Combustion characteristics of direct injection hydrogen in noble gases atmosphere

Norhidayah Mat Taib¹, Mohd Radzi Abu Mansor*¹ and Wan Mohd Faizal Wan Mahmood¹

¹ Department of Mechanical Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia.

*E-mail: radzi@ukm.edu.my

Abstract. Hydrogen combustion in the internal combustion engine (ICE) has currently taken part in the transportation industry due to its environmentally friendly and high engine thermal efficiency. Hydrogen direct injection introduction in the internal combustion engine eliminates the harmful emission from carbon and improves engine stability. The substitution from nitrogen to noble gases for the intake will solve the high auto-ignition temperature of hydrogen in compression ignition (CI) engine problem. This paper intended to study the combustion characteristics of direct injection hydrogen in oxygen-noble gas atmosphere such as argon and helium to find the suitable engine and injection parameters for the optimum engine efficiency.

The simulation conducted using Converge CFD V2.4 software based on Yanmar NF19K direct injection CI engine. The simulation was done for different oxygen-noble gases such as argon, neon, and helium, while the injection timing and ambient temperature were modified to optimize the hydrogen combustion characteristics. The study found that noble gases help to increase the in-cylinder temperature and ignite the hydrogen. The study also found that early injection timing results in the highest in-cylinder pressure. Besides, increasing ambient temperature for intake decreases the in-cylinder pressure and lengthen the ignition delay. Therefore, the most suitable injection parameter for the most optimum hydrogen combustion characteristics is 380 K ambient temperature, early injection timing at -10°CA, and higher injection pressure. Helium produced higher in-cylinder peak pressure compared to argon due to its high specific heat ratio. Hence, further consideration of helium and good injection strategies should be applied for better engine thermal efficiency.

Keywords: Argon, Helium, Compression Ignition, Ignition Delay, Heat Release Rate
1. Introduction

Hydrogen is renewable energy sources and has great potential as an alternative fuel. Previously, hydrogen has widely used in fuel cell vehicles application with the ability to travel as far as almost 500 km with full tank [1]. However, its high operating cost and low power operation not able to beat the low operation cost and high compression power of the compression ignition engine, although the production cost of hydrogen is considerably high [2]. However, diesel fuel combustion leads to a serious carbon emission problem. Malaysia aims to become the regional hub for energy-efficient vehicles (EEV). Hence, the carbon emissions should minimize to the lowest scale through the development of hydrogen in compression ignition engine. This development solves the problem by eliminates the emission of carbon. However, high auto-ignition temperature of hydrogen causes another problem to the hydrogen ignition in normal air condition.

Therefore, noble gases are suggested as the best working gas to help the ignition of hydrogen by replacing the nitrogen in the air while eliminating the NOx emissions. Noble gases are known as non-reactive gas with the ability to raise the compression temperature and solve the hydrogen ignition problem due to its high specific heat ratio. Besides, noble gases also can increase the cycle efficiency by 1.3 -1.4 times higher than air [2]. However, noble gases are rare gases, so noble gas recirculation is designed to reuse the gas from the exhaust into the intake manifold through the condensation process of water vapor. From the previous study, the combustion of hydrogen in compression ignition engine focused on argon as the working gas. The study is conducted experimentally and computationally. Figure 1 shows the hydrogen combustion in argon recirculation schematic chart.

![Noble gases recirculation engine schematic diagram](image)

A high specific heat ratio of argon help in increasing engine efficiency, and the study of the other noble gases has not yet been focused. It is because the production of other noble gases is expensive. The study of xenon gas in CI engine has been computationally conducted to study the jet development of hydrogen in argon and xenon atmosphere. However, there is no information about other gases such as helium as the working gas in hydrogen combustion application. Other than that, research about combustion characteristics of hydrogen combustion in argon gas also are very limited.

Hence, this paper aims to study the combustion characteristics of hydrogen combustion in different oxygen-noble gases atmosphere focusing on argon and helium gases. Helium is compared and suggested as another good working gas since it is widely used in many applications and has a lower cost. Although the market price of helium is slightly higher than argon, the high specific heat ratio of helium promised the high thermal efficiency to the engine [4]. In this study, few parameter changes also were made to study the effect of injection timing, and intake temperature to the hydrogen combustion progress in argon atmosphere. The study was conducted computationally using the Converge CFD software on a Yanmar NF19SK compression ignition engine parameter. The injection strategies and new noble gases application other than argon provides a new information on the potential of hydrogen combustion in internal combustion engine.
2. Methodology
In this study, a simulation work on hydrogen in the oxygen-noble gases atmosphere was conducted. Simulation was conducted using Converge CFD software based on Yanmar NF19SK compression ignition engine parameter. Converge CFD Software is equipped with adaptive mesh refinery (AMR) function that able to eliminates the time required for the grid generation because it can automatically generate the mesh with perfect orthogonal and grid during simulation [5]. The specification of the engine is explained in Table 1 and the combustion chamber 3D model is shown in Figure 2. Hydrogen was injected at the edge of the cylinder wall marked in Figure 1 for 5°CA duration and injected at -10°CA. The engine was operated at 600 RPM started from the intake valve closed (IVC) at -179°CA until the exhaust valve open (EVO) at 179°CA. SAGE combustion model was used in this simulation work to simulate the ignition and combustion process.

![Figure 2. Yanmar NF19SK combustion chamber model](image)

| Engine specification                      |
|------------------------------------------|
| **Engine Type**                          | Compression ignition |
| **Engine model**                         | Yanmar NF19SK        |
| **Bore x Stroke (mm)**                   | 110 x 106            |
| **Compression ratio**                    | 10                   |
| **Nozzle diameter (mm)**                 | 0.8                  |
| **Intake valve close (°CA)**             | -179                 |
| **Exhaust valve open (°CA)**             | 179                  |

| Operation condition                      |
|------------------------------------------|
| **Engine speed (RPM)**                   | 600                  |
| **Injection pressure (MPa)**             | 8                    |
| **Intake pressure (MPa)**                | 0.114                |
| **Intake temperature (K)**               | 380, 400             |
| **Oxygen ratio**                         | 0.21                 |
| **Injection duration (°CA)**             | 5°CA                 |
| **Injection timing (°CA)**               | -10, -3              |
| **Working gases**                        | (O<sub>2</sub>-Ar), (O<sub>2</sub>-He) |

*underlined parameter is the experiment condition

The simulation for cold-flow compression expansion process was compared to the experimental results conducted by Rey, 2014 [3], where the study investigated the combustion characteristics and jet development of hydrogen combustion in argon atmosphere. The experiment was conducted on the
Rapid Compression Expansion Machine (RCEM), which describes the one-shot firing to visualize the combustion process [7]. The cold-flow was set up without any hydrogen injection running at 600 RPM, and the initial temperature and pressure of 370K and 0.114 MPa. The grid-independent test also conducted to identify the optimum grid size, and 0.0005 m grid size is chosen for the most converged simulation results. The simulation were conducted on hydrogen in oxygen-argon and oxygen-helium atmosphere. Each noble gas has different thermodynamic properties, which influenced the combustion progress of hydrogen after injected into the combustion chamber. High specific heat ratio of noble gas requires no heating during intake since it is capable of increasing the in-cylinder temperature for the hydrogen ignition. However, the initial condition of the engine was also modified with the different ambient temperatures at 380K and 400K to study its combustion characteristics. The injection timing also varied at -10 °CA and -3°CA. The injection duration was maintained at 5°CA.

3. Results and Discussion
Hydrogen combustion in different oxygen-noble gases atmosphere leads to different combustion characteristics due to its thermo-physical properties. Few modifications to injection parameters and initial conditions such as injection timing and intake temperature also influenced the combustion progress for better engine parameters strategies.

3.1 Hydrogen-argon model validation
Validation is conducted by comparing the cold-flow results from simulation to the experiment conducted by Rey 2014 [3]. Figure 3 shows the comparison of in-cylinder pressure of cold-flow condition of argon atmosphere from experiment and simulation works. The engine runs at 600 RPM, with initial temperature and pressure of 370 K and 0.114 MPa. The result shows that the pressure from the simulation is slightly higher than the experiment with the percentage difference at top dead center (TDC) around 10.8%. The lower pressure from experiment shows that there may be pressure or temperature loss during the compression. RCEM not representing the real engine; the lack of adequate turbulence level and slow charging process may become another reason for lower pressure during compression [8].

![Figure 3. In-cylinder pressure of cold-flow simulation validation](image)

3.2 Combustion analysis of hydrogen combustion at different intake temperature
Figure 4 shows the in-cylinder pressure of hydrogen combustion in the argon atmosphere run at different initial temperatures. Results show that increasing the ambient temperature reduces in-cylinder pressure. At the same time, the ignition of hydrogen at lower intake temperature also caused the late ignition compared to ambient temperature at 400K. This small ignition difference occurs in the combustion with different ambient temperatures. It is because the in-cylinder temperature rises and reaches the auto-ignition temperature of hydrogen faster.
3.3 Effect of injection timing on combustion characteristics of hydrogen combustion in oxygen-noble gases

Figure 5 shows the in-cylinder pressure of hydrogen combustion in the argon atmosphere running at 600 RPM with different hydrogen injection timing. The injection timing is delayed from -10 °CA to -3 °CA due to the delay of hydrogen ignition from the experiment. Rapid ignition of hydrogen proved that delayed injection also delayed the ignition of the fuel. From the graph, the ignition timing difference between simulation and experiment occurs proved, that the injection timing from the experiment was not started at -10°C. Hence, delaying the injection will delay the ignition. However, the pressure and heat release rate also decreases. Therefore, delaying the injection is not a good solution without increasing the amount of hydrogen injected. In future, further study needs to find a good strategy to improve the combustion of hydrogen in oxygen-noble gases atmosphere.

3.4 Combustion characteristics of hydrogen combustion in different oxygen-noble gases atmosphere

Figure 6 shows the in-cylinder pressure of hydrogen combustion in different oxygen-noble gases atmosphere. The result shows that the hydrogen combustion in helium has higher pressure than argon. Previously, most of the researchers focused on argon due to its availability and low-cost gases. Compared to air, oxygen-argon was proved to able to improve the hydrogen ignitability [9]. However, results proved that in helium atmosphere resulting in higher pressure and leads to better engine thermal efficiency compared to argon. Based on the properties of noble gases, helium has smaller atomic mass and higher specific heat capacity at constant pressure. Although helium and argon have the same specific heat ratio, due to the low molecular weight of helium, the specific heat capacity of helium at constant volume is higher than argon, which resulting in higher entropy and enthalpy. Hence, helium is recognized as another good potential noble gases and need further injection and operation strategies for future works.
Figure 6. In-cylinder of hydrogen combustion in different oxygen-noble gases atmosphere

4. Conclusion
In this study, hydrogen combustion in argon atmosphere is simulated by using the Converge CFD software to study its combustion characteristics while obtaining the correct setup for validation purpose. The study found that increasing the intake temperature does not helpful for the combustion efficiency and 380K is enough to ignite the hydrogen in argon atmosphere. However, due to the hydrogen rapid ignition, the ignition timing from experiment does not start at -10°C BTDC but delayed with 7CA. Therefore, future experiment conducted should consider the correct injection timing shifting. Other than argon, helium is found to be another good option for the hydrogen ignition in ICE. In future, detail investigation of hydrogen combustion in helium atmosphere also should be conducted to find the suitable condition.

Acknowledgement
The authors would like to thank Universiti Kebangsaan Malaysia for supporting this research with grant GUP-2018-099 and Ministry of Education Malaysia for supporting this research with grant FRGS/1/2017/TK07/UKM/02/1.

References
[1] Kurtz J, Sprik S, Saur G and Onorato S 2019 Fuel Cell Electric Vehicle Driving and Fueling Behavior Fuel Cell Electric Vehicle Driving and Fueling Behavior.
[2] Dibble RW, Aznar MS, Sennott TB and Chen J-Y 2017 Recirculating Noble Gas Internal Combustion Power Cycle. US 2017/0211515 A1.
[3] Rey S 2014 Study on the SI-CI Combustion and the Spontaneous Ignition of Hydrogen Jets using a Rapid Compression Expansion Machine. Kyoto University.
[4] Abo El Ela AM, Eldrainy YA, Elkasaby MM and Nour AM 2016 Effect of replacing nitrogen with helium on a closed cycle diesel engine performance. Alexandria Eng J 55 2251–2256.
[5] Dhyani V, Kumar D, Ganji PR and Raju V 2014 Numerical Experiment of CI Engine Combustion Using CONVERGE Software. FIRE 2014.
[6] Hafiz NM, Mansor MRA and Wan Mahmood WMF 2018 Simulation of the combustion process for a CI hydrogen engine in an argon-oxygen atmosphere. Int J Hydrogen Energy 43 11286–11297.
[7] Ishibashi R and Tsuru D 2017 An optical investigation of combustion process of a direct high-pressure injection of natural gas. J Mar Sci Technol 22 447–458.
[8] Kammermann T, Koch J, Wright YM, Soltic P and Boulouchos K 2017. Generation of Turbulence in a RCEM towards Engine Relevant Conditions for Premixed Combustion Based on CFD and PIV Investigations. SAE Tech Pap 2017.
[9] Hafiz NM, Mansor MRA, Wan Mahmood WMF, Ibrahim F, Abdullah S and Sopian K 2016 Numerical Study of Hydrogen Fuel Combustion in Compression Ignition Engine Under Argon-Oxygen Atmosphere. J Teknol 78 77–83.