Insight into Emissions and Combustion Efficiency of Hydrogen-Diesel Dual Fuel Engine with Exhaust Gas Recirculation Using Chemical Equilibrium Analysis

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Abstract

This paper presents theoretical analysis of the hydrogen-diesel dual fuel combustion with exhaust gas recirculation. A chemical equilibrium method is employed to estimate exhaust gas products from diesel and hydrogen-diesel mode combustion in a presence of exhaust gas portion. The combustion products, e.g. unburned hydrocarbons (in terms of methane, CH_4), hydrogen (H_2), carbon dioxide (CO_2), carbon monoxide (CO), etc. from those are comparatively investigated, based upon equivalent specific energy input. Subsequently, those products are subsequently used to calculate combustion efficiency, based upon chemical energy left in the waste exhaust gases. The main findings are associated with the reduction in CH_4, CO_2, and CO corresponding to the increase in combustion efficiency in hydrogen-diesel combustion mode. Meanwhile, hydrogen content in flue gas may increase in some operating conditions.

***Keywords**:* equilibrium analysis, hydrogen, dual fuel, diesel engine, emissions, combustion efficiency, exhaust gas recirculation.

1. Introduction

Compression ignition (diesel) engines can be operated by using a wide range of fuels under a variety of operating conditions. Comparing to spark ignition (gasoline or petrol) engine, diesel engine can offer better engine durability and higher thermal efficiency. The latter reflects lower fuel consumption resulting in less carbon dioxide emission which is considered to be a major source of greenhouse effect gas. In transportation, a huge amount of energy is consumed, mostly in form of fossil fuels as their flue gases are a main cause of environmental issues. Therefore, using alternative fuels is part of a sustainable solution to energy and ecological crisis. Hydrogen is a choice among other promising fuels that can be added to the diesel engine, running on dual fuel mode [1]. Although industrial hydrogen in massive container to be carried in vehicle is considered to be expensively improper, alternative ways to produce hydrogen on-board being exhaust gas fuel reforming [2], water electrolysis [3], etc. are also of interest. Diesel engines in dual fuel mode have shown experimentally a viable technology as seen in literatures [4-5].

The main aim of the present work is to determine the theoretical effects when exhaust gas recirculation (EGR) is in use with hydrogen-diesel combustion. Influences of hydrogen addition without EGR on combustion products and temperature are firstly investigated in fuel-lean condition. Subsequently, exhaust gas composition alteration and combustion efficiency when hydrogen and different EGR portions are added is studied and discussed.

2. Calculation Method

2.1 The Chemical Equilibrium Calculation

The chemical equilibrium method is often used to find the final products of chemical reaction processes. 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:

$$G^t = \sum_{i=1}^{N} n_i g_i \qquad (1)$$

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 n_i 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:

$$G^t = \sum_{i=1}^{N} n_i \Delta\overline{G}^o_{f,i} + \sum_{i=1}^{N} n_i \overline{R} T \ln\left(\frac{n_i}{n_{tot}}\right) \qquad (2)$$

Where $\Delta\overline{G}^o_{f,i}$ 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:

$$\Delta\overline{G}^o_{f,i} + \overline{R} T \ln\left(\frac{n_i}{n_{tot}}\right) + \sum_k \lambda_k a_{ik} = 0 \qquad (3)$$

where a_{ik} is the number of atom of the k^{th} element in a mole of the i^{th} species. λ represents the Lagrange multipliers. The desired solution can be achieved be solving Eq. (3) with constraint equations.

2.2 The Combustion Temperature

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

$$\sum_{r=react} n_r \overline{H}_r(T_r) = \sum_{p=prod} n_p \overline{H}_p(T_p) \qquad (4)$$

In Eq. (4), the energy loss from combustion system is assumed as zero. $\overline{H}_r$ and $\overline{H}_p$ represent the enthalpies of reactants and products, respectively. The combustion temperature, T_p is implicitly obtained from the enthalpy of product mixture.

2.3 The Calculation Scheme

A computer program was developed following two main concepts, e.g. the chemical equilibrium method and the energy balance. The input of the model is chemical composition of diesel fuel oil ($C_{15}H_{27}$), hydrogen and air under stoichiometric and fuel-lean combustion condition. In this work, the engine load can be characterized by the relative air-to-fuel ratio (lambda). The lambda value is defined on mass basis as the air-to-fuel ratio actually used by the engine over the air-to-fuel ratio theoretically combusted. The higher the value of lambda, the greater the amount of air induced to the engine. Therefore, the higher lambda values indicate lighter engine loads. The exhaust gas components deliberated in this model are CO_2, CO, H_2, H_2O, O_2, N_2, and NO. CH_4 represents the hydrocarbon in the exhaust gas.

The calculation starts with assuming the reaction temperature and then, solving the exhaust gas compositions by chemical equilibrium method. The exhaust gas components are substituted to compute the energy balance. The reaction temperature is found and compared with the assumed value. If the difference of both temperatures is higher than 1K, the reaction temperature is adjusted and the composition of exhaust gas is calculated again. The checking of the energy balance is also done. This calculation procedure is repeated until the difference of temperature in present step and temperature in previous step is less than 1K. The result of this calculation is used as input information for the case of using EGR. The same calculation algorithm is repeated again until the final solution is obtained.

2.4 Combustion efficiency determination

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 Eq. (5):

$$\eta_c = \left(1 - \frac{\sum_i x_i Q_{HV_i}}{\left[\frac{\dot{m}_f}{\dot{m}_a + \dot{m}_f} \right] Q_{HV_f}} \right) \times 100 \quad (5)$$

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 and discussion

3.1 Effects of hydrogen addition without EGR

The temperature and products from diesel-fuelled combustion in fuel-lean condition are numerated in Table 1. It has seen that there were traces of unburned combustible portions (CH_4, CO and H_2) left in the exhaust gas even in the lean condition; the figures tend to reduce with lambda. Other combustion products such as CO_2 and H_2O were lower with the increasing lambda while O_2 and N_2 were higher in the exhaust gas. For temperature-dependent species, the NO emission decreased with the reduction of lambda in this lean condition.

Table. 1 Combustion temperature and exhaust gas composition from diesel-fuelled engine

Lambda	Combustion temperature (K)	Mole fraction							
		CH_4	CO	H_2	CO_2	H_2O	O_2	N_2	NO
1.0	2336.1	Very low	0.0180	0.0032	0.1166	0.1179	0.0089	0.7320	0.0045
1.1	2264.8	Very low	0.0076	0.0013	0.1162	0.1101	0.0202	0.7402	0.0044
1.2	2168.4	Very low	0.0030	0.0005	0.1113	0.1024	0.0327	0.7456	0.0034

When 5% hydrogen was added to diesel combustion (dual fuel mode) without exhaust gas recirculation (EGR) based on equivalent energy input, there were subtle changes in combustion products and temperature. Fig. 1 shows the alteration in unburned combustible products e.g. CH_4, CO and H_2. The H_2 in the exhaust gas increased while CO reduced without changes in CH_4 composition. The trends of the changes in H_2 and CO were increased with the increasing lambda.

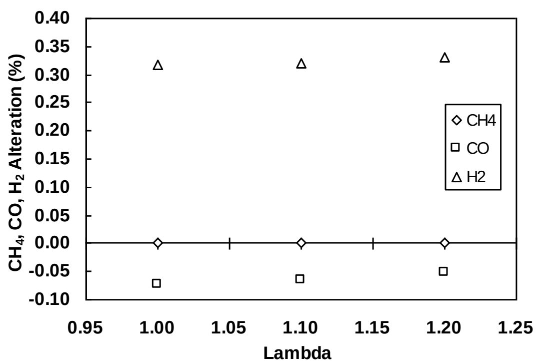

Fig. 1 The alteration in unburned combustible products from dual fuel engine without EGR

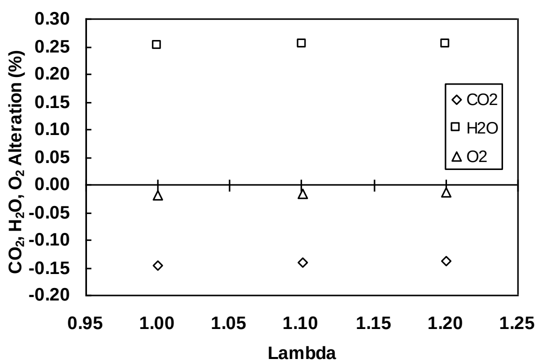

Fig. 2 The alteration in combustion gaseous products from dual fuel engine without EGR

Fig. 2 shows the alteration in combustion gaseous products e.g. CO_2, H_2O and O_2. It was founded that CO_2 and O_2 decreased with hydrogen addition while H_2O increased. All the trends of changes were in higher levels corresponding to the increasing lambda.

The NO emission corresponding to the combustion temperature was found to increase with the hydrogen addition as shown in Fig. 3. These trends of changes increased with the increasing lambda.

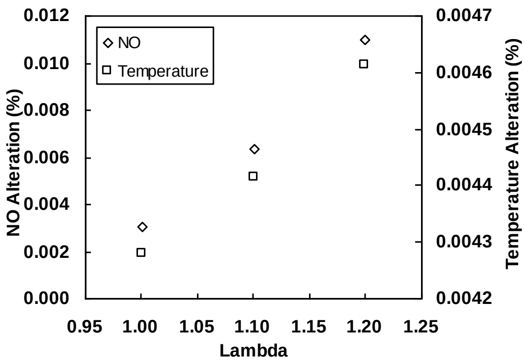

Fig. 3 The alteration in temperature-dependent nitric oxide emission from dual fuel engine without EGR

3.2 Effects of EGR addition to hydrogen-diesel dual fuel engine

The effects of EGR on alteration in unburned combustible products from dual fuel engine are depicted in Fig. 4. They have shown obviously that the dual fuel combustion with EGR resulted in the reduction of combustible products i.e. CH_4, CO and H_2. With the higher extent of EGR, the more reduction of these products was observed.

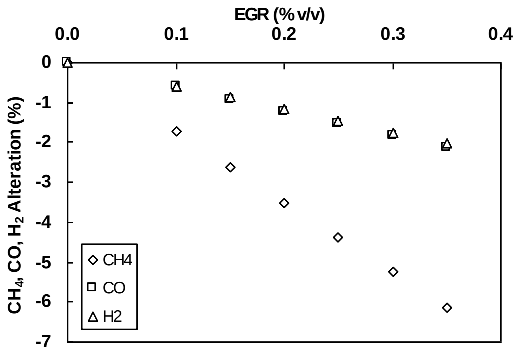

Fig. 4 The effects of EGR on alteration in unburned combustible products from dual fuel engine at lambda 1.1

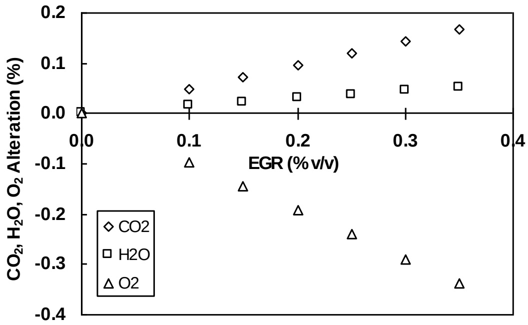

Fig. 5 The effects of EGR on alteration in combustion gaseous products from dual fuel engine at lambda 1.1

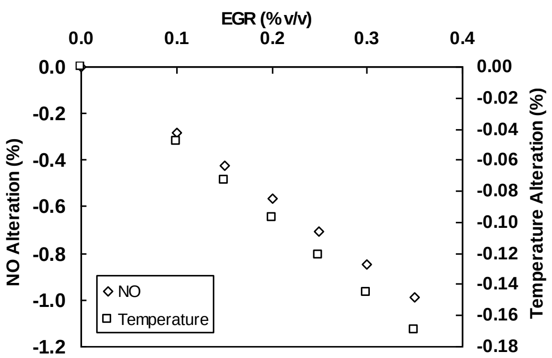

Fig. 6 The effects of EGR on alteration in temperature-dependent nitric oxide emission from dual fuel engine at lambda 1.1

Fig. 5 shows the impacts of EGR on combustion gaseous products from dual fuel engine. CO_2 and H_2O are found to increase with EGR while O_2 decreased. This indicated more complete combustion was taken place.

The EGR addition to the dual fuel combustion has influenced the NO emission as shown in Fig. 6. The NO emission reduced with the increase in EGR percentage. This corresponds with the combustion temperature which is the main cause of the NO formation in the combustion.

3.3 Combustion efficiency

The combustion efficiency calculated base on energy left in unburned combustible products were calculated and are compared in Fig. 7. It has seen that the dual fuel combustion without EGR addition results in the decrease in combustion efficiency. This is as there was hydrogen left in the exhaust gas as already discussed and shown in Fig. 1.

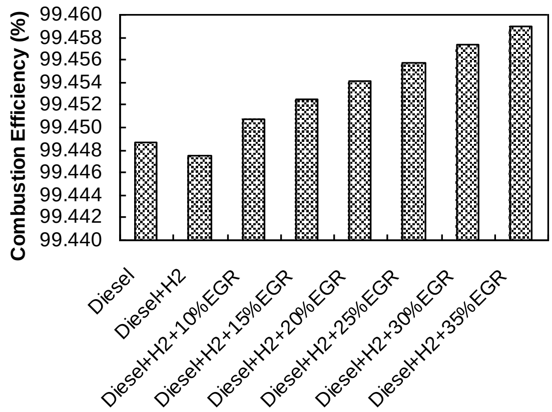

Fig. 7 Combustion efficiency in different combustion modes at lambda 1.1

Fig. 7 also shows that the EGR addition to the dual fuel combustion enhanced combustion efficiency. This confirms the reduction of all unburned combustible products

(Fig. 4) that pronounces more complete combustion (Fig. 5).

4. Conclusions

The emissions and combustion efficiency of hydrogen-diesel dual fuel engine with exhaust gas recirculation was investigated in this paper using chemical equilibrium analysis. It can be concluded that the use of 5% hydrogen-diesel dual fuel lowered carbon monoxide, carbon dioxide and oxygen while increasing hydrogen and vapor in the exhaust gas. When the EGR was in use with dual fuel combustion, all combustible products including temperature-dependent nitric oxide emission were lowered while enhancing combustion efficiency. This benefits not only in terms of exhaust emissions but reserving fossil diesel fuel.

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6. References

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