

Exhaust Gas Simulation of Hydrogen–Ethanol Dual Fuel

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ABSTRACT The drawback of lean burn with ethanol is reduced power output. Lean operation of ethanol fuelled engines has additional drawbacks. Lean mixtures are hard to ignite, despite the mixture being above the low fire (point) limit of the fuel. This results in misfire, which increases unburned hydrocarbon emissions, reduces performance and wastes fuel. Hydrogen can be used in conjunction with ethanol provided it is stored separately. Mixing hydrogen with a oxygenated hydrocarbon fuel such as ethanol reduces all of these drawbacks. The low ignition energy limit of hydrogen combined with a high burning speed makes the hydrogen-ethanol mixture easier to ignite, reducing misfire and thereby improving emissions, performance and fuel economy. The current study involved generating simulation software that provides the mole fraction of each of the exhaust species when hydrogen is combusted 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 a combination of 80% hydrogen and 20% ethanol by volume.

KEYWORDS Combustion, dissociation reaction, dual fuel, equivalence ratio, mole fraction.

Introduction

Among alternative fuels, hydrogen and alcohol are very attractive substances for many practical applications in the energy sector [Baghdadi, 2001]. While conventional energy sources such as natural gas and oil are non-renewable, hydrogen and alcohol can be coupled to act as a renewable energy source [Veziroglu and Barbir, 1991; Yousufuddin and Nawazish, 2008; Yousufuddin and Masood, 2009].

Combustion is a chemical reaction between fuel and oxygen, which is accompanied by the production 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. Using principles of thermodynamics, it is possible to predict the equilibrium state that results from burning an air-fuel mixture given only the initial conditions. A lean mixture has $\Phi < 1$ A rich mixture has $\Phi > 1$. The mixture is said to be stoichiometric if $\Phi = 1$.

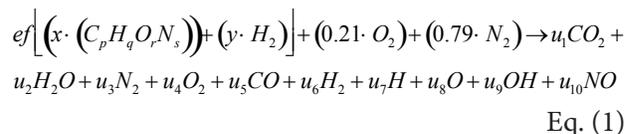
The heat of combustion of a fuel is defined as the heat transferred out of a system per unit mass or mole of fuel when the initial and final states are at the same temperature and pressure. Based on theories of stoichiometric combustion, a computer program was developed for fuel blends to calculate the mole fractions of the exhaust gases [Masood and Ishrat, 2008]. 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 [Stull and Prophet, 1971]. For single component fuels the data presented by Stull, Westrum and Sinke is in the same format as that of JANAF tables [Stull, Westrum and Sinke, 1969]. A compilation by Rossini is useful for hydrocarbon fuels at temperatures as high as 1500 K [Rossini, 1953].

Inputs to the Program

The fuel was specified in terms of the C, H, O, and N atoms in the fuel. For the blend of the two fuels considered, ethanol and hydrogen, their respective percentages by volume in the mixture was also specified. The other parameters specified were equivalence ratio, pressure and temperature. For the calculation of equilibrium constant, the data for constants was considered from JANAF tables. The molar air-fuel ratio is calculated from the number of C, H, N and O atoms present in the fuel.

Formation of equations

The mixture was blend of fuels, with the composition $C_p H_q O_r N_s$ and hydrogen. Considering that there are ten constituents, the combustion reaction is written as [Masood and Ishrat, 2008],



The molar air-fuel ratio is given by:

$$e = \left(x \cdot \left(\frac{0.210}{(p + (0.25 \cdot q) - (0.5 \cdot r))} \right) \right) + (y \cdot 0.42) \quad \text{Eq. (2)}$$

Convenient approximations for lean and rich combustion are:

$$\begin{aligned} f < 1 \quad u_5 = u_6 = 0 \\ f > 1 \quad u_4 = 0 \end{aligned}$$

The mole fractions are obtained for the products are obtained by:

$$\begin{aligned} y_i &= n_i / \sum n_i \\ i &= 1 \text{ to } 6 \end{aligned}$$

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

$$u = x \cdot (p \cdot f \cdot e) \quad \text{Eq. (3)}$$

$$u_2 = \left(x \cdot \left(q \cdot f \cdot \left(\frac{e}{2} \right) \right) \right) + \left(y \cdot \left(q \cdot f \cdot \left(\frac{e}{2} \right) \right) \right) \quad \text{Eq. (4)}$$

$$u_3 = \left(x \cdot \left(0.79 + \left(s \cdot f \cdot \left(\frac{e}{2} \right) \right) \right) \right) + (y \cdot 0.79) \quad \text{Eq. (5)}$$

$$u_4 = \left(x \cdot (0.21 \cdot (1 - f)) \right) + \left(y \cdot (0.21 \cdot (1 - f)) \right) \quad \text{Eq. (6)}$$

$$u_5 = 0 \quad \text{Eq. (7)}$$

$$u_6 = y \cdot 42 \quad \text{Eq. (8)}$$

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

$$u_5 = \left(-b + \left(\text{sqr}t \left(\frac{(b \cdot b) - (4 \cdot a \cdot c)}{(2 \cdot a)} \right) \right) \right); -(8a) \quad \text{Eq. (9)}$$

where:

$$a = (x \cdot (1 - k)) + (y \cdot (1 - k)) \quad \text{Eq. (10)}$$

$$b = (x \cdot (0.42 - (f \cdot e \cdot (2 - r))) + (k \cdot ((0.42 \cdot (f - 1)) + (p \cdot f \cdot e)))) + (y \cdot (0.42 - (2 \cdot f \cdot e) + (k \cdot (0.42 \cdot (f - 1)))))) \quad \text{Eq. (11)}$$

$$c = -(x \cdot (0.42 \cdot p \cdot f \cdot e \cdot (f - 1) \cdot k)) \quad \text{Eq. (12)}$$

and:

$$k = \exp(0.273 - (1.761/t) - (1.611/t^2) + (0.283/t^3)); \quad \text{Eq. (13)}$$

$$u = (x \cdot ((p \cdot f \cdot e) - v5)) + (y \cdot v5); \quad \text{Eq. (14)}$$

$$u_2 = (x \cdot (0.42 + (f \cdot e \cdot ((2 \cdot p) - r)) + v5)) - (y \cdot (0.42 + v5)); \quad \text{Eq. (15)}$$

$$u_3 = (x \cdot (0.79 + (s \cdot f \cdot (e/2)))) + (y \cdot 0.79); \quad \text{Eq. (16)}$$

$$u_4 = 0; \quad \text{Eq. (17)}$$

$$u_6 = (x \cdot ((0.42 \cdot (f - 1)) - v5)) + (y \cdot 0.42); \quad \text{Eq. (18)}$$

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:

$$y_7 = C_1 \cdot (y_6)^{0.5}; \quad \text{Eq. (19)}$$

$$y_8 = C_2 \cdot (y_4)^{0.5}; \quad \text{Eq. (20)}$$

$$y_9 = C_3 \cdot (y_4)^{0.5} \cdot (y_6)^{0.5}; \quad \text{Eq. (21)}$$

$$y_{10} = C_4 \cdot (y_4)^{0.5} \cdot (y_3)^{0.5}; \quad \text{Eq. (22)}$$

where:

$$C_1 = K_1 / P^{1/2}; \quad \text{Eq. (23)}$$

$$C_2 = K_2 / P^{1/2}; \quad \text{Eq. (24)}$$

$$C_3 = K_3; \quad \text{Eq. (25)}$$

$$C_4 = K_4; \quad \text{Eq. (26)}$$

Where K_p value is obtained from equation:

$$\log K_p = \exp \left[\left(\frac{A}{T} \right) + \left(\frac{B+C}{T} \right) \ln(T) + D \right] \quad \text{Eq. (27)}$$

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.

Results and discussion

As shown in Fig. 1, for an 80% hydrogen substitution, with higher temperature of 1800 K, the CO_2 value was higher than that obtained at 1200 K 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. This incomplete combustion results in higher amounts of CO_2 emissions in the beginning, but as the hydrogen substitution is increased, complete and rigorous combustion reduces the emissions of CO_2 as dissociation increases with temperature.

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

Fig. 3 shows the change in mole fraction of Nitrogen (N_2) for various percentages of hydrogen

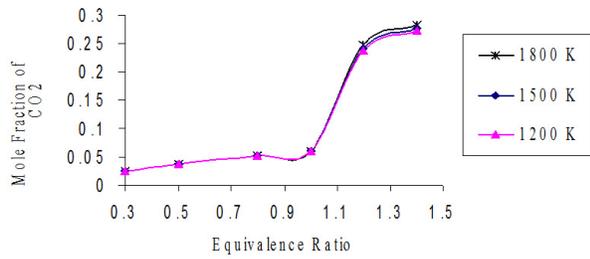


Figure 1 Mole fraction of CO₂ against the equivalence ratio, for 80% hydrogen, at T=1200 K, 1500 K and 1800 K.

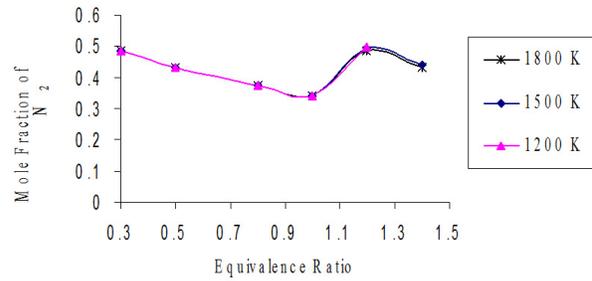


Figure 5 Mole fraction of N₂ against the equivalence ratio, for 80% hydrogen at T=1200 K, 1500 K and 1800 K.

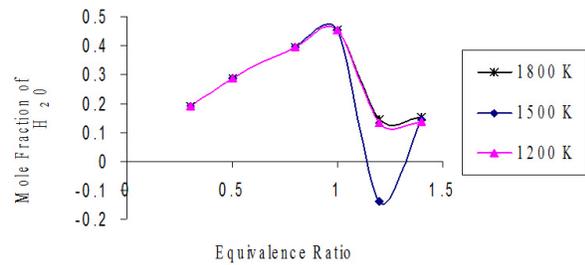


Figure 2 Mole fraction of H₂O against the equivalence ratio, for 80% hydrogen at T=1200 K, 1500 K and 1800 K.

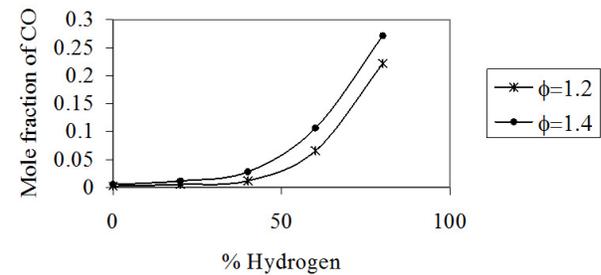


Figure 6 Mole fraction of CO against the percentages of hydrogen at T=1200 K and P= 50 bar.

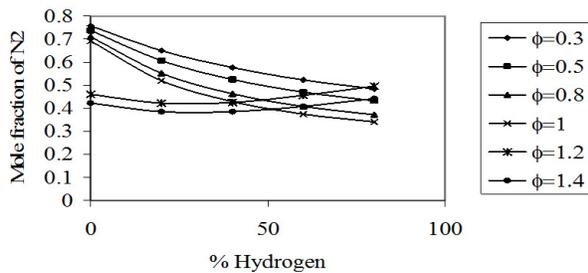


Figure 3 Mole fraction of N₂ against the percentage substitutions of hydrogen at T=1200 K and P= 50 bar.

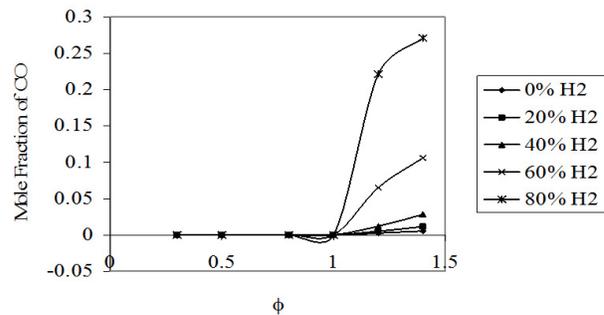


Figure 7 Mole fraction of CO against equivalence ratio at T=1200 K.

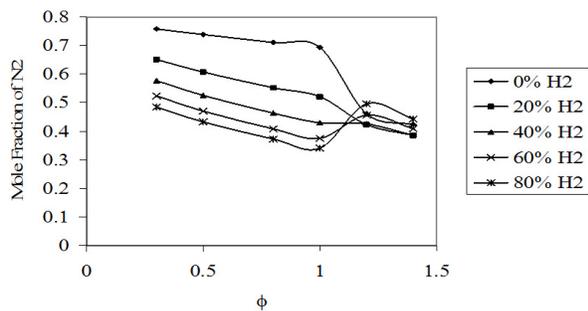


Figure 4 Mole fraction of N₂ against equivalence ratio at T=1200 K.

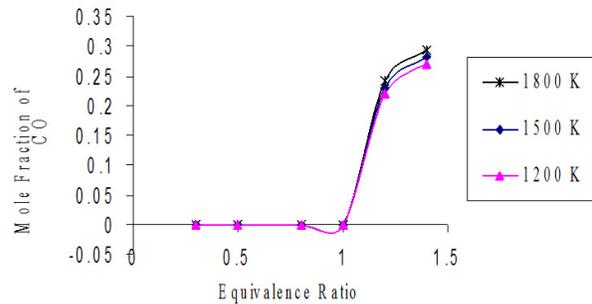


Figure 8 Mole fraction of CO against the equivalence ratio, for 80% hydrogen at T=1200 K, 1500 K and 1800 K

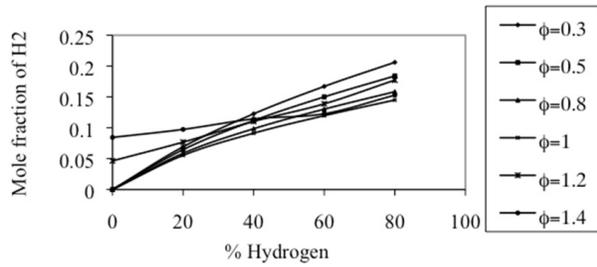


Figure 9 Mole fraction of H₂ against the different percentages of hydrogen at T=1200 K and P = 50 bar.

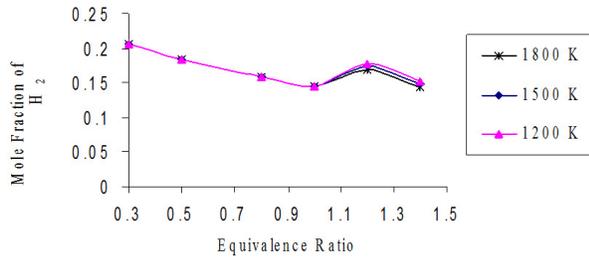


Figure 10 Mole fraction of H₂ against the equivalence ratio, for 80% hydrogen at T=1200 K, 1500 K and 1800 K.

substitutions for different constant equivalence ratios for temperatures of 1200 K, 1500 K and 1800 K. It is observed that mole fraction of N₂ 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 N₂ decreases. However, slight increase in mole fraction value corresponding to 60 and 80% hydrogen addition was seen at an equivalence ratio of 1.0 (Fig. 4). For 80% Hydrogen substitution (Fig. 5) it is seen that for temperatures of 1200 K, 1500 K, and 1800 K, the mole fraction of N₂ first decreases at an equivalence ratio of 1 and then again increases at equivalence ratio of 1.2. Further decrease was observed at an 1.4 equivalence ratio.

Fig. 6 shows the change in the mole fraction of carbon monoxide (CO) for various percentages of hydrogen substitutions for different constant equivalence ratios for temperatures of 1200 K, 1500 K, and 1800 K. It can be noted that as the hydrogen percentage increased, the mole fraction of CO increased sharply for equivalence ratio values of 1.2 and 1.4 and for other equivalence ratios, no increase was found in the mole fraction of CO. In Fig. 7, it is seen that

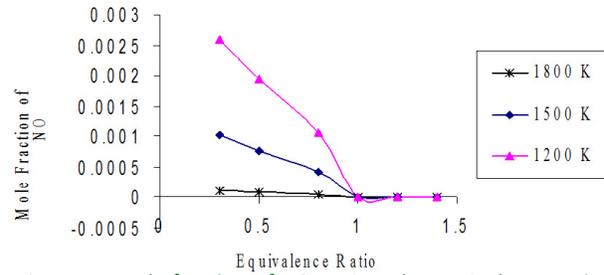


Figure 11 Mole fraction of NO against the equivalence ratio, for 80% hydrogen at T=1200 K, 1500 K and 1800 K.

maximum deviation for mole fraction of CO is for 80% hydrogen when compared to 60% hydrogen. The value of the mole fraction of CO was greater at higher temperatures for 80% hydrogen substitution (Fig. 8). Therefore, it is clear that the CO₂ and CO concentrations decrease as the percentage of hydrogen in the ethanol blend increase. This is due to the reduction in the concentration of carbon atoms in the blended fuel and the high molecular diffusivity of hydrogen, which improves the mixing process thus providing higher combustion efficiency [Desoky and El Emam, 1985].

The variations of mole fractions of hydrogen (H₂) for various percentages of hydrogen substitutions for different constant equivalence ratios at temperatures of 1200 K, 1500 K, and 1800 K is depicted in Fig. 9. It is seen that with an increase in hydrogen percentage substitution, the mole fraction of H₂ increases. As shown in Fig. 10, all fractions of hydrogen showed a decreasing trend until an equivalence ratio of 1.0. Subsequently, an appreciable increase in mole fraction of hydrogen was observed until equivalence ratio of 1.4. Fig. 11 shows that the mole fraction for 80% hydrogen is higher at lower temperatures (i.e.1200 K) with an increase in equivalence ratio. The adiabatic flame temperature calculated on the available theory gave higher values of peak temperature. The higher adiabatic temperature is because of the higher heating values of hydrogen. It does not theoretically take into account the formation of moisture. However, the exhaust simulation code takes into account the formation of exhaust products along with the moisture that forms during combustion. Therefore, as the percentage of hydrogen increases, the formation of

H₂O during combustion increases, which maintains a lower peak temperature, and reduces the formation of NO and N₂ [Abd Alla, 2001].

Conclusions

1. At equivalence ratio of 1.4, the molar fraction of CO₂ decreases for lean equivalence ratios due to a reduction in fuel carbon.

2. For 80% hydrogen substitution, with a temperature of 1800 K, the CO₂ value is higher than that obtained at 1200 K and 1500 K.

3. As the percentage of hydrogen increases in the blend, the mole fraction of H₂O also increases, and has a higher value for an equivalence ratio of 1.0. Furthermore, with the increase in equivalence ratio, the mole fraction of H₂O falls considerably.

4. For an 80% hydrogen substitution, with a temperature of 1800 K the mole fraction of H₂O is higher than that obtained at 1200 K and 1500 K.

5. The mole fraction of N₂ decreases for all hydrogen fractions except for 60% and 80% hydrogen substitutions.

6. Maximum deviation for mole fraction of CO is of 80% hydrogen when compared to 60% hydrogen. The value of the mole fraction of CO was larger at higher temperatures for an 80% hydrogen substitution.

7. With an increase in the hydrogen substitution percentage, the mole fraction of H₂O increases. All fractions of hydrogen showed decreasing trend until an equivalence ratio of 1.0. A subsequent increase in the hydrogen mole fraction was observed until equivalence ratio of 1.4.

8. As the percentage of hydrogen increases, the formation of H₂O during combustion increases, which keeps the peak temperature low and thus reduces the formation of NO and N₂.

The code developed gave reasonably good results. However, many areas exist which are not addressed 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 shows

the limitation of the model and opens the doors for further investigation. The best results were obtained for a combination of 80% hydrogen and 20% ethanol by volume.

Nomenclature

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
n_i	: Coefficient describing product composition of i^{th} species
x	: Percentage of ethanol in ethanol-hydrogen fuel blend
y	: Percentage of hydrogen in ethanol-hydrogen fuel blend
y_i	: Mole fraction of i^{th} species
f	: Equivalence ratio
e	: Molar air-fuel ratio

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