Simulation of Hydrogen Combustion Characteristics in Argon-Oxygen Compression Ignition Engine using Large Eddy Simulation (LES) Turbulence Model

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Abstract. Hydrogen combustion in a noble gas atmosphere will increase thermal efficiency because of higher specific heat ratio. During the compression stroke, noble gas produces a higher temperature at the same compression ratio compared to standard air compression. Argon is the best noble gas in this study because it is abundant and readily available. In this study, argon replaced the nitrogen and formed the argon-oxygen atmosphere in a compression ignition engine. The objectives of this study are to determine the suitable initial temperature for simulation work based on the experimental value and to study the effect of injection parameter changes towards combustion and emission characteristics. This study uses Converge V2.4 CFD simulation based on Yanmar NF19SK engine parameter. The turbulence model used Large Eddy Simulation (LES) due to accessibility in extensive eddies calculation that has a significant fraction of energy. Thus, combustion analysis accuracy also increased. Base grid of 5mm with adaptive mesh refinement (AMR) and fix embedding is chosen based on simulation time and computer storage. Combustion simulations involve changing of initial temperature, the start of injection (SOI) and injection pressure to obtain pressure and heat release rate data. At intake temperature of 370K, hydrogen combustion shows the highest peak pressure, and for intake temperature at 500K, SOI of 700°CA produces the highest peak pressure for the combustion. Ignition delay increases as the temperature and injection pressure decrease.

1. Introduction
Fossil fuel is a major contributor of toxic emissions into the atmosphere as a result of combustion in the engine. Transport industry depends on fossil fuel and contributes to the production of greenhouse gases such as carbon dioxide [1]. Carbon dioxide will cause air pollution and global climate change.

The combustion of diesel fuel in the air atmosphere (N2-O2) causes the release of NOx and hydrocarbons resulting in pollution [2]. Based on this issue, the researchers examined the use of hydrogen as a fuel in compression ignition engine. Hydrogen is a clean fuel, and renewable and results of combustion using hydrogen will avoid carbon emissions and but at the same time increases NOx because of the high temperature [3].

The main challenge is the hydrogen has high auto-ignition temperature at 858K compared to diesel at a temperature of 525K [4,5]. High auto-ignition temperature leads to long ignition delay and knocks [6]. Hydrogen has minimum ignition energy. Also, the low ignition energy causes the backfire and the issue of pre-ignition. The use of direct injection can prevent backfire phenomena and improve volumetric efficiency.
Ignition of hydrogen is compulsory at high temperature. Thus, the noble gas, which has a higher specific heat ratio at 1.67 compared to normal air, will result in higher in-cylinder temperature achievement at the same compression ratio [7]. Moreover, it will eliminate NOₓ problems. In this study, argon gas is chosen instead of other noble gases because argon is abundant and high accessibility. The use of argon gas replaces nitrogen to form Ar-O₂ atmosphere requires argon circulated hydrogen engine.

Simulation of an internal combustion engine using Converge V2.4 requires selection of turbulence modelling. Turbulence increases momentum, energy, and species mixing rates. Turbulence in a combustion engine is important to ensure the accuracy of the simulation [8]. Large Eddy Simulation (LES) is used instead of Reynolds-averaged Navier–Stokes (RANS) for turbulence model. LES is a large vortex scale solution approach to reduce the number of grid points that need. Thus, the small eddies must briefly explain in the semi-empirical sub-capital. Large whirlpool in the integral length scale fraction containing large energy and more important in the transport of small quantities of the preserved compared vortex. Small vortex is more isotropic and easily resolved by DNS [9].

2. Methodology
Simulations were conducted using the engine parameters similar to Rey [10]. Table 1 shows the engine parameter used for this study. The simulation conducted in a closed cycle system started from intake valve closure (IVC) at 540°C until the exhaust valve opening (EVO) at 900°C.

| Table 1. Yanmar NF19SK Engine specification |
|--------------------------------------------|
| Parameter | Specification |
| Engine speed (rpm) | 600 |
| Cylinder head type | Disc |
| Bore (mm) x stroke (mm) | 110 x 106 |
| Fuel | Hydrogen |
| Compression ratio, r | 10:1 |
| Start of injection [°CA] | 10 BTDC |
| Injection duration [°CA] | 5 |
| Nozzle diameter (mm) | 0.8 |
| Nozzle location | 90° symmetry |

This study used Converge V2.4 that comes with adaptive mesh refinement (AMR). AMR is a special function developed for internal combustion engine simulation to generate the auto-meshing and eliminate grid generation problems during the simulation. The injection duration is kept constant at 5°CA for all three different starts of injection of 700°C, 705°C, 710°C. Meanwhile, the equivalence ratio is kept constant at 0.08. Table 2 explained the simulation parameter setup. The geometry preparation of the simulation is shown in figure 1 followed by the case setup, processing, and data analysis.

| Table 2. Simulation parameter |
|--------------------------------|
| Parameter | Specification |
| Oxygen Concentration (%) | 21 |
| Initial Pressure (MPa) | 0.114 |
| Initial Temperature, Ti (K) | 300, 370, 500 |
| Compression ratio, r | 10:1 |
| Injection Pressure (MPa) | 4, 8, 12 |
| Injection duration [°CA] | 5 |
| Nozzle diameter (mm) | 0.8 |
| Equivalence ratio (φ) | 0.08 |
3. Results and Discussion

3.1. Cold flow

Comparison between experiments from the past study needs [10] to further verified before changing the other parameters in the simulation. Figure 2 shows the in-cylinder pressure results without the injection of hydrogen fuel. The simulation results show the peak pressure for initial temperature, $T_i$, that closely approached to the initial temperature of the experiment is for $T_i=500K$. The peak pressure generated at the TDC is 3.31 MPa. $T_i=300K$ generated peak pressure of 3.87 MPa and difference of 16.8% compared with the experimental result for peak pressure. $T_i=370K$ generated a peak pressure of 3.64 MPa with a difference of 9.97%. The initial temperature of $T_i=300K$, 370K, and 500K will be used to study the further effect of changing the parameter of the injection of hydrogen that will affect the combustion process in this study.

![Figure 2. Peak in-cylinder pressure for cold flow simulation](image)
3.2. Effect of initial temperature

Figure 3 shows the combustion process is carried out at the beginning of $T_i=300K$, $370K$, and $500K$ with an injection pressure of 8 MPa. After the hydrogen injected at crank angle $710^{\circ}\text{CA}$, the graph shows a sharp increase in pressure at $T_i=370K$ and $T_i=500K$. This sudden change of pressure happened due to the occurrence of combustion in the combustion chamber [11]. $T_i=300K$ does not show any sudden increase in pressure after the hydrogen injection due to the long ignition delay.

Once the piston passes through the after top dead center (ATDC), the pressure also decreased due to the decrease in combustion and volume expansion of the combustion chamber. $T_i=370K$ generate the highest pressure of 4.60 MPa, followed by $T_i=500K$ with a pressure of 4.09 MPa and the initial temperature of $T_i=300K$ with a pressure of 3.92 MPa. The pressure at $T_i=500K$ is lower than $T_i=370K$ because combustion occurs at an early stage before the top dead center (TDC). Early combustion in the chamber with a large volume prevents the movement of the piston during the compression stroke, thereby inhibiting the production of high pressure [8].

![Figure 3](image_url)

**Figure 3.** Effect of initial temperature on pressure

3.3. Effect of the start of injection

This study aims to improve combustion efficiency at $T_i=500K$. During the study, hydrogen injection started at $700^{\circ}\text{CA}$, $705^{\circ}\text{CA}$, and $710^{\circ}\text{CA}$ with a constant injection duration of $5^{\circ}\text{CA}$. The parameter selection decided after reviewing the injection timing properties of hydrogen gas has a high auto-ignition temperature but has low ignition energy.

Figure 4 shows the start of injection (SOI) of $705^{\circ}\text{CA}$ generate the highest pressure at 4.18 MPa, followed by $700^{\circ}\text{CA}$ SOI at 4.17 MPa and $710^{\circ}\text{CA}$ SOI at 4.09 MPa. Different SOI results in longer ignition delay and all combustion show diffusion combustion throughout the process. SOI at $700^{\circ}\text{CA}$ result in the longer combustion process.
3.4. Effect of injection pressure

Figure 5 shows the combustion characteristics of hydrogen at an injection pressure of 4 MPa, 8 MPa, and 12 MPa. The effect of the injection pressure at $T_i=300$K, 370K, and 500K are studied. The results showed that the injection pressure and temperature to produce a minimum difference of pressure.

4. Conclusions

Simulation result for initial temperature, $T_i=500$K is closed to the experimental result in term of in-cylinder peak pressure. Peak pressure at $T_i=500$K is 3.31 MPa. The higher the initial pressure, the lower the pressure. $T_i=370$K produced the highest pressure, followed by $T_i=500$K and $T_i=300$K. At $T_i=500$K, SOI 705°CA produced the highest peak pressure, followed by SOI 700°CA and 710°CA.

Different injection pressure provides a minimum effect on the pressure and heat release rate produced. Overall changing of SOI and injection pressure parameter results to the changes of the combustion process and ignition delay of hydrogen in argon-oxygen combustion. Changes in the combustion process were more significant in changing of SOI compared to injection pressure. Further changes of some other parameter needs to investigate further to supply the fundamental data for this type of combustion.
In order to utilize this type of engine, argon needs a good recirculation system to separate the argon from the other combustion products. Since the end product of combustion is only water (H$_2$O), further development of argon and water separation technology need to be study.

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References
[1] Acar C and Dincer I 2018 Comprehensive Energy Systems Hydrogen Energy 1–5(April): 568-605.
[2] Tan Q and Hu Y 2016 A study on the combustion and emission performance of diesel engines under different proportions of O$_2$ and N$_2$ & CO$_2$ Appl. Therm. Engin. 108 508-515
[3] Mansor M R A and Shioji M 2016 Investigation of the combustion process of hydrogen jets under argon-circulated hydrogen-engine conditions Combustion and Flame 173 245-57
[4] Kumar V, Gupta D and Kumar N 2016 Hydrogen Use in Internal Combustion Engine: a Review The Int. J. Adv. Culture Technol. 3(2) 87-99
[5] Dhole A E, Yarasu R B, Lata D B and Baraskar S S 2014 Mathematical modeling for the performance and emission parameters of dual fuel diesel engine using hydrogen as secondary fuel Int. J. Hydrogen Energy 39(24) 12991-13001
[6] Hafiz N M, Mansor M R A, Mahmood W M F W and Shioji M 2016 Simulation of the Effect of Initial Temperature and Fuel Injection Pressure on Hydrogen Combustion Characteristics in Argon-Oxygen Compression Ignition Engine SAE Technical Paper 2016-01-2227.
[7] Shahsavan M, Morovatiyan M and Mack J H 2018 A numerical investigation of hydrogen injection into noble gas working fluids Int. J. Hydrogen Energy 43(29) 13575-82
[8] Hafiz N M, Mansor M R A and Mahmood W M F W 2018 Simulation of the combustion process for a CI hydrogen engine in an argon-oxygen atmosphere Int. J. Hydrogen Energy 43(24) 11286-97
[9] Stiesch W A 2008 Modeling Engine Spray and Combustion Processes Springer New York.
[10] Rey S 2014 Study on the SI-CI Combustion and the Spontaneous Ignition of Hydrogen Jets using a Rapid Compression Expansion Machine (Japan: Kyoto University)
[11] Ishiyama T, Shioji M and Inoue T 2003 Characteristics of Spontaneous Ignition and Combustion in Unsteady High-Speed Gaseous Fuel Jets SAE Technical Paper 2003-01-1922.