

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

Index terms— combustion, dissociation reaction, dual fuel, equivalence ratio, mole fraction.

1 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, Westrum and Sinke (1969) is in the same format as that

99 mole fraction for 80% hydrogen is higher at lower temperatures (i.e.1200K) with increase in equivalence ratio.
100 The adiabatic flame temperature calculated on the available theory gives higher values of peak temperature. The
101 higher adiabatic temperature is because of the higher heating values of hydrogen. It does not take into account
102 the formation of moisture theoretically. However, exhaust simulation code takes into account the formation of
103 complete exhaust species along with the moisture that forms during combustion. Therefore, as the percentage of
104 hydrogen increases the formation of H₂O during combustion increases which keeps the peak temperature down
105 and reduces the formation of NO and N₂ [6].

106 V.

107 9 Conclusions

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

110 2. For 80% hydrogen substitution, with higher temperature of 1800K the CO₂ value is higher than that
111 obtained at 1200K and 1500 K. 3. As the percentage hydrogen increases, the mole fraction of H₂O also
112 increases, and has higher value for equivalence ratio of 1.0. Further, with the increase in equivalence ratio the
113 mole fraction of H₂O falls down considerably. 4. For 80% hydrogen substitution, with higher temperature of
114 1800K the mole fraction of H₂O value is higher than that obtained at 1200K and 1500 K. 5. Mole fraction of
115 N₂ decreases for all hydrogen fractions except for 60% and 80% hydrogen substitutions. 6. Maximum deviation
116 for mole fraction of CO is for 80% hydrogen when compared to 60% hydrogen. The value of mole fraction of
117 CO found to be higher at higher temperatures for 80% hydrogen substitution. 7. With increase in hydrogen
118 percentage substitution the mole fraction of H₂ increases. All fractions of hydrogen showed decreasing trend until
119 equivalence ratio of 1.0 and then afterwards appreciable increase in mole fraction of hydrogen was observed until
120 equivalence ratio of 1.4. 8. As the percentage of hydrogen increases, the formation of H₂O during combustion
121 increases which keeps the peak temperature down and thus reduces the formation of NO and N₂.

122 The code developed gave reasonably good results. However, there exist many areas which are unaddressed
123 by the code. At low and high percentages of hydrogen and during transition between ethanol and hydrogen
124 the model predictions are not very clear, this eventually shows the limitation of the model and opens Fig. ??
125 shows the change in mole fraction of carbon monoxide (CO) for various percentages of hydrogen substitutions
126 for different constant equivalence ratios for temperatures of 1200 K, 1500K and 1800 K. It can be noted that
127 as the hydrogen percentage is increasing the mole fraction of CO increases sharply for equivalence ratio values
128 of 1.2 and 1.4 and for other equivalence ratios, no increase is found in mole fraction of CO. From Fig. ??, it is
129 seen that maximum deviation for mole fraction of CO is for 80% hydrogen when compared to 60% hydrogen.
130 The value of mole fraction of CO found to be higher at higher temperatures for 80% hydrogen substitution (Fig.
131 ??). Therefore, it is clear that the CO₂ and CO concentrations decrease as the percentage of hydrogen and
132 ethanol blending are increased. This is due to the reduction in carbon atoms concentration in the blended fuel
133 and the high molecular diffusivity of hydrogen, which improves the mixing process and, hence, provides higher
134 combustion efficiency [5].

135 10 Global Journal of Researches in Engineering

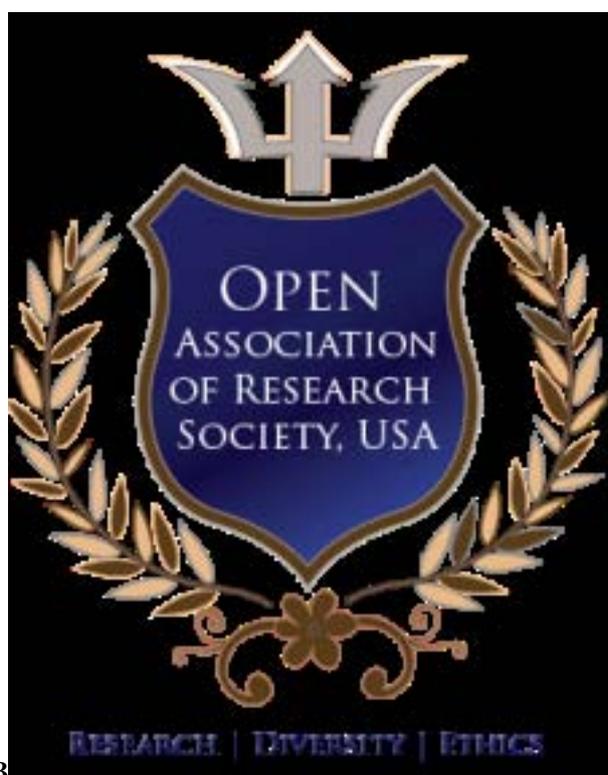


Figure 1: ? 3 =

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