Jurnal Kejuruteraan SI 6(2) 2023: 239 – 247
https://doi.org/10.17576/jkukm-2023-si6(2)-25

Ignition Stability of Hydrogen in Noble Gases Atmosphere in Compression Ignition Engine

(Kestabilan Pencucuhan Hidrogen dalam Persekitaran Gas Adi dalam Enjin Pencucuhan Mampatan)

Norhidayah Mat Taib[a,b], Wan Mohd Faizal Wan Mahmood[a,b], Hasan Koten[c] & Mohd Radzi Abu Mansor[a,b,*]

[a] *Department of Mechanical and Manufacturing Engineering,*

[b] *Centre of Automotive Research*

Faculty of Engineering & Built Environment, Universiti Kebangsaan Malaysia, Malaysia

[c] *Department of Nanoscience and Nanoengineering, Istanbul Medeniyet Universitesi, 34700 Istanbul, Turkey*

**Corresponding author: radzi@ukm.edu.my*

Received 30 July 2022, Received in revised form 14 October 2023
Accepted 24 November 2023, Available online 30 December 2023

ABSTRACT

Hydrogen fuel promises a high engine efficiency and the ability to eliminate harmful emissions in an internal combustion engine. However, the ignition stability of hydrogen in compression ignition engine is unstable due to the high-auto ignition temperature of hydrogen. Noble gases such as argon, krypton and xenon have a larger molecular weight compared to nitrogen. Therefore, replacing nitrogen with noble gases appears to be a promising option due to their high specific heat ratio. This paper aims to investigate the ignition stability in a heavy molecular noble gases atmosphere in a CI engine. In this study, Converge CFD software simulates a single-cylinder compression ignition engine model based on the Yanmar NF19SK engine parameters. Hydrogen combustion in a noble gas atmosphere resulted in low ignition stability when operated at low intake temperature. Based on this study, we found that increasing intake temperature improves the ignition stability. As a result, argon is the most preferable among other noble gases. Nevertheless, future research should investigate the other noble gases' capability under different parameters to improve the engine's thermal efficiency.

Keywords: Ignitability; Combustion characteristics; Combustion stability

ABSTRAK

Pembakaran hidrogen menjanjikan kecekapan enjin yang tinggi dan keupayaan untuk menghapuskan emisi berbahaya dalam enjin pembakaran dalaman. Walau bagaimanapun, kestabilan pencucuhan bahan api hidrogen dalam enjin pembakaran mampatan adalah tidak stabil disebabkan suhu pencucuhan hidrogen yang tinggi. Gas adi seperti argon, kripton, dan xenon mempunyai berat molekul yang lebih tinggi berbanding gas nitrogen. Oleh itu, penggantian nitrogen dengan gas adi merupakan sebagai pilihan yang tepat kerana nisbah haba tentunya yang tinggi akan meningkatkan suhu ketika mampatan. Kajian ini bertujuan untuk menyiasat kestabilan pencucuhan dalam persekitaran gas adi yang mempunyai berat molekul yang tinggi dalam enjin pembakaran dalaman. Dalam kajian ini, perisian Converge CFD digunakan untuk simulasi sebuah model enjin pembakaran dalam silinder tunggal berdasarkan parameter enjin Yanmar NF19SK. Pembakaran hidrogen dalam persekitaran gas adi menghasilkan kestabilan penyalaan yang rendah apabila beroperasi pada suhu kemasukan yang rendah. Kajian juga mendapati bahawa peningkatan suhu kemasukan mampu meningkatkan kestabilan pencucuhan. Hasil dari perbandingan, argon merupakan gas yang disarankan berbanding gas adi yang lain. Namun, penyelidikan akan datang juga akan meneliti keupayaan gas adi yang lain menggunakan parameter enjin yang lebih sesuai untuk meningkatkan kecekapan haba enjin.

Kata Kunci: Kebolehnyalaan; Ciri-ciri pembakaran; Kestabilan pembakaran

INTRODUCTION

Hydrogen is well known as the most environmentally friendly fuel in many applications. Hydrogen fuel has high energy density, zero carbon emissions and durable in storage (Yang et al. 2022). In the transportation sector, hydrogen is commonly used in fuel cells and internal combustion engines (ICE), promising the cleanest emission products. The development of hydrogen in ICE, particularly in compression ignition (CI) engines, is more reliable for heavy-duty and high-performance operations due to the high energy efficiency. CI engine has the advantages of high compression power, low operational cost and long lifespan (Dibble et al. 2017; Luo et al. 2019; Dimitriou 2017). However, the high auto-ignition temperature of hydrogen around 858 K, is a significant challenge when operated in a CI engine, especially if the engine is operated in a normal ambient air atmosphere (Annamalai 2013; Szwaja 2009). Moreover, the higher in cylinder temperature with hydrogen combustion results in the formation of NOx emissions (Kadir et al. 2020).

The suggestion to replace nitrogen with noble gases is a great solution to solve these problems. Noble gas, which is the non-reactive element, is the most suitable gas for preventing harmful emissions. Noble gases have a higher specific heat ratio compared to nitrogen. Table 1 compares the thermo-physical properties of noble gases argon, krypton and xenon and also the properties of hydrogen and nitrogen.

Specific heat ratio is the most important criteria in determining the effectiveness of gas to offer higher temperatures during compression. The compression of a higher specific heat ratio's gas can increase the in-cylinder temperature to reach the auto-ignition temperature of hydrogen Equation 1 represents the relationship between the thermal efficiency and specific heat ratio, k (Cengel 2007; Dibble et al. 2017) which indicates that the thermal efficiency during the gas compression for higher specific heat ratio gas which is aroundof 1.66 to 1.68 is much greater than nitrogen, which has a value of 1.40.

$$\eta_{th,Diesel} = 1 - \frac{r^{1-k}(r_c^k - 1)}{k(r_c - 1)} \tag{1}$$

TABLE 1. Thermo-physical properties of noble gases (Rayleigh 1997)

Properties	Hydrogen	Nitrogen	Argon	Krypton	Xenon
Molecular weight (kg/mol)	2.016	28.014	39.95	83.3	131.29
Density (kg/m3) @ 32 ^{o}C	0.08375	1.165	1.7818	3.708	5.851
Boiling point (K)	20.25	77.15	87.29	120.85	166.1
Melting point (K)	13.95	63.15	83.6	115.8	161.7
Specific heat capacity (J/kg.K)	10.16	1040	519	247	159
Specific heat ratio	1.41	1.40	1.67	1.68	1.66

Several studies discussed the evolution of hydrogen combustion in noble gases. The molecular weight and specific heat capacity of each noble gas are the most significant differences. According to a study reported by Shahsavan in 2017, noble gases such as argon and xenon play an important role in increasing the combustion temperature. In the study, it also discovered that the diffusivity of hydrogen in argon is better than in nitrogen and xenon (Shahsavan 2017). However, the study was carried out in a constant volume combustion chamber (CVCC), where the ignition is stabilized by a source of ignition. In a real compression ignition engine application, the hydrogen ignition is completely reliant on the compression power to enhance the ignition. However, there are no detail study on these noble gas has been discussed. Hydrogen is preferred for the high power generation due to the high amount of energy from hydrogen (Zhu et al. 2020). Therefore, in internal combustion engine, high fuel consumption needed if the operation worked for low power vehicles.

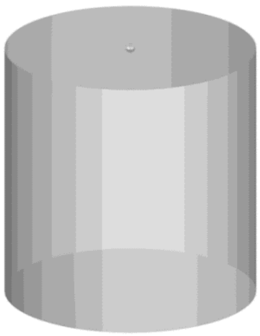
This paper aims to investigate the ignition stability of hydrogen in noble gases in a compression ignition engine. A numerical approach is employed on a combustion chamber model based on a Yanmar NF19SK direct injection compression ignition engine. The noble gases such as argon, krypton and xenon replaced the 79% nitrogen in the air, operated in a low compression ratio engine at a high intake temperature.

MATERIALS AND METHOD

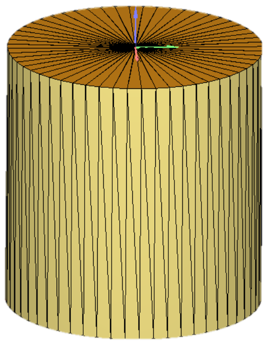
This study conducts a numerical approach by using Converge Computational Fluid Dynamic (CFD) software. Converge CFD is a software equipped with an adaptive mesh refinery (AMR) tool to refine the mesh grid size. The refinery process is unique in that the mesh is automatically refined based on the combustion progress, allowing it to improve the mesh quality and combustion analysis accuracy (Morovatiyan et al. 2019; Hafiz et al. 2018).

VALIDATION AND GRID INDEPENDENCE TEST

This study validates an experiment conducted by (Rey 2014). The experiment is carried out on Yanmar NF19SK direct injection compression ignition engine. Hydrogen is directly injected into the argon-oxygen atmosphere. Based on the same engine specification, the software transformed the 3D model of the combustion chamber into a triangulated model, as illustrated in Figure 2. The simulation operates on a closed combustion system, starting with the intake valve close (IVC) at 179 ^{o}CA BTDC (before top dead centre) and ending with the exhaust valve open (EVO) at 179 ^{o}CA ATDC (after top dead centre). The injector is located at the centre of the cylinder head. An injector located in the centre of the cylinder's head injects hydrogen direct into the combustion chamber at 3 ^{o}CA BTDC for 5 ^{o}CA at an 8 MPa pressure. The intake temperature is kept constant at 380 K. Table 2 lists the engine specifications and parameters used in this study.



(a) NF19SK 3D model



(b) NF19SK triangulated model

FIGURE 2. Yanmar NF19SK engine 3D model dan triangulated model (Hafiz et al. 2018)

TABLE 2. Engine specification (Rey 2014; Hafiz et al. 2018)

Specification	
Engine model	Yanmar NF19SK
Engine type	Compression ignition
Bore x stroke	110 mm x 106 mm
Engine speed	600 RPM
Intake valve close (IVC)	179 ^{o}CA BTDC
Exhaust valve open (EVO)	179 ^{o}CA ATDC
Compression ratio	10
Intake pressure	0.114 MPa
Injection pressure	8 MPa
Nozzle diameter	0.8 mm
Injection timing	3 ^{o}CA BTDC
Injection duration	5 ^{o}CA
Intake temperature	380 K
Noble gas	Air, Argon, krypton, xenon

The combustion model used in this study is SAGE detailed chemistry solver, which works to accelerate the simulation. The turbulence model used in this simulation is Reynolds-averaged Navier-Stokes (RANS) because of its small memory spaces, which shortened the operating time The Navier-stokes equation can solve all the models and equations based on PISO solver. Models of base grid with size of 0.003 m, 0.004 m, 0.005 m and 0.006 m tested. Results found that the most suitable grid size for this study is 0.005 m with the lowest percentage error of 9.89%, compared to the experiment conducted by (Rey 2014). Numerical studies by Hafiz

2018, and Shahsavan 2020 support the results of this study (Hafiz et al. 2018; Shahsavan et al. 2020). Table 3 shows the error percentage of pressure obtained from different grid size which finalize that grid size of 0.005 is chosen as the best grid as its give the small error percentage with reasonable simulation duration and file sizes.

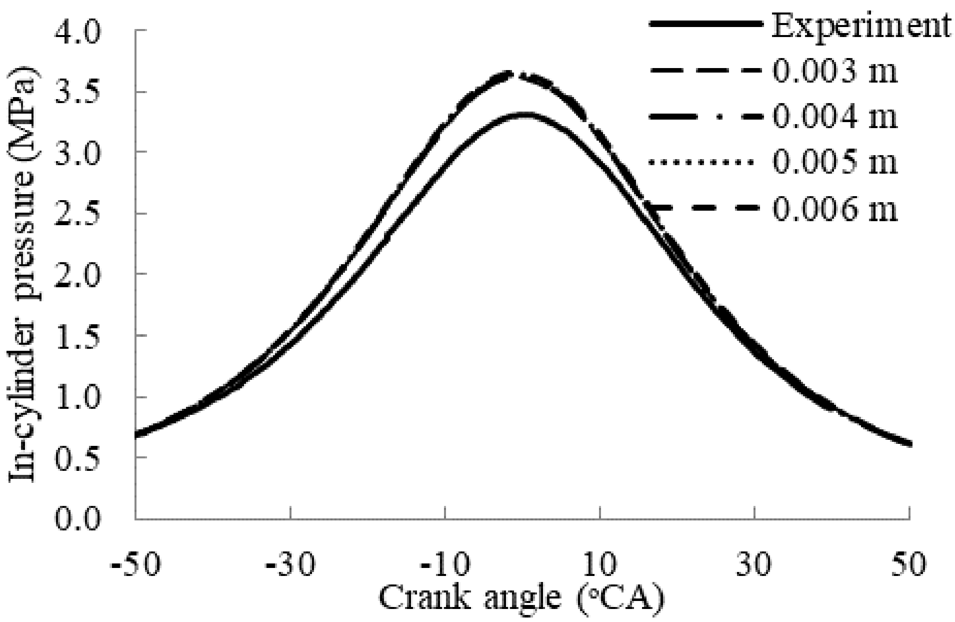


FIGURE 3. In-cylinder pressure of hydrogen combustion in the argon-oxygen atmosphere with different grid size

SIMULATION OF HYDROGEN IN NOBLE GASES ATMOSPHERE

The potential of argon in replacing 79% of the nitrogen in air for the hydrogen combustion application was actively discussed. In this study, noble gas such as argon, krypton and xenon are also discussed, which have a larger molecular weight and density than nitrogen. The simulation is conducted for all the noble gases selected, operated at high intake temperature due to the ignition stability problem of hydrogen if operated in low intake temperature conditions (Hafiz et al. 2016; Rey 2014). Throughout the studies, the initial pressure, engine speed, nozzle diameter, compression ratio, and injection timing were all kept constant. Based on the combustion characteristics analysis obtained from the simulation, the ignitability of hydrogen is discussed.

TABLE 3. Error percentage of grid independence test

Grid size	In-cylinder at TDC	Error percentage compared to 0.003m	Duration	File's size	Number of cells
0.003 m	3.61 MPa	-	93.48 hours	19.7 GB	2717000
0.004 m	3.62 MPa	0.28%	24.01 hours	8.83 GB	1146000
0.005 m	3.63 MPa	0.55%	18.35 hours	5.27 GB	600000
0.006 m	3.66 MPa	1.39%	15.03 hours	2.94 GB	350000

RESULTS AND DISCUSSION

Figure 4 shows the compression of noble gases-oxygen and air, in the absence of hydrogen. The result shows that the compression of argon produced the highest pressure followed by krypton, xenon and air. It indicates that when the molecular weight of the gas decrease, the compression pressure increases. Even though nitrogen has a lower molecular weight than argon, krypton and xenon, its low specific heat ratio results in extremely low compression pressure. The compression results of argon-oxygen and air are consistent with a study by Hafiz 2016, which indicated that the compression pressure of argon is higher than air due to its lower specific heat capacity compared to nitrogen (Hafiz et al. 2016). Despite the facts that nitrogen has lower molecular weight compared to argon, xenon and krypton, the specific heat ratio of these noble gases gives better compression results compared to nitrogen in air. The potential behind these gases should be discovered.

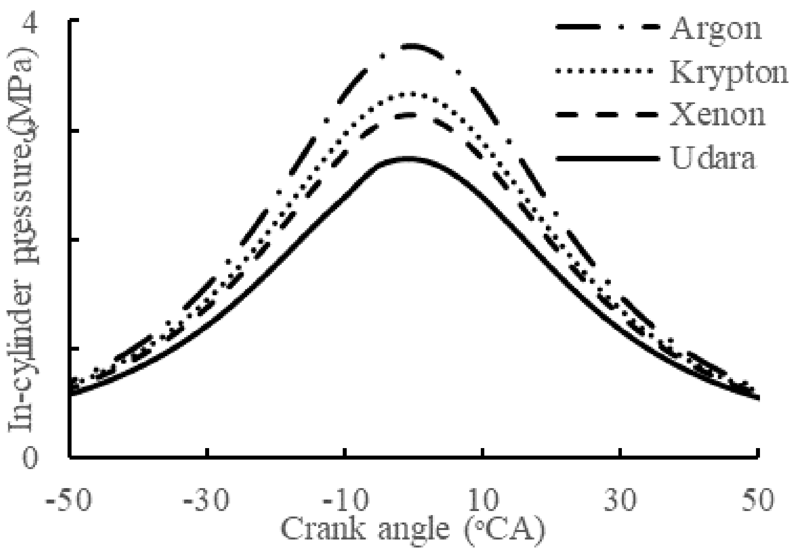
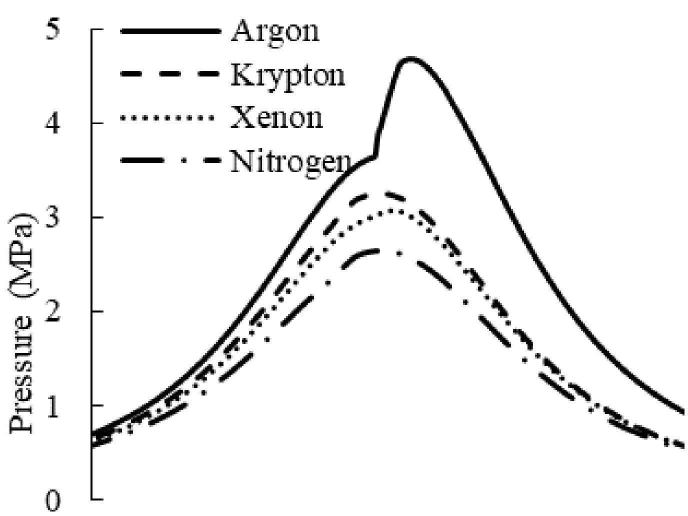


FIGURE 4. Compression pressure of noble gases atmosphere at ambient intake temperature

Figure 5 shows the in-cylinder pressure and temperature of hydrogen combustion in noble gases-oxygen and air atmosphere at the intake temperature of 380 K. When the hydrogen fuel is injected, the pressure rises exclusively in the argon-oxygen atmosphere, indicating that the ignition of hydrogen occurs only in the argon-oxygen atmosphere with a maximum pressure of 4.69 MPa. The ignition timing of hydrogen is found to be at 1.98 °CA BTDC, with a very short delay of 0.004 ms. Hence argon is suggested as the stable working gas for hydrogen combustion in low compression ratio engine (Taib, 2021).



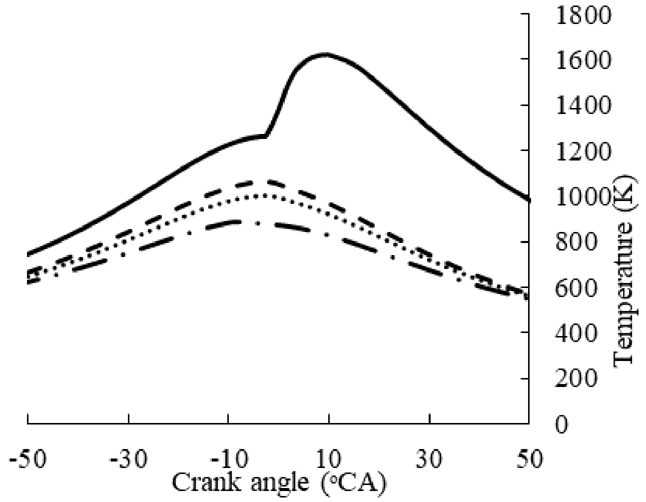


FIGURE 5. Compression pressure of noble gases atmosphere at intake temperature of 380 K

Based on the temperature plotted, the maximum temperature achieved by the compression of nitrogen is insufficient to reach the required auto-ignition temperature of hydrogen. Meanwhile, although the in-cylinder temperature of krypton and xenon compression has reached the required minimum, the temperature required to break the OH radicals to initiate the ignition of hydrogen is far too low. Figure 6 shows the temperature distribution of hydrogen flame in argon, krypton and xenon-oxygen atmosphere at an intake temperature of 380 K.

The in-cylinder temperature of hydrogen combustion in krypton-oxygen and air shows a decreasing trend before the piston reaches the TDC position. As a result, the temperature distribution in the krypton-oxygen atmosphere is narrower compared to the xenon-oxygen atmosphere. The ability of the argon-oxygen atmosphere to produce higher temperatures is supported by a study from Shahsavan (2017). The study found that the temperature distribution of hydrogen combustion in argon-oxygen is higher than in air, but the combustion temperature in the xenon-oxygen atmosphere is found higher than in argon-oxygen. The fundamental explanation was due to the lower specific heat capacity of noble gases compared to the lighter ones. However, in the study presented, the ignition is supplied from the ignition sources, which initiates and enhances the combustion (Shahsavan 2017).

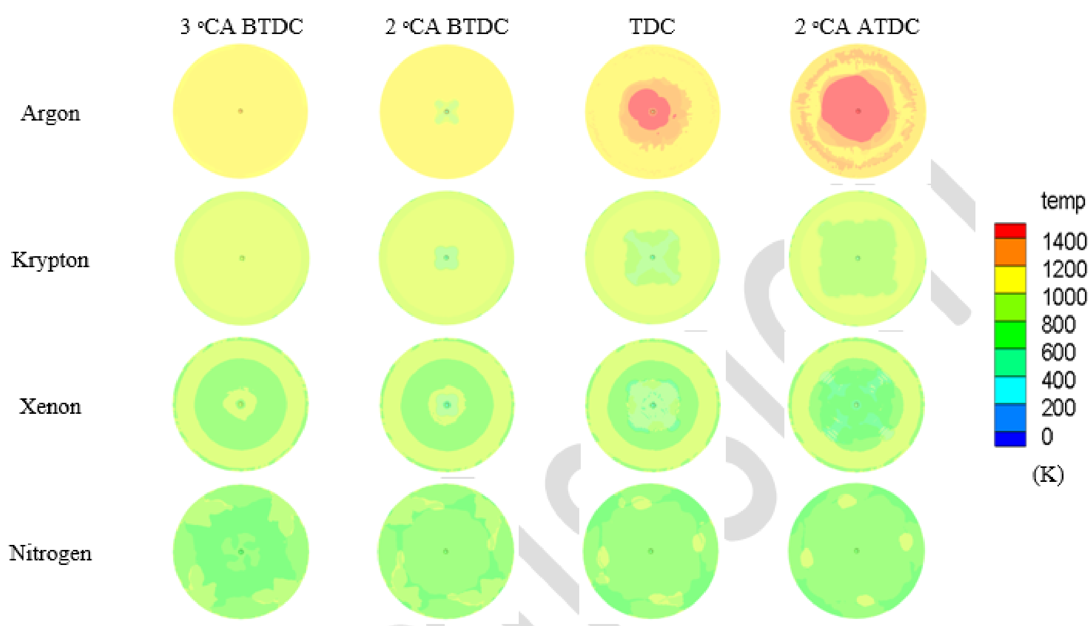


FIGURE 6. Flame temperature distribution of hydrogen combustion in noble gases atmosphere

Based on the study, the activation of OH radicals is a very important indicator for ignition (Shahsavan et al. 2020; Blocquet et al. 2013). Figure 7 shows the comparison of the OH mass fraction of hydrogen combustion in noble gases and air. The result shows that the OH radicals only rapidly increased in the argon-oxygen atmosphere, with a maximum value of 0.0011. The OH radicals of the other noble gases are very low, indicating the ignition does not occur. According to a study by Stankovic 2011, the threshold for proving the ignition of hydrogen is when the temperature or pressure rise exceeds 1% of the value in cold flow operation. The second criteria for ignition are the OH mass fraction must be greater than 0.0002 (Stanković 2011). Therefore, based on the figure, the OH mass fraction of hydrogen in argon meets both the ignition criterion.

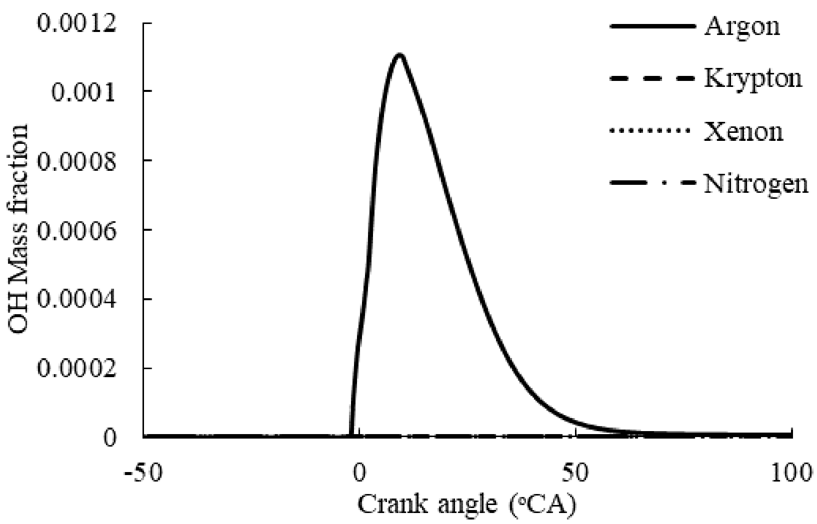


FIGURE 7. Mass fraction of OH radical during the combustion in noble gases atmosphere at intake temperature 380 K

Figure 8 shows the relationship between minimum intake temperature and the molecular weight of noble gases when operating with low compression ratio of 10 in the engine. The intake temperature is varied to determine the minimum required intake temperature, and it was found that the minimum intake temperature for heavy noble gases increases with the molecular weight. As depicted in the graph, operation in kyrpton and xenon atmospheres require temperatures higher than the 380K baseline mentioned in this paper. This is attributed to the lower energy during compression due to their weight.

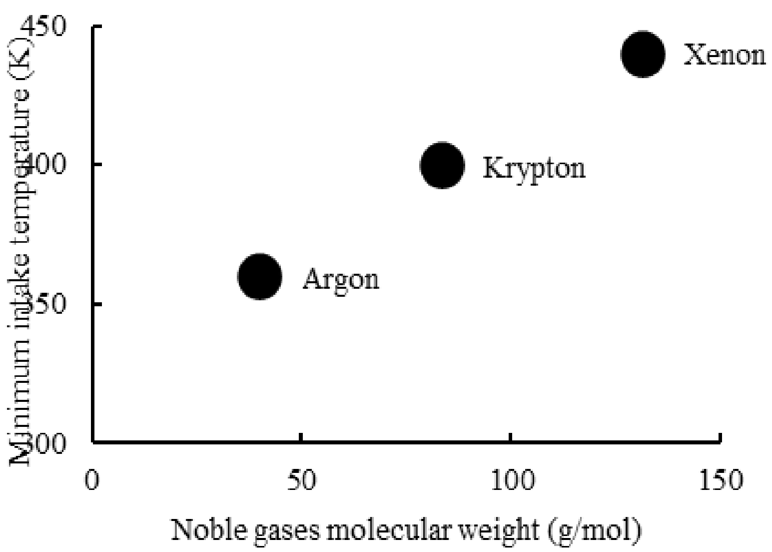


FIGURE 8. Minimum intake temperature needed for noble gases based on their molecular weight when operating at compression ratio of 10

CONCLUSION

The study found that the noble gases atmosphere reduces the hydrogen's ignition stability when operated at low intake temperature and low compression ratio. High molecular weight of xenon and krypton shows that the compression of these gases results in higher compression temperature and pressure. However, further suitable setup is needed to identify the stable ignition. The study proves that argon-oxygen atmosphere is the most promising working gas for hydrogen combustion in compression ignition engines, compared to krypton and xenon-oxygen atmosphere. Future studies should study the engine operation with a high compression ratio and a suitable hydrogen injection parameter for the noble gas atmosphere to improve engine thermal efficiency. In future, suitable parameter for these noble gases should be discovered.

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

Annamalai, K, and A R Pradeepkumar. 2013. Using hydrogen as a fuel in automotive engines - An investigation. *International Journal of Innovative Technology and Research* 1(1): 90–93. https://doi.org/http://www.ijitr.com/index.php/ojs/article/view/28.

Blocquet, M., Schoemaecker, C., Amedro, D., Herbinet, O., Battin-Leclerc, F. and Fittschen, C. 2013. Quantification of OH and HO2 radicals during the low-temperature oxidation of hydrocarbons by fluorescence assay by gas expansion technique. *Proceedings of the National Academy of Sciences of the United States of America* 110(50): 20014–17. https://doi.org/10.1073/pnas.1314968110.

Cengel, Yunus A. 2007. *Thermodynamics An Engineering Approach*. Mc-Graw Hill publisher.

Dibble, R. W., Aznar, M. S., Sennott, T. B. and Jyh-Yuan Chen. 2017. Recirculating Noble Gas Internal Combustion Power Cycle. US 2017/0211515 A1, issued 2017.

Dimitriou, P. and Taku, T. 2017. A review of hydrogen as a compression ignition engine fuel. *International Journal of Hydrogen Energy* 42(38): 24470–86. https://doi.org/10.1016/j.ijhydene.2017.07.232.

Hafiz, Nik Muhammad, Mohd Radzi, Abu Mansor, and Wan Mohd Faizal, Wan Mahmood. 2018. Simulation of the Combustion Process for a CI Hydrogen engine in an argon-oxygen atmosphere. *International Journal of Hydrogen Energy* 43(24): 11286–97. https://doi.org/10.1016/j.ijhydene.2018.05.022.

Hafiz, Nik Muhammad, Mohd Radzi, Abu Mansor, Wan Mohd Faizal, Wan Mahmood, and Masahiro Shioji. 2016. Simulation of the effect of initial temperature and fuel injection pressure on hydrogen combustion characteristics in argon-oxygen compression ignition engine. *SAE Technical Papers* 2016-Octob: 1–8. https://doi.org/10.4271/2016-01-2227.

Hafiz, Nik Muhammad, Mohd Radzi, Abu Mansor, Wan Mohd Faizal, Wan Mahmood, Fadzli Ibrahim, Shahrir Abdullah, and Kamaruzzaman Sopian. 2016. Numerical study of hydrogen fuel combustion in compression ignition engine under argon-oxygen atmosphere. *Jurnal Teknologi* 78 (6–10): 77–83. https://doi.org/10.11113/jt.v78.9192.

Kadir, Murat, Yesilyurt Zeki, and Yilbasi Mustafa. 2020. *The Performance , Emissions , and Combustion Characteristics of an Unmodified Diesel Engine Running on the Ternary Blends of Pentanol / Safflower Oil Biodiesel / Diesel Fuel*. *Journal of Thermal Analysis and Calorimetry*. Springer International Publishing. https://doi.org/10.1007/s10973-020-09376-6.

Luo, Qing he, Ji Bin Hu, Bai Gang Sun, Fu Shui Liu, Xi Wang, Chao Li, and Ling zhi Bao. 2019. Experimental investigation of combustion characteristics and NOx emission of a turbocharged hydrogen internal combustion engine. *International Journal of Hydrogen Energy* 44 (11): 5573–84. https://doi.org/10.1016/J.IJHYDENE.2018.08.184.

Morovatiyan, Mohammadrasool, Martia Shahsavan, and John Hunter Mack. 2019. Numerical study on direct injection of hydrogen-methane blends into a constant volume combustion chamber. In *11th U.S. National Combustion Meeting*, 1–11. Pasadena, California. https://doi.org/10.31224/osf.io/ebvah.

Rayleigh, L. 1997. The Noble Gases: Helium, Neon, Argon, Krypton, Xenon and Radon. In *Chemistry of the Elements*, edited by N.N. Greenwood, 888–904. https://doi.org/10.1016/b978-0-7506-3365-9.50024-9.

Rey, Sopheak. 2014. Study on the SI-CI Combustion and the Spontaneous Ignition of Hydrogen Jets Using a Rapid Compression Expansion Machine. Kyoto University.

Shahsavan, M, and Mack, J. H. 2017. The Effect of Heavy Working Fluids on Hydrogen Combustion. In *10th U.S. National Combustion Meeting*, 2017-April:1–7. Maryland: Eastern States Section of the Combustion Institute. https://doi.org/10.31224/osf.io/94s8d.

Shahsavan, M., Mohammadrasool Morovatiyan, Mammadbaghir Baghirzade, and J. Hunter Mack. 2020. Implementing natural gas in a compression ignition cycle using noble gas addition. In *ASME 2019 Internal Combustion Engine Division Fall Technical Conference, ICEF 2019*, 1–9. Chicago, USA: American Society of Mechanical Engineers (ASME). https://doi.org/10.1115/ICEF2019-7159.

Stanković, I., and B. Merci. 2011. Analysis of auto-ignition of heated hydrogen-air mixtures with different detailed reaction mechanisms. *Combustion Theory and Modelling* 15 (3): 409–36. https://doi.org/10.1080/13647830.2010.542830.

Szwaja, Stanislaw, and Karol Grab-Rogalinski. 2009. Hydrogen combustion in a compression ignition diesel engine. *International Journal of Hydrogen Energy* 34(10): 4413–21. https://doi.org/10.1016/j.ijhydene.2009.03.020.

Taib, Norhidayah Mat, Mohd Radzi Abu Mansor, and Wan Mohd Faizal Wan Mahmood. 2021. Combustion characteristics of hydrogen in a noble gas compression ignition engine. *Energy Reports* 7 (May): 200–218. https://doi.org/10.1016/j.egyr.2021.07.133.

Yang, Fusheng, Jing Wang, Yang Zhang, Zhen Wu, Zaoxiao Zhang, Fengqi Zhao, Jacques Huot, Jasmina Grobivć Novaković, and Nikola Novaković. 2022. Recent progress on the development of high entropy alloys (HEAs) for solid hydrogen storage: A review. *International Journal of Hydrogen Energy* 47 (21): 11236–49. https://doi.org/10.1016/j.ijhydene.2022.01.141.

Zhu, Pengfei, Jing Yao, Chenhui Qian, Fusheng Yang, Ekambaram Porpatham, Zaoxiao Zhang, and Zhen Wu. 2020. High-efficiency conversion of natural gas fuel to power by an integrated system of SOFC, HCCI engine, and waste heat recovery: thermodynamic and thermo-economic analyses. *Fuel* 275 (March): 117883. https://doi.org/10.1016/j.fuel.2020.117883.