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A simulation and experimental study of the effect of hydrogen added to diesel fuel on performance and exhaust emissions in diesel engine

J.Zareei [1]*, A. Rohani[1]

1 Department of Biosystems Engineering, Faculty of Agriculture, Ferdowsi University of Mashhad, Mashhad, Iran

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A B S T R A C T

Diesel engines are the most trusted sources in the transportation industry. They are also widely used in the urban transportation system. Most pollutants are related to these engines. Therefore, it is important to increase the performance and reduce exhaust emissions of these engines. Alternative fuels are key to meeting upcoming targets. An experimental and numerical study was performed to investigate the effect of diesel fuel and hydrogen addition to diesel fuel from 0 to 30% on performance and exhaust emissions. Also in this research for changing diesel fuel, an indirect injection engine converted to direct injection engine. The simulation study was conducted by Star cd codes and experimental investigation was carried out on a diesel engine (Perkins 1103A-33TG1), three- cylinders, and four-stroke with maximum engine power 72.3hp at 1800 rpm. The results from this study showed that the increase of hydrogen to diesel fuel improves the thermal efficiency, resulting in lower specific fuel consumption. Also, the results showed that adding hydrogen until 30%, the cylinder pressure increase by about 9% and occurred the delay of peak pressure about 8 degrees of a crank angle compared to diesel fuel. The other obtained results in emission with 30%H2+Diesel showed the soot emission reduced 11.3%, HC and CO reduced nearly 36%, but NOx increased by about 8.3% due to high combustion temperature.

1. Introduction

The increasing production of fossil-fuel powered cars in the world and consequent increase in pollutants in major cities have caused serious concerns about increased respiratory diseases. Consequently, experts believe that non-fossil fuels can be used as a viable solution for reducing vehicle emissions. The use of hydrogen fuel as a synthetic fuel not only improves engine performance by increasing the flame speed in the combustion chamber but also reduces emissions.

The recent years have witnessed an increase in the use of different fuels such as combinations of hydrogen mixed with gasoline, diesel, and natural gas, liquefied petroleum gas (LPG), and biodiesel fuels in gasoline and diesel vehicles, leading researchers to further study using laboratory methods and simulations to further decrease emissions and increase the engines' efficiency (Tsolakis and Megaritis 20005; Porpatham et al. 2007; Adnan et al. 2009; Ceviz et al. 2012; Köse and Ciniviz 2013; Banapurmath et al. 2015; Zareei et al. 2018a, 2018b; Karagöz and Ebrahimi Jazayeri 2019; Loganathan et al. 2020).

A number of researchers in the University of Calgary (Li et al. 2005), in a laboratory

*Corresponding Author: *Tel: +985138805819; fax: +985138804686*

Email Address: *javadzareei@um.ac.ir*

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investigation on the effect of hydrogen-gas fuel mixture in a spark ignition engine, found less changes in NOx and significant reductions in CO and CO2 quantities.

Another fuel used in vehicles is ethanol. It is considered an alternative fuel for spark ignition engines; however, it is difficult to evaporate ethanol due to its high latent heat. Therefore, to enhance the ignition process, the hydrogen mixed with ethanol, gasoline, and biofuels have been investigated (Wang et al. 2010; Park et al. 2010; Serin and Yıldızhan 2018; Zareei et al.2020). The results indicate that the HC and CO values initially fall and then rise after adding hydrogen due to the high heat transfer and reduced manifold temperature. In addition, the thermal efficiency and output power of the engine improve.

The addition of hydrogen to gasoline increases the NOx quantity due to the higher ignition temperature of hydrogen compared to gasoline. This issue can be solved by using Exhaust Gas Recirculation (EGR) to retard ignition in indirect injection engines. Lots of research has been conducted on this topic (Du et al.2017; Ji et al.2018; Manigandan et al.2019; Kim eta l. 2018; Zhao et al.2020, Akal et al. 2020), all indicating adding hydrogen to gasoline fuel along with using EGR in both direct and indirect injection vehicles improves the performance and reduces the engine emissions.

Some experimental and computational fluid dynamics (CFD) research has been performed on the addition of hydrogen with different percentages to diesel fuel in the light-duty commercial diesel vehicles. The results indicated that adding hydrogen decreases NOx quantity while it increases the exhaust gas temperature (EGT) (Shirk et al. 2020; Masood et al. 2007; Miyamoto et al. 2011).

An experimental study by Toru et al. (2012) on a four-cylinder diesel engine showed that adding a 10 vol% hydrogen to diesel fuel along with EGR reduces the NOx emission and soot.

Another remarkable study has been conducted on hydrogen as an alternative fuel in diesel engines (Lata et al. 2012). The autoignition temperature of hydrogen is 858K, while that of diesel fuel is 525K. Therefore, diesel can be used as a pilot fuel for hydrogen ignition (Sahoo et al. 2009). The impact of adding hydrogen to diesel fuel in a marine engine showed that fuel consumption increase by about 2.6% at 75% load and adding 22% hydrogen results in a peak heat release rate of 25.77% (Pan et al. 2014; Karagöz et al. 2016), leading to a rise in output power of the engine.

Hydrogen cannot be utilized as an alternative fuel in diesel vehicles due to its high autoignition temperature. It, therefore, requires an ignition source in compression ignition engines. High ignition temperature and high ignition delay are the most important barriers for using hydrogen as an alternative fuel in diesel vehicles. Reviews indicate that the hydrogen quantity, the use of advanced technologies such as EGR, and the injection and combustion timing play significant roles in reducing emission and improving engine performance (Koten 2018; Karagöz 2018; Nag et al. 2019; Tutak et al. 2020; Vijayaragavan and Ramachandran 2020).

The present work studies the effect of hydrogen added to diesel fuel on performance and exhaust emissions by experimental and simulation investigation. So that in this work investigates the relationship between the thermal efficiency, specific fuel consumption, power output and exhaust emissions like soot, NOx, CO and HC as an output and the operating condition (hydrogen level, full load condition) for hydrogen/diesel fuel engine. There are very few investigations that how much hydrogen in the blend of diesel fuel can improve engine performance and exhaust emission. A multidimensional software package was implemented in this work. Experimental work was also carried out to verify the accuracy of the simulation results.

2. Simulation, geometry, and engine mesh generation

The engine used in the simulation was a 3.3L, three cylinders four-stroke indirect-injection compression ignition engine. The fuel used was diesel with a cetane number of 57 and additive fuel was hydrogen with different percentages. The operating conditions and engine specifications were summarized in Table 1. This engine is equipped with a turbocharger and an intercooler. To examine the performance and emissions of the engine, it was modeled using CATIA, meshed in GAMBIT, and simulated in STAR-CD. Moreover, the engine was converted from an indirect injection type to a direct injection type.

Table 1. Specification of the diesel engine

Engine	Value	Unit	Engine	Val	Unit
Maximu	53.9/1800	KW/RP	Boost	1.2	bar
Combusti	Indirect		Air/Fue	40:1	
Bore and	105*127	mm	Start of	24°	bTD
Connectin	104	mm	Injectio	20°	
Aspiratio	Turbochrge				
Compress	17.25:1	-			
Fuel	Diesel+ Hydrogen				

To model the engine, the geometrical data of the engine, including the manifold, cylinders, and valves were taken from the actual geometry of the engine, similar to the engine input data. The performance parameters such as the engine operating speed, environmental conditions, ignition timing, and injection timing, were considered as input data. The engine performance, outlet emission, the time average of momentum, the energy required for combustion simulation, and droplet diffusion were determined by simultaneously solving the continuity equations using the mentioned software.

In modeling, the governing instability, density, multiple-component equations of mixtures were solved using the CFD program for reactions that are a mixture of several gases with the dynamic flow of fuel injection from the air valve closing timing to soot valve opening timing.

The turbulent flow inside the combustion chamber was modeled by simulating the k-ε turbulent defined variable for density currents. In this model, the initial turbulence on the surface of fuel spray is proportional to its wavelength and other physical and dynamic variables of the fuel injected in the flow amplitude. The drops were injected with a specified size equal to the outlet diameter of spray.

The ignition process starts from 12 degrees before top dead center (BTDC) to 6 degrees after top dead center. The Dukowicz model was used to initiate heat transfer and droplet evaporation, in which the droplet temperature is assumed to be uniform.

The eddy-break-up model of the ignition process was simulated based on turbulent mixing. *Stochastic turbulence modeling* was applied to the interactions between turbulent particles by adding an *oscillating velocity* to the average velocity of the gas. Wall Jet simulation was applied to predict the fuel droplets-wall *collision (*Halstead et al. 1977*).*

The Shell auto ignition modeling as a multi-stage motion pattern was applied to vortex turbulence ignition modeling. The Zeldovich mechanism was used for Nitrogen oxide (*NOx*) pollution formation and the Hiroyasu and Magnussen mechanism was used for soot formation (Patterson et al. 1994).

The above mechanisms were simultaneously solved to model the diffusion and ignition of fuel droplets in the turbulent flow field, and then, fuel spray-wall collision and fuel ignition were numerically analyzed.

Finally, the numerical results from modeling were compared with the experimental results. It should be mentioned that the thermophysical properties of hydrogen-diesel fuel depend on the raw materials required to its production, and thus, our results are valid just for diesel fuel with the cetane number of 57. The thermophysical properties of hydrogen-diesel fuel were listed in Table 2.

Table 2. Diesel and hydrogen fuel properties

Properties	Diesel	Hydrogen
Density (Kg/m^3)	850	0.09
Molecular Formula	$C_{10}H_{22}$	H_2
Molecular weight (Kg/Kmol)	142.3	2.01
Stoichiometric fuel-air ratio	0.0777	0.093
Auto ignition temperature (°C)	280	858

2.1. Initial and boundary conditions

Calculations were performed on a closed system from the air valve closing timing at the *crank angle of 150º before the* bottom dead center (BDC) to the exhaust valve opening timing at the *crank angle of 125º* after BDC.

Figs.1 and 2 represent the geometry of the engine and the network numerically designed for the engine. To satisfy independence from the network, a computational network composed of at least 218000 cells at the *crank angle of 150º before the* top *dead center* (TDC) was considered.

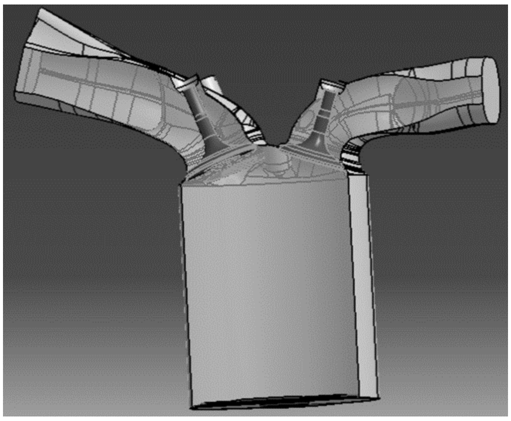


Fig 1. The geometry of the model designed for a diesel engine.

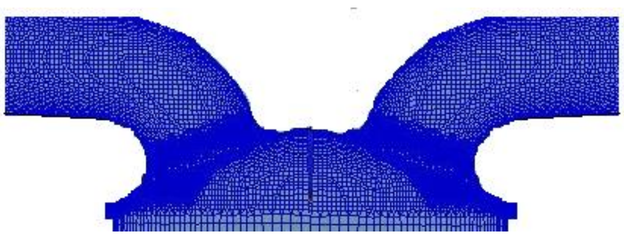


Fig 2. A section of the diesel engine network

Study of network independence in fluid software is one of the most important parts of any simulation. For this purpose, different mesh values were considered in three different cases. The obtained results showed that the desired results can be achieved with proper accuracy with this number of meshes. This can be accessed in references (Zareei et al. 2014).

2.2. Modeling the nitrogen oxide formation

In this research, a multi-point ignition model was used to calculate the rate of releasing heat and also to examine the engine function. In the hydrogen-diesel fuel mixture, 10 main components were considered in the reaction according to the following equation. In this reaction, the components O, H, OH, and NO are decomposed.

$$x\emptyset\varepsilon C_\alpha H_\beta O_\gamma N_\delta + yH_2 + 0.21O_2 + 0.79N_2 \rightarrow v_1\,CO_2 + v_2\,H_2O + v_3\,N_2 + v_4\,O_2 + v_5\,CO + v_6\,H_2 + v_7\,H + v_8\,O + v_9\,OH + v_{10}\,NO \tag{1}$$

. In above equation N is total mole numbers Where: (is the number of C atoms, (is the number of H atoms, (is number of O atoms, (is number of N atoms, x is percentage of diesel in diesel–hydrogen fuel blend, why is percentage of hydrogen in diesel–hydrogen fuel blend, (is the fuel–air equivalence ratio, (is stoichiometric molar fuel–air ratio, v_i is a coefficient describing the product composition of I-the species.

One of the main issues in the field of pollutants in diesel engines is the rate of emitted NOx. The Zeldovich mechanism was used for NOx formation, which includes three main steps (Missen et al. 1999).

$$O_2 \rightarrow 2O \tag{2}$$
$$N_2 + O \rightarrow NO + N \tag{3}$$
$$N + O_2 \rightarrow NO + O \tag{4}$$

The key reaction is reaction No. 4, nitric oxide. The rate of this reaction depends on the *oxygen atom concentration*. The governing equation to calculate the nitric oxide concentration in ignition products is expressed as follows:

$$\frac{d[NO]}{d\theta} = \frac{p \times 2.33 \times 10^7 \times e^{\frac{38020}{Tz}} [N_2]_e [O]_e \{1 - ([N}{R \times T_z \left[1 + \frac{2365}{T_z} \times e^{\frac{2365}{T_z}} \times \frac{[No]}{[O_2]}\right]} \times \frac{1}{rps} \quad (5)$$

2.3. modeling of soot formation

Incomplete combustion of hydrocarbons is the main source of soot. Under normal conditions, the soot concentration in the exhaust gas is expressed by the Razleytsev equation (Razleytsev 1980):

$$[C] = \int_{\theta B}^{480} \frac{d[C]}{dt} \cdot \frac{d\theta}{6n} \left(\frac{0.1}{p}\right)^{\frac{1}{\gamma}} \quad (6)$$

Where $\gamma = 1.333$ is the adiabatic power of the exhaust gas, *C* is the soot concentration in the cylinder, and *p* is the cylinder pressure at *60º (crank angle) before* BDC. The Hartridge number of soot is calculated as follows:

$$hartridge = 100\left[1 - 0.9545 \times e^{(-2.4226[C])}\right] \quad (7)$$

The soot number is measured using experimental diagrams as a function of Eq. (7). The particle emission determined from the Alkidas equation is a function of the Bush soot number (Alkidas 1984).

3. Test method

To confirm the simulation accuracy, an engine with the specifications mentioned above was installed on the test bed. To measure the changed engine performance at different speeds, *different hydrogen* quantities were added to the diesel fuel using the installed system as shown in Fig. 3.

Fig 3. Control panel and test engine on dynamometer

A short-term test was conducted aimed at comparing engine efficiency between hydrogen-diesel fuel mixtures. The controlled variables of load applied by the dynamometer to the engine are speed, fuel type, and percent hydrogen added to the diesel fuel. All tests were performed at the standard temperature and humidity conditions. First, the engine operated with diesel fuel as the main fuel for 15 minutes to rich steady state conditions without load, then, according to the test table, the values of load, speed, and the desired fuel mixture were applied through dynamometer control panel, and finally, the values for the engine performance test were read.

Also, a piezoelectric pressure transducer installed on engine body, was used to measure the engine in–cylinder gas pressure. Since the in-cylinder pressure transducer was of the piezoelectric type, the inlet manifold pressure was measured to measure the absolute pressure by adjusting the in-cylinder pressure at every engine cycle when the piston was at the top dead center. These pressure readings, in addition to several control and operation temperatures, were logged by PCs utilizing National Instruments (NI) data acquisition systems. The flow of air introduced to inside of cylinder was measured using a Romet positive displacement volumetric air flow metre. Pressure and temperature measurements, taken immediately adjacent to the air flow metre inlet, were used to convert the volumetric air flow rate to air mass flow rate. The oil and coolant water were circulated around the engine head and crankcase. Diesel fuel direct injection inside of cylinder with the injection pressure, injection timing and duration controlled using an engine control system.

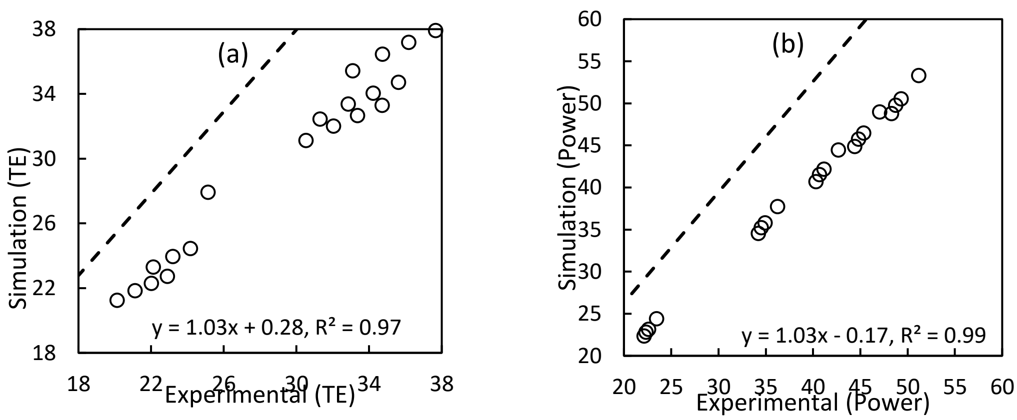
Hydrogen gas was supplied from a compressed hydrogen gas cylinder with 300 bar pressure and was injected into the engine inlet manifold upstream of the inlet valves. The flow of H_2 was controlled using a Bronkhorst thermal mass flow controller, to an accuracy of ±0.08 L/min.

The pollution results were recorded using an *AVL DiGas 4000* pollutant analyzer. In this test, the engine speed was changed from 1000 RPM to 1800 RPM. The percent hydrogen added to diesel fuel was 0%, 10%, 20%, and 30%, respectively.

4. Validation of simulation data with experimental data

In this study, the effect of hydrogen added to diesel fuel with different percentages of 10%, 20%, and 30% was examined on the engine performance and exhaust emissions. To evaluate the accuracy of the simulation data, a comparison was made between the simulation and experimental data. Fig. 4 represents that there is an agreement between values obtained from experimental tests for engine performance parameters and simulation results. As can be seen, in all cases, there is a slight difference between the relationship these two data sets and the best fitting line (y = 1.00x + 0.00, R2 = 0.99). In all cases, the coefficient of determination (R^2) between experimental and simulation data is greater than 99%. Therefore, the results from modeled engine operating conditions are completely consistent with experimental conditions, indicating the reliability of simulation data.

In figures below, the curves of (a), (b), (c), (d), (e), (f), (g) and (h) are, respectively, Thermal efficiency, Power, Specific fuel consumption, NOx, Soot, HC, CO and Pressure.



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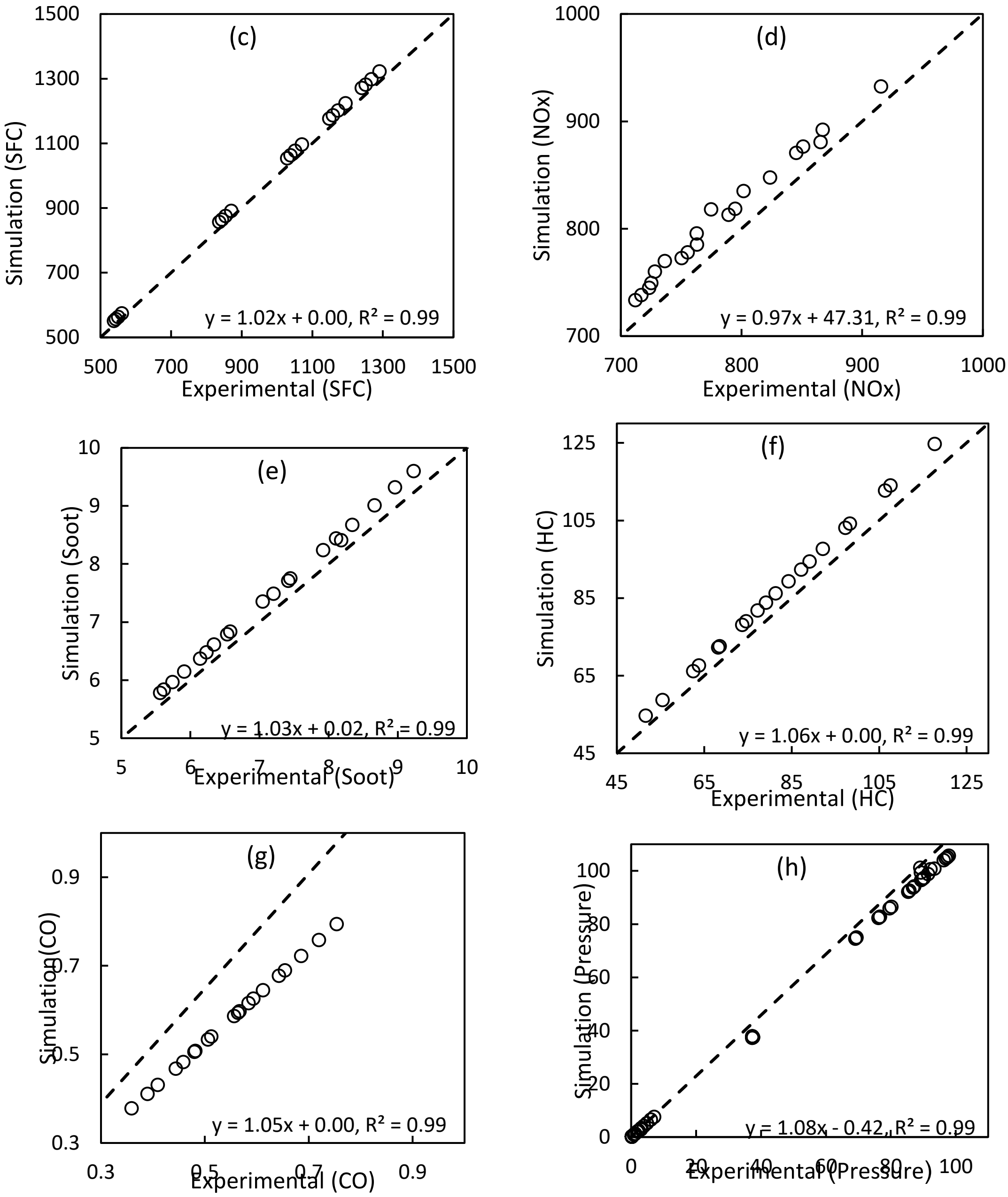

Fig.4 comparison between simulation and experimental data

5. Results and discussion

5.1. Effect of hydrogen addition to diesel fuel on engine performance

5.1.1.Engine efficiency

Fig. 5 represents the changes in engine thermal efficiency versus engine speed for pure diesel and the percent hydrogen added to diesel fuel. The maximum thermal efficiency at full load for pure diesel is 33.1% at 1800rpm. By adding hydrogen to diesel fuel with percentages of 10%, 20%, and 30%, the maximum efficiencies are 34.74%, 36.19%, and 37.66%, respectively; indicating thermal efficiency can be increased by 13.77% in the case of adding 30% hydrogen to diesel fuel. Therefore, as the rate of diesel fuel flow decreases in the combustion chamber, the hydrogen increases in the fuel composition. However, the thermal efficiency increases due to higher hydrogen flame speed (Zareei et al. 2019). The trend of increasing the thermal efficiency induced by 10%, 20%, and 30% hydrogen added to diesel fuel in high speeds is almost the same, while the thermal efficiency with 30% hydrogen increases significantly compared to 10% and 20% at the lower speeds. This suggests that greater thermal efficiency can be

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achieved by increasing the percent hydrogen at lower speeds in a diesel engine.

Fig. 6 represents the variation of the cylinder pressure versus crank angle in full load condition. It can also be seen that the peak cylinder pressure increases by 8.26 bar by adding hydrogen fuel to the diesel fuel composition. Although the injection initiation and the injection duration are the same in all diesel compositions, the peak pressure and the crank angle are not the same as the maximum pressure. The delay of peak pressure of 30% hydrogen added to the diesel fuel composition is about 8º due to a higher ignition temperature of hydrogen as compared to pure diesel. This issue helps in reduction of power drop when the piston goes down in the power generation stroke. In addition, the increased pressure of hydrogen-diesel fuel blend is due to high flame speed of hydrogen fuel.

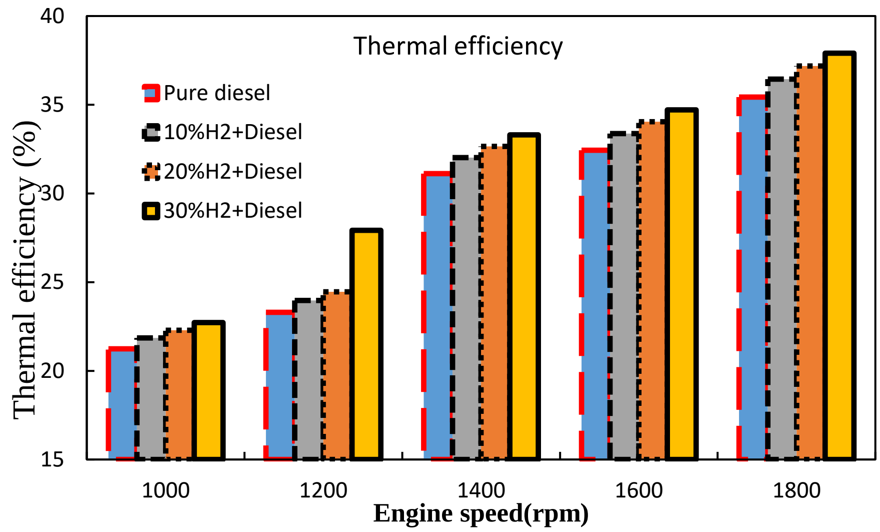

Fig 5. Variations of thermal efficiency versus engine speed with adding hydrogen to diesel fuel

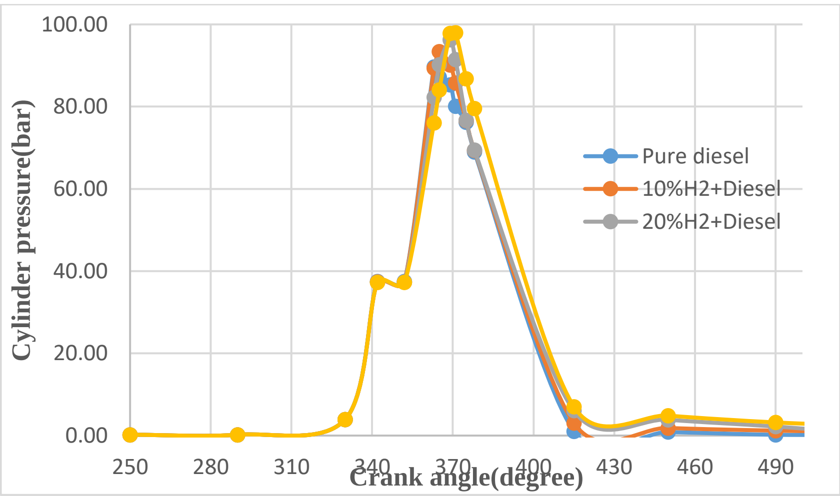

Fig 6. Variation of cylinder pressure versus crank angle with adding hydrogen to diesel fuel

5.1.2. Engine power output and specific fuel consumption

Figs. 7 and 8 represent the changes in power and specific fuel consumption with pure diesel, 10%, 20%, and 30% hydrogen added to diesel fuel at different engine speeds at full load. According to the figures, the engine power increases by increasing the percent hydrogen added to the diesel

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fuel, while the maximum engine power is 51.15 kW with 30%H_2+diesel fuel under experimental conditions, indicating an increase of 5.9% in power compared to pure diesel. It also can be mentioned that the specific fuel consumption decreases with increasing the percent hydrogen in the diesel composition due to the increased power. Thus, the maximum specific fuel consumption occurs when only diesel fuel is used. In general, special fuel consumption decreases and engine power increases as the hydrogen quantity increases in the diesel composition. This is true for all three modes of 10%, 20% and 30% hydrogen added to diesel fuel. This is due to the more complete combustion of the hydrogen-diesel fuel mixture.

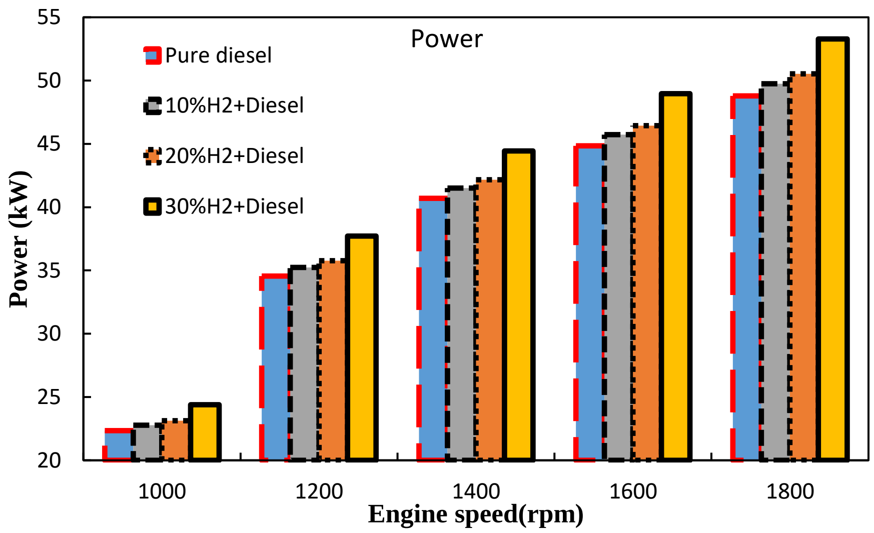

Fig 7. Variation of engine power versus engine speed with adding hydrogen to diesel fuel

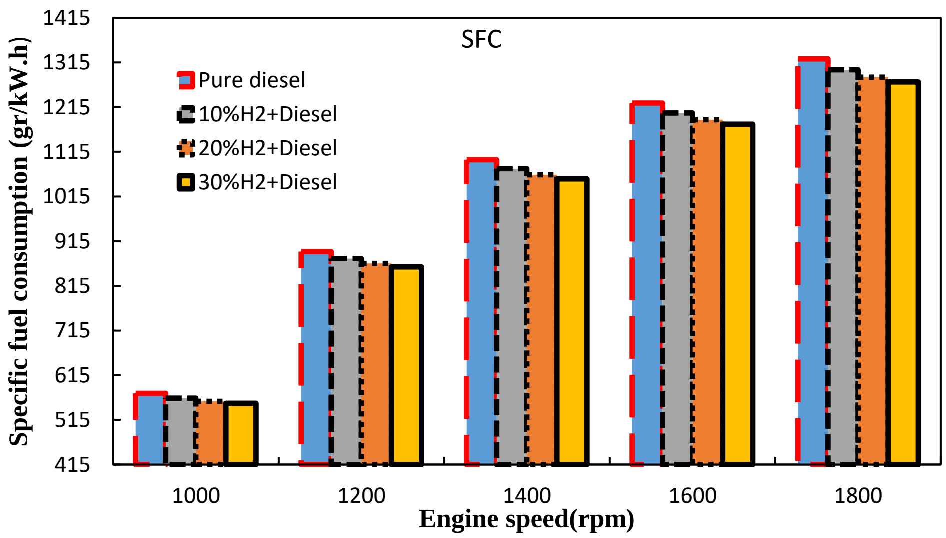

Fig 8. Variation of engine specific fuel consumption versus engine speed by adding hydrogen to diesel fuel

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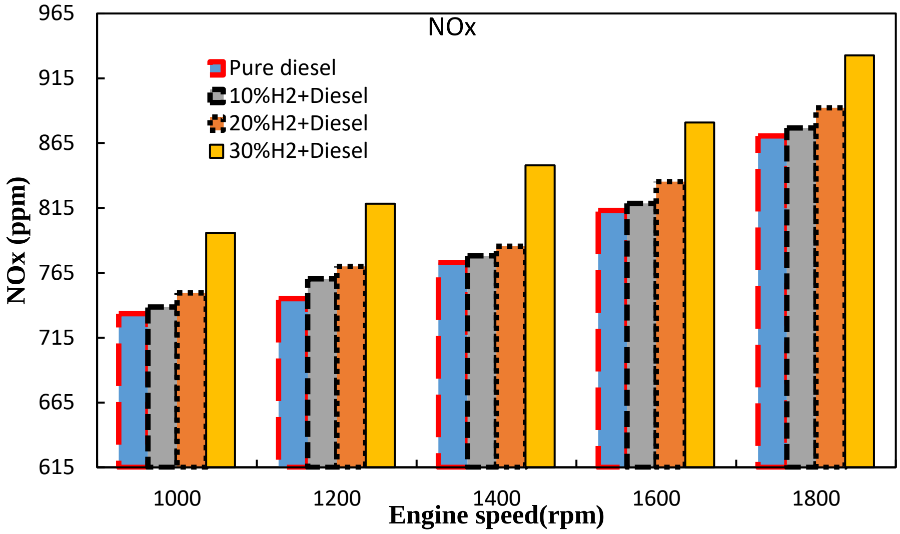

Fig 9. Variation of NOx emissions versus engine speed with adding hydrogen to diesel fuel

5.2. Effect of blend of hydrogen and diesel fuel on exhaust emissions

5.2.1.NOx and soot emissions

According to Figs. 9 and 10, NOx increases by adding hydrogen to the base fuel (diesel) and increasing the engine speed, and also soot increases as the engine speed decreases. In general, NOx is caused by high ignition temperature. Thus, increased NOx in this engine is due to the high ignition temperature induced by adding hydrogen to diesel fuel. As a pressure increase is required in the combustion chamber to produce more power, more complete fuel combustion is required in the combustion chamber to produce more pressure. The flame speed and ignition temperature increase by adding hydrogen to fuel. Therefore, NOx increases by about 8.3% by adding 30% hydrogen to diesel fuel.

The reason for increased soot in the diesel engine is the increased rate of diesel fuel flow input to the combustion chamber. The diesel fuel flow decreases as the hydrogen quantity increases in diesel fuel. Therefore, more complete combustion occurs and eventually the quantity of formed soot decreases by adding more hydrogen to diesel fuel. Fig. 10 represents the maximum soot reduction of 11.3% with 30% hydrogen at 1200 RPM.

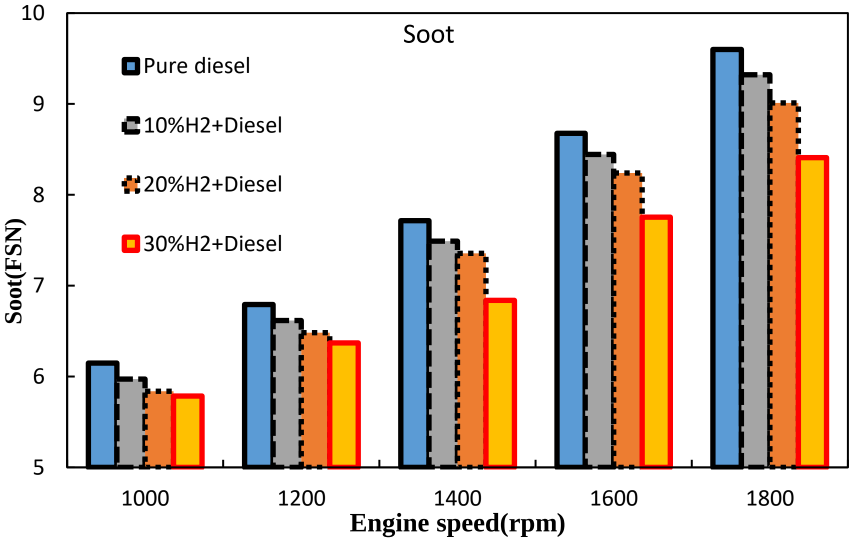

Fig 10. Variation of soot emissions versus engine speed with adding hydrogen to diesel fuel

5.2.2.HC and CO emissions

The variation of HC emission versus engine speed by adding hydrogen to diesel fuel at full load condition is shown in Fig. 11.

Since hydrogen fuel cannot contain carbon, unburned hydrocarbons reduce by adding hydrogen to diesel fuel. The minimum HC was achieved with 30% hydrogen in the fuel composition, which shows a decrease of about 36% compared to diesel fuel. Therefore, according to the results of the previous research (Talibi et al. 2014; Nag et al.2019; Tutak et al. 2020), it can be said that such reduced hydrocarbons can be a good achievement in reducing diesel vehicle emissions.

Fig. 12 shows the variation of CO emission versus engine speed by adding hydrogen to diesel fuel at full load condition. The trend of HC variations is like CO emission. CO production is induced by incomplete combustion in the combustion chamber. Although the CO production in the diesel engines is less, it can be reduced more by using the synthetic hydrogen-diesel fuel compared to pure diesel due to higher ignition temperature and more complete combustion so that the minimum CO with about 36% reduction belongs to the 30%h_2+diesel fuel.

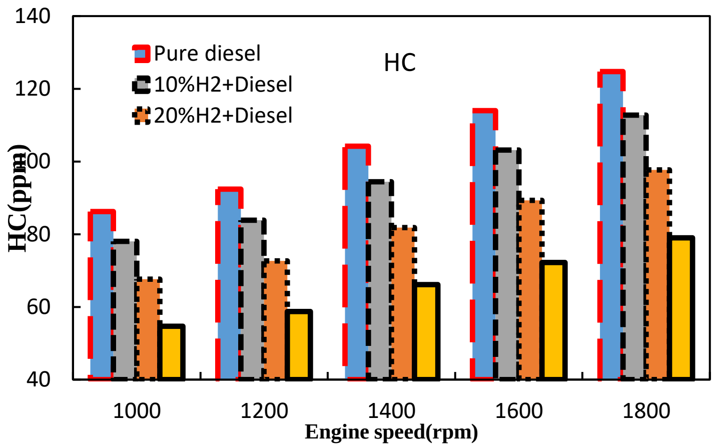

Fig 11. Variation of HC emissions versus engine speed with adding hydrogen to diesel fuel

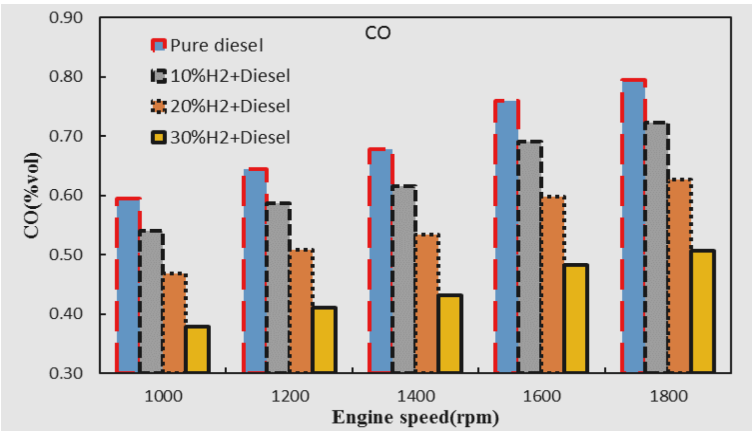

Fig 12. Variation of CO emissions versus engine speed with adding hydrogen to diesel fuel

6. Conclusions

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The main conclusions in this study are listed as below.

1- The engine thermal efficiency was increased by adding hydrogen to diesel fuel due to the increased flame speed inside the combustion chamber. The maximum increase in thermal efficiency with 30% hydrogen added to diesel fuel was 13.77% compared to pure diesel at 1800 RPM.
2- Adding hydrogen to the diesel fuel composition increased the pressure inside the combustion chamber by about 8.26 bar and a delayed peak pressure was achieved at the *crank angle of* 8º due to the degree of hydrogen ignition higher than pure diesel.
3- The engine power increased by 5.9% by increasing the hydrogen quantity in the diesel fuel composition due to more complete combustion, while the specific fuel consumption decreased as the engine power increased.
4- The effects of adding hydrogen to diesel fuel were reduced soot by 11.3% with H_2+diesel fuel and increased NOx by 8.3% due to high ignition temperature.
5- The trend of reducing HC and CO emissions was the same by increasing the hydrogen quantity in the diesel fuel composition so that HC and CO emissions decreased by about 36% by adding 30% hydrogen.
6- The general result was that if 30% hydrogen is added to diesel fuel, the engine performance improves and the emissions would be significantly reduced while the NOx quantity increases. It was also demonstrated that new technologies such as EGR and catalysts can solve this problem.

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