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6 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 8 the mixture being above the low fire (point) limit of the fuel. This result in misfire, which 9 increases unburned hydrocarbon emissions, reduces performance and wastes fuel. Hydrogen 10 can be used in conjunction with ethanol provided it is stored separately. Mixing hydrogen 11 with oxygenated hydrocarbon fuel like ethanol reduces all of these drawbacks. Hydrogen's low 12 ignition energy limit and high burning speed makes the hydrogen-ethanol mixture easier to 13 ignite, reducing misfire and thereby improving emissions, performance and fuel economy. This 14 paper involves generating the simulation software that provides the mole fraction of each of 15 the exhaust species when the hydrogen is burnt along with ethanol. The proportion of 16 hydrogen in the hydrogen-ethanol blend affecting the mole fraction of the exhaust species is 17 also simulated. The program code developed gave reasonably good results for the present 18 hydrogen-ethanol dual fuel. At low and high percentages of hydrogen and during transition 19 between ethanol and hydrogen the model predictions are not very clear. The best results were 20 obtained for for a combination of 80 21

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

24 1 Introduction

mong 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 nonrenewable, 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 28 a considerable amount of heat. The composition of the exhaust gas produced is a function of temperature as 29 well as equivalence ratio (ratio of actual fuel ratio to theoretical fuel air ratio). Many components are present 30 in the exhaust gas because of dissociation of some species. Thermodynamics is able to predict the equilibrium 31 state that results from burning a fuel-air mixture given only the initial conditions. Combustion is a chemical 32 reaction between a fuel and oxygen, which is accompanied by the production of a considerable amount of heat. 33 The composition of the exhaust gas produced is a function of temperature as well as equivalence ratio (ratio of 34 35 actual fuel ratio to theoretical fuel air ratio). A lean mixture has ?<1 A rich mixture has ?>1. The mixture is 36 said to be stoichiometric if ?=1. 37 Many components are present in the exhaust gas because of dissociation of some species. The heat of

a 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.

46 **2** II.

47 **3** 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.

53 4 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?? [(x * (C p H q O r N s))+ (y * H 2)] + (0.21 * O 2) + (0.79 * N 2) ? 1 CO 2 + ? 2 ? 2 ? + ? 3 ? 2 + ? 4 ? 2 + ? 5 CO + ? 6 H 2 + ? 7 H + ? 8 ? + ? 9 ?? + ? 10 ??

The molar fuel -air ratio is given by ? = (x * (0.210 / (p + (0.25 * q) - (0.5 * r)))) + (y * 0.42)Convenient approximations for lean and rich combustion are? < 1 ? 5 = ? 6 = 0 ? >1 ? 4 = 0

- The mole fractions are obtained for the products are obtained by i = ?i / ??i i = 1 to 6
- For a lean mixture the coefficients of combustion products are obtained as ? $1 = x^*(p^*?^*?)$; ? $2 = x^*(p^*?^*?)$
- 61 $(x^{(q^{??}(?/2))})+(y^{(q^{??}(?/2))});$ The mole fractions for all the remaining species is obtained in terms of y 3, y 62 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
- (33); 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 $C_1 = K_1 / P_{1/2}$; $C_2 = K_2 / P_{1/2}$; $C_3 = K_3$; $C_4 = K_4$;
- 65 Where K p value is obtained from equation

$_{^{66}}$ 5 log K p = exp [(A / T) + (B+C/T) ln(T) +D]

⁶⁷ where T is in Kelvin. The value of A, B, C and D are obtained from the JANAF tables based upon the reaction ⁶⁸ of the species with oxygen.

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

70 **6** IV.

71 7 Results and Discussion

As shown in Fig. ?? for 80% hydrogen substitution, with higher temperature of 1800K the CO 2 value is higher 72 than that obtained at 1200K and 1500 K. Under the stoichiometric conditions the mole fractions of CO 2 is at 73 its peak and decreases when the mixture becomes either richer or leaner due to presence of other products. As 74 the temperature increases, the mole fraction of CO 2 decreases as the dissociation increases with temperature. 75 As explained earlier under heat release rate explanation the peak heat release rate (i.e. the peak combustion at 76 77 low outputs is considerably low in dual fuel mode) with different hydrogen substitutions when compared to the 78 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 79 in the beginning, but as the hydrogen substitution is increased, rigorous and strong As shown in Fig. 2 for 80% 80 hydrogen substitution with higher temperature of 1800K the mole fraction of H 2 O value is higher than that 81 obtained at 1200K and 1500 K. As the mole fraction of H 2 O increases with hydrogen substitution, this brings 82 down the combustion temperature, and hence the reason of reduction in the values of NO and N 2 at higher 83 percentages of hydrogen substitution. 84

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Figs. 3 show the change in mole fraction of Nitrogen (N 2) for various percentages of hydrogen substitutions for 86 different constant equivalence ratios for temperatures of 1200 K, 1500K and 1800 K. It is Exhaust Gas Simulation 87 of Hydrogen-Ethanol Dual Fuel observed that mole fraction of N 2 decreases for all hydrogen fractions except for 88 60 and 80% hydrogen substitutions. Fig. ?? shows that with the increase in equivalence ratio the mole fraction 89 90 value of N 2 decreases. However, slight increase in mole fraction value corresponding to 60 and 80% hydrogen 91 addition could be seen at equivalence ratio of 1.0 (Fig. ??). For 80% Hydrogen substitution (Fig. ??) it is seen 92 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. 93

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. ??. It is seen that with increase in hydrogen percentage substitution the mole fraction of H 2 increases. As shown in Fig. ??0 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. ??1 shows 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 H 2 O during combustion increases which keeps the peak temperature down ¹⁰⁵ and reduces the formation of NO and N 2 [6].

107 9 Conclusions

V.

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108 1. At equivalence ratio of 1.4, the molar fraction of CO 2 decreases for lean equivalence ratios due to a reduction 109 in fuel carbon.

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

The code developed gave reasonably good results. However, there exist many areas which are unaddressed 122 by the code. At low and high percentages of hydrogen and during transition between ethanol and hydrogen 123 the model predictions are not very clear, this eventually shows the limitation of the model and opens Fig. ?? 124 shows the change in mole fraction of carbon monoxide (CO) for various percentages of hydrogen substitutions 125 for different constant equivalence ratios for temperatures of 1200 K, 1500K and 1800 K. It can be noted that 126 as the hydrogen percentage is increasing the mole fraction of CO increases sharply for equivalence ratio values 127 of 1.2 and 1.4 and for other equivalence ratios, no increase is found in mole fraction of CO. From Fig. ??, it is 128 seen that maximum deviation for mole fraction of CO is for 80% hydrogen when compared to 60% hydrogen. 129 The value of mole fraction of CO found to be higher at higher temperatures for 80% hydrogen substitution (Fig. 130 ??). Therefore, it is clear that the CO 2 and CO concentrations decrease as the percentage of hydrogen and 131 132 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 133 combustion efficiency [5]. 134

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Figure 1: ? 3 =

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