Exhaust Gas Simulation of Hydrogen–Ethanol Dual Fuel

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This paper involves generating the simulation software that provides the mole fraction of each of the exhaust species when the hydrogen is burnt along with ethanol. The proportion of hydrogen in the hydrogen–ethanol blend affecting the mole fraction of the exhaust species is also simulated. The program code developed gave reasonably good results for the present hydrogen-ethanol dual fuel. At low and high percentages of hydrogen and during transition between ethanol and hydrogen the model predictions are not very clear. The best results were obtained for for a combination of 80% hydrogen and 20% ethanol by volume.

Keywords : combustion, dissociation reaction, dual fuel, equivalence ratio, mole fraction.

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EXHAUST GAS SIMULATION OF HYDROGENETHANOL DUAL FUEL

Strictly as per the compliance and regulations of :

Exhaust Gas Simulation of Hydrogen–Ethanol Dual Fuel

Dr. Syed Yousufuddin [α], Dr. Sultan Ali [σ], Naseeb Khan [ρ] & Dr. Syed Nawazish Mehdi [ω]

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I. Introduction

Among the various alternative fuels, hydrogen and alcohol are very attractive substances for many practical applications in the energy sector [1]. While conventional energy sources such as natural gas and oil are non-renewable, hydrogen and alcohol can be coupled to act as renewable energy sources [2, 3].

Combustion is a chemical reaction between a fuel and oxygen, which is accompanied by the production of a considerable amount of heat. The composition of the exhaust gas produced is a function of temperature as well as equivalence ratio (ratio of actual fuel ratio to theoretical fuel air ratio). Many components are present in the exhaust gas because of dissociation of some species. Thermodynamics is able to predict the equilibrium state that results from burning a fuel-air mixture given only the initial conditions. Combustion is a chemical reaction between a fuel and oxygen, which is accompanied by the production of a considerable amount of heat. The composition of the exhaust gas produced is a function of temperature as well as equivalence ratio (ratio of actual fuel ratio to theoretical fuel air ratio). A lean mixture has $\Phi < 1$ A rich mixture has $\Phi > 1$. The mixture is said to be stoichiometric if $\Phi = 1$.

Many components are present in the exhaust gas because of dissociation of some species. The heat of combustion of a fuel is defined as the heat transferred out of a system per unit mass or mole of fuel when the initial and final states are at the same temperature and pressure. Based on the combustion stoichiometric theory a computer program had been developed for blend fuels to calculate the mole fractions of the exhaust gases [4]. Thermodynamic data for elements, combustion products and many pollutants are available in a compilation published by the National Bureau of Standards called the JANAF (Joint Army-Navy-Air Force) tables (1971). For single component fuels the data presented by Stull, We strum and Sinke (1969) is in the same format as that of JANAF tables. A compilation by Rossini (1953) is useful for hydrocarbon fuels at temperatures as high as 1500K.

II. Inputs to the Program

The fuel is to be specified in terms of the C, H, O, and N atoms in the fuel. For the blend of two fuels considered i.e., Ethanol and Hydrogen, the percentage with which they blend in the mixture also has to be specified. The other parameters that need to be, specified are equivalence ratio, pressure and temperature. For the calculation of equilibrium constant, the data for constants is considered from JANAF tables. The molar-air fuel ratio is calculated from the number of Carbon, Hydrogen, Nitrogen and Oxygen atoms present in the fuel.
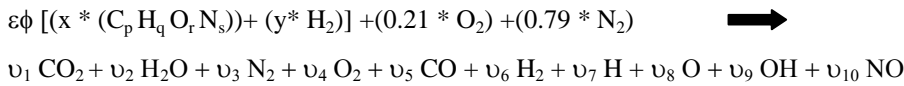
III. Formation of Equations

The mixture is blend of fuel of composition $C_p H_q O_r N_s$ and Hydrogen. Considering that there are ten constituents the combustion reaction is written as

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$\epsilon\phi \; [(x * (C_p H_q O_r N_s))+ (y* H_2)] +(0.21 * O_2) +(0.79 * N_2)$ ⟶

$\upsilon_1 \, CO_2 + \upsilon_2 \, H_2O + \upsilon_3 \, N_2 + \upsilon_4 \, O_2 + \upsilon_5 \, CO + \upsilon_6 \, H_2 + \upsilon_7 \, H + \upsilon_8 \, O + \upsilon_9 \, OH + \upsilon_{10} \, NO$

The molar fuel –air ratio is given by

$\epsilon = (\, x * (\, 0.210 \, / \, (\, p + (\, 0.25 * q \,) - (\, 0.5 * r \,) \,) \,) \,) +(\, y * 0.42)$

Convenient approximations for lean and rich combustion are

$\phi < 1 \qquad \upsilon_5 = \upsilon_6 = 0$

$\phi > 1 \qquad \upsilon_4 = 0$

The mole fractions are obtained for the products are obtained by

$y_i = v_i / \; \Sigma \, v_i$

$i = 1 \text{ to } 6$

For a lean mixture the coefficients of combustion products are obtained as

$b=(x*(0.42-(\phi*\epsilon*(2-r)) + (k*((0.42*(\phi-1)) + (p*\phi*\epsilon))))) + (y*(0.42-(2*\phi*\epsilon) + (k*(0.42*(\phi-1)))));$

$c=-(x*(0.42*p*\phi*\epsilon*(\phi-1)*k));$

and

$k = \exp (\, 0.273 - (\, 1.761 \, / \, t \,) - (\, 1.611 \, / \, t^2 \,) + (\, 0.283 \, / \; t^3)); $

$\upsilon_1 =(x*((p*\phi*\epsilon)-v5))+(y*v5);$

$\upsilon_2 = (x*(0.42+(\phi*\epsilon*((2*p)-r))+v5))-(y*(0.42+v5));$

$\upsilon_3 = (x*(0.79+(s*\phi*(\epsilon/2))))+(y*0.79);$

$\upsilon_4 = 0;$

$\upsilon_6 = (x*((0.42*(\phi-1))-v5))+(y*0.42);$

The mole fractions for all the remaining species is obtained in terms of y_3, y_4 and y_6 i.e, the mole fractions of N_2, O_2 and H_2 respectively as

$y_7=C_1*(y_6)^{0.5};$

$y_8=C_2*(y_4)^{0.5};$

$y_9=C_3*(y_4)^{0.5}*(y_6)^{0.5};$

$y_{10}=C_4*(y_4)^{0.5}*(y_3)^{0.5};$

where

$C_1 = K_1 / P^{1/2} \; ;$

$C_2 = K_2 / P^{1/2} \; ;$

$C_3 = K_3 \; ;$

$C_4 = K_4 \; ;$

Where K^p value is obtained from equation

$\log K_p = \exp [(A / T) + (B+C/T) \ln(T) +D]$

where T is in Kelvin. The value of A, B, C and D are obtained from the JANAF tables based upon the reaction of the species with oxygen.

With the variation in the input parameters various results and plots can be obtained.

$\upsilon_1 =x*(\, p * \phi * \epsilon \;);$

$\upsilon_2 = (x*(q*\phi*(\epsilon/2)))+(y*(q*\phi*(\epsilon/2)));$

$\upsilon_3 = (x*(0.79+(s*\phi*(\epsilon/2))))+(y*0.79);$

$\upsilon_4 = (x*(0.21*(1-\phi)))+(y*(0.21*(1-\phi)));$

$\upsilon_5 = 0;$

$\upsilon_6 = y*0.42;$

For a rich mixture the coefficients of combustion products are obtained as

$\upsilon_5 = (-b+(\mathrm{sqrt}((b*b)-(4*a*c))))/(2*a); \quad –(8a)$

Where

$a=(x*(1-k))+(y*(1-k));$

IV. RESULTS AND DISCUSSION

As shown in Fig.1 for 80% hydrogen substitution, with higher temperature of 1800K the CO_2 value is higher than that obtained at 1200K and 1500 K. 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 presence of other products. As the temperature increases, the mole fraction of CO_2 decreases as the dissociation increases with temperature. As explained earlier under heat release rate explanation the peak heat release rate (i.e. the peak combustion at low outputs is considerably low in dual fuel mode) with different hydrogen substitutions when compared to the ethanol mode. This is the reason for the reduced brake thermal efficiency and reduced rate of pressure rise as compared to ethanol at low outputs. This incomplete combustion results in higher amounts of CO_2 emissions in the beginning, but as the hydrogen substitution is increased, rigorous and strong complete combustion reduces the emissions of CO_2 as the dissociation increases with temperature

As shown in Fig.2 for 80% hydrogen substitution with higher temperature of 1800K the mole fraction of H_2O value is higher than that obtained at 1200K and 1500 K. As the mole fraction of H_2O increases with hydrogen substitution, this brings down the combustion temperature, and hence the reason of reduction in the values of NO and N_2 at higher percentages of hydrogen substitution.

Figs. 3 show the change in mole fraction of Nitrogen (N_2) for various percentages of hydrogen substitutions for different constant equivalence ratios for temperatures of 1200 K, 1500K and 1800 K. It is

observed that mole fraction of N_2 decreases for all hydrogen fractions except for 60 and 80% hydrogen substitutions. Fig.4 shows that with the increase in equivalence ratio the mole fraction value of N_2 decreases. However, slight increase in mole fraction value corresponding to 60 and 80% hydrogen addition could be seen at equivalence ratio of 1.0 (Fig.4). For 80% Hydrogen substitution (Fig.5) it is seen that for temperatures of 1200K, 1500K and 1800K the mole fraction of N_2 first decreases at equivalence ratio of 1 and then again increases at equivalence ratio of 1.2 and further decrease is observed at 1.4 equivalence ratio.

Fig.6 shows the change in mole fraction of carbon monoxide (CO) for various percentages of hydrogen substitutions for different constant equivalence ratios for temperatures of 1200 K, 1500K and 1800 K. It can be noted that as the hydrogen percentage is increasing the mole fraction of CO increases sharply for equivalence ratio values of 1.2 and 1.4 and for other equivalence ratios, no increase is found in mole fraction of CO. From Fig.7, it is seen that maximum deviation for mole fraction of CO is for 80% hydrogen when compared to 60% hydrogen. The value of mole fraction of CO found to be higher at higher temperatures for 80% hydrogen substitution (Fig.8). Therefore, it is clear that the CO_2 and CO concentrations decrease as the percentage of hydrogen and ethanol blending are increased. This is due to the reduction in carbon atoms concentration in the blended fuel and the high molecular diffusivity of hydrogen, which improves the mixing process and, hence, provides higher combustion efficiency [5].

The variations of mole fractions of hydrogen (H_2) for various percentages of hydrogen substitutions for different constant equivalence ratios at temperatures of 1200 K, 1500K and 1800 K is depicted in Fig. 9. It is seen that with increase in hydrogen percentage substitution the mole fraction of H_2 increases. As shown in Fig.10 all fractions of hydrogen showed decreasing trend until equivalence ratio of 1.0 and then afterwards appreciable increase in mole fraction of hydrogen was observed until equivalence ratio of 1.4. Fig.11 shows that mole fraction for 80% hydrogen is higher at lower temperatures (i.e.1200K) with increase in equivalence ratio. The adiabatic flame temperature calculated on the available theory gives higher values of peak temperature. The higher adiabatic temperature is because of the higher heating values of hydrogen. It does not take into account the formation of moisture theoretically. However, exhaust simulation code takes into account the formation of complete exhaust species along with the moisture that forms during combustion. Therefore, as the percentage of hydrogen increases the formation of H_2O during combustion increases which keeps the peak temperature down and reduces the formation of NO and N_2 [6].

V. CONCLUSIONS

1. At equivalence ratio of 1.4, the molar fraction of CO_2 decreases for lean equivalence ratios due to a reduction in fuel carbon.

2. For 80% hydrogen substitution, with higher temperature of 1800K the CO_2 value is higher than that obtained at 1200K and 1500 K.

3. As the percentage hydrogen increases, the mole fraction of H_2O also increases, and has higher value for equivalence ratio of 1.0. Further, with the increase in equivalence ratio the mole fraction of H_2O falls down considerably.

4. For 80% hydrogen substitution, with higher temperature of 1800K the mole fraction of H_2O value is higher than that obtained at 1200K and 1500 K.

5. Mole fraction of N_2 decreases for all hydrogen fractions except for 60% and 80% hydrogen substitutions.

6. Maximum deviation for mole fraction of CO is for 80% hydrogen when compared to 60% hydrogen. The value of mole fraction of CO found to be higher at higher temperatures for 80% hydrogen substitution.

7. With increase in hydrogen percentage substitution the mole fraction of H_2 increases. All fractions of hydrogen showed decreasing trend until equivalence ratio of 1.0 and then afterwards appreciable increase in mole fraction of hydrogen was observed until equivalence ratio of 1.4.

8. As the percentage of hydrogen increases, the formation of H_2O during combustion increases which keeps the peak temperature down and thus reduces the formation of NO and N_2.

The code developed gave reasonably good results. However, there exist many areas which are unaddressed by the code. At low and high percentages of hydrogen and during transition between ethanol and hydrogen the model predictions are not very clear, this eventually shows the limitation of the model and opens the doors for further investigations. The best results were obtained for a combination of 80% hydrogen and 20% ethanol by volume.

Notation:

k_p	specific heat ratio of the products
k_r	specific heat ratio of the reactants
K	equilibrium constant
p	number of C atoms
P	pressure in bar
q	number of H atoms
r	number of O atoms
s	number of N atoms
T	temperature in K

v_i coefficient describing product composition of ith species

x   percentage of Ethanol in Ethanol- Hydrogen fuel blend

Y   percentage of hydrogen in Ethanol- Hydrogen fuel blend

y_i mole fraction of ith species

☐   Equivalence ratio

☐   Molar air-fuel ratio

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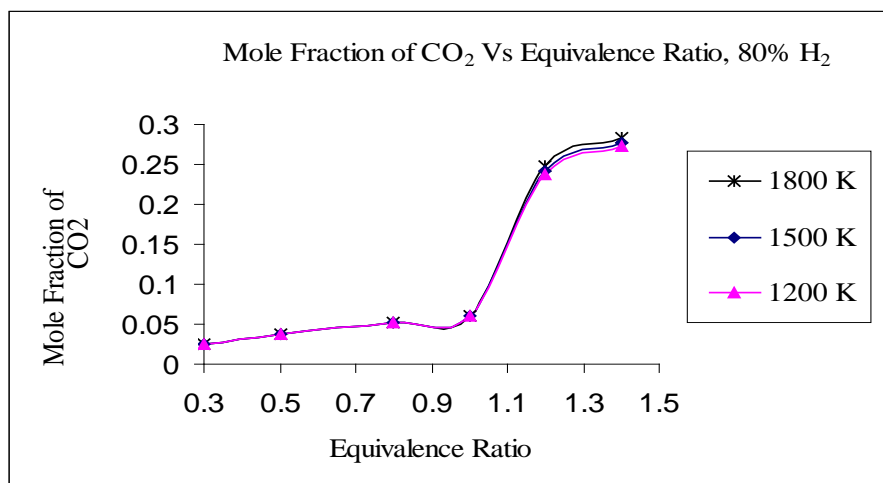6. Abd Alla, G.H., "Computer Simulation of a Four-Stroke Spark Ignition Engine", SAE, (2001), 571-578.

Figure 1 : Mole fraction of CO_2 against the Equivalence ratio, for 80% Hydrogen and at T=1200K, 1500K and 1800K

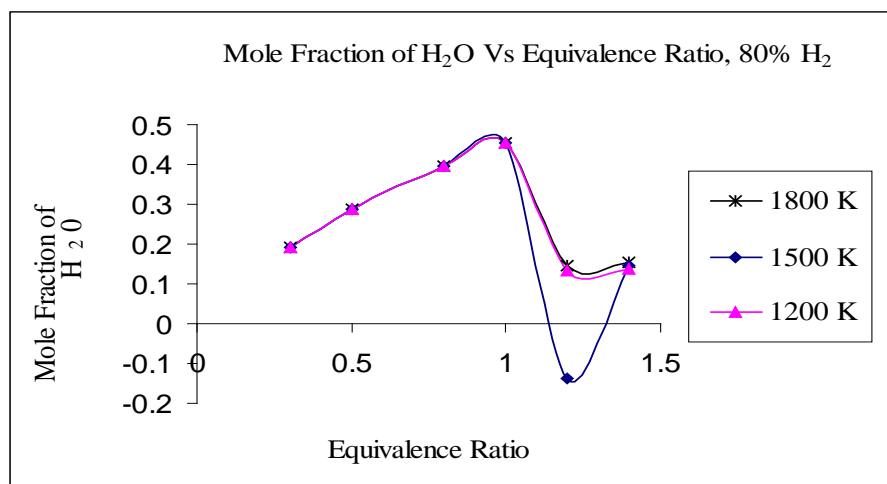Figure 2 : Mole fraction of H_2O against the Equivalence ratio, for 80% Hydrogen and at T=1200K, 1500K and 1800K

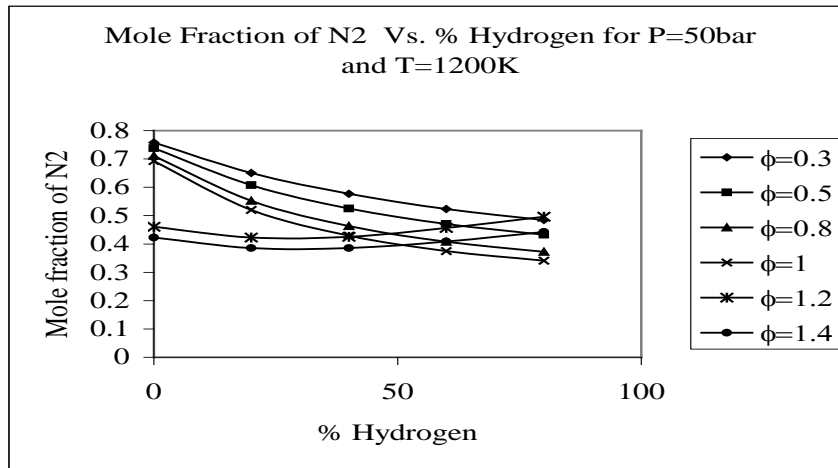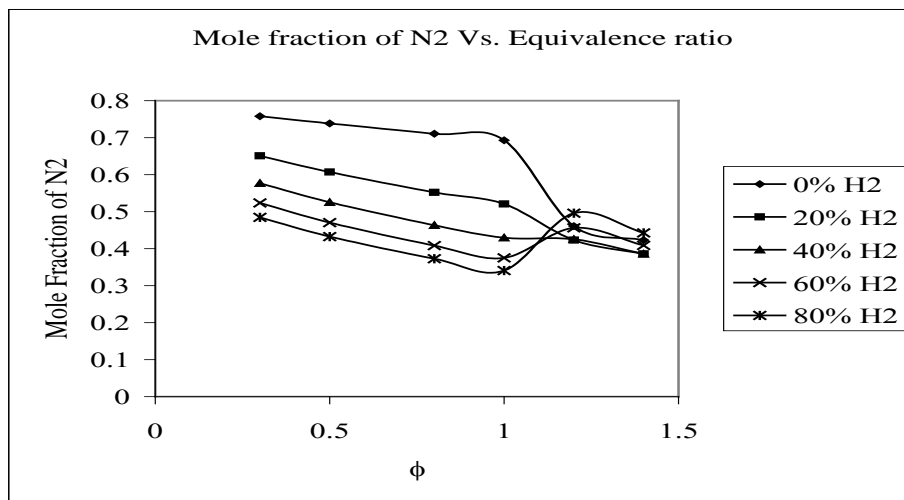*Figure 3 :* Mole fraction of N_2 against the percentage substitutions of hydrogen at T=1200K

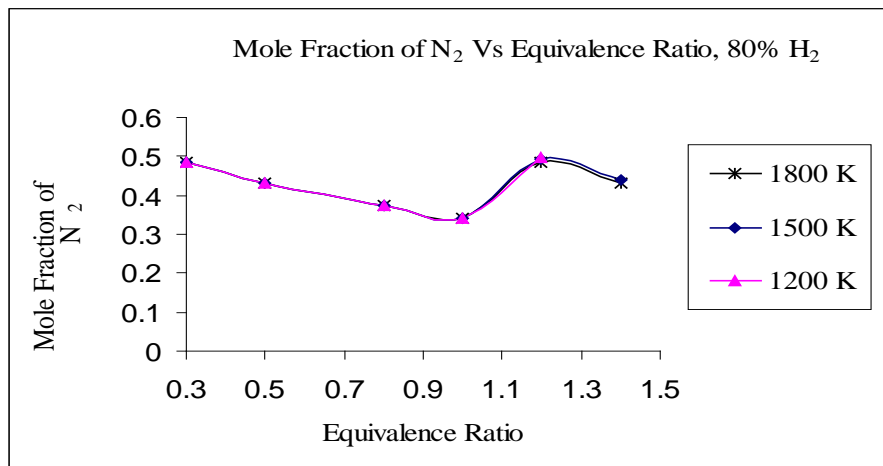*Figure 4 :* Mole fraction of N_2 against equivalence ratio at T=1200K

Figure 5 : Mole fraction of N_2 against the Equivalence ratio, for 80% Hydrogen and at T=1200K, 1500K and 1800K
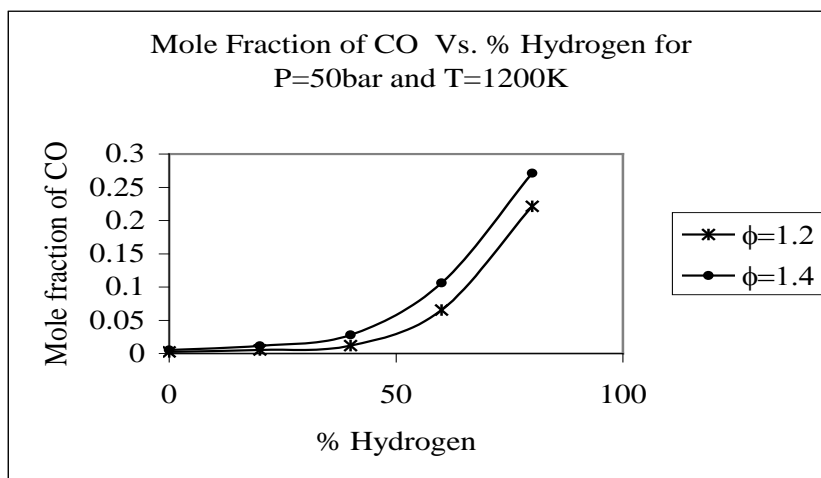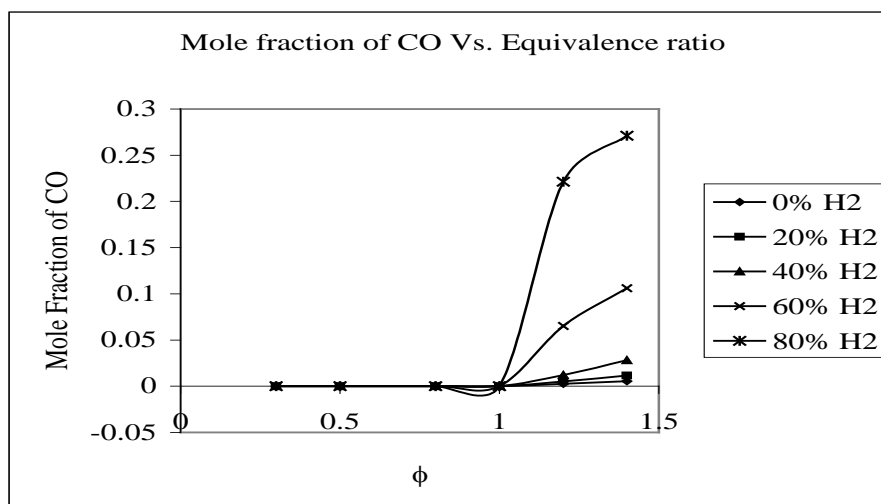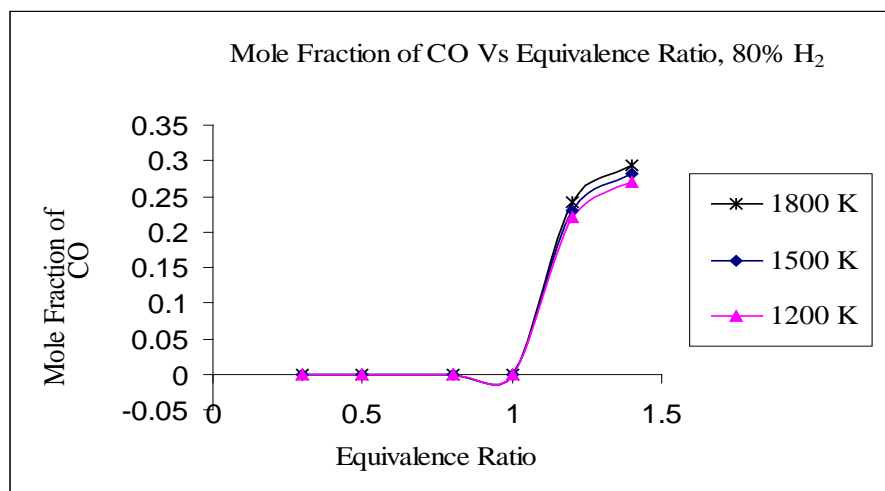
Mole Fraction of CO Vs. % Hydrogen for P=50bar and T=1200K

Figure 6 : Mole fraction of CO against the percentages of hydrogen at T=1200K

Mole fraction of CO Vs. Equivalence ratio

Figure 7 : Mole fraction of CO against equivalence ratio at T=1200K

Mole Fraction of CO Vs Equivalence Ratio, 80% H$_2$

Figure 8 : Mole fraction of CO against the Equivalence ratio, for 80% Hydrogen and at T=1200K, 1500K and 1800K
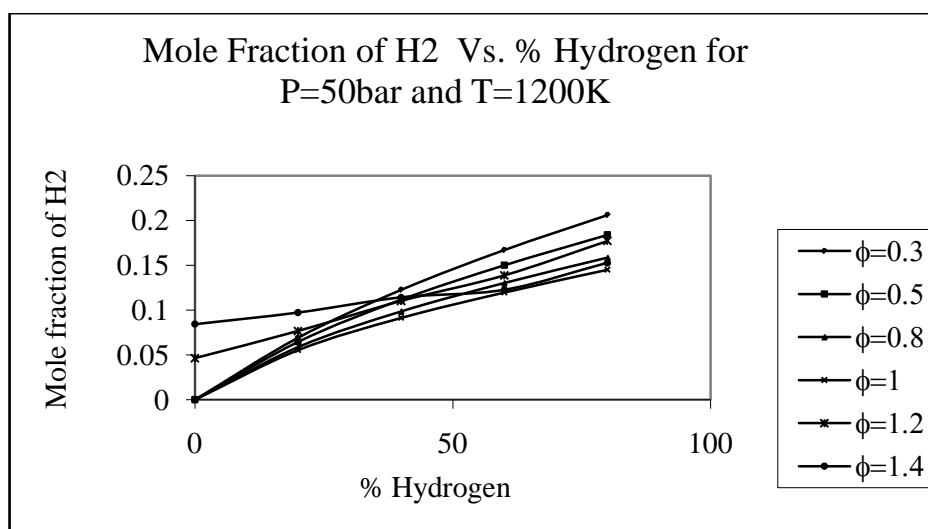
Figure 9 : Mole fraction of H_2 against the different percentages of hydrogen at T=1200K
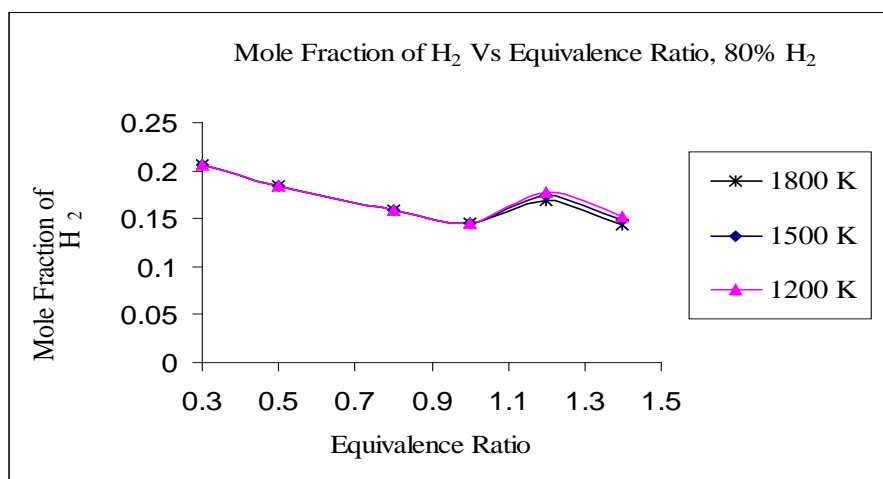

Figure 10 : Mole fraction of H_2 against the Equivalence ratio, for 80% Hydrogen and at T=1200K, 1500K and 1800K
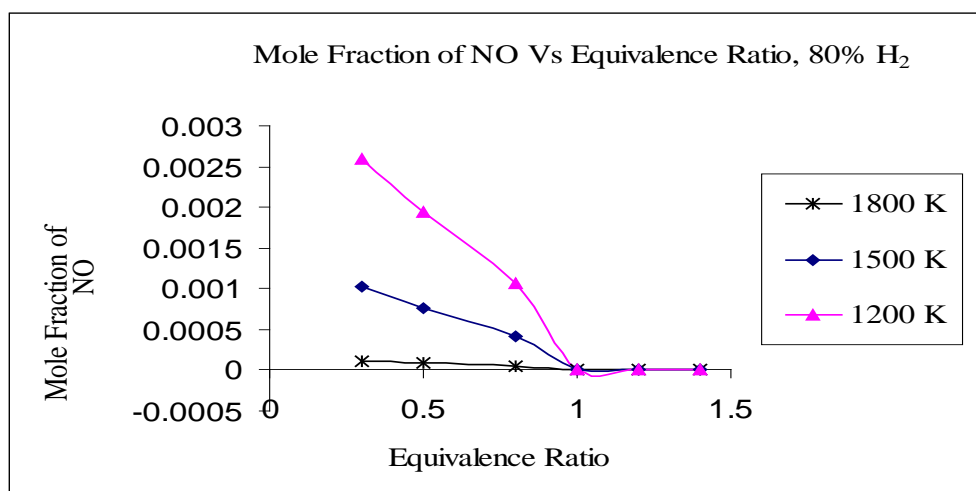

Figure 11 : Mole fraction of NO against the Equivalence ratio, for 80% Hydrogen and at T=1200K, 1500K and 1800K

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