Exhaust Gas Simulation of Hydrogen–Ethanol Dual Fuel

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Abstract - The drawback of lean operation with ethanol is a 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 result 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 oxygenated hydrocarbon fuel like ethanol reduces all of these drawbacks. Hydrogen’s low ignition energy limit and high burning speed makes the hydrogen-ethanol mixture easier to ignite, reducing misfire and thereby improving emissions, performance and fuel economy.

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 Hydrogen–Ethanol Dual Fuel

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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 Φ<1. A rich mixture has Φ>1. The mixture is said to be stoichiometric if Φ=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 Cp Hq Or Ns and Hydrogen. Considering that there are ten constituents the combustion reaction is written as
\[ \varepsilon \phi = [(x \cdot (C_1 H_2 O, N_2)) + (y \cdot H)] + (0.21 \cdot O_2) + (0.79 \cdot N_2) \]

\[ v_1 \text{ CO}_2 + v_2 \text{ H}_2 \text{O} + v_3 \text{ N}_2 + v_4 \text{ O}_2 + v_5 \text{ CO} + v_6 \text{ H}_2 + v_7 \text{ H} + v_8 \text{ O} + v_9 \text{ OH} + v_{10} \text{ NO} \]

The molar fuel–air ratio is given by

\[ \varepsilon = (x \cdot \frac{0.210}{p} + (0.25 \cdot q) - \frac{0.5}{r}) + (y \cdot \frac{0.42}{r}) \]

Convenient approximations for lean and rich combustion are

\[ \phi < 1 \quad \varepsilon = \varepsilon_0 = 0 \]

\[ \phi > 1 \quad \varepsilon = \varepsilon_0 = 0.42 \]

The mole fractions are obtained for the products are obtained by

\[ y_i = \sum v_i \quad \text{i = 1 to 6} \]

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

\[ b = (x \cdot (0.42 - (\phi \cdot \varepsilon \cdot (2 - r)) + (k \cdot (0.42 \cdot (\phi - 1) + (p \cdot \phi \cdot c)))) + (y \cdot (0.42 - (2 \cdot \phi \cdot c) + (k \cdot (0.42 \cdot (\phi - 1))))) \]

\[ c = -x \cdot (0.42 \cdot p \cdot \phi \cdot c \cdot (\phi - 1) \cdot k) \]

and

\[ k = \exp \left(0.273 - (1.761/t) - (1.611/t^2) + (0.283/t^3)\right) \]

\[ v_1 = x \cdot ((p \cdot \phi \cdot c) - v_5) + (x \cdot v_5) \]

\[ v_2 = (x \cdot (0.42 + (\phi \cdot \varepsilon \cdot (2 - r)) - v_5) - y_4(0.42 + v_5)) \]

\[ v_3 = (x \cdot (0.79 + (s \cdot \phi \cdot (\varepsilon / 2))) - y_4(0.79)) \]

\[ v_4 = 0 \]

\[ v_5 = (x \cdot (0.42 \cdot (\phi - 1)) - v_5) + (y \cdot (0.42 - (2 \cdot \phi \cdot c) + (k \cdot (0.42 \cdot (\phi - 1))))) \]

\[ \text{IV. Results and Discussion} \]

As shown in Fig.1 for 80% hydrogen substitution, with higher temperature of 1800K the CO\textsubscript{2} value is higher than that obtained at 1200K and 1500K. Under the stoichiometric conditions the mole fractions of CO\textsubscript{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\textsubscript{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\textsubscript{2} emissions in the beginning, but as the hydrogen substitution is increased, rigorous and strong complete combustion reduces the emissions of CO\textsubscript{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\textsubscript{2}O value is higher than that obtained at 1200K and 1500K. As the mole fraction of H\textsubscript{2}O increases with hydrogen substitution, this brings down the combustion temperature, and hence the reason of reduction in the values of NO and N\textsubscript{2} at higher percentages of hydrogen substitution.

Figs. 3 show the change in mole fraction of Nitrogen (N\textsubscript{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 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 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 N₂ 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 CO₂ 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 (H₂) 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 H₂ 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 H₂O during combustion increases which keeps the peak temperature down and reduces the formation of NO and N₂ [6].

V. 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 higher temperature of 1800K the CO₂ value is higher than that obtained at 1200K and 1500 K.
3. As the percentage hydrogen increases, the mole fraction of H₂O also increases, and has higher value for equivalence ratio of 1.0. Further, with the increase in equivalence ratio the mole fraction of H₂O falls down considerably.
4. For 80% hydrogen substitution, with higher temperature of 1800K the mole fraction of H₂O value is higher than that obtained at 1200K and 1500 K.
5. 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 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 H₂ 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 H₂O during combustion increases which keeps the peak temperature down and thus reduces the formation of NO and N₂.

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:

- kₚ: specific heat ratio of the products
- kₗ: 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 \( i \)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

**References Références Referencias**


**Figure 1**: Mole fraction of \( \text{CO}_2 \) against the Equivalence ratio, for 80% Hydrogen and at \( T = 1200 \text{K}, 1500 \text{K} \) and \( 1800 \text{K} \)

**Figure 2**: Mole fraction of \( \text{H}_2\text{O} \) against the Equivalence ratio, for 80% Hydrogen and at \( T = 1200 \text{K}, 1500 \text{K} \) and \( 1800 \text{K} \)
**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
Figure 6: Mole fraction of CO against the percentages of hydrogen at T=1200K

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

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 H₂ against the different percentages of hydrogen at T=1200K

Figure 10: Mole fraction of H₂ 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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