

SIMULATION OF PERFORMANCE AND NITROGEN OXIDE FORMATION OF A HYDROGEN-ENRICHED DIESEL ENGINE WITH THE STEAM INJECTION METHOD

by

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In the present study, steam injection method is implemented to a hydrogen-enriched Diesel engine in order to improve the levels of performance and NO emissions. As hydrogen enrichment method increases effective efficiency, NO emissions could be increased. However, the steam injection method is used to control NO emissions and improve the engine performance. Due to these positive effects, hydrogen enrichment and the steam injection method are applied into a Diesel engine by using a two-zone combustion model for 30% hydrogen enrichment of the fuel volume and 20% steam ratio of the fuel mass at full load conditions. The results obtained are compared with conventional Diesel engine, steam injected Diesel engine, hydrogen-enriched Diesel engine, and hydrogen-enriched Diesel engine with steam injection in terms of performance and NO emissions. In the results, the effective efficiency and effective power improve up to 22.8% and 3.1%, as NO emissions decrease up to 22.1%. Hence, the hydrogen enrichment with steam injection method is more environmentally friendly with better performance.

Key words: *hydrogen-enriched engine, engine performance, steam injection, nitrogen oxide emission, combustion, Diesel engine*

Introduction

In recent years, the attention of alternative fuel using for Diesel engines has rapidly increased. The essential reasons of this attention are uncertainty of oil availability in the future and environmental regulations focused on reducing pollutant emissions released from engines [1]. The NO_x, particulate matter and smoke emissions are primary pollutants emitted from Diesel engines [2]. In order to decrease these detrimental emissions, the use of alternative fuels is proposed such as liquid petroleum gas, compressed natural gas, liquefied natural gas, producer gas, bio gas, hydrogen, and vegetable oils as substitutes for hydrocarbon-based fuels. One of renewable energy resources is hydrogen and when it burns, complete combustion occurs and just water is emitted with NO_x emissions [3]. Although, natural gas and bio fuels are expected as the essential short term alternative fuels in the European Commission's White Paper, hydrogen would become long term solution for meeting goals of energy demand and environmental requirements [4]. Because of these reasons, so many studies have been carried out on hydrogen as an alterna-

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tive fuel in vehicle engines, especially for gasoline engines, since hydrogen could be burned as single fuel in spark ignition engines [5]. However, as it has higher self-ignition temperature (858 K) compared to pure diesel fuel (553 K), it is not convenient as a single fuel in Diesel engines [6]. It may be used in just dual fuel mode in Diesel engine operations. Because of knocking problem, hydrogen could not be burnt in large ratios [7]. One of the known methods is to burn hydrogen by mixing air, which is called hydrogen enrichment, in Diesel engines. Researches show that hydrogen-enriched engines give almost the same brake power and higher thermal efficiency than conventional Diesel engines thanks to complete combustion of hydrogen by mixing well with air [3, 7, 8].

Naber and Siebers [9] performed an investigation on the combustion and auto ignition of hydrogen in a direct injection Diesel engine using variable parameters such as ambient gas pressure, temperature and composition, injection pressure and temperature, and orifice diameter. It was observed from results that ignition delay of hydrogen strongly depends on temperature. Hydrogen combustion is insensitive to concentrations of oxygen quantities. Yi *et al.* [10] showed that hydrogen-fuelled engines are more efficient when the intake port injection method is applied to the engine at low loads. Also, Saravanan *et al.* [11] obtained higher efficiency with hydrogen-fuelled Diesel engine than that of conventional Diesel engine using timed port injection technique. Masood and Ishrat [12] developed a simulation program which defines the mole fraction of the exhaust species for the combustion of hydrogen-diesel blends. It is stated that the simulation program gives a good approximation between the calculated and experimental results. Saravanan and Nagarajan [3] carried out an experimental study on hydrogen-enriched air systems in Diesel engines by using different rates of hydrogen in the suction air and they investigated the performance and emission characteristics of the hydrogen-enriched engine. In the results, NO_x emissions were seriously decreased with 90% hydrogen enrichment at 70% engine load. While NO_x emissions slightly raise compared to conventional diesel, the brake thermal efficiency increased by 22.5% with 30% hydrogen enrichment condition at full load due to decreasing equivalence ratio. It was emphasized that hydrogen-enriched Diesel engine is more eco-friendly with higher performance.

Although hydrogen enrichment provides better engine performance, it is not suitable so as to minimize NO_x emissions at full load conditions. In order to decrease NO_x emissions, there are various methods such as exhaust gas re-circulation (EGR), water and steam injection into combustion chamber [13-19]. Nevertheless, EGR method is commonly used to decrease NO_x emissions it is well known that performance is got worse [13-15]. Another NO_x reduction technique is water injection into the engine cylinder with various methods [16, 17]. However, one of the essential disadvantages of water injection methods is that condensed water in the cylinder downgrades the quality of lubrication oil and raises the attrition rate of moving parts of engine. In order to prevent this adverse effect of water injection method, water could be injected into suction manifold in the vapor phase [18]. Murthy *et al.* [19] performed a study on the effects of steam injection solar generated into a Diesel engine and it was observed from the study that NO_x emissions and exhaust temperature diminish, soot emissions, power, and SFC raises with steam injection method at full load conditions.

In the present study, aside from the former studies, the effects of steam injection into a hydrogen-enriched Diesel engine have been computationally investigated in terms of performance and NO_x emissions using a two-zone combustion model. The optimum proportions have been used for steam injection and hydrogen enrichment as 20% and 30% of injected fuel by mass, respectively. In the literature, there is no study on the simultaneous application of hydro-

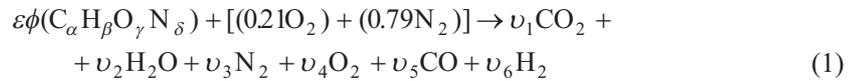
gen and the steam injection method (SIM) into a Diesel engine. Thus, this work presents a substantial novelty on the utilization of hydrogen and the SIM methods together in Diesel engines.

Theoretical model

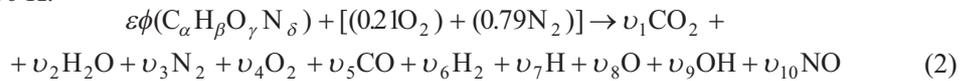
In this part, two-zone combustion model [20-29] is used by adding hydrogen into the reactants in order to calculate NO emissions, effective efficiency and power. The combustion reaction used in the modified program is given:

For single fuel and without steam condition [27-29]:

if $T \leq 1000$ K:

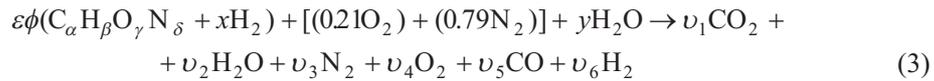


if $T > 1000$ K:



For the dual fuel and with steam injection condition at the modified code:

if $\phi < 1$ and $T \leq 1000$ K:



where from chemical equation balancing for atoms:

$$\begin{aligned} \nu_1 &= \varepsilon\phi\alpha, & \nu_2 &= \frac{\varepsilon\phi(\beta + x2)}{2} + y, & \nu_3 &= \frac{\phi\varepsilon\delta}{2} + 0.79, \\ \nu_4 &= \phi(-0.21) + 0.21, & \nu_5 &= 0, & \nu_6 &= 0 \end{aligned} \quad (4)$$

if $\phi \geq 1$ and $T \leq 1000$ K:

$$\begin{aligned} \nu_1 &= \varepsilon\phi\alpha - \nu_5, & \nu_2 &= \frac{\varepsilon\phi(\beta + x2)}{2} + y - \nu_6, \\ \nu_3 &= \frac{\phi\varepsilon\delta}{2} + 0.79, & \nu_6 &= \phi\left(\frac{-\gamma}{2\alpha} + 0.42\right) - 0.42 - \nu_5, & \nu_4 &= 0 \end{aligned} \quad (5)$$

Equilibrium constant:



therefore,

$$K = \frac{\nu_5 \nu_2}{\nu_1 \nu_6} \quad (7)$$

where $\ln K = 2.743 - 1.761/t - 1.611/t^2 + 0.2803/t^3$, $t = T/1000$, ν_5 could be found by solving next equation:

$$\nu_5 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad (8)$$

where

$$a = 1 - K \quad (9)$$

$$b = K(\varepsilon\phi\alpha) + (K - 1) \left[\phi \left(\frac{-\gamma}{\alpha} + 0.42 \right) - 0.42 \right] + \left(\frac{\varepsilon\phi(\beta + x2)}{2} + y \right) \quad (10)$$

$$c = -K(\varepsilon\phi\alpha) \left[\phi \left(\frac{-\gamma}{\alpha} + 0.42 \right) - 0.42 \right] \quad (11)$$

where

$$x = \frac{M_d m_{\text{hyd}}}{\varepsilon\phi M_{\text{hyd}} m_d} \quad (12)$$

$$y = \frac{K_{\%} \varepsilon\phi (M_d + M_{\text{hyd}})}{M_{\text{ste}}} \quad (13)$$

where m_d [20-24, 30, 31] and m_{hyd} are the masses of diesel fuel and hydrogen, respectively, and M_{ste} , M_d , and M_{hyd} are the total molecular weights of the steam, diesel, and hydrogen, respectively. The α , β , γ , and δ are atomic numbers of carbon, hydrogen, oxygen, nitrogen in diesel, respectively. The ε is the molar fuel-air ratio and $K_{\%}$ is the ratio of the steam mass to the total fuel mass where:

$$M_d = \alpha M_C + \beta M_H + \gamma M_O + \delta M_N, \quad M_{\text{hyd}} = 2M_H \quad (14)$$

$$K_{\%} = \frac{m_{\text{ste}}}{m_d + m_{\text{hyd}}} \quad (15)$$

$$\varepsilon = \frac{0.21}{\left(\alpha - \frac{\gamma}{2} + \frac{(\beta + x2)}{4} \right)} \quad (16)$$

where ϕ is equivalence ratio and it can be written:

$$\phi = \frac{\frac{m_d + m_{\text{hyd}}}{m_a}}{F_{\text{st}}} \quad (17)$$

where m_a is air mass per cycle. F_{st} is the stoichiometric fuel-air ratio and it is given for single fuel [27]:

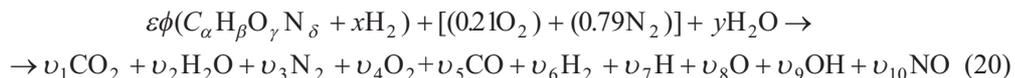
$$F_{\text{st}} = \frac{\varepsilon(12.01\alpha + 1.008\beta + 16\gamma + 14.01\delta)}{28.85} \quad (18)$$

where F_{st} can be written for dual fuel mode:

$$F_{\text{st}} = \frac{\varepsilon(12.01\alpha + 1.008\beta(\beta + 2b) + 16\gamma + 14.01\delta)}{28.85} \quad (19)$$

For the condition of high combustion temperature:

$$T \geq 1000K$$



where from chemical equation balancing for atoms:

$$\varepsilon\phi\alpha = (y_1 + y_5)NY \\ \varepsilon\phi(\beta + x2) + 2y = (2y_2 + 2y_6 + y_7 + y_9)NY \\ \varepsilon\phi\gamma + 2 \cdot 0.21 + y = (2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10})NY \\ \varepsilon\phi\delta + 2 \cdot 0.79 = (2y_3 + y_{10})NY \quad (21)$$

where NY is the total mole number and could be defined:

$$NY = \sum_{i=1}^{10} v_i \quad \text{and} \quad \sum_{i=1}^{10} y_i - 1 = 0 \quad (22)$$

$$2y_2 + 2y_6 + y_7 + y_9 - (y_1 + y_5) \frac{\varepsilon\phi(\beta + x2) + 2y}{\varepsilon\phi\alpha} = 0$$

$$2y_1 + y_2 + 2y_4 + y_5 + y_8 + y_9 + y_{10} - \frac{\varepsilon\phi\gamma + 2 \cdot 0.21 + y}{\varepsilon\phi\alpha} (y_1 + y_5) = 0 \quad (23)$$

$$2y_3 + y_{10} - \frac{\varepsilon\phi\delta + 2 \cdot 0.79}{\varepsilon\phi\alpha} (y_1 + y_5) = 0$$

The mole fractions of the species are given with respect to $y_3, y_4, y_5,$ and y_6 :

$$y_7 = c_1 \sqrt{y_3}, \quad y_8 = c_2 \sqrt{y_4}, \quad y_9 = c_3 \sqrt{y_4} \sqrt{y_6},$$

$$y_{10} = c_4 \sqrt{y_4} \sqrt{y_3}, \quad y_2 = c_5 \sqrt{y_4} y_6, \quad y_1 = c_6 \sqrt{y_4} y_5$$

$$c_1 = \frac{K_1}{\sqrt{P}}, \quad c_2 = \frac{K_2}{\sqrt{P}}, \quad c_3 = K_3,$$

$$c_4 = K_4, \quad c_5 = K_5 \sqrt{P}, \quad c_6 = K_6 \sqrt{P} \quad (24)$$

where K_i is the equilibrium constant and calculated by using:

$$\log K_i = A \ln \left(\frac{T}{1000} \right) + \frac{B}{T} + C + DT + ET^2 \quad (25)$$

The A, B, C, D, and E constants are taken from JANAF tables and these equations are solved with Newton-Raphson iteration method and results are obtained in [27]. The NO emissions are calculated by using extended Zeldovich mechanism taking into account ten combustion products including ($\text{CO}_2, \text{H}_2\text{O}, \text{N}_2, \text{O}_2, \text{CO}, \text{H}_2, \text{H}, \text{O}, \text{OH}, \text{NO}$) [27-29]. The three reaction steps of NO formation are given in tab. 1. and the rate constant is written:

$$k = A_A T^{B_A} e^{E_A/T} \quad (26)$$

Table 1. Reactions of NO formation [28]

No.	Reaction	Forward/Backward		
		A_A [$\text{cm}^3\text{mol}^{-1}\text{s}^{-1}$]	B_A	E_A [$\text{kcalmol}^{-1}\text{K}^{-1}$]
1	$\text{N}_2 + \text{O} \leftrightarrow \text{NO} + \text{N}$	$7.6 \cdot 10^{13} / 1.6 \cdot 10^{13}$	0/0	-38000/0
2	$\text{O}_2 + \text{N} \leftrightarrow \text{NO} + \text{O}$	$6.4 \cdot 10^9 / 1.5 \cdot 10^9$	0/0	-3150/-19500
3	$\text{OH} + \text{N} \leftrightarrow \text{NO} + \text{H}$	$4.1 \cdot 10^{13} / 2 \cdot 10^{14}$	0/0	0/-23650

The rate of NO formation [$\text{molcm}^{-3}\text{s}^{-1}$] is given [28]:

$$\frac{d[\text{NO}]}{dt} = \frac{2R_1(1 - \zeta^2)}{1 + \frac{\alpha R_1}{R_2 + R_3}} \quad (27)$$

where $\zeta = [\text{NO}]/[\text{NO}]_e$ and $[\]_e$ stands for equilibrium concentration. The other constants written in eq. (27) are expressed:

$$R_1 = k_{+1}[N_2]_e[O_2]_e = k_{-1}[NO]_e[N]_e \quad (28)$$

$$R_2 = k_{+2}[O_2]_e[N]_e = k_{-2}[NO]_e[O]_e \quad (29)$$

$$R_3 = k_{+3}[OH]_e[N]_e = k_{-3}[NO]_e[H]_e \quad (30)$$

The effective power output and thermal efficiency can be obtained, respectively:

$$P = \frac{WN}{120} \quad \text{and} \quad \eta = \frac{W}{m_d \text{LHV}_d + m_{\text{hyd}} \text{LHV}_{\text{hyd}}} \quad (31)$$

where W is the cycle work and it can be investigated in the previous works [20-32]. N is the engine revolution per minute. LHV_d and LHV_{hyd} are the lower heat values of diesel and hydrogen, and their values are taken as 45730 kJ/kg and 120700 kJ/kg, respectively.

Results and discussion

In order to investigate the influences of steam injection on the performance and NO formation of a hydrogen-enriched Diesel engine, a simulation has been carried out and figures obtained from the analysis have been presented. The two-zone combustion model has been run with the properties of superstar model engine given in tab. 2. Other model running parameters are given in the previous studies [21-26] in detailed. The optimum steam rate is 20% of injected fuel by mass

Table 2. Engine specifications

Cylinder number	1
Primary fuel	Diesel ($C_{14.4}H_{24.9}$)
Secondary fuel	Hydrogen (H_2)
Injection	Direct injection
Stroke volume	0.92 dm ³
Engine speed range	1200-2400 rpm
Bore	10.8 cm
Stroke	10 cm
Compression ratio	17
Power	13 kW
Ambient pressure – P_1	1 bar
Ambient temperature – T_1	300 K
T_{ste}	406 K

in terms of maximum NO reduction and maximum performance increase [18, 22-24] and the optimum hydrogen rate is 30% of fuel by mass in terms of maximum performance increase [3] defined by experimental data. The results obtained from the model have been compared with each other. The consequences of four engine modes have been examined which are diesel engine (D), steam injected diesel engine (D + S20), hydrogen enriched diesel engine (D + H30), and hydrogen enriched diesel engine with steam injection (D + H30 + S20).

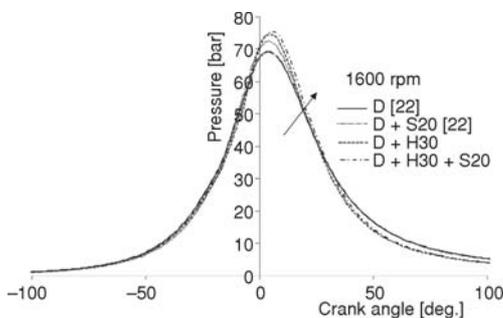


Figure 1. Variation of in-cylinder pressure with crank angle for different engine modes at 1600 rpm

Figure 1 depicts the variation of in-cylinder pressures depending on crank angle for different engine modes. It could be seen from the figure that peak pressures increase with steam injection and in-cylinder pressure is the maximum in the mode of hydrogen enrichment with steam injection. It can be said that hydrogen enrichment leads to late combustion slightly as peak pressures of hydrogen fuel operations happens later compared to diesel fuel modes. Because, diesel-hydrogen mixture burn faster than pure diesel condition. It is fairly clear that the compression and expansion works decrease in hydrogen enrichment modes. However, net total work and also effective power are close to other engine modes.

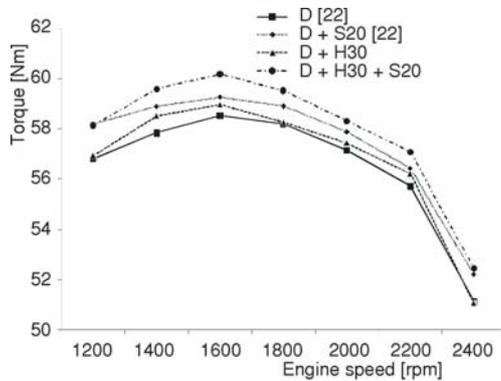


Figure 2. Variation of torque with engine speed for different engine modes

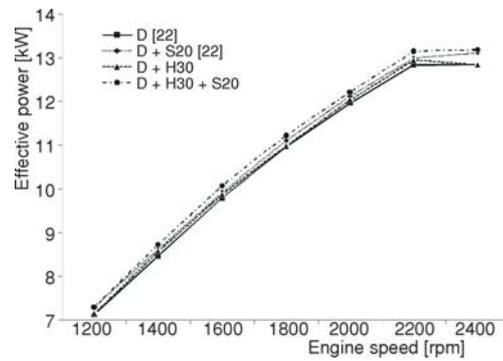


Figure 3. Variation of effective power with engine speed for different engine modes

The engine torques and effective powers of different engine modes are illustrated in figs. 2 and 3, respectively. As could be observed from the figures, application of steam injection into the engine improves the torque and effective power at all engine modes and engine speeds. It is clear that hydrogen enrichment does positively influence the torque and effective power. In hydrogen enrichment mode, the maximum torque reached with steam injection is 60.2 Nm, as it is 58.9 Nm without steam injection at 1600 rpm and the increase rate is 2.2% at this speed. The maximum increase rate is 3.1% with hydrogen enrichment and steam injection at 1400 rpm, the minimum increase rate 2.1% at 2000 rpm, increasing to 58.3 Nm and 57.1 Nm, respectively. The maximum effective power with steam injection and hydrogen enrichment is 13.2 kW at 2400 rpm while the minimum effective power is 7.3 kW at 1200 rpm with improvement of 2.7% and 2.4%, respectively.

Figure 4, comparatively, presents the variation of effective efficiency depending on engine speed for different engine modes. It is clear that the effective efficiency raises at all engine speeds with steam injection. The essential reason for this increment in the effective efficiency, effective power and torque with steam injection is possibly improvement in the atomization of the fuel droplets, suppression of thermal dissociation and the increment in enthalpy of cylinder charge [18, 22-24]. Because, specific heat of steam is greater than that of exhaust gases. The specific heat of the steam absorbs more heat. Therefore, as the engine performance increases, combustion temperature decreases. In the hydrogen enrichment mode, the effective efficiency is considerably increased as hydrogen has more rapid burning characteristics and it mixes well with the air [3]. The maximum effective efficiency with steam injection and hydrogen enrichment is 37.8%, the rate of increase is 2.3% compared to hydrogen enrichment mode without steam injection at 1600 rpm and also it is minimum increase rate. The high-

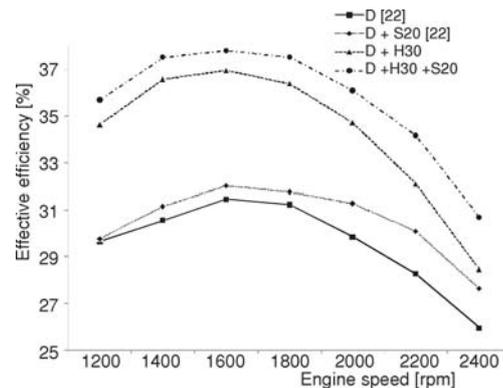


Figure 4. Variation of effective efficiency with engine speed for different engine modes

est increase rate of hydrogen enrichment mode with steam injection is 7.8% at 2400 rpm, compared to hydrogen enrichment mode without steam injection, the effective efficiency is reached to 30.7%. When the model results of hydrogen enrichment mode compared with those of neat diesel mode, it is seen that the rates of increase of effective efficiency rise up to 19.7% and 22.8% without and with steam injection, respectively.

The NO formation rate strongly depends on peak temperature and higher oxygen concentrations [33]. Water injection applications positively influence the NO_x emissions and combustion efficiency. The water droplets which have good atomization vaporize rapidly in the combustion chamber. This vaporization of the water absorbs the heat of the cylinder charge owing to its high heat capacity and increases partial pressure of oxygen in the cylinder. Consequently, these reactions reduce the peak combustion temperature and hence put down NO emissions [18, 24, 34]. Figures 5 and 6 depict variation of in-cylinder temperature and NO formation with engine speed. As could be observed from the figures, as hydrogen enrichment causes slight increase, the steam injection leads to reduction in NO emissions compared to modes without steam injection at all engine speeds, as the peak combustion temperatures decrease.

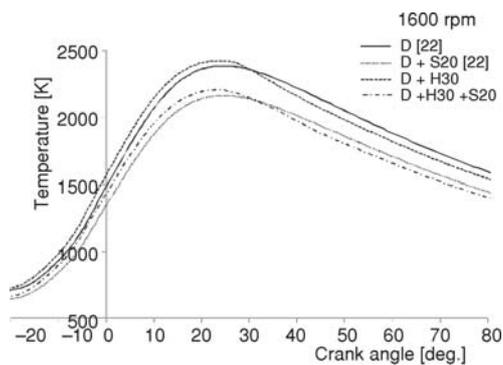


Figure 5. Variation of in-cylinder temperature with crank angle for different engine modes at 1600 rpm

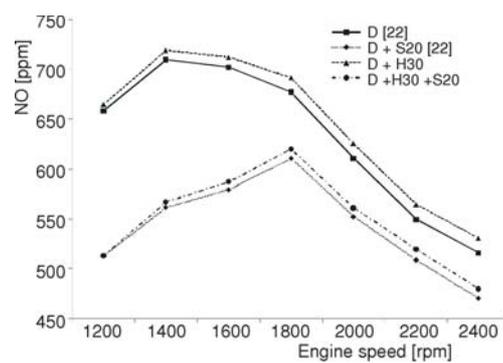


Figure 6. Variation of NO emissions with engine speed for different engine modes

In the hydrogen enrichment mode, the minimum NO with steam injection is 480 ppm, as it occurs 530 ppm without steam injection at 2400 rpm. The maximum reduction rate with hydrogen enrichment and steam injection is 22.1% compared to standard condition at 1200 rpm, the minimum reduction rate is 5.5% at 2200 rpm, decreasing to 513 ppm and 519 ppm, respectively. It obviously seems that the results give a fine approximation for hydrogen-enriched Diesel engines when compared to other studies [3, 7, 22, 23].

Conclusions

In this study, the influences of steam injection on the performance and NO emissions of a hydrogen-enriched Diesel engine have been simulated and investigated with a two zone combustion model. When the modes of hydrogen-enriched Diesel engine compared with those of standard Diesel engine, a substantial increment in the effective efficiency and a little increase in NO emissions have been observed. However, the torque and effective power have been found very close to those of standard and steam injected engines. The main reason of increase in the effective efficiency is the total energy given with diesel fuel and hydrogen into the cycle is less than the energy given with pure diesel. Application of steam injection into hydrogen-enriched

Diesel engine gives the highest effective efficiencies compared to other modes. The effective efficiency rises up to 22.8% at 1600 rpm compared to standard condition. The maximum increase rate with hydrogen enrichment and steam injection in the effective efficiency is 7.8% compared to hydrogen enrichment mode without steam injection at 2400 rpm. The maximum torque is 60.2 Nm at 1600 rpm and the highest increase rate is 3.1% at 1400 rpm. The highest effective power with steam injection is 13.2 kW at 2400 rpm. The minimum NO is 480 ppm at 2400 rpm and the highest reduction rate is 22.1% at 1200 rpm.

As a result, hydrogen-enrichment with steam injection gives the best results in terms of the effective efficiency with a noticeable reduction in NO emission. Thus, hydrogen-enrichment with steam injection combination can be applied to the Diesel engines in order to provide fuel economy and to decrease NO emissions.

Nomenclature

F	– fuel-air ratio	γ	– atomic number of oxygen for diesel fuel
$K_{\%}$	– ratio of the steam mass to the fuel mass	δ	– atomic number of nitrogen for diesel fuel
LHV	– lower heating value, [kJ/kg]	ε	– molar fuel-air ratio
M	– molecular weight	η	– thermal efficiency
m	– mass, [g]	ϕ	– equivalence ratio
NY	– total mole number		
P	– power, [W]		
T	– temperature, [K]		
W	– cycle work, [kJ]		

Greek symbols

α	– atomic number of carbon for diesel fuel
β	– atomic number of hydrogen for diesel fuel

Subscripts

a	– air
d	– diesel fuel
hyd	– hydrogen
st	– stoichiometric
ste	– steam

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