$$

$$[C : x = b \;\rightarrow b = x]$$

$$\left[H : y = 2C \;\rightarrow C = \frac{y}{2}\right]$$

$$O_2 : a = b + \frac{C}{2} \quad ,so \;\; a = x + \frac{y}{4}$$

So the equation

$$C_x\,H_y + \left(x + \frac{y}{4}\right)\,O_2 + xCO_2 + \frac{y}{2}\,H_2\,O$$

The oxygen is accompanied by nitrogen when air is supplied for combustion then this nitrogen should be included in the combustion equation.

Since with one mole of O_2 there are 3.76 mole of N_2 hence

$$C_x\,H_y + a(O_2 + 3.76O_2) \;\rightarrow bCO_2 + cH_2\,O + dN_2$$

$$[\,C : x = b \;\rightarrow b = x\,]$$

$$\left[\,H : y = 2C \;\rightarrow C\,\frac{y}{2}\right]$$

$$O_2 : a = b\,\frac{C}{2} \;\rightarrow a = x + \frac{y}{4}$$

$$N_2 : 3.76\,a = d \;\rightarrow d = \;3.76\,a$$

So

$$C_x\,H_y + \left(x + \frac{y}{4}\right)(O_2 + 3.76N_2) \;\rightarrow xCO_2 + \frac{y}{2}\,H_2\,O + 3.76\,aN_2$$

- Stoichiometric (or theoretical air) : defined as the minimum of air needed for the complete combustion a fuel
- Air – fuel ratio (A/F) : defined as the ratio of the mass of air to the mass of fuel

$$\frac{A}{F} = \frac{m_a}{m_f} \;\text{ or }\; \frac{F}{A} = \frac{m_f}{m_a} = \frac{M_f}{M_a}$$

Where

m_f , m_a _ mass of fuel and air . $[k_g]$

M_f , M_a _ mass flow rate of fuel and air $[k_g/s]$

- The stoichiometric air – fuel ratio can be founds as

$$\left(\frac{A}{F}\right)_s = \left(\frac{m_a}{m_f}\right)_s = \frac{M_a}{M_f}$$

Where , m_i = n .Mw

n _ mole number m_{ol} , k_{mol}

Mw _ molecular weight [k_g/k_{mol}]

m= n .Mw

$k_{mol}\frac{k_g}{k_{mol}} = k_g$

So

$\left(\frac{A}{F}\right)_s = \frac{(4.76a)Mw_a}{(1)Mw_f}$

Equivalence ratio (Ǿ):

Defined as the ratio of actual $(F/A)_a$ to the stoichiometric ratio $(F/A)_s$

Ǿ = $\frac{(A/F)_s}{(A/F)_a} = \frac{(F/A)_a}{(F/A)_s}$

Where

- Ǿ = 1 : stoichiometric

$C_xH_y + a(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dN_2$

- Ǿ > 1 : rich mixture – deficiency of air

$C_xH_y + a(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dN_2 + eCO$

- Ǿ < 1 : lean mixture – excess of air

$C_xH_y + a(O_2 + 3.76N_2) \rightarrow bCO_2 + cH_2O + dN_2 + eO_2$

- Excess air is the amount of extra air then the stoichiometric

Excess air = $\frac{1-\text{Ǿ}}{\text{Ǿ}}$ ×100

We can relate a to excess air by the following equation

$a = [1 - fraction\ excess\ air] \times \left[x + \frac{y}{4}\right]$

So the equation becomes

$$C_xH_y + (1+FE)\left(x + \frac{y}{4}\right)(O_2 + 3.76N_2) \rightarrow bCO_2 + \frac{y}{2}\,H_2O + FE\,\left(x + \frac{y}{4}\right)O_2 + 3.76\,(1+FE)\,\left(x + \frac{y}{4}\right)N_2$$

Also we can relate a to Ǿ as following

$a = \frac{x + \frac{y}{4}}{\text{Ǿ}}$

2.1 Formation Of Equation

Combustion is a chemical reaction in which hydrocarbon fuel combines with air liberating heat energy and causing an increase in temperature of gases.

In present work, the mixture is a blend of fuel of composition Cp Hq Or Ns and hydrogen. Considering that there are 10 constituents the combustion reaction is written as:

$$\begin{aligned} &equ \times sto \times \{(1-x) \times C_pH_qO_rN_s + (x \times H_2)\} + (0.21 \times O_2) + (0.79 \times N_2) \\ &\quad \rightarrow n_1CO_2 + n_2H_2O + n_3N_2 + n_4O_2 + n_5CO + n_6H_2 + n_7O + n_8H + n_9OH \\ &\quad + n_{10}NO \qquad (1) \end{aligned}$$

Here, stoichiometric fuel-air ratio:

$$sto = 0.21 \times \left(\frac{1-x}{p + 0.25q - 0.5r} + 2x\right) \qquad (2)$$

Balancing of atoms lead to:

$$C: equ \times sto \times (1-x) \times p = n_1 + n_5 \qquad (3)$$

$$H: equ \times sto \times (1-x) \times q + 2x = 2n_2 + 2n_6 + n_8 + n_9 \qquad (4)$$

$$O: equ \times sto \times (1-x) \times r + 0.42 = 2n_1 + n_2 + 2n_4 + n_5 + n_7 + n_9 + n_{10} \qquad (5)$$

$$N: equ \times sto \times (1-x) \times s + 1.58 = 2n_3 + n_{10} \qquad (6)$$

Applying the following approximations, we developed the equations:

For $equ < 1: n_5 = 0$ (7)

For $equ > 1: n_4 = 0$ (8)

The equations of products for equivalence fuel air ratio < 1 are:

$$n_1 = (1-x) \times p \times equ \times sto \qquad (9)$$

$$n_2 = 1 \times q \times equ \times sto \div 2 \qquad (10)$$

$$n_3 = 1 \times 0.79 + (1-x) \times s \times equ \times sto \div 2 \qquad (11)$$

$$n_4 = (1) \times 0.21 \times (1 - equ) \qquad (12)$$

$$n_5 = 0 \qquad (13)$$

$$n_6 = 0.42x \qquad (14)$$

And for equivalence fuel air ratio > 1;

In this case, considering the equilibrium constant for the water gas reaction [3] and taking values from JANAF tables [7] we get the following equations:

$$k = e^{0.273 - \left(1.761 \div \frac{t}{1000}\right) - \left(1.611 \div \left(\frac{t}{1000}\right)^2\right) + \left(0.283 \div \left(\frac{t}{1000}\right)^3\right)} \qquad (15)$$

$$a = \times (1 - K) \qquad (16)$$

$$\begin{aligned} b = (1-x) \times \big(0.42 - equ \times sto \times (2-r) + k \times \big(0.42 \times (equ-1)\big) + p \times equ \times sto\big) + x \\ \times \big(0.42 - 2 \times equ \times sto + K \times 0.42(equ-1)\big) \qquad (17) \end{aligned}$$

$$c=-(1-x)\times(0.42\times equ\times sto\times p\times(equ-1)\times k) \quad (18)$$

$$n_5=\frac{-b\pm\sqrt{b^2-4ac}}{2a} \quad (19)$$

$$n_1=(1-x)\times(p\times equ\times sto-n_5)+x\times n_5 \quad (20)$$

$$n_2=(1-x)\times(0.42+equ\times sto\times(2p-r)+n_5)-x\times(0.42+n_5) \quad (21)$$

$$n_3=(1-x)\times(0.79+s\times equ\times sto\div 2)+0.79x \quad (22)$$

$$n_4=0 \quad (23)$$

$$n_6=(1-x)\times(0.42\times(equ-1)-n_5)+0.42x \quad (24)$$

Mole fractions of these products are found out using the equation:

$$y_{i\,=}\; n_i/\sum n_i \quad (25)$$

$$\log_{10}=K_i\times\ln\frac{t}{1000}+\frac{B_i}{t}+C_i+D_i\times t+E_i\times t^2 \quad (26)$$

$$y_7=\frac{k_1}{preg^{0.5}}\times {y_6}^{0.5} \quad (27)$$

$$y_8=\frac{k_2}{preg^{0.5}}\times {y_4}^{0.5} \quad (28)$$

$$y_9=K_3\times {y_6}^{0.5}\times {y_4}^{0.5} \quad (29)$$

$$y_{10}=K_4\times {y_4}^{0.5}\times {y_2}^{0.5} \quad (30)$$

3. Results discussion

The simulations are done for pure diesel and diesel-Hydrogen mixture under various conditions as discussed before. The results are presented below:

3.1 Pure diesel:

The simulation was carried out at pure diesel with different equivalence ratios. Carbon dioxide, carbon monoxide, water vapor and oxygen in the exhaust were determined.

The simulation was carried out at pure diesel with different equivalence ratios. Carbon dioxide, carbon monoxide, water vapor and oxygen in the exhaust were determined.

3.1.1 Carbon dioxide emission

The higher carbon dioxide emission in the exhaust is indication of better combustion of fuel. Figure 1 shows the variation of CO_2 mole fraction in different equivalence ratios. As it can be seen in the figure, with increasing equivalence ratio from 0.2 to 1 and approaching to the stoichiometry mode, the CO_2 mole fraction increase. With increasing the equivalence ratio from 1 to 1.2 CO_2 mole fraction decreases which is due to the increase in the ratio of fuel to air and the fact that we are away from the Stoichiometry state.

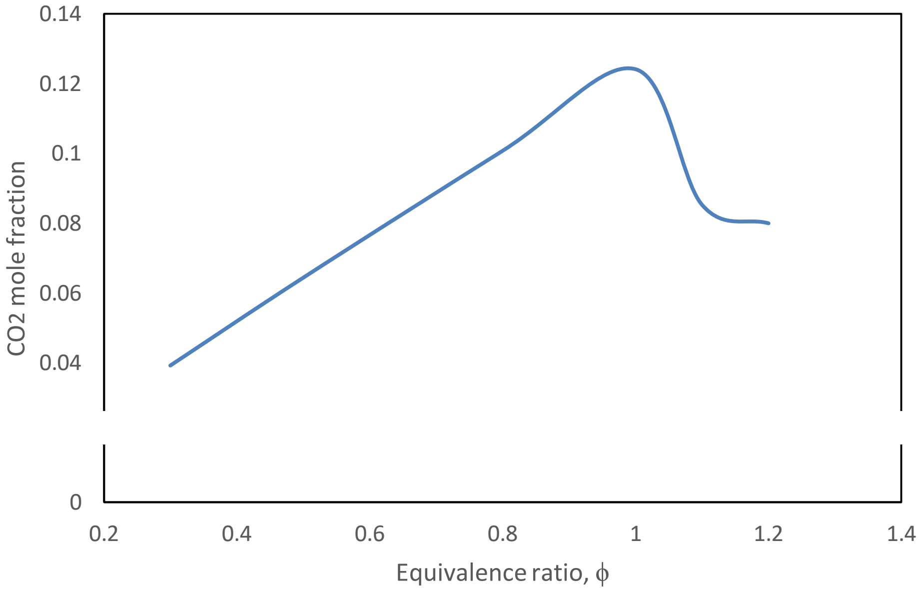


Figure 1. Effect of equivalence ratio on CO2 mole fraction, for pure diesel at T=1500 K

3.1.2 Carbon monoxide emission

Carbon monoxide results from the incomplete combustion where the oxidation process does not occur completely. This concentration is largely dependent on air/fuel mixture. Figure 2 shows the variation of CO mole fraction in different equivalence ratios. It can be observed that in lean side the CO mole fraction was negligible. However, in the rich side, it can be noted that as the equivalence ratio is increasing the mole fraction of CO increases sharply. This can be attributed to the incomplete combustion of diesel due to deficient in the air with rich mixture ($\phi > 1$).

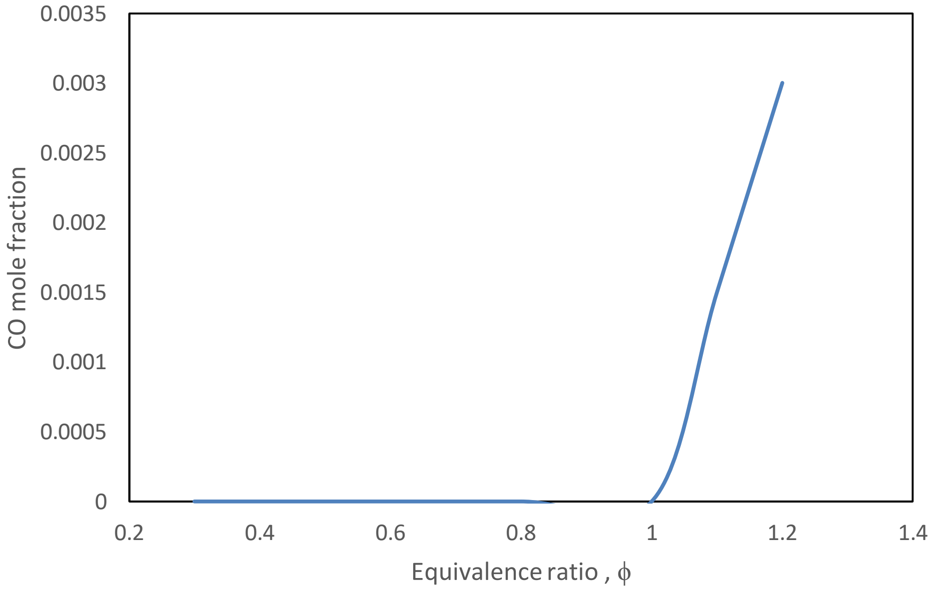


Figure 2. Effect of equivalence ratio on CO mole fraction, for pure diesel at T=1500 K

3.1.3 Oxygen emission

Figure 3 demonstrates the oxygen mole fraction variations as a function of equivalence ratio. It can be seen that the oxygen emission in the exhaust gases decreases with the increasing equivalence ratio. The reason for this phenomenon lies in the fact that the mixture is approaching the stoichiometric situation.

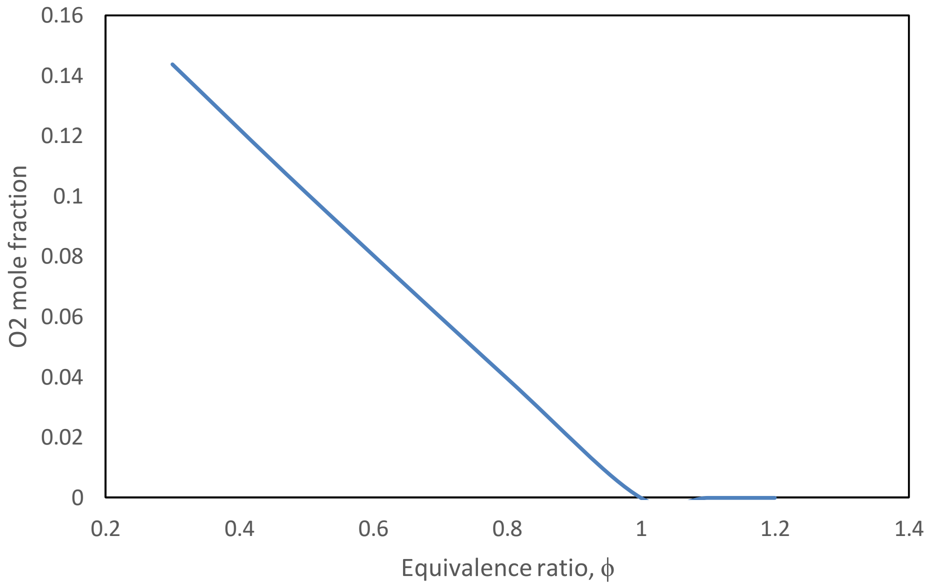


Figure 3. Effect of equivalence ratio on O_2 mole fraction, for pure diesel at T=1500 K

3.1.4 Water vapor emission

Figure 4 demonstrates the H_2O mole fraction variations as a function of equivalence ratio. It can be seen that the H_2O in the exhaust gases increase with the increasing equivalence ratio; it has highest value at equivalence ratio of 1. If the equivalence ratio is further increased, the mole fraction of H_2O falls down considerably, due to incomplete combustion.

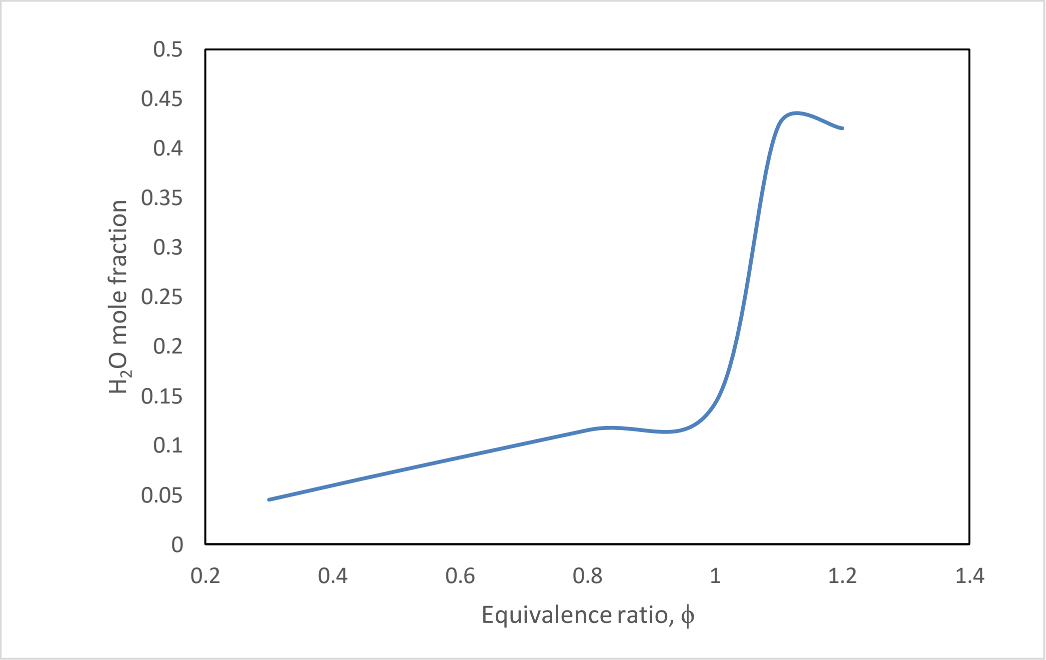


Figure 4. Effect of equivalence ratio on H_2O mole fraction, for pure diesel at T=1500 K

3.2 Diesel-hydrogen mixture

The simulation was carried out at diesel-hydrogen mixture with various percentage hydrogen substitutions at different constant equivalence ratios.

The mole fraction of each of the exhaust species such as carbon dioxide (CO_2), carbon monoxide (CO), water vapor (H_2O), nitrogen (N_2) and oxygen (O_2) in the exhaust were determined

3.2.1 Carbon Dioxide

Figure 5 shows the change in mole fraction of CO_2, for various percentage hydrogen substitutions at different constant equivalence ratios. It can be noted that for all equivalence ratios, the mole fraction of CO_2 increases between 20% and 40% hydrogen substitution and then decreases with further increase in hydrogen percentage, however for equivalence ratios of 1.1 and 1.2, it increases continuously.
Under the stoichiometric conditions the mole fractions of CO_2 is at its peak and decreases when the mixture becomes either richer or leaner due to simultaneous presence of other products.

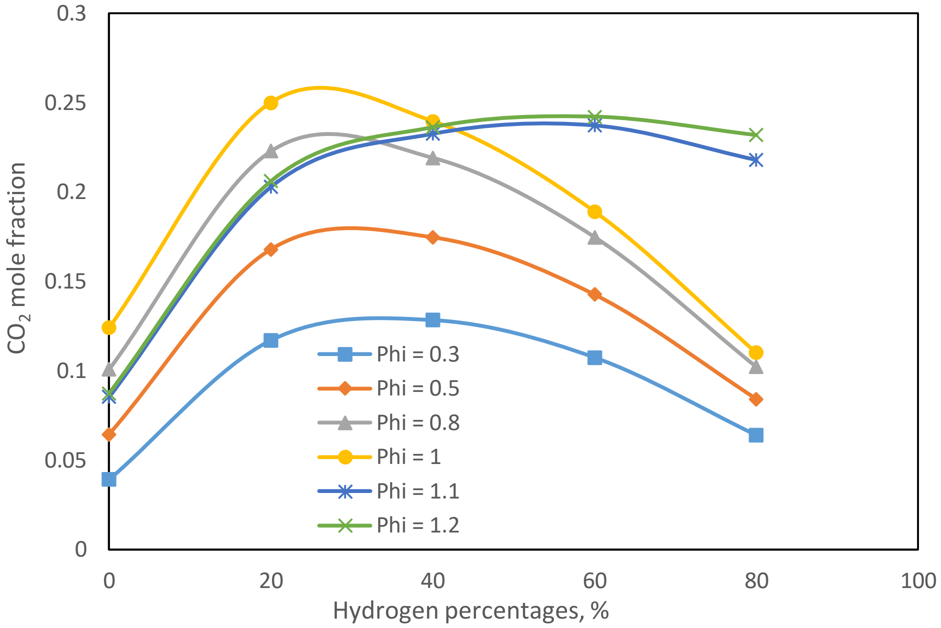


Figure 5. Effect of hydrogen substitution on CO_2 mole fraction with different equivalence ratios, at T=1500 K

3.2.2 Carbon monoxide

Figure 6 demonstrates the various CO mole fraction levels for various percentage hydrogen substitutions at different constant equivalence ratios. It can be observed that in lean side the CO mole fraction was negligible. However, it can be noted that as the hydrogen percentage is increasing the mole fraction of CO increases sharply for equivalence ratio values of 1.1 and 1.2.

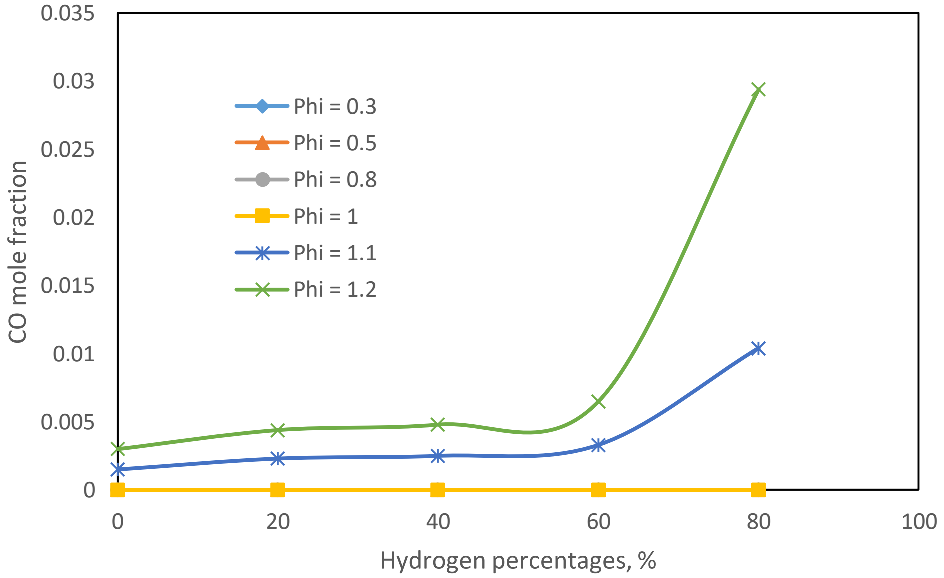


Figure 6. Effect of hydrogen substitution on CO mole fraction with different equivalence ratios, at T=1500 K

3.2.3 Water vapor emission

Figure 7 demonstrates the various H_2O mole fraction levels for various percentage hydrogen substitutions at different constant equivalence ratios. It can be observed that with increase in equivalence ratio the mole fraction of H_2O increases. This due to the increase in the fuel amount in fuel-air mixture

Also, it is seen that with increase in hydrogen percentage substitution the mole fraction of H_2O increases; it has highest value at equivalence ratio of 1. If the equivalence ratio is further increased, mole fraction of H_2O falls down considerably.

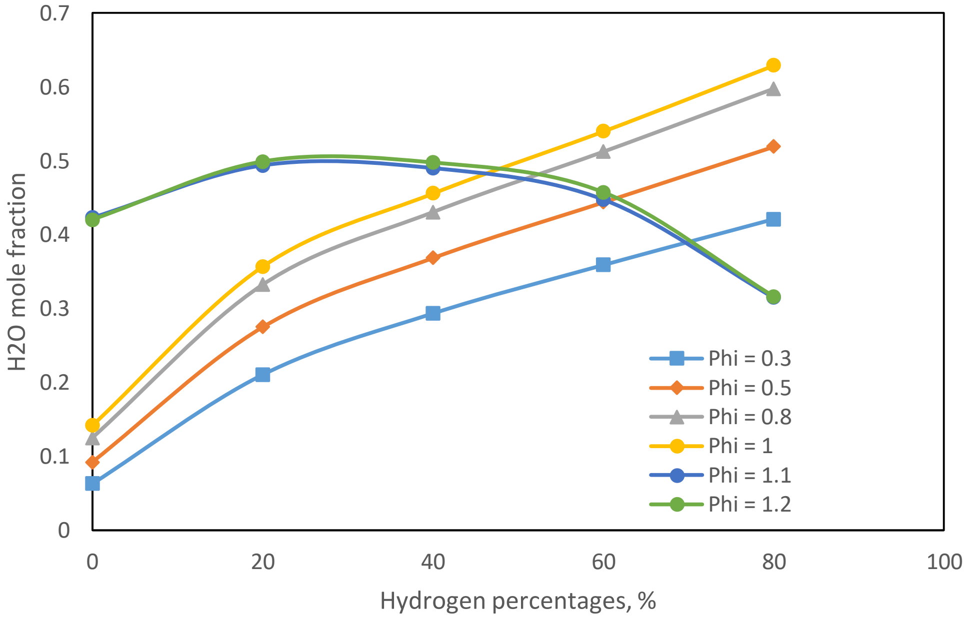


Figure 7. Effect of hydrogen substitution on H_2O mole fraction with different equivalence ratios, at T=1500 K

3.2.4 Nitrogen emission

Figure 8 demonstrates the various nitrogen mole fraction levels for various percentage hydrogen substitutions at different constant equivalence ratios. It can observed that with increase in equivalence ratio the mole fraction of N_2 decreases. This due to the decrease in the air amount in fuel-air mixture.

Also, it can be observed that as the hydrogen percentage is increasing the mole fraction of N_2 decreases. However, slight increase in mole fraction value corresponding to 60 and 80% hydrogen addition could be seen at equivalence ratios of 1.1 and 1.2.

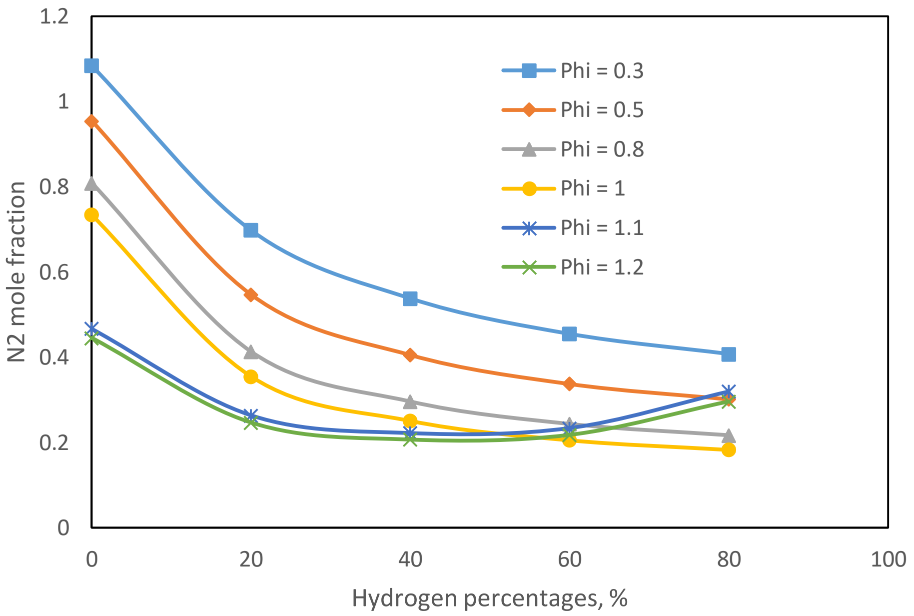


Figure 8. Effect of hydrogen substitution on N_2 mole fraction with different equivalence ratios, at T=1500 K

Conclusions

The following conclusions can be drawn from the investigation.

- The code developed gave reasonably good results which are in good agreement with the experimental values.
- For all equivalence ratios except for 1.2 and 1.4, the mole fraction of CO_2 increases between 20% and 40% hydrogen substitution and then decreases with further increase in hydrogen percentage. However for equivalence ratios of 1.2 and 1.4, it increases continuously.
- As the hydrogen percentage increases the mole fraction of CO increases, and for more than 1 equivalence ratio, the increase is sharp.
- The mole fraction of H_2O increases with hydrogen substitution;

Acknowledgments

The author are thankful to the Libyan government for financial support and Tobruk University for providing the necessary facilities.

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