American Journal of Applied Sciences 9 (9): 1472-1478, 2012
ISSN 1546-9239

Effect of Hydrogen Addition on Diesel Engine Operation and NO_x Emission: A Thermodynamic Study

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Abstract: Problem statement: The worldwide increasing energy demand and the environmental problem due to greenhouse gas emission, especially produced from fossil fuel combustion, have promoted research work to solve these crises. Diesel engine has proven to be one of the most effective energy conversion systems. It is widely used for power generation, land vehicles and marine power plant. To reduce diesel fuel consumption, an alternative energy sources, such as Hydrogen (H_2), is promoted to use as dual-fuel system. H_2 is considered as a fuel for future because it is more environmental friendly compared to carbon-based fuel. However, the most exiting diesel engines were designed for using diesel fuel. Feeding H_2-diesel dual fuel to the engine, it is required to study its effect on engine operation parameters. Moreover, it is also an interesting point to observe the engine emission when H_2-diesel dual fuel is used. **Approach:** The thermodynamic modeling was used to simulate the operating parameters, i.e., cylinder pressure and gas temperature. Finite different method was employed to find the solution. The H_2 supply and EGR were varied. The pressure and temperature were observed. For NO_x emission, which is a major problem for use of diesel engine, the thermodynamic equilibrium calculation was conducted to find the mole fraction of gas species in the exhaust gas. The mole fraction of NO and NO_2 were combined to present as the mole fraction of NO_x. **Results:** The simulation showed that at 5% EGR, increase of H_2 caused increasing of cylinder pressure and temperature. It also increased NO_x in exhaust gas. However, when H_2 was fixed at 10%, increasing EGR led reducing of cylinder pressure and temperature. The mole fraction of NO_x decreased with increasing EGR. **Conclusion:** The H_2 supplied to the engine provided positive effect on the engine power indicated by increasing pressure and temperature. However, it showed the negative effect on NO_x emission. Use of EGR was recommended for controlling NO_x emission when H_2 is supplied.

Key words: Thermodynamic modeling, nitrogen oxide, dual-fuel, hydrogen, diesel engine, Hydrogen (H_2), Exhaust Gas Recirculation (EGR)

INTRODUCTION

Due to energy crisis and environmental problem, more efficient and cleaner engines have been developed. Diesel engines are widely used, especially for transportation and power generation because of their higher thermal efficiency. However, it is well known that NO_x and smoke emissions are the important problems for use of diesel engine. Therefore, many researches have been done in order to improve diesel engines efficiency and lower their emission. One of the most frequently used methods to control NO_x is supplying Exhaust Gas Recirculation (EGR) into the intake manifold of engine. Maiboom *et al*. (2008) investigated the effect of EGR on the diesel engine emission. They found that EGR was more effective way to control NO_x emission. The simulation of NO formation in diesel engine has been done. The NO emission at different equivalence ratio, which was predestined by the single zone zero dimensional model, agreed with the experimental results.

Hydrogen is one of the most promising energy carriers fulfilling energy, environment and sustainable development needs. Since hydrogen is a carbon-free fuel, hydrogen combustion does not generate CO_2 and smoke (Miyamoto *et al*., 2011). Using hydrogen and diesel fuel in diesel engine, called dual-fuel diesel engine, it has been interested by many researchers. Varde and Frame (1983) studies the effect of hydrogen added in the intake of a diesel engine. The result showed that smoke decreased with the increase in hydrogen addition. Dual-fuel operation of biodiesel with hydrogen was studied by Geo *et al*. (2008). They found that NO_x emission increased with increase in

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hydrogen. The diesel engine combustion process and knocking behavior was investigated by Szwaja and Grab-Rogalinski (2009) when the proportion of hydrogen and diesel fuel was varied. They reported that the hydrogen addition affected the ignition delay. The simulation of exhaust emission for diesel engine using diesel blended with hydrogen was conducted by Masood and Ishart (2008). The conclusion of their study showed that NO_x emission was depended on the equivalent ratio.

In this study, the thermodynamic simulation for diesel engine was developed. The amount of H_2 supply was varied while the fraction of Exhaust Gas Recirculation (EGR) was fixed in order to study the effect of H_2 on the engine operation parameters i.e., cylinder pressure and temperature and NO_x emission. To investigate the effect of EGR on hydrogen-diesel dual fuel engine, the amount of EGR was changed and H_2 supply was fixed. The cylinder pressure and gas temperature were found. The effect o f EGR at constant H_2 supply was also observed in this study.

MATERIALS AND METHODS

To find the Pressure (P) and the Temperature (T) of working fluid in the engine cylinder, the first law of thermodynamics for closed system was applied and it can be expressed as:

$$\frac{dQ_{in}}{dt}-\frac{dQ_{out}}{dt}-P\frac{dV}{dt}=\frac{dU}{dt} \tag{1}$$

where, Q and U represent heat and internal energy, respectively. For the ideal gas, the differentiation of internal energy, shown on the right side of Eq. 1, can be written as:

$$\frac{dU}{dt}=mc_v\frac{dT}{dt} \tag{2}$$

Considering the equation of state, a differentiation of gas temperature can be obtained as:

$$\frac{dT}{dt}=\frac{1}{mR}\frac{d(PV)}{dt} \tag{3}$$

where, R is the gas constant. Substituting Eq. 3 into Eq. 2, it leads to the following equation:

$$dU=\frac{c_v}{R}\left(P\frac{dV}{dt}+V\frac{dP}{dt}\right) \tag{4}$$

By substituting Eq. 4 into Eq. 1, the following equation is obtained.

$$\frac{dQ_{in}}{dt}-\frac{dQ_{out}}{dt}-P\frac{dV}{dt}=\frac{c_v}{R}\left(P\frac{dV}{dt}+V\frac{dP}{dt}\right) \tag{5}$$

Using chain rule of differentiation, Eq. 5 can be rewritten as:

$$\begin{aligned}&\frac{dQ_{in}}{dt}\cdot\frac{dt}{d\theta}-\frac{dQ_{out}}{dt}\cdot\frac{dt}{d\theta}-P\frac{dV}{dt}\cdot\frac{dt}{d\theta}=\\&\qquad\frac{c_v}{R}\left(P\frac{dV}{dt}\cdot\frac{dt}{d\theta}+V\frac{dP}{dt}\cdot\frac{dt}{d\theta}\right)\end{aligned} \tag{6}$$

where, θ is the crank angle and $\frac{d\theta}{dt}=\omega$ is the crank angle angular velocity which is related to the engine speed. Rearranging Eq. 6, it is finally obtained an equation describing the relationship between the cylinder pressure and the crank angle as Eq. 7:

$$\frac{dP(\theta)}{d\theta}=\frac{\gamma-1}{V(\theta)}\left(\frac{dQ_{in}}{d\theta}-\frac{\dot{Q}_{out}}{\omega}\right)-\gamma\frac{P(\theta)}{V(\theta)}\frac{dV(\theta)}{d\theta} \tag{7}$$

where, γ is the specific heat ratio ($\gamma = c_p/c_v$). The heat release rate due to combustion of fuel, $\frac{dQ_{in}}{d\theta}$, can be calculated by using Eq. 8 (Gogio and Baruah, 2010):

$$\frac{dQ_{in}}{d\theta}=Q_{LHV}\frac{dx_b}{d\theta} \tag{8}$$

x_b is the mass fraction burned obtained from the Weibe function which is defined as:

$$x_b=1-\exp\left[-a\left(\frac{\theta-\theta_{sc}}{\Delta\theta}\right)^{m+1}\right] \tag{9}$$

where, θ_{sc} is the start of combustion and $\Delta\theta$ is the combustion duration. a and m are the parameters that characterizes the combustion process in the engine cylinder. In Eq. 9, the coefficients a and m are 5.0 and 2.0, respectively (Ferguson and Kirkpatrick, 2001). For rate of heat transfer from gas in cylinder to cylinder wall, $\frac{\dot{Q}_{out}}{\omega}$, it can be estimated by using Eq. 10:

$$\frac{\dot{Q}_{out}}{\omega}=\frac{h_gA(\theta)}{\omega}\left(T(\theta)-T_w\right) \tag{10}$$

The convective heat transfer coefficient, h_g, is expressed as shown in Eq. 11 (Heywood, 1988):

Table 1: Engine geometry and operational conditions used in simulation

Cylinder bore [m]	8.75×10^{-2}
Stoke [m]	1.1×10^{-1}
Connecting rod length [m]	2.34×10^{-3}
Clearance volume [m^3]	5.50×10^{-6}
Engine speed [rpm]	2,000
Air Fuel ratio [-]	1.1
Injection timing [degree BTDC]	-20
Wall temperature [K]	450

$$h_g = 3.26D^{-0.2}P^{0.8}T^{-0.55}w^{0.8} \tag{11}$$

where, w is the velocity of the burned gas given by Eq. 12 :

$$w = c_1S_p + c_2\frac{V_dT_r}{P_rV_r}\left(P(\theta)\text{-}P_m\right) \tag{12}$$

The coefficient $c_1 = 2.28$ whereas $c_2 = 0$ during the compression process and $c_2 = 0.00324$ during the combustion and the expansion processes. S_p is the piston speed. V_d is the displacement volume. The quantities V_r, T_r and P_r are reference state properties at closing of inlet valve and P_m is the pressure value in cranking.

The instantaneous cylinder volume, area and displacement are given as Eqs. 13-15, respectively:

$$V(\theta) = V_c + \frac{\pi D^2}{4}X(\theta) \tag{13}$$

$$A(\theta) = \frac{\pi D^2}{4} + \frac{\pi DS}{2}\left(a+1\text{-}\cos\theta+\left(a^2\text{-}\sin^2\theta\right)^{1/2}\right) \tag{14}$$

$$X(\theta) = \left(L+a\right)\text{-}\left(a\cos\theta+\left(L^2\text{-}\sin^2\theta\right)^{1/2}\right) \tag{15}$$

where, a is crank radius, S is stoke and L is connecting rod length.

For the working fluid temperature, the calculation was done by using Eq. 16, which is derived from the ideal gas equation of state.

$$T(\theta) = \frac{P(\theta)V(\theta)}{mR} \tag{16}$$

In this study, the interested result is not only the thermodynamic state, represented by pressure and temperature, but also the chemical compositions of exhaust gas. To show the effect of added hydrogen and EGR on the engine emission, the thermodynamic equilibrium method based on the minimization of Gibbs free energy described in Ref. (Jarungthammachote, 2011) was used. This method is based on that at equilibrium state, the total Gibbs free energy of the system is minimized. The total Gibbs free energy of system is defined in Eq. 17:

$$G^t = \sum_{i=1}^{N} n_iG_i = \sum_{i=1}^{N} n_i\mu_i \tag{17}$$

where, n_i and μ_i are the number of moles and the chemical potential of species i, respectively. G_i represents the partial molar Gibbs free energy of species i.

If all gases are assumed as ideal gas, the chemical potential of species i can be obtained from Eq. 18:

$$\mu_i = \Delta\bar{G}^o_{f,i} + RT\ln\left(y_i\right) \tag{18}$$

where, R and T are the universal gas constant and temperature, respectively. y_i is The mole fraction of gas species i and it is the ratio of n_i and the total number of moles in the reaction mixture. $\Delta\bar{G}^o_{f,i}$ represents the standard Gibbs free of formation of species i. The Lagrange multiplier method is conducted with constraint of mass balance, i.e.:

$$\sum_{i=1}^{N} a_{ij}n_i = A_j,\ j = 1,2,3,\ldots,k \tag{19}$$

where, a_{ij} is the number of atom of the j-th element in a mole of the i-th species. A_j is defined as the total number of atom of j-th element in the reaction mixture.

The solutions n_i have to be real numbers in the boundary such that $0 \le n_i \le n_{tot}$. In this study, there are the number of mole of CH_4, CO, CO_2, H_2, H_2O, O_2, N_2, NO and NO_2. The summation of NO and NO_2 is presented in terms of NO_x. The Newton-Raphson method is used to find the solution. The data from Jarungthammachote (2011) is employed to calculate all thermodynamic properties in this model.

The engine and operational conditions used in this simulation are presented in Table 1. The thermal properties of diesel fuel, ignition delay and duration of combustion were assumed following the information obtained from (Heywood, 1988).

RESULTS

The simulation results were obtained by solving Eq. 7 which is differential equation. The numerical method called finite difference technique was employed. The mole fraction of fed hydrogen was varied while the EGR was fixed. Then, the results were observed.

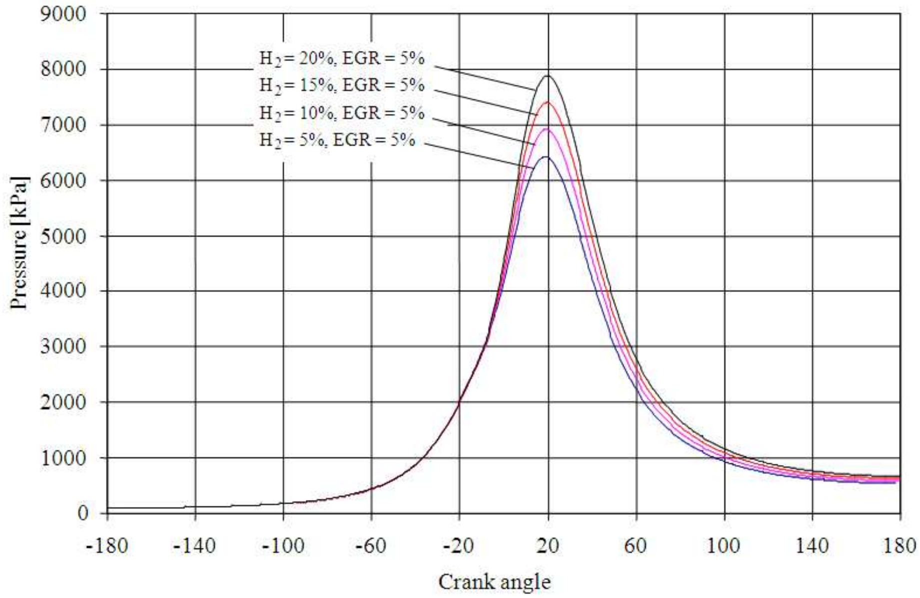

Fig.1: Effect of hydrogen supply on cylinder pressure

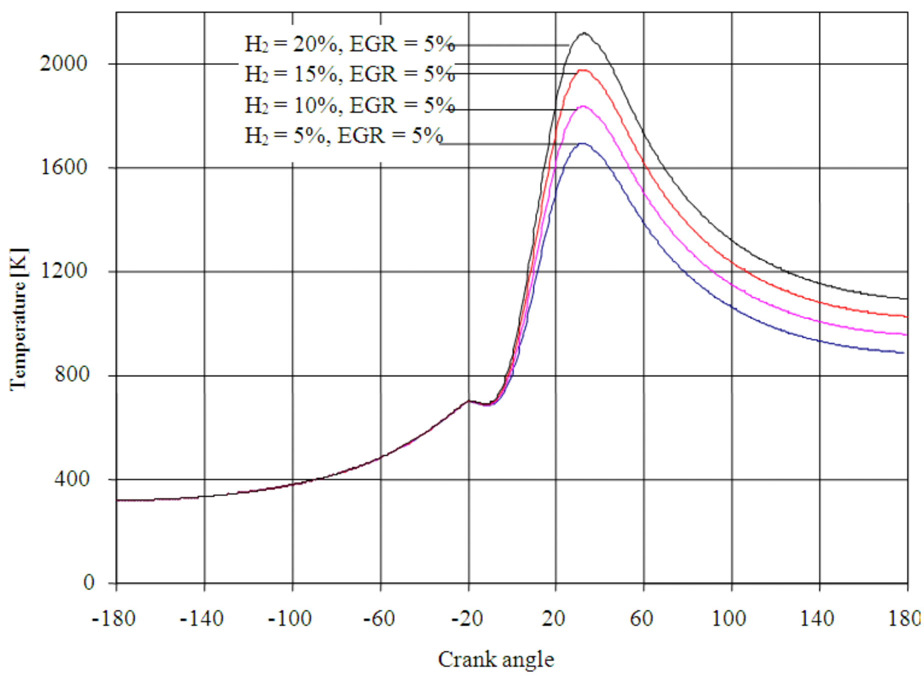

Fig. 2: Effect of hydrogen supply on working fluid temperature

To investigate the effect of EGR on the engine operation and emission, the amount of hydrogen was fixed and the mole fraction of EGR was changed. The results of simulation are given in Fig. 1-6. Figure 1 and 2 present the effect of hydrogen supply on cylinder pressure and gas temperature, respectively. For the effect of EGR, Fig. 3 and 4 shows the cylinder pressure and gas temperature, respectively at different EGR rates. The last two figures elucidate the variation of NO_x due to the change of hydrogen supply and EGR.

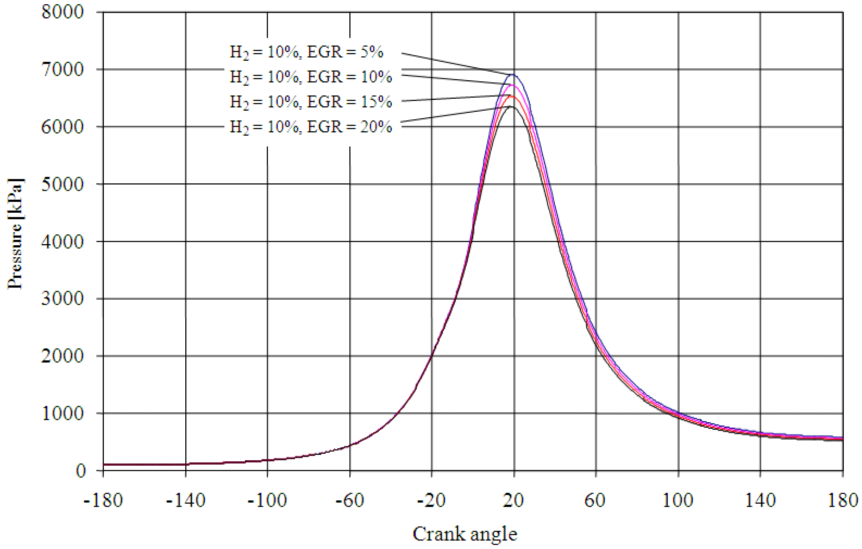

Fig. 3: Effect of EGR on cylinder pressure

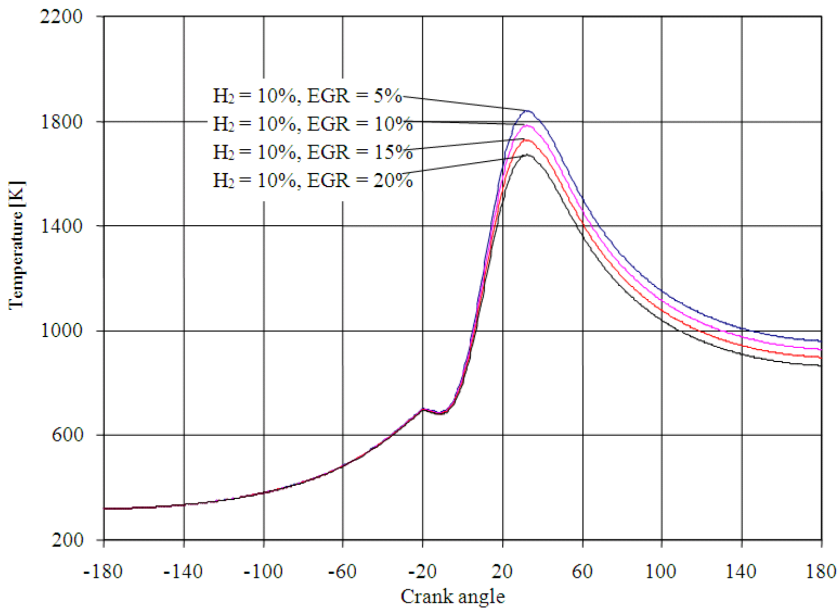

Fig. 4: Effect of EGR on working fluid temperature

DISCUSSION

In the first case, EGR was fixed at 5% and H_2 supply was varied. From the simulation results, Fig. 1 and 2 clearly show that increasing H_2 supply causes increase of cylinder pressure and temperature. As shown in Fig. 1 the peak of cylinder pressure is 6.4 MPa for 5% H_2 supply while 20% H_2 supply raises the peak of pressure up to 8.0 MPa. As observed from the simulation results, for each 5% increase of H_2 supply, the peak of cylinder pressure gains about 490 kPa. For the gas temperature, it can be increased with increasing H_2 supply. The peak of gas temperature for 5% H_2 supply is about 1700 K and it reaches 2120 K when H_2 is fed with 20%. 5% H_2 fed into engine can increase the peak of gas temperature about 140 K. From the results, it can be explained that more H_2 induced into the cylinder increases releasing energy from combustion process. Thus, combustion gas has higher pressure and temperature.

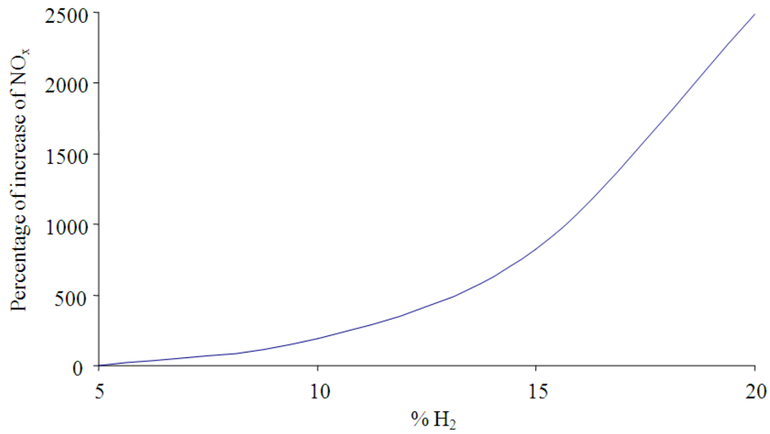

Fig. 5: Effect of hydrogen supply on NOx in exhaust gas

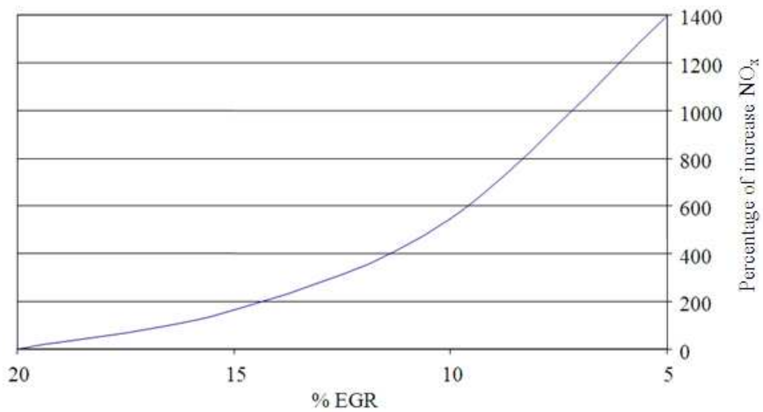

Fig. 6: Effect of EGR on NO_x in exhaust gas

The relationship between cylinder pressure and EGR is expressed in Fig. 3. The H_2 supply was fixed at 10% while EGR was varied from 5-20%. The result shows that the cylinder pressure decreases with increasing EGR. The same effect can be observed for the gas temperature. Reduction of gas temperature is found when EGR fraction is increased, as presented in Fig. 4. From the results, it can be implied that EGR acts as combustion dilutor. Most of gas species in EGR do not react with H_2 and diesel fuel.

To study NO_x emission, chemical equilibrium calculation was simultaneously done with pressure and temperature simulation. Figure 5 indicates that NO_x fraction in exhaust gas increases with increasing H_2 supply. At 20% H_2 supply, the NO_x emission is higher than that at 5% H_2 supply with 2500%. This is the effect of rising temperature due to increasing H_2 supply. The same effect was observed by Varde and Frame (1983). Miyamoto *et al*. (2011) demonstrated that at the energy per cycle of 0.9 kW/cycle, NO first decreased, attained minimum at 4% of H_2 supply and then NO increased with increasing H_2 supply. In contrast, increase of EGR reduces the NO_x emission, as shown in Fig. 6, because EGR lower the gas temperature. Comparing with NO_x emission at 20% H_2 supply, it is 1400% lower than that at %5 H_2 supply.

CONCLUSION

In this study, the thermodynamic model for diesel engine was developed to simulate the effects of H_2 addition and EGR on the operation condition and NO_x emission. The chemical equilibrium method was used to find the mole fraction of NO_x in the exhaust. The result showed that increasing H_2 caused increases of cylinder pressure and temperature. Therefore, the NO_x emission was grown due to increasing temperature. Therefore, it should be make sure that the engine structure can handle the increasing pressure and the engine cooling system can control the temperature to protect the overheat damage. In contract, EGR could reduce the cylinder pressure and temperature. To control NO_x emission, use of higher EGR was recommended to diesel engine added H_2 to the intake air.

ACKNOWLEDGEMENT

The study is a part of research project "The application of hydrogen with multi-cylinder diesel engine for energy saving and pollution reduction" which was financially supported by The Kasetsart University Si Racha Campus Research Committee.

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