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Simulation of Hydrogen Combustion in Neon-Oxygen Compression Ignition Engine



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ARTICLE INFO	ABSTRACT
Article history: Received 21 October 2020 Received in revised form 22 December 2020 Accepted 22 December 2020 Available online 30 December 2020	The elimination of nitrogen oxide (NO _x) emissions for hydrogen combustion in the compression ignition (CI) engine is the primary concern, therefore replacing nitrogen with noble gas is one of the solutions to eliminate the NO _x emission and improve the engine thermal efficiency. The current research trend focuses on oxygen-argon as the most suitable working. However, external heating for intake is required if operated in low compression ratio (CR) engines. Hence, neon is another option because the specific heat ratio is as high as other noble gasses, and the lower density of neon gas provides a higher temperature during compression. This paper aims to acknowledge neonoxygen gas as the working gas for stabilization of the hydrogen ignition in the standard ambient intake condition. Besides, the optimum intake temperature and suitable CR were also determined from the analysis of the combustion properties. A computational analysis was performed using Converge CFD software with specific initial temperature and CR conditions base on Yanmar NF19SK engine parameters. The study showed that the minimum initial hydrogen temperature in the neon-oxygen atmosphere was lower than that of oxygen-argon. However, the initial minimum temperature needed for compression ratio 10:1 is 310 K, with the unstable ignition and potential of detonation. Considering the detonation phenomena, the most suitable initial temperature selected is at 380K For operation in ambient condition, pre-heating of intake. The neonoxygen atmosphere is proved as the good working gas in CI engine hydrogen combustion when operated at a higher compression ratio and requires no modification. Analysis of the injection parameters and control of heat loss in the neonoxygen atmosphere is needed in the future for hydrogen combustion strategies for this type of engine.
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1. Introduction

Hydrogen as alternative energy can solve the issue of carbon emissions and reduce the dependency on fossil fuels. Hydrogen is an excellent energy carrier and has been widely used in many applications. In Malaysia, biomass contributes to the most promising hydrogen production which makes hydrogen is an environmentally friendly fuel and an excellent energy carrier [1]. Hence, the sources can provide enough supply for many hydrogen application sectors, mainly in transportation and power generation.

The new trend of hydrogen in the transportation sector has used the fuel cell system to provide the cleanest and most powerful vehicles. However, it will require higher costs, shorter lifespan, and limited engine power compared to hydrogen in an internal combustion engine [2-3]. Since the 80th century, many car manufacturers have proposed the application of hydrogen in the internal combustion engine by dual-fuel and pre-mixed mode [4]. This solved the carbon problem from the conventional ignition compression (CI) engine and delivered more power for the vehicles that are reliable for heavy-duty work. Due to the very wide flammability limit and high flame speed, hydrogen combustion can deliver more power for the engine [5].

However, hydrogen has a high auto-ignition temperature and it becomes the challenge for hydrogen development in compression ignition (CI) engine [6]. Table 1 shows hydrogen thermophysical characteristics. CI engine ignition works based on the piston's compression power to increase the in-cylinder temperature to ignite the fuel. The compression of natural air to ignite the hydrogen is slightly difficult due to the high auto-ignition temperature. For this situation, the engine needs a very high compression ratio and requires the installation of an intake manifold pre-heating system to raise the initial gas temperature [7].

Thermo-physical characteristics of hydrogen [8]			
Properties			
Molecular weight (kg/mole)	2.01		
Density (kg/m3)	0.0838		
Flashpoint (K)	585		
Flame speed (cm/s)	270-325		
Octane number	130		
Stoichiometric Fuel air ratio	34.4		
Auto-ignition temperature (K)	858		

Tabla 1

Therefore, the noble gas are a great option to solve the ignition problem of hydrogen. Noble gas is non-reactive gas with a high specific heat ratio. The compression of high specific heat ratio noble gas can rise the in-cylinder temperature and reach the required auto-ignition temperature [9]. In this type of engine design, the noble gas replaced the nitrogen by 79 % by mass and another 21% of oxygen during the intake stroke. Oxygen and noble gas are supplied from the gas tank into the intake chamber, and then the water vapour from the exhaust is separated from noble gas by using the condenser [10]. Noble gas has higher production cost and challenges in storage. Hence, the recirculation of exhaust gas is needed to reduce the gas operational costs. Recirculation of exhaust not only suggested in noble gas work but also proposed in the conventional diesel engine to control the emission of NO_x [11]. The good combination of the exhaust system, recirculation of heat to the intake pre-heating, sensible heat recovery, direct injection of hydrogen, and suitable gas storage management can produce a very high thermal efficiency and reduce the total operation costs [12]. Since the noble gas did not react to other gas during the combustion process, it will be easily separated and recirculated after the combustion process.



The previous study about hydrogen in the direct injection compression ignition engine has based primarily on the argon-oxygen atmosphere. The first study about hydrogen combustion in the argon-oxygen atmosphere is conducted in a spark-ignition engine, investigated by de Boer *et al.*, [13] in 1980. The hydrogen, argon, and oxygen gas are readily premixe. Meanwhile, direct injection hydrogen combustion in CI engine is developed by Ikegami *et al.*, [14] in 1982 and found a great improvement in thermal efficiency from the mixture. The key of interest in hydrogen combustion on argon-oxygen atmosphere continued by Mansor *et al.*, [9] and Shahsavan *et al.*, [15] which studied the flame propagation of hydrogen in control volume combustion in the argon-oxygen atmosphere in low compression require the intake manifold pre-heating to increase the temperature during compression to reach the hydrogen auto-ignition temperature. However, this method includes additional costs for heating installation and also decreases the thermal efficiency of the engine.

Therefore, other noble gas with a high specific heat ratio such as neon were studied to prove the feasibility for hydrogen ignition. Neon is the second-lightest noble gas element after helium, which is followed by argon. The specific heat ratio of neon is slightly lower than argon. However, the low molecular mass of neon able to provide a better combustion environment for hydrogen since it will allow the hydrogen jet to penetrate better due to its low density. The theory is supported by research from Shahsavan *et al.*, [15] which compared the penetration of hydrogen in argon and xenon. The research found that the density difference of these two gases provides better jet development of hydrogen in argon compared to xenon. Good penetration gas allows the fuel and the gas to mix well. Based on the finding, neon can be concluded as better working gas to raise the temperature higher. The summary of thermo-physical properties of neon, nitrogen, and argon are explained in Table 2.

Table 2				
Thermo-physical properties of neon, argon, and air [6,18]				
Properties	Neon	Nitrogen	Argon	
Density (g/dm3)	0.9002	1.165	1.7818	
Boiling point (K)	27.3	77.15	87.4	
Melting point (K)	24.7	63.15	83.6	
Atomic number	10	7	18	
Specific heat capacity	1030	1040	519	
Specific heat ratio	1.64	1.40	1.76	

This paper aims to study the neon-oxygen atmosphere as the working gas to enhance the ignitability of hydrogen at the state of the ambient atmospheric intake. The simulation was performed using Converge CFD software, based on the Yanmar NF19SK direct injection compression ignition engine parameter. The quality of neon compression in cold flow and hydrogen injected state is compared to the hydrogen combustion characteristics in the argon-oxygen atmosphere and normal air atmosphere. At 10°CA BTDC, hydrogen was injected directly into the combustion chamber operated in low compression ratio condition. The minimum initial temperature is tested and identified to investigate the need for intake manifold pre-heating in the neon-oxygen atmosphere to ignite the hydrogen. The simulation was conducted on a low and high compression ratio set up to achieve the optimum hydrogen combustion condition set up in the neon-oxygen atmosphere. The ability of the neon-oxygen atmosphere is highlighted and suitable parameters for hydrogen combustion in neon-oxygen atmosphere operation are proposed. In the future, apart from the suitable parameter of and proper investigation of hydrogen combustion in the neon-oxygen atmosphere directly in the neon-oxygen atmosphere.



2. Methodology

The simulation was performed on a model of a direct injection Yanmar NF19SK ignition compression engine. Table 3 displays the specification of the engine and the injection setup. The model of the combustion chamber was adapted from Hafiz *et al.*, [17]., and the parameter of the experiment was obtained by research from Rey [16]. The engine was run at a constant engine speed of 600 RPM and simulated from the intake valve close (IVC) until the exhaust valve open (EVO). Parameters for injection such as injection timing, injection duration, and injection pressure were held constant during simulation research. The hydrogen was injected through a 0.8 mm diameter nozzle, which begins at 10°CA BTDC for 5°CA duration. Before the injection begins, the cylinder was filled with 79% neon gas and 21% oxygen by mass. Upon injection, hydrogen mixed with neon-oxygen gas with the equivalence ratio of 0.08 [6].

Table 3				
Specification of Yanmar NF19SK engine [16-17]				
Specification				
Borexstroke (m)	0.11x 0.106			
Compression ratio	10,12,14			
Connecting rod length (m)	0.15			
Engine operation speed (RPM)	600			
Intake valve close, IVC (°CA)	-179			
Exhaust valve open, EVO (°CA)	179			
Injection timing (°CA)	-10			
Top dead center, TDC (°CA)	0			
Injection duration (°CA)	5			
Injection pressure (MPa)	8			
Nozzle diameter (m)	0.0008			
Initial pressure (MPa)	0.114			
Initial temperature (K)	300, 320, 340, 360, 380			

The hydrogen gas was injected from the position shown in Figure 1 based on the position and injection parameter from Rey [16], and Hafiz *et al.*, [17]. The injector is located at a radial position, 0.0058 m from the cylinder axis, 90° from the y-axis, and 0.0052 m below the x-axis. The position was selected in the experiment due to the diagnostic setup application on top of the cylinder head. Therefore, the simulation set up was based on the experimental setup, with a compression ratio (CR) of 10 [16]. However, compression ratio 10 is considered low for the normal compression ignition engine. The normal compression ignition engine has a compression ratio of between 12:1 and 24:1[19].

Figure 1 shows the 3D combustion chamber model built and generated in the software before and after the meshing. In order to get the accurate velocity profile, the embedding region also covered the cylinder and spray area with scales 2 and 4. The embedding region improves the grid resolution based on the time and position of the embedding at the given embedding cylinder and inflow region.







From the experiment, the intake manifold pre-heating system was applied to the machine to raise the initial temperature to 380K. A pre-heating system in the engine indicates that more energy required to heat the intake gas and the thermal efficiency of the engine will be decreased. Therefore, this simulation work will discuss the hydrogen combustion behaviour in the neon-oxygen atmosphere in low intake temperature to avoid as much as possible the need for pre-heating intake. Hence, the simulation is conducted at different intake temperatures, to identify the minimum intake temperature for hydrogen ignition in a low compression ratio engine. After that, if the minimum intake temperature is not matched with ambient, the suitable compression ratio for the hydrogen combustion in the ambient temperature intake also is investigated. The engine's compression ratio is varied based on the standard compression ratio of a conventional CI engine which is typically from 12 to 24. With the correct compression ratio of the engine at the standard ambient intake temperature, no intake pre-heating will be needed. For better understanding, the flow chart of the selected parameter is shown in Figure 2.

The simulation was performed by using the Converge CFD software, which exclusively builds for internal combustion engine analysis. Converge CFD software equipped with adaptive mesh refinery (AMR) feature that can refine the mesh automatically depending on the combustion chamber situation. AMR feature was activated with the target cell number of 5 million cells. Hence, the meshing quality is improved as it produces automatic orthogonal meshing. Besides, based on the same model from the previous study, the independent grid test was performed to determine the correct grid size input for the mesh by comparing the three different grid sizes of 3 mm, 4 mm, 5 mm, and 6 mm. From the study, the grid size of 5 mm was the most appropriate with an error of 6.5% when the AMR activated [6].





Fig. 2. Parameter selection flow chart

The simulation was performed in the full hydrodynamic mode, and the compressible solver was developed with the help of the PISO convergence algorithm to solve the momentum Eq. (1) before it was transformed into pressure, Eq. (2) and correction pressure, Eq. (3). The other solver equation was solved from the minimum and the maximum number of corrections calculated. PISO solver is an important input for the simulation. The accuracy and the iteration of simulation data rely on information from these inputs.

$$\frac{\rho^n u_i^n}{dt} - \frac{\rho^n u_i^n}{dt} = -\frac{\partial P^n}{\partial x_i} + H_i^* \tag{1}$$

$$\frac{\partial^2}{\partial x_i \partial x_i} \left(P^* - P^n \right) - \frac{(P^* - P^n) \Phi^n}{dt^2} = \left(\frac{\partial \rho^n u_i^*}{\partial x_i} - S \right) \frac{1}{dt}$$
(2)



$$\frac{\partial^2}{\partial x_i \partial x_i} (P^{**} - P^*) - \frac{(P^{**} - P^*)\phi^*}{dt^2} - \frac{(\phi^* - \phi^n)P^*}{dt^2} - \frac{(P^* - P^n)}{dt^2} = \left(\frac{\partial \rho^* u^{**}}{\partial x_i} - S\right) \frac{1}{dt}$$
(3)

The equation of successive over-relaxation solver was used in this work to result in faster convergence work for pressure, momentum, density, and equation species [20]. The law of wall has been applied to all boundaries, including hydrogen in-flow, liner, piston, and head of the engine. The SAGE detail-chemistry solver model was used as the combustion model by activating the adaptive zoning starting from 10 °CA before the injection until the end of combustion. Reynolds Averaged Navier-Stokes (RANS) model was used as the turbulence model by applying the O'Rourke and Amsden as wall heat transfer model. Flame development was viewed from Tecplot software. Flame development of hydrogen in the neon-oxygen atmosphere at low compression ratio and high intake temperature condition was matched with air and argon atmosphere.

3. Results and Discussion

In this paper, the neon-oxygen atmosphere was selected as working gas in the compression ignition engine for hydrogen combustion with neon consist of 79% by mass. Previous researches were mainly focused on the combustion of hydrogen in the argon-oxygen atmosphere in the CI engine. Intake manifold pre-heating and a high compression ratio are therefore needed to improve the ignition of hydrogen.

3.1 Compression of the Neon-Oxygen Atmosphere in Low Compression Ratio Engine

Figure 3 displays the in-cylinder pressure graphs from the simulation of the cold flow compression operating at 600 RPM with the intake temperature, T_i of 370K. The in-cylinder pressure of argon in the engine with a compression ratio of 10 was compared with the experimental results of argon obtained from Rey [16]. The in-cylinder pressure from the simulation was validated with in-cylinder pressure from the experiment with a 6.5% error difference when the AMR is activated as reported by Hafiz *et al.*, [6].

The result shows that neon-oxygen compression has resulted in a higher in-cylinder pressure compared to air (nitrogen-oxygen) and argon-oxygen atmosphere. Neon gas has a significantly lower specific heat ratio compared to argon. However, the compression of the neon-oxygen atmosphere results in higher pressure due to the low molecular mass of neon gas. The molecules of lower density gas travel faster and generate more energy. The energy from the molecule motion releases the heat during the compression. The compression of the ideal gas tends to heat the combustion chamber due to the work done by the motion of the molecules [21]. The specific heat ratio of neon is smaller than that of argon and neon specific heat capacity is as high as nitrogen. Gas with light molecular mass allow the hydrogen to travel faster during combustion, which results in higher pressure and temperature due to its high diffusion ratio [22]. The compression of low molecular mass gas increases the heat since the gas molecule collides rapidly.





Fig. 3. In-cylinder pressure of cold flow simulation of air, neon, and argon compared to the experiment in argon with the initial temperature of 370K and compression ratio of 10

3.2 Effects of Initial Temperature on Combustion Characteristics in Low Compression Ratio Engine

Figure 4 shows the hydrogen combustion in-cylinder pressure, temperature, and HRR in the neonoxygen atmosphere. Simulation at 600 RPM was set up with a compression ratio of 10 at various intake temperatures. Hydrogen was unable to ignite at low compression ratio engine condition without the intake manifold pre-heating for nitrogen-oxygen. During the compression stroke, the maximum temperature rise is about 1080K. Although the maximum temperature of the neon-oxygen atmosphere reached the auto-ignition temperature of hydrogen, the results presented do not show any sign of ignition.

The minimum intake temperature needed for neon-oxygen to increase the temperature that reaches hydrogen auto-ignition temperature is 310K. However, the ignition delay is too long, and the ignition that occurred after TDC is not stable. The rapid increase in temperature and pressure during ignition indicates that the explosion happens during the expansion stroke which also indicates detonation [23-24] as observed from the in-cylinder pressure increasing rate in Figure 5. The incylinder pressure increasing rate of combustion in the ambient temperature of 310K has exceeded the knock boundary. The pressure increasing rate of a conventional engine should not exceed 1.0MPa/°CA [25-26]. Therefore, the intake temperature of 310K is not suggested for the engine to produce efficient combustion. This condition also leads to several issues with the engine components due to overheating.

In addition, in-cylinder pressure and HRR of hydrogen combustion controlled at 380K and 340K intake temperature are approaching each other, as observed from the graphs. High intake temperature shortened the ignition delay of hydrogen and resulting in low HRR and progressive mixing-controlled combustion. The premixed combustion phase change at high intake temperature conditions is very low [9]. However, there is a slight rapid change of temperature and pressure at the beginning of injection with a rate of 1.66 MPa/°CA. At 340K, the combustion also experienced detonation. From all the considerations, the most suitable intake temperature for a low compression ratio engine is 380K with a peak temperature of 1729K. The results obtained proved that the intake manifold pre-heating is still needed for the neon-oxygen atmosphere for the engine to operate in low



compression ratio condition, For optimal performance, the higher compression ratio and optimum intake temperature must be considered in the future.



Fig. 4. In-cylinder pressure, temperature, and heat release rate of hydrogen combustion in neon-oxygen atmosphere operated in various intake temperature in low compression ratio engine





Fig. 5. In-cylinder pressure increasing rate against intake temperature of hydrogen combustion in the neon-oxygen atmosphere in low compression ratio

Figure 6 displays the 3D view plotted at standard ambient (300K), 320K, 340K, and 380K intake condition for hydrogen combustion in the neon-oxygen atmosphere. Results show that at high intake temperature conditions, the ignition occurs immediately after the injection. However, the ignition cannot occur at standard ambient intake temperature.



Fig. 6. Ignition progress of hydrogen in the neon-oxygen atmosphere at 300K (ambient), 320K, 340K, and 380K intake temperature in the low compression ratio engine



As observed from the figure, the minimum intake temperature to reach the ignition of hydrogen is 320K. However, at -2 °CA BTDC, the flame propagates rapidly occupied the right side of the cylinder, which is caused by the rapid pressure and temperature rise as explained in Figure 3. This phenomenon is called as detonation or explosion [23]. It can be concluded that increasing the temperature of the intake manifold resulting in high in-cylinder temperature during compression and shortened the ignition delay of hydrogen and this condition can also result in a significant loss of heat. Hydrogen flame travels directly from the injector to the cylinder wall due to the injector location and can result in further heat dissipation at the surface of the right side of the cylinder. A new injection position is suggested to have better flame distribution and to improve the thermal efficiency of the engine [6].

3.3 Effect of Compression Ratio on Hydrogen Combustion in Neon-Oxygen Atmosphere Standard Ambient Condition

The neon-oxygen atmosphere has been proved to enhance the ignition of hydrogen. However, hydrogen in the neon-oxygen atmosphere requires a slight intake manifold pre-heating effort. External energy is needed to heat the intake gas, which has caused the thermal efficiency of the engine to reduce overall efficiency. The adjustment of the compression ratio is needed in increasing the temperature during compression for better ignition of hydrogen.

Figure 7 shows the cold flow simulation result of in-cylinder temperature operating at 300K and 370K intake temperature with varying compression ratio. The graph shows that increasing of compression ratio increased the in-cylinder temperature. For 300K, increasing the compression ratio to 14 will result in a similar temperature pattern for the in-cylinder temperature of an engine operated in a low compression ratio with an intake temperature of 370K. This compression ratio is sufficient to ignite the hydrogen at standard ambient intake conditions for the engine.



Fig. 7. Pressure and temperature of cold flow simulation of neon-oxygen gas compression at different intake temperature and compression ratio

Figure 8 shows the in-cylinder pressure of hydrogen combustion in the neon-oxygen atmosphere at the initial standard ambient temperature conditions and varying compression ratio. Hydrogen combustion in the neon-oxygen atmosphere in a low compression ratio with standard ambient intake conditions could not ignite the hydrogen. The alternative way to improve the ignition is to increase



the compression ratio. As observed from the graph, CR11 at standard ambient intake condition is sufficient to ignite the hydrogen. However, the rapid rise of pressure or overpressure occurs near the TDC. The explosion that occurs near the TDC is the result of the rapid rise of pressure and HRR. This condition indicates that the knock is occurred since the in-cylinder pressure increasing rate exceeds the knock boundary, as shown in Figure 9.

The rapid rise of the heat release rate from the pre-mixed combustion region, which reached a value of 958 J/°CA shows that the combustion is unstable, as the heat transfer during this process is too high. In the premixed combustion, the combustion typically only evolved one-third of the whole combustion process [27]. Therefore, CR 14 is the sufficient compression ratio for the application for hydrogen combustion in the neon-oxygen atmosphere without intake manifold pre-heating. Due to the high specific heat ratio of neon, increasing the engine compression ratio increased the temperature and pressure peaks limits. There are often limited peak temperatures and pressures in the simulation, which cause the simulation to stop [12].



Fig. 8. In-cylinder pressure of hydrogen combustion in the neon-oxygen atmosphere, with standard ambient intake condition in various compression ratios





Fig. 9. In-cylinder pressure increasing rate against the engine compression ratio of hydrogen combustion in the neon-oxygen atmosphere at ambient intake condition

The compression ratio was increased to ensure a stable hydrogen ignition. Figure 10 displays the 3D image of the hydrogen combustion in the neon-oxygen atmosphere in various compression ratio in standard ambient intake conditions. The compression ratio was increased and hydrogen was possible to ignite with the lowest compression ratio of 11. The sudden ignition occurs at -2 °CA, just before the TDC.



Fig. 10. Ignition progress of hydrogen in the neon-oxygen atmosphere in various compression ratios in the standard ambient intake condition

The high-temperature distribution indicates that rapid ignition has occurred. The explosion that occurs near the TDC causes the flame to spread to the injector region since the strongest explosion occurs when the piston near the TDC. The high speed of flame forced the piston down but the force from the piston resists the movement and leads to uneven flame propagation. For engine reliability,



this condition is not preferable. Therefore, at standard ambient temperatures, CR11 is not suitable for the combustion of hydrogen in the neon-oxygen atmosphere. Hydrogen combustion in CR14 was successfully ignited at -9 °CA, which is immediately after the start of the injection. In this compression ratio, hydrogen shows good combustion progress.

4. Conclusions

This paper study the hydrogen combustion in the neon-oxygen atmosphere by 79% of mass for the neon-oxygen atmosphere. This paper aims to obtain the optimum setup to operate for standard ambient intake temperature conditions for hydrogen combustion and to improve the ignitability of hydrogen. Simulation of hydrogen combustion in a direct injection CI engine was carried out by using Converge CFD software, controlled at a low compression ratio. It can be concluded that:

- I. Neon is one of the noble gas elements that show great potential for enhancing the ignition of hydrogen. The low molecular mass and high specific heat ratio give the engine advantage to improve the hydrogen ignition stability.
- II. At a low compression ratio engine, the minimum intake temperature needed to ignite the hydrogen is 310K. This parameter, however, results in a knocking during combustion. Under the consideration of ignition behaviour and combustion, the most suitable intake temperature for the neon-oxygen atmosphere is 380K.
- III. The minimum compression ratio required in the neon-oxygen atmosphere for the ignition of hydrogen is 11. In the state of standard ambient intake condition, the most suitable compression ratio for the engine is 14 and intake manifold pre-heating is no longer needed at this stage.

The outcomes of neon-oxygen atmospheric hydrogen combustion are only in the preliminary stage. Therefore, further analysis of the neon-oxygen atmosphere should be carried out. There is currently no actual engine configuration of the compression ignition system for the noble gas. Therefore, laboratory tests for hydrogen combustion in the neon-oxygen atmosphere should be considered as well. In this preliminary result, the neon-oxygen atmosphere is indicated as one of a possible working gas for hydrogen combustion in a CI engine. With the suitable parameters as suggested in this paper, a proper investigation of hydrogen combustion in the neon-oxygen atmosphere will be useful for engine optimization and design. Further analysis should also be considered about its effect on heat loss.

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