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NUMERICAL STUDY OF HYDROGEN FUEL COMBUSTION IN COMPRESSION IGNITION ENGINE UNDER ARGON-OXYGEN ATMOSPHERE

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Abstract

Gas emissions from automobiles are one of the major causes of air pollution in our environment today. In fact, emissions of carbon dioxide (CO_2), a product of complete combustion, has become a significant factor of the global warming effect. Hydrogen, which is a renewable energy, is regarded as a promising energy to solve this problem since the final product of hydrogen (H_2) combustion, is water (H_2O). However, the reaction of hydrogen fuels in the air under high temperature conditions produces a high volume of harmful nitrogen oxide (NOx). Furthermore, the high auto-ignition temperature of H_2 makes it difficult to ignite in a compression ignition engine in normal air. In this research, argon (Ar) is used to replace nitrogen (N_2), in order to eliminate NOx and enhance combustion. Simulation for this research was conducted using Converge, computational fluid dynamics software that is based on Yanmar TF90M compression ignition engine parameters. The simulation process was initially conducted with normal air (N_2-O_2) as the medium of combustion; but later it was replaced with an argon-oxygen (Ar-O_2) atmosphere to investigate the ignition possibility of hydrogen fuel. Hydrogen was injected at 9.95 MPa at the start of injection (SOI) at 18° BTDC. The results show that, by employing the same parameters for both simulations in normal air and argon-oxygen mediums, the combustion of hydrogen only occurred in the argon-oxygen medium. However, no combustion took place in normal air. It is therefore concluded that an argon-oxygen medium is applicable for direct hydrogen injection in a compression ignition engine.

Keywords: Energy efficient vehicle, hydrogen, argon, CFD, direct injection compression ignition

Abstrak

Pengeluaran gas daripada ekzos kenderaan merupakan punca utama kepada pencemaran alam sekitar. Malah, hasil daripada pembakaran lengkap di dalam enjin juga turut mengeluarkan gas CO_2 yang diklasifikasikan sebagai gas rumah hijau. Gas ini akan memberi kesan kepada pemanasan global. Hydrogen, sebagai punca tenaga yang boleh diperbaharui dianggap sebagai penyelesaian kepada masalah ini berdasarkan hasil utama pembakaran adalah wap air (H_2O). Walau bagaimanapun, tindak balas pembakaran gas hidrogen di dalam udara turut menghasilkan gas yang berbahaya iaitu nitrogen oksida (NOx). Selain itu, sifat hidrogen yang mempunyai suhu auto-pencucuhan yang tinggi menyukarkan pembakaran gas ini di dalam enjin pembakaran dalaman jenis pencucuhan mampatan. Di dalam kajian ini, gas argon (Ar) dipilih untuk menggantikan gas Nitrogen (N_2) di dalam udara bagi menyingkirkan NOx dan sebagai pemangkin pembakaran di dalam enjin. Converge, perisian dinamik bendalir komputeran telah digunakan dalam kajian ini berlandaskan kepada parameter enjin pencucuhan mampatan Yanmar TF90M. Bagi mengkaji nyalaan bahan api hidrogen, simulasi pembakaran hidrogen dijalankan dengan menggunakan udara (N_2-O_2) sebagai medium dan kemudiannya ditukar kepada argon-oksigen (Ar-O_2). Di dalam simulasi ini, gas hidrogen disuntik pada tekanan 9.95 MPa pada 18°BTDC. Keputusan kajian menunjukkan pembakaran gas hidrogen berlaku di dalam medium argon-oksigen manakala tiada pembakaran berlaku di dalam medium udara. Dapat disimpulkan bahawa dengan menggantikan medium pembakaran kepada argon-oksigen, pembakaran gas hidrogen secara pencucuhan mampatan boleh dilaksanakan di dalam enjin.

Kata kunci: Kenderaan cekap tenaga, hidrogen, argon, CFD, pencucuhan mampatan

1.0 INTRODUCTION

The transportation industry depends primarily on petroleum fuels. Worldwide, a huge number of engines burn a vast amount of fuel. Indeed, 70% of the 88.13 million barrels of crude oil that we consume every day is used for internal combustion engines [1]. Reciprocating internal combustion engines are used in a wide range of sizes; from small handheld model engines, to gigantic marine engines which can stand as high as four-storey building. Consequently, research on engines (both petrol and diesel) has been performed, and small improvements in their efficiency have had major positive impacts on economy and pollution.

Important tasks related to petroleum fuels mainly focus on emissions. Petroleum contains mostly hydrocarbon chains, which, during the burning process, produce various exhaust pollutants that include nitrogen oxides (NOx), carbon monoxide (CO), hydrocarbons (HC), particulate matter (PM), among other products. Even in a complete combustion product, CO_2 is believed to contribute to the 'Greenhouse Effect' or global warming. This has led to environmental health implications; and thus, most governments have imposed stringent vehicle emission regulations that are continually being tightened. In line with this issue, the International Energy Agency road map's vision is to reduce worldwide fuel use per kilometre by 30–50% in new road vehicles by 2030 and in all vehicles by 2050. The goal is to limit the global average temperature rise, which some climatologists project for 2050 [2]. In Malaysia, the government's target is to become the regional hub for Energy Efficient Vehicles (EEV) through strategic investments and the adaptation of high technology for the domestic market; and to penetrate regional and global markets by 2020. Based on global practices, EEV is defined as vehicles that meet a set of specifications in terms of carbon emission level (CO_2/km) and fuel consumption (L/km). EEV includes fuel-efficient internal combustion engine (ICE) vehicles, hybrid, electric vehicles (EV) and alternative fuelled vehicles; such as compressed natural gas (CNG), liquefied petroleum gas (LPG), biodiesel, ethanol, hydrogen and fuel cell [3]. Further than these immediate issues, fossil fuels are a finite energy source that cannot be renewed. As time passes, these crude oil and natural gas reserves will be depleted. Huge efforts have been made to improve drilling technologies, which will certainly help to increase fossil fuel reserves. However, fossil fuels do not appear to be a sustainable option at the current rapid rate that they are being consumed.

Much work has been done in the search for alternative fuel sources for powering vehicles and coping up with current regulatory demands. For this reason, renewable hydrogen energy is regarded as a promising energy storage form for vehicles. This ultimate carbon-free fuel has high energy content per unit mass, is easily combustible due to low ignition energy, and has water as its major product; thus making it one of the best potential fuels. Future demands for power units with high thermal efficiency and low pollutant emission levels have motivated the researcher to develop hydrogen fuelled reciprocating internal combustion engines. In line with this research, most efforts have been given to the types of engine spark ignition. It is widely accepted that an un-throttled lean-burn operation and reduced NOx emissions in the exhaust may be attainable. However, a common problem with the use of hydrogen and air in an internal combustion engine is the low amount of heat produced per unit volume. For example, in a stoichiometric mixture, the heat released per unit volume for a hydrogen-air mixture is only approximately 83% of that for a petrol-air system. A solution to this is to use direct injection fuel gas into the cylinder. This eliminates the loss in suction, and improves the volumetric efficiency, thus increasing the power output. It also provides additional advantages, in other respects, by removing the abnormalities of hydrogen combustion [4-5]. However, the spark ignition engine of pure premixed type can only serve as a compact power unit; it is not feasible for the requirements of larger output power, like heavy machines, ships, and other stationary power supplies that are normally worked by diesel engines [5].

In order to achieve high thermal and volumetric engine efficiency, increased power output while simultaneously being able to eliminate combustion abnormalities, compression ignition (CI) engines operating with hydrogen fuel are strongly recognized [5]. An engine with the capability to operate in high compression ratios will result in a higher power output than a spark ignition (SI) engine. However, the high auto-ignition of hydrogen fuel requires a high compression ratio to burn. This high compression ratio also leads to a higher combustion temperature and encourages the formation of nitrogen oxide (NOx) emissions [6-7]. Thus, to avoid such problems, a monoatomic gas, argon, is suggested to replace the air, in order to increase in-cylinder temperature for ignition purposes and simultaneously solve the NOx problem; since the major product of this reaction is water [8]. Argon was selected because it is abundantly available, easy to obtain, and facilitates the creation of gas tight seals [7]. In engine applications, the storage and portability of an adequate mass of hydrogen for practical applications remains one of the most difficult problems to overcome. In this research, argon with low heat capacity (Cp), is used to replace nitrogen in normal air, with the purpose of eliminating NOx and enhancing the combustion of hydrogen that was identified with high auto-ignition temperature. The research was conducted using Converge simulation software based on Yanmar TF90M compression ignition engine. The first simulation used air as the combustion medium and the next used an argon-oxygen medium.

2.0 METHODOLOGY

For this article, Converge CFD software, based on Yanmar TF90M compression ignition engine parameters, was used to investigate the combustion process. The software came with Adaptive Mesh Refinement (AMR) that could be applied to the velocity field or any scalar field to automatically increase the resolution, when or where needed. The maximum number of cells could be specified by the user in order to maintain reasonable runtimes. The AMR algorithm prioritizes and adds resolution where it is needed the most [9].

Table 1 Engine specifications for Yanmar TF90M

Parameter	Specifications
Engine type	Horizontal
Displacement	0.493 l
Bore x stroke	85 x 87 mm
Compression ratio	18
Injection Timing	18° CA BTDC
Fuel injection pressure	9.95 MPa

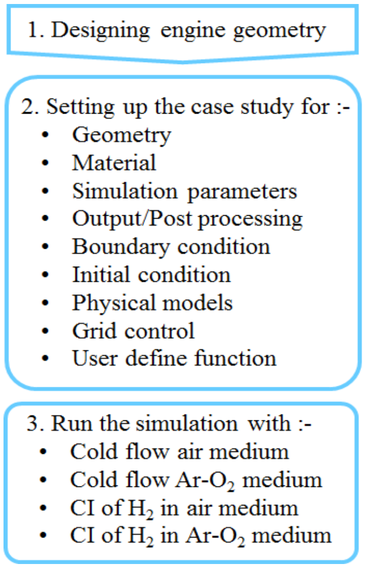

Figure 1 Workflow

The simulation runs on a direct injection compression ignition (DICI) engine, with an injection pressure and start of injection (SOI) of diesel fuel fixed at 9.95 MPa and 18° BTDC, respectively.

Table 1 shows the specification details for the base model engine. Figure 1 shows the workflow of the study simulation. At the beginning, the engine geometry, which was designed using 3D CAD software, was exported to Converge for the case set-up process. Next, the simulation was run with different initial conditions to obtain the results from two different parameters, namely air and argon-oxygen mediums. Detailed simulation parameters for each simulation set-up are shown in Table 2.

Table 2 Simulation parameters for region and initialization in case set-up

Simulation Conditions	Region Names	Temperature [K]	Pressure [kPa]	Species (Mass Fraction)
Cold Flow Air	Cylinder	300	103	O_2 23% N_2 77%
Cold Flow Ar-O_2	Cylinder	300	103	O_2 23% Ar 77%
H_2 injection in Air	Cylinder	300	103	O_2 23% Ar 77%
H_2 injection in Ar-O_2	Cylinder	300	103	O_2 23% Ar 77%

2.1 Gas Simulation

Redlich-Kwong equation of state was selected for the gas simulation model. Momentum and mass transport can be solved for both compressible and incompressible flows. For compressible flows, an equation of state is also required to couple density, pressure and temperature. The equation for this model is shown in Equation (1).

$$P = \frac{RT}{v-b} - \frac{a}{v^2 + bv}$$
$$b = \beta\, v_c$$
$$a = \alpha\, \frac{p_c v_c^2}{\sqrt{T_r}}$$
$$v_c = \frac{RT_c}{p_c};$$
$$\alpha = 0.42748, \beta = 0.08664; \quad (1)$$

where

v_c is critical volume,

T_c is the critical temperature,

P_c is the critical pressure,

α is attractive forces between molecules,

β is volume of the molecules

2.2 Combustion Modelling

SAGE combustion model, which is included in Converge, was selected for this research. The model has the capability to solve detailed chemical kinetics during the combustion process. SAGE can also determine kinetically-limited phenomena, including knock and emissions levels in combustion. This combustion model reads in a chemical reaction mechanism in a Chemkin format, and solves the ODEs to identify the cell reaction rate.

In order to speed up the Converge software calculation, SAGE comes with options, such as solving temperature, which can be excluded from the chemistry solver (assumed constant), and also allow the solver to pass an analytically-calculated Jacobian process.

2.3 Turbulence Modelling

In this research, Reynolds-Averaged Navier–Stokes (RANS) was selected as the turbulence model. This model's approach is to solve the averaged quantities of turbulent motion. This approach does not require large computing resources and has been the backbone of industrial CFD applications for several decades, due to its modest computing requirements [10-11].

3.0 RESULTS AND DISCUSSIONS

In this research, argon was studied to replace nitrogen in normal air for hydrogen fuel combustion. A great deal of research has been carried out that focused on spark ignition engine [5,7,12]. However, the potential of efficiency, power density and safety advantages of a direct injection hydrogen fuelled diesel engine, over a premixed spark-ignited, provided the motivation to further study the compression ignition engine.

3.1 Validation Of Simulation Results

In order to obtain accurate results, the simulation was validated against theoretically thermodynamic results. Since the simulation was conducted from the condition of intake valve close (IVC) to exhaust valve open (EVO), the temperature and pressure obtained during compression and expansion processes can be calculated using equation (2). Where, T is the temperature, V is the volume and κ is the specific heat ratio. The combustion process occurred under the isentropic compression of an ideal gas, where specific heats were constant [13].

$$T_2 = T_1\left(\frac{V_1}{V_2}\right)^{k-1}$$
$$P_2 = P_1\left(\frac{V_1}{V_2}\right)^{k} \quad (2)$$

Cold flow simulation in an air medium was selected for validation with a theoretically thermodynamic calculation for this research. Detailed boundary conditions are shown in Table 1 and Table 2. The simulation time started form IVC at 552° CA to EVO at 858° CA, and the simulation results for pressure and temperature were compared with the thermodynamic theory (as shown in Figure 2). From the graph, it can be observed that pressure and temperature showed a strong agreement between simulation and theory. The maximum value for pressure in the simulation was recorded as 5.4 MPa and temperature as 864K. However, the maximum value for temperature and pressure for the theoretically thermodynamic calculations were 924 K and 5.7 MPa, respectively; slightly higher than the value obtained in the simulation.

The discrepancies between maximum values for pressure and temperature were 5% and 6%, respectively. Due to this validation process, it was deemed practical to proceed to the next step of the simulation with hydrogen fuel direct injection in air and argon-oxygen mediums.

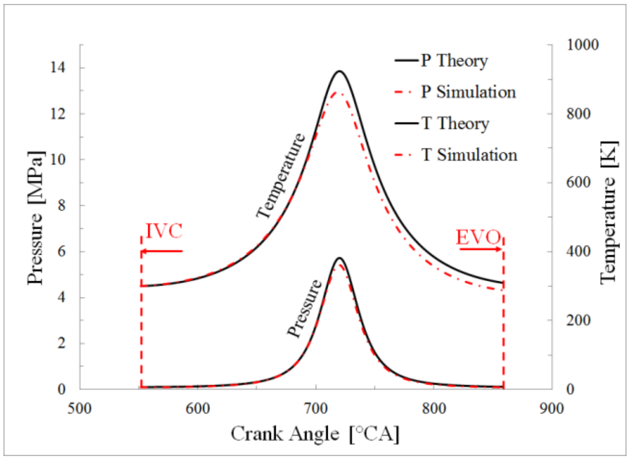

Figure 2 Pressure and temperature for simulation and theory results

3.2 Direct Injection Of Hydrogen In Compression Ignition Engine With Air Medium

The simulation process continued with hydrogen fuel injected into a compression ignition engine at 702° CA to 712° CA. Figure 3 shows the pressure and temperature results from the simulation. Pressure increased and decreased proportionally with the decrease and increase of in-cylinder volumes. The same trend was also observed for temperature. The maximum pressure and temperature obtained was 847 K and 5.5 MPa, respectively. Figure 4 shows a very small value of heat release rate with a maximum value of 1.54 X 10^{-5}[J/CA]. It can be concluded that no combustion occurred throughout the process. The maximum temperature of 847 K (as shown in Figure 4) prevented the hydrogen fuel from igniting, because the auto-ignition temperature for hydrogen is 858K [14].

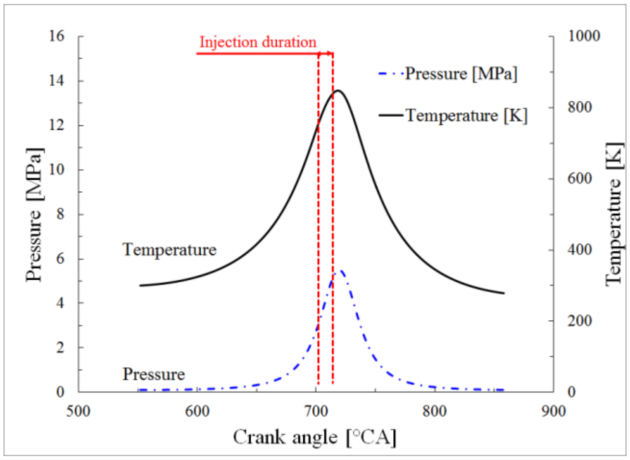

Figure 3 Pressure and temperature for H_2 direct injection in air atmosphere

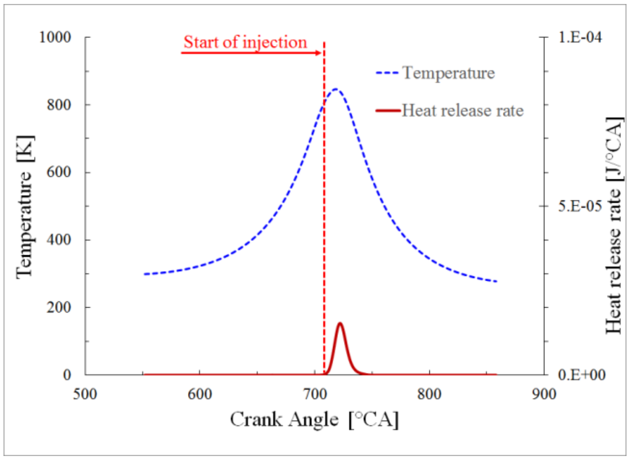

Figure 4 Temperature and heat release rate for H_2 DI in air medium

3.3 Direct Injection Of Hydrogen In Compression Ignition Engine With Argon-Oxygen Medium

Figure 5 shows the values of temperature between three different conditions, which are cold flow simulation with air, cold flow simulation with argon-oxygen, and hydrogen direct injection with argon-oxygen medium. From the graph, it is understood that temperature increase in the cold flow simulation with argon-oxygen medium was higher than in the air medium because the low specific value of argon generated a higher temperature during the compression stroke in the engine. The maximum temperature obtained for the cold flow simulation in argon-oxygen medium was 1,286 K; instead of 847 K for the simulation in air medium. This condition is suitable for hydrogen to ignite in a compression ignition engine; whereby the temperature achieves 1,245 K at 702°CA while the hydrogen is being injected during the simulation process. As a result, the maximum temperature obtained for hydrogen direct injection in argon-oxygen medium was1,545 K.

Figure 6 shows the heat release rate value for hydrogen fuel combustion in argon-oxygen medium. Even though the injection began at 702 °CA, the fuel started to ignite with a premixed combustion at 710 °CA. The maximum heat release rate was recorded at 908 J/degree and an ignition delay (τ) of 8.8° CA (9.17 ms). Mansor et al. [15] performed an experiment using a constant volume combustion chamber with ambient temperature 1,200 K. They obtained a value of ignition delay of 0.3 ms; which is much shorter than the duration obtained in the simulation. This discrepancy was due to the differences of oxygen concentration and equivalence ratio between the experiment and the simulation [15-16].

From the simulation results, the value of heat release rate shown in Figure 6 is very high compared with the value shown in Figure 4. Longer ignition delay provides sufficient time for the hydrogen fuel and the oxygen to mix properly and allow the gas mixture to burn under premixed combustion [17]. Moreover, high fuel injection pressure, at 9 MPa, and the potential of

H_2 gas with higher flame speed and faster combustion velocity [18], induces the high premixed combustion phase and produces a high heat release rate.

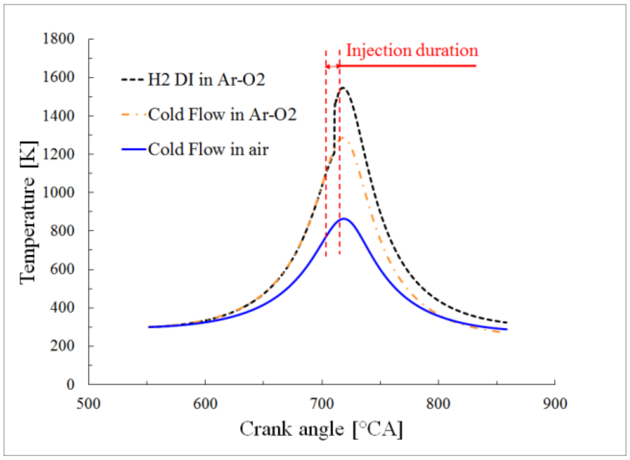

Figure 5 Temperature for H_2-DI in Ar-O_2 compared to cold flow temperature in air and Ar-O_2

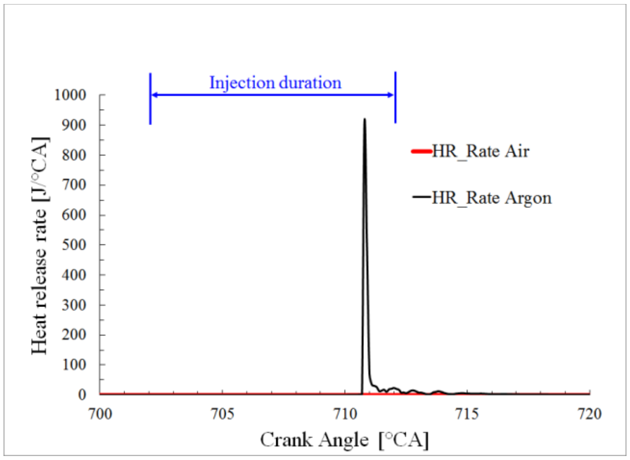

Figure 6 Heat release rate for H2-DI in Ar-O2 atmosphere

Figure 7 shows the species mass of reactant and product during the simulation process from the beginning at 552°CA until the end at 858° CA. Major products for hydrogen combustion with argon-oxygen medium are oxygen (O_2) and water (H_2O). Besides that, other species, such as O, OH, HO_2 and H_2O_2, contribute only a very minimum mass value. It was observed that O_2 remained high in volume and proved that the combustion occurred under lean combustion. Since argon gas reacts with no other gases during the simulation, it is proposed that this gas is recirculated back to the engine when designing and producing a concept engine in the future [7].

Figure 8 shows the simulation results of temperature for hydrogen direct injection in argon-oxygen medium, compared with normal air. The result was obtained using EnSight software. Contour of temperature was compared at 552°CA (IVC), 662°CA (before injection), 702°CA (during injection) and 792°CA (during combustion). At the beginning of the simulation process, at 552°CA and 662°CA, only small differences in temperature values were obtained. Later, during the injection period at 702°CA, the values of temperature in argon-oxygen medium had already reached the hydrogen auto-ignition temperature; but a different situation occurred in the medium in normal air. At 792°CA, the temperature remained high in the argon-oxygen medium due the combustion process; however, the temperature in normal air had already decreased towards the ambient temperature. Detailed values for pressure and temperature between hydrogen direct injection in argon-oxygen and normal air medium are shown in Table 3.

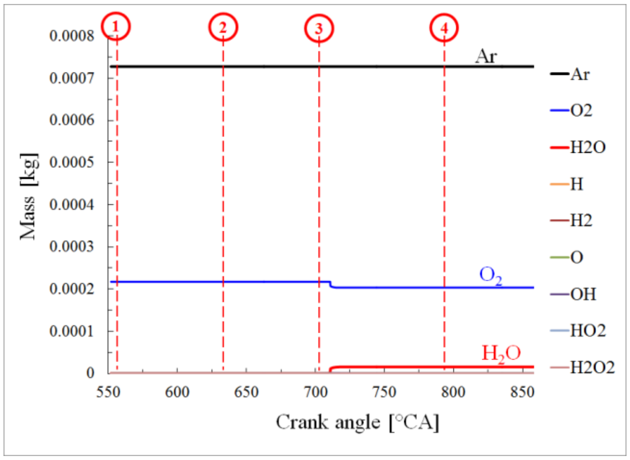

Figure 7 Mass of combustion product

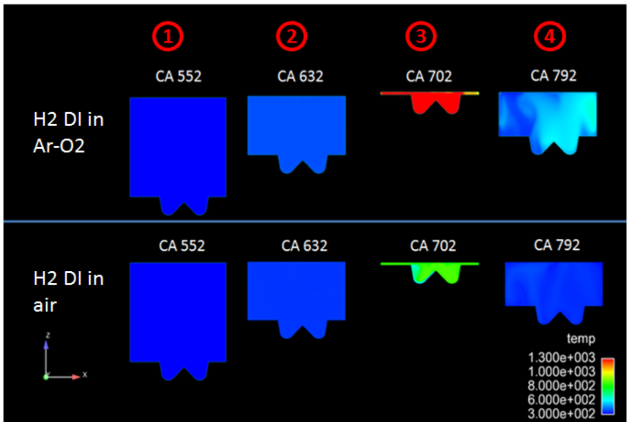

Figure 8 Comparison temperature image for DI H_2 in Ar-O_2 and air atmosphere

Table 3 Temperature and pressure at 552°CA, 632°CA, 702°CA, and 792°CA

Medium		**1** 552°CA	**2** 632°CA	**3** 702°CA	**4** 792°CA
Ar-O$_2$	Pressure [MPa]	0.10	0.23	4.30	0.36
	Temperature [K]	300	402	1,071	473
Air	Pressure [MPa]	0.10	0.21	3.04	0.29
	Temperature [K]	300	370	755	365

4.0 CONCLUSIONS

In this research, the possibility to replace nitrogen in normal air with the mono atomic noble gas argon, for direct injection of hydrogen fuel in compression ignition engine, is studied using numerical Converge software. The following conclusions were obtained from the results:

1. Hydrogen direct injection in normal air medium with maximum temperature of 848 K does not ignite as shown in the simulation results, even though the obtained temperature was close to the hydrogen auto-ignition temperature.
2. Replacing the combustion medium from air to argon-oxygen caused an increasing in-cylinder temperature and allowed the hydrogen fuel to ignite and burn.
3. The ignition delay for hydrogen combustion at the start of injection at 702 °CA was 9.17 ms.
4. Product of hydrogen fuel combustion in an argon-oxygen medium is mainly oxygen and water.

In this study, only the preliminary data was obtained. More detailed analysis, with more variables confirmed by simulation and experimentation, is needed. Hence, in order to realize this mission, much more work should be done by many researchers, in terms of gas portability for hydrogen, oxygen and argon, and the safety and delivery of these gasses. All of these issues will remain as new challenges for the next research.

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