Gaseous Emissions and Combustion Efficiency Analysis of Hydrogen-Diesel Dual Fuel Engine under Fuel-Lean Condition

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ABSTRACT

Exhaust gas emissions from diesel engine combustion using alternative fuel may change in their quantities that can affect exhaust gas after-treatment devices and environmental ambient. This study presents theoretical analysis of combustion generated emissions and efficiency of hydrogen-diesel duel fuel in fuel-lean condition. A chemical equilibrium method by minimizing Gibbs free energy is employed to estimate exhaust gas products from diesel and hydrogen-diesel mode combustion. The combustion products, e.g., unburned hydrocarbons (CH_4), hydrogen (H_2), carbon dioxide (CO_2), carbon monoxide (CO) are comparatively investigated, based upon similar specific energy input. Subsequently, the obtained combustible products (CH_4, H_2 and CO) are used to calculate combustion efficiency, based upon chemical energy left in waste exhaust gases. The main findings are associated with the reduction in CO_2 corresponding to the increase in combustion efficiency in hydrogen-diesel combustion mode, depending on relative air-to-fuel ratios. Meanwhile, the CH_4, H_2 and CO contents in the flue gas increase in the operating conditions used.

Keywords: Equilibrium Analysis, Hydrogen, Dual Fuel, Diesel Engine, Emissions, Combustion Efficiency

1. INTRODUCTION

In present, diesel engines are applied in many works such as industrial, agriculture and transportation. Some advantages comparing to spark ignition (gasoline) engine are mainly to offer better fuel conversion efficiency. Moreover, diesel engine exhibits in fuel flexibility under various operating conditions, superior engine durability, higher thermal efficiency and lower fuel consumption.

However, the diesel engines also have a few disadvantages. Firstly, the exhaust gas consists of hydrogen (H_2), carbon monoxide (CO), unburned hydrocarbons (uHCs), excess oxygen (O_2) and carbon dioxide (CO_2). The latter is considered as a major source of greenhouse effect. Secondly, the lack of fossil fuel makes it expensive in the diesel fuel price. From these reasons, diesel engine vehicles, used in industry and transportation have involved environmental problems and need remediation.

An alternative energy such as hydrogen is becoming a choice among others due to its positive effects. It contains no carbon and has higher energy density when compared to fossil diesel as well as its global availability. Moreover, a trend of increasing use of hydrogen is prospectively observed towards the future.

Hydrogen can be found in chemical compounds, e.g., natural gas, coal, biomass, water, as it does not exist by itself on Earth (Williams, 1980). Nowadays, the most hydrogen production is by reforming natural gas process (Pohl, 1995). In addition, pure hydrogen from water electrolysis is produced by fossil fuel burning generated electricity (Marrero-Alfonso *et al*., 2007), hydroelectric, wind energy and solar energy (Khaselev and Turner, 1998). Among such renewable resources, biomass conversion is also a technique usually used for hydrogen production (Cortright *et al*., 2002). Padro and Lau (2000) listed some other advanced techniques for hydrogen generation.

A number of research works apply hydrogen for reducing the fossil fuels. Tomita *et al*. (2001) and Tsolakis *et al*. (2005) presented their experimental findings on exhaust emission effects from dual fuel diesel engine operation using H_2. Kumar *et al*. (2003) listed a

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viable technology in hydrogen usage. Recently, Jarungthammachote *et al.* (2012) studied on thermodynamics of hydrogen addition effects on diesel engine operation, some combustion characteristics and nitrogen oxides emissions, using finite difference method.
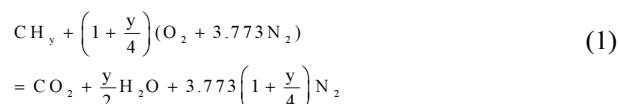
From the aforementioned reasons, there are yet some aspects of using hydrogen as dual fuel with fossil diesel in terms of theoretical analysis. Therefore, the main aim of this study is to analyze the combustion generated exhaust gas emissions and efficiency of hydrogen-diesel duel fuel mode.

2. MATERIALS AND METHODS

The combustion of hydrogen-diesel dual fuel was studied through the chemical equilibrium method. The concept of minimization of Gibbs free energy combined with the energy balance was used. The amount of added hydrogen was varied to study its effect on the combustion process. Moreover, the result of changing relative air/fuel ratio was also observed. In every case, the compositions of exhaust gas, which are CO_2, CO, H_2O, H_2, N_2, O_2 and HC represented by CH_4 and the combustion temperature were found. Then, the combustion efficiency was evaluated. However, the calculations in all cases were carried out based on similar total energy input.

2.1. Combustion Reaction of Hydrocarbon Fuel

For diesel fuel with the empirical formula CH_y, the composition of the unburned and burned gas fractions can be theoretically calculated using a stoichiometric combustion equation, showing in Equation 1:
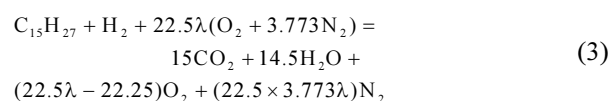
$$CH_y + \left(1 + \frac{y}{4}\right)(O_2 + 3.773N_2)$$
$$= CO_2 + \frac{y}{2}H_2O + 3.773\left(1 + \frac{y}{4}\right)N_2 \tag{1}$$

In such circumstances the combustion can also be in fuel-rich or fuel-lean condition. Therefore, the relative air/fuel ratio (λ) defined in Equation 2 are used:

$$\lambda = \frac{(A/F)_{actual}}{(A/F)_{stoichiometric}} \tag{2}$$

where, $(A/F)_{actual}$ is air-to-fuel ratio on mass basis used in real combustion and $(A/F)_{stoichiometric}$ is chemically correct or theoretical proportion of air and fuel on mass basis (Chuepeng and Komintarachat, 2010).

2.2. Chemical Equilibrium Analysis

The diesel-hydrogen combustion equation is shown in Equation 3:

$$C_{15}H_{27} + H_2 + 22.5\lambda(O_2 + 3.773N_2) =$$
$$15CO_2 + 14.5H_2O + \tag{3}$$
$$(22.5\lambda - 22.25)O_2 + (22.5 \times 3.773\lambda)N_2$$

where, λ is relative air/fuel ratio. From Equation 1, it can be observed that, for lean fuel combustion, the major gas species in exhaust gas are CO_2, H_2O, excess O_2 and N_2. The amount of each gas species can be obtained by using mole balance concept. However, in the real combustion process, CO and H_2 can also be found in significant amount in the exhaust gas. Considering CO, H_2 and incomplete cracked hydrocarbon represented by CH_4, the simple mole balance method cannot find the number of mole of each gas species. To evaluate the final product in complex chemical reaction, like combustion process, the chemical equilibrium method is often used.

This method is based on the concept that at equilibrium state, the total Gibbs free energy of the system has minimum value. For the multi-reaction, single phase system, the total Gibbs free energy (G^t) can be expressed as Equation 4:

$$G^t = \sum_{i=1}^{N} n_i g_i \tag{4}$$

where, g_i and n_i are the chemical potential and the number of mole of specie i, respectively. The problem is to find the set of which minimizes the total Gibbs free energy of system. In combustion system, the ideal gas assumption can be applied because of high temperature. Thus, the total Gibbs free energy for ideal gas system can be calculated by Equation 5:

$$G^t = \sum_{i=1}^{N} n_i \Delta \overline{G}_{f,i}^{\circ} + \sum_{i=1}^{N} n_i \overline{R}T \ln\left(\frac{n_i}{n_{tot}}\right) \tag{5}$$

where, $\Delta \overline{G}_{f,i}^{\circ}$ is the standard Gibbs free of formation of species i and $\overline{R}$ is the universal gas constant. To find the minimum value of G^t, an optimization method, called Lagrange multipliers, is used. The mass balance of each chemical element is carried out and it is set as the constraint of this problem. The obtained final equation is as Equation 6:

$$\Delta \overline{G}_{f,i}^{\circ} + \overline{R}T \ln\left(\frac{n_i}{n_{tot}}\right) + \sum_{k} \Pi_k a_{ik} = 0 \tag{6}$$

where, a_{ik} is the number of atom of the kth element in a mole of the ith species. The values of Π_k represent the Lagrange multipliers. The desired solution can be achieved be solving equation 6 with constraint equations. In this problem, the mass balance equations of chemical elements found in reactants were applied as constraint equations.

To predict the combustion temperature, the energy balance equation is formed as Equation 7:

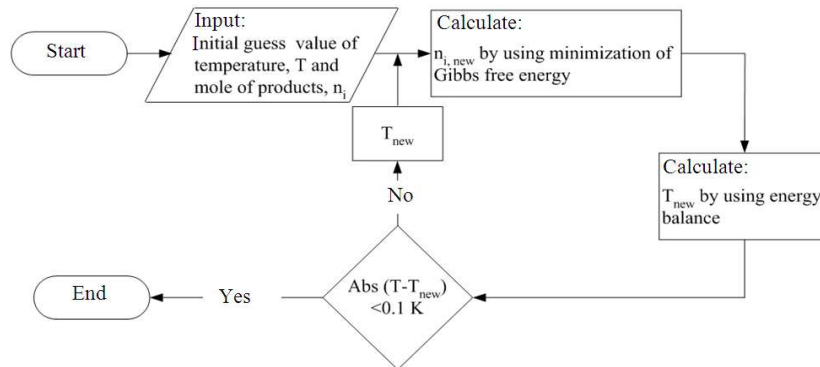$$\sum_{r=react} n_r \overline{H}_r(T_r) = \sum_{p=prod} n_p \overline{H}_p(T_p) \tag{7}$$

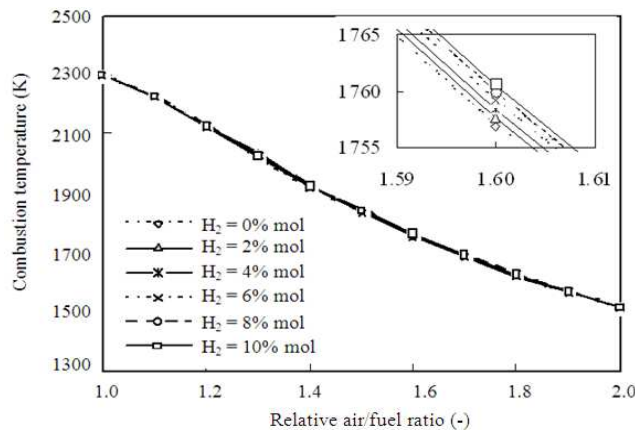**Fig. 1.** Combustion temperature determining diagram

Fig. 2. The alteration in combustion temperature from hydrogen dual fuel engine

In Equation 7, the energy loss from combustion system is assumed as zero. $\bar{H}_r$ and $\bar{H}_p$ represent the enthalpies of reactants and products, respectively. The combustion temperature, T_p is implicitly obtained from the enthalpy of product mixture. The step of calculation can be shown as in **Fig. 1**.

2.3. Combustion Efficiency

Generally, there are still combustible species left in exhaust gas i.e., CO, H_2 and unburned hydrocarbon. The higher amounts of these species reflect combustion inefficiency. The combustion efficiency (η_c) can be calculated using Equation 8:

$$\eta_c = \left(1 - \frac{\sum_i x_i Q_{HVi}}{\left[\frac{\dot{m}_f}{\dot{m}_a + \dot{m}_f} \right] Q_{HVi}} \right) \times 100 \qquad (8)$$

where, x_i are the mass fractions of CO, H_2 and CH_4 (obtained from chemical equilibrium analysis), Q_{HVi} are the lower heating values of each species and the subscripts a and f denote air and fuel, respectively.

3. RESULTS

3.1. Combustion Temperature

The temperature variation of the diesel-H_2 duel fuel combustion under fuel lean conditions is shown in **Fig. 2**. It has seen that the temperatures tend to reduce with relative air-to-fuel ratios. However, there is only a subtle increase in the temperature when hydrogen is added to the combustion at constant relative air-to-fuel ratio.

3.2. Exhaust Gas Emissions

The combustion generated exhaust gas variations, i.e., H_2, CO, unburned hydrocarbon (CH_4) and CO_2 are shown in **Fig. 3-6**, respectively. When hydrogen added to the engine increases, the amounts of H_2, CO and CH_4 in the exhaust gas are increased, depending on relative air-to-fuel ratios. Meanwhile, the CO_2 composition in the exhaust gas is reduced when the increasing hydrogen is added to the engine.
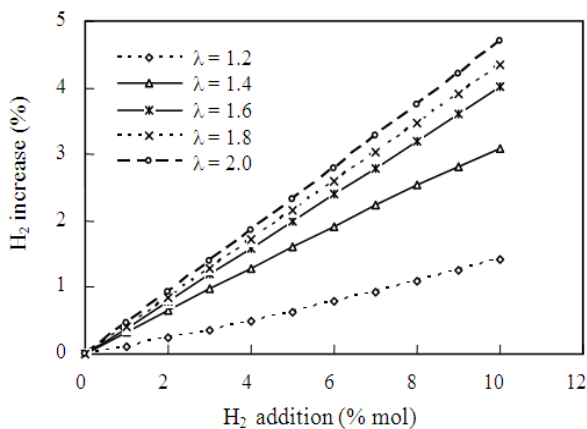
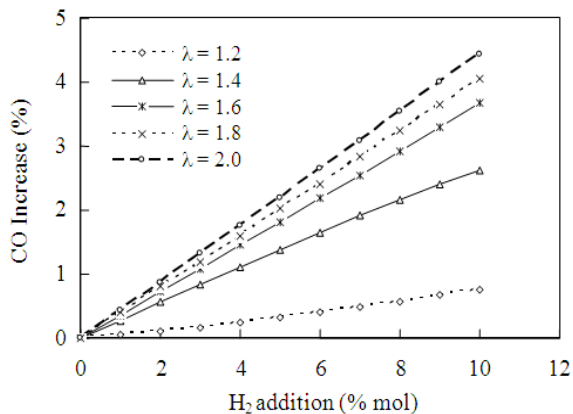**Fig. 3.** The alteration of H_2 emission from hydrogen dual fuel engine

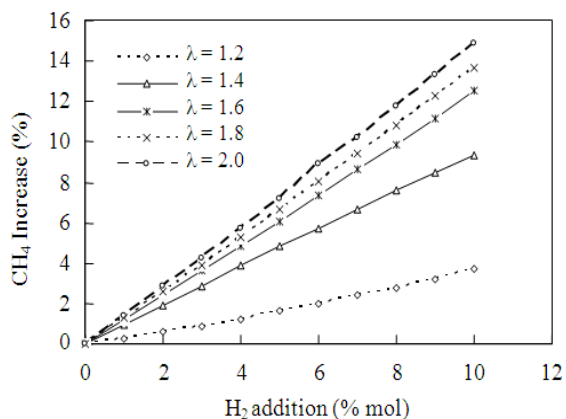**Fig. 4.** The alteration of CO emission from hydrogen dual fuel engine

Fig. 5. The alteration of CH_4 emission from hydrogen dual fuel engine
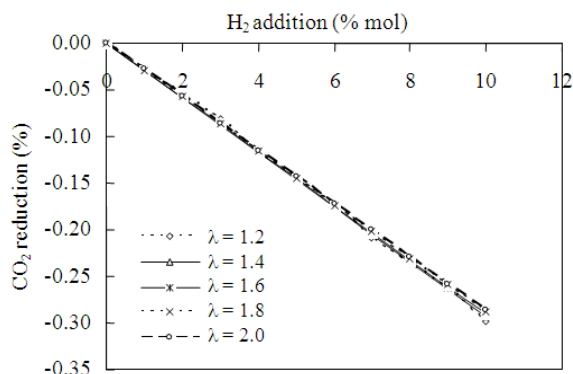

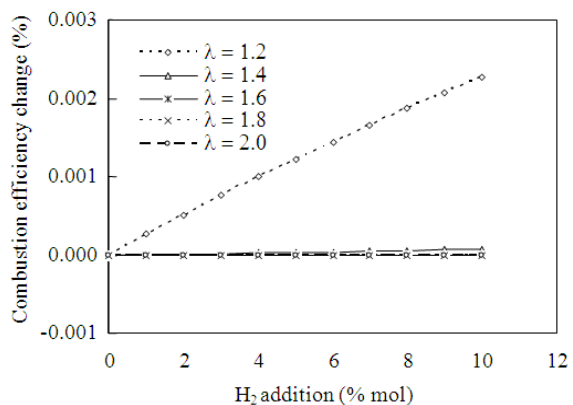**Fig. 6.** The alteration of CO_2 emission from hydrogen dual fuel engine

Fig. 7. The alteration of combustion efficiency from hydrogen dual fuel engine

3.3. Combustion Efficiency

The combustion efficiencies on the basis of energy left in unburned combustible products were calculated and are compared in **Fig. 7**. It has seen that almost all the efficiencies of the combustion are subtle increased when hydrogen is added, depending on the relative air-to-fuel ratios.

4. DISCUSSION

In **Fig. 2** the combustion temperature strongly depends on the fuel composition in the mixture to be combusted. As the relative air-to-fuel ratios increase, more air is induced in to the combustion chamber, resulting in lesser fuel proportion for burning and thus, the reduced combustion temperature. Even the calculation was accomplished on the equivalent energy basis, the hydrogen added up to 10 molar percentage as a dual fuel

operation can generate the increase in temperature within 5 K as seen in the magnified section in **Fig. 2.**

In **Fig. 3-5,** at a constant relative air-to-fuel ratio, the hydrogen addition to the engine results in CO, H_2 and CH_4 left in the exhaust gas due to incomplete combustion even in global fuel lean condition. At lower relative air-to-fuel ratios in **Fig. 3,** the lesser amount of the air is induced to the engine while hydrogen is also added to the engine. This results in greater proportion of H_2 in the exhaust gas composition. This effect is also applied to **Fig. 4 and 5** for the CO and CH_4, respectively.

Figure 6 shows, at a constant relative air-to-fuel ratio that the reduction of CO_2 when increasing in H_2 addition is as a result of lesser amount of diesel that was substituted by hydrogen is combusted. At lower relative air-to-fuel ratios, the lesser amount of the air is induced to the engine during hydrogen addition. This results in greater reduction proportion of CO_2 in the exhaust gas composition.

It is to note in **Fig. 7** that the combustion efficiency change is apparently at lower relative air-to-fuel ratios while showing only subtle amount within 0.03% over the relative air-to-fuel ratios investigated.

5. CONCLUSION

The combustion of hydrogen-diesel dual fuel is analyzed using a chemical equilibrium model of Gibbs free energy minimization and energy balance to first determine combustion temperatures. The subsequent combustion temperatures and chemical elements are input to the solver to obtain gas-phase species i.e., CO_2, CO, H_2O, H_2, N_2, O_2 and CH_4. Combustible species (CO, H_2 and CH_4) in the exhaust gases are combustion inefficiency. It is found that CO_2 was reduced while CO, H_2 and CH_4 increased. H_2 addition increases combustion efficiency in majority while maintaining the efficiency in very fuel-lean conditions.

6. ACKNOWLEDGMENT

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