NUMERICAL INVESTIGATION ON THE COMBUSTION PERFORMANCE AND EMISSION FORMATION OF AMMONIA SPARK IGNITION ENGINE USING DIRECT INJECTION AND MULTI COILS SPARK-IGNITION STRATEGY

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ABSTRACT

Future internal combustion engines can achieve zero carbon emissions by using ammonia, an efficient hydrogen energy carrier with a greater energy density and a more sophisticated production-storage-transportation lifecycle. Ammonia fuel's laminar flame speed is comparatively sluggish, nevertheless, which leads to less than ideal combustion performance. Investigating the impact of direct injection and the multi-coil method on ammonia spark ignition engine performance was the goal of this study. The simulation's output was then verified using standard diesel fuel and the literature on combustion performance for RCEM engines. At four SOIs between 40° and 0° BTDC, with varying multi-coil spark timing of ignition under high compression ratio of 17, the combustion performance and emission production of ammonia direct injection were examined using the created numerical model. As the timing of the spark increased, there was a tendency for the velocity and turbulence intensity to rise and then decline. Increased spark timing can improve ignition stability, reduce combustion time, reduce cooling loss, and boost output power. Ammonia flame propagation is sensitive to temperature and flow field. Regretfully, when the spark timing increases, the NOx emission progressively increases. By offering a basic ignition method for ammonia engines, this result holds promise for the transition of internal combustion engines to zero carbon ammonia engines.

KEYWORDS ammonia spark ignition engine; direct injection; multi coils; combustion performance; emission.

INTRODUCTION

People are exploring new alternative fuels in an era of diminishing energy supplies (Sonker et al., 2022) and the damaging effects of their combustion products on the environment (Kalghatgi et al., 2018). Ammonia has recently been proposed as the fuel that spark ignition (SI) engines can run on. With its many advantageous qualities, ammonia is seen to be a good substitute for fossil fuels. Being one of the most produced chemicals in the world, it has a well-established infrastructure, a decent energy density, no carbon, which contributes to the generation of carbon dioxide (CO2), and is relatively easy to store (Chai et al., 2021). However, using ammonia to feed ICEs has two significant issues. Its toxicity and causticity are the root of the first issue (Valera-Medina et al., 2018). The second issue emerges from the chemical properties of ammonia, which include its sluggish laminar flame propagation speed and high ignition energy need (J. Lee et al., 2024).

Ammonia has two important drawbacks in spark ignition (SI) engines, which are primarily made for gasoline, despite its potential (J. Liu & Liu, 2024). First of all, ammonia requires a large spark energy to initiate combustion (Kurien & Mittal, 2023). Furthermore, compared to traditional fuels such as gasoline, its laminar flame speed is significantly slower. The narrow flammability limitations and low flame speed of ammonia, which result in incomplete combustion, restrict its employment in SI engines (Mounaïm-Rousselle et al., 2021), (X. Liu et al., 2024). Port injection or direct injection are the two methods available for introducing ammonia into the cylinder, much like with gasoline. In doing so, the engine's volumetric efficiency is decreased as the air that was brought to the combustion chamber is displaces. It is necessary to overcome the in-cylinder pressure by raising the injection pressure when injecting gaseous ammonia straight into the cylinder, which presents additional challenge (El-Adawy et al., 2024). Unfortunately, the operational range of the injection pressure is somewhat small because gaseous ammonia liquefies if the pressure is higher than the saturation pressure (e.g. 1 MPa at 298 K) (J. Lee et al., 2024). Several investigations have demonstrated that ammonia combustion in SI engines is feasible if the appropriate combustion strategy (D. Lee & Song, 2018) is implemented together with the necessary fuel delivery system adjustments (Min et al., 2024). The viability of employing ammonia as an engine fuel is the main finding from earlier research (Gross & Kong, 2013). For optimal combustion performance in direct injection engines, fuel and air should be evenly distributed throughout the combustion chamber (Schramm et al., 2020). In order to achieve rapid dispersion and atomization in combustion chambers, particularly in large-bore engines, it is necessary to increase the injection pressure of liquid ammonia (Fang et al., 2023).

In light of these facts, a novel approach to combustion is required in order to get high efficiency like to a diesel engine and lower emissions akin to a SI engine. The amount of discharge energy transmitted to the spark plug in a SI system depends on both the spark duration and the discharge current. Previous research has indicated that greater spark energy is beneficial for producing flames; this effect is also impacted by the flow stream that generates vortices close to the spark plug. Both the length of the spark and the discharge currents affect the amount of energy delivered to the spark gap since the spark energy is the result of the discharge voltage and discharge current convergent within the spark discharge period. Nevertheless, a detailed investigation of the relative impacts of the discharge length on the RCEM in-cylinder pressure is still lacking. Simultaneous computational fluid dynamics modeling is carried out to investigate the effects of spark ignition and ammonia direct injection on the combustion and performance of a diesel-fueled RCEM. Furthermore, the effect of the spark discharge energy on the ignition discharge energy process is examined, as is the reciprocal relationship between the spark discharge energy and flow field. In order to identify the proper relationships during this ignition process, CFD modeling was used to examine the effects of the in-cylinder flow field on spark channel operation and the multi-coil spark plug discharge energy on the in-cylinder performance of RCEM with a spark ignition ammonia direct injection strategy. However, techniques implementing the conventional coil ignition system are the main focus of the study.

RESEARCH METHOD

Methodology

CFD simulations of CONVERGE® were conducted utilizing ammonia direct injection and fuel injection pressures ranging from 150 to 200 bar. The RCEM research engine model includes features that are comparable to those of a gasoline spark ignition engine. 20 degrees before top dead center (BTDC), 1000 µs injection time, and a 17 engine compression ratio were all established.

In order to predict the performance of internal combustion engines (ICEs) and provide information that can be used to improve the design of future combustion systems, computational fluid dynamics, or CFD, is presently a widely used approach in both industry and research. Depending on user-specified grid control settings, CONVERGE® will produce an entirely orthogonal and ordered grid at runtime.

Fuel Preparation

Table 1 shows the characteristics of ammonia in comparison to other fuels. Like liquid propane, it is readily liquefied for storage at low pressure at room temperature or chilled to -33°C for ambient pressure storage. Ammonia (NH_3) is easily kept in a liquid condition at a pressure of 10.3 bar, despite not being a pure hydrogen component. When compared to pure hydrogen, ammonia has a higher energy density per unit volume due to its liquid state storage capacity. To put it another way, for tanks of equal capacity, more hydrogen is kept in liquid ammonia than in a tank of gaseous or liquid pure hydrogen. It is very resistant to autoignition and has a high-octane rating of 110. Compared to liquid hydrogen, it retains 30% more energy by volume and has 17.8 weight percent hydrogen. Additionally, it dissociates more readily, requiring just 16% of the fuel's energy and negating the need for energy during the last stage of hydrogen purification. Although ammonia has a very high ignition temperature of 650 °C, its characteristics are similar to those of liquid propane (C_3H_8). The densities, boiling points (-33.3°C for ammonia and -42.0°C for propane), and octane values of ammonia and propane are almost identical.

Ammonia is a trigonal pyramidal molecule made up of three hydrogen atoms and one unshared pair of electrons attached to the nitrogen atom. Due to strong hydrogen bonds between molecules, this polar molecule has a high degree of association. Ammonia works better as a solvent for organic compounds because its dielectric constant (22 at 239.2 K) is lower than water's (81 at 298.2 K). Ammonia may nevertheless function as a somewhat effective ionizing solvent because of its high dielectric constant. Though not as much as water, ammonia also self-ionizes. The stoichiometric formula for propane in air is as follows:

$$4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O + \text{heat}$$

In contrast, the equivalency ratio, or ϕ, is the ratio of the fuel/oxidizer ratio in the stoichiometric formula, as indicated in equation (1), to the actual fuel/oxidizer ratio.

$$\phi = \frac{(A/F)_{stoic}}{A/F} = \frac{X_{NH_3}/X_{O_2}}{\left(X_{NH_3}/X_{O_2}\right)_{stoich}} = 3\left(X_{X_{NH_3}}/X_{O_2}\right) \quad (1)$$

Table. 1 Properties of various internal combustion fuels. Adapted from ref. (Reiter & Kong, 2011)

	Fuel name			
	Gasoline	**Propane**	**Gaseous H_2**	**Ammonia**
Formula	C_8H_{18}	C_3H_8	H_2	NH_3
Storage method	Liquid	Liquid	Compressed	Liquid
Approximate AKI*Octane rating	87 – 93	103	RON > 130	110
Storage temperature (°C)	25	25	25	25
Storage pressure (kPa)	101.3	1020	24,821	1030
Fuel density (kg/m^3)	698.3	492.6	17.5	602.8
LHV (MJ/kg)	42.5	45.8	120.1	18.8
LHV (MJ/L)	29.7	22.6	2.1	11.3

Table. 2 Combustion properties of various internal combustion fuels. Adapted from ref. (Kobayashi et al., 2019)

	Fuel name			
	Gasoline	**Propane**	**Gaseous H_2**	**Ammonia**
Flammability limits	C8H18	C3H8	H_2	NH_3
Flame speed	Liquid	Liquid	Compressed	Liquid
Autoignition temperature	87 – 93	103	RON > 130	110
Minimum ignition energy	25	25	25	25
Latent heat of vaporization	29.7	22.6	2.1	11.3

Spark Discharge Energy

An ignition driver controller, ten spark coils, and a single spark plug were used to construct a high-energy inductive ignition system for this study. Two sets of ignition coils were linked and paralleled with a single spark plug, as seen in Figure 1. The ICD-212 ignition driver was linked to each discharge coil. The ICD-212 ignition driver features three modes of ignition control: pair mode, which pairs two coil channels; individual mode, which displays a sequence of separate outputs for each coil channel; and simultaneous mode, which displays all coil channels simultaneously. It is possible to adjust the timing of the ignition signals between channels from 1.0 to 65.4 ms.

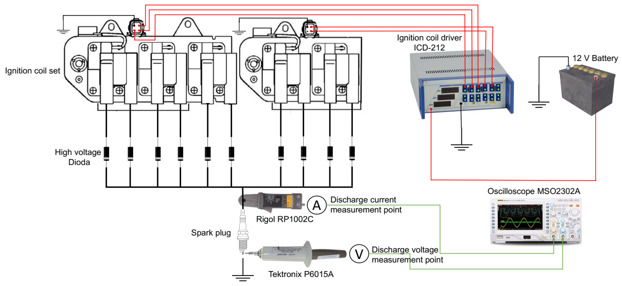

Fig. 1 Schematic of enhanced ignition system

CFD Simulation

A Windows computer with an Intel (R) Core (TM) i7 77003.60 GHz CPU and 32 GB of RAM was used to conduct CONVERGE®. The computation technique, graphics preprocessor surface treatment, computer network computations, beginning and boundary conditions, and post-treatment are all included in this simulation. The outcomes are also shown in a Tecplot. As seen in Fig. 2, all restrictions were seen as permanent, with the exception of the piston, which was thought of as a moveable boundary. At the input, the pressure and temperature were set to 1 bar and 383 K, respectively. To ensure simulation quality, the grid size was set to 4 mm, and the automated mesh refinement (AMR) tool was used to update the major area valves. The models used in this study are listed in Table 3.

Table 3. CONVERGE key processes used in this study

Physical Model	**Physical process**	**Model**
Turbulence Modeling	Renormalization group (RNG) k-ε	Reynolds-averaged Navier-Stokes (RANS)
	Wall heat transfer	O'Rourke and Amsden
Ignition Spark Modeling	Source	Energy
	Shape	Sphere type
	Motion	Move with flow
Combustion Modeling	Chemistry solver	SAGE
	Emissions	Extended Zeldovich
	SOOT	Hiroyasu SOOT
Spray Modeling	Spray break up	Kelvin-Helmholtz (KH) – Rayleigh-Taylor (RT)
	Drop drag	Dynamic drop drag
	Collision	NTC
	Turbulent dispersion	O'Rourke model
	Spray wall interaction	Wall film

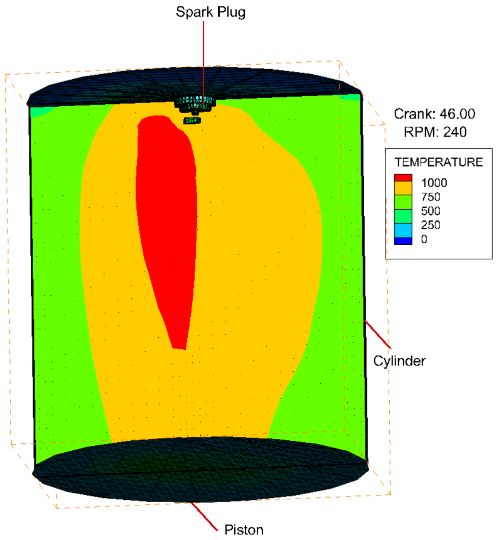

Fig. 2 RCEM spark modelling

RESULT AND DISCUSSION

One key factor defining an engine's power performance is its in-cylinder pressure. A comparison of the engine's cylinder pressure with several ignition procedures is shown in Fig. 2. The ignition methods that functioned with the spark running at about 20 °CA BTDC at roughly 11.3 MPa produced the highest maximum in-cylinder pressure. It shows how the cylinder's pressure curve changes as the CR 17. The reason for this is that when the CR rises, the fuel and air in the cylinder are compressed to a smaller volume, which raises the mixture's pressure and temperature. The combination burns more quickly thanks to the spark from the spark plug. Pressure within the cylinder rises as a result of the quick combustion and energy release. In nearby areas of the TDC, more ammonia burns as the spark duration increases. As a result, the pressure within the cylinder increases continuously due to the piston's upward movement, rapidly raising the pressure curve. Less combustion happens after the TDC when the piston is going lower, and the cylinder volume is rising. The cylinder pressure curve thus drops off quickly.

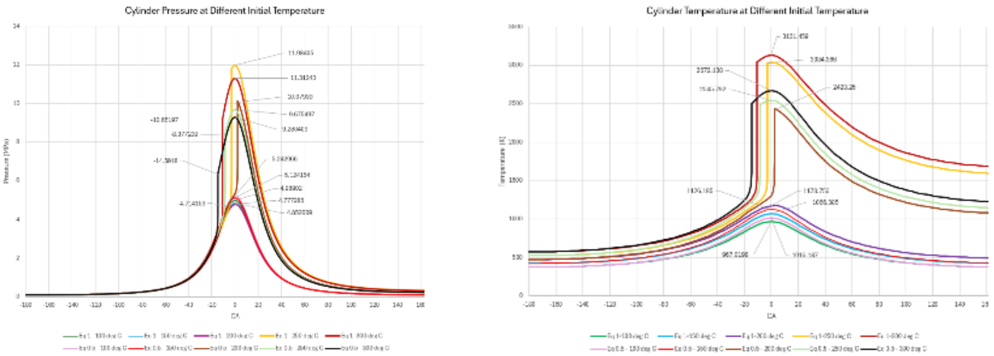

Fig. 2 Pressure and temperature inside the RCEM in-cylinder model

Fig. 3 shows the results of the simulations that have been spatially averaged throughout the flame growth field close to the spark plug with differing discharge energy. Thus, these measurements provide low-pass spatially filtered values surrounding the spark plug as the energy of the spark discharge increases. It is incorrect to say that the measurement plane crosses the spark plug exactly. Apart from exposing the kernel growth to a greater range of varied velocities, the creation of an ammonia layer around the spark plug in conjunction with spark energy discharge may facilitate quicker flame generation. The growth of the flame kernel and the subsequent combustion process plug are impacted by the flow conditions surrounding the spark plug gap because they raise the spark discharge energy upon ignition. The nitrogen element in NH_3 and the oxygen element produce nitrogen oxides at high temperatures when the cylinder's temperature rises.

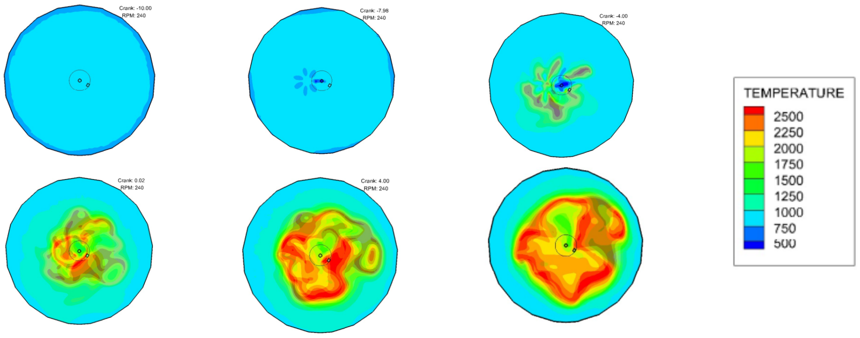

Fig. 3 Flame temperature distribution (z-axis direction*)* with the discharge energy of single coil

Fig. 4 shows spray development from -10 CA to 5 CA. Reproducing SMD trends required adjusting the parameters of the KH-RT breakdown model as it moved from the flash boiling regime to the non-flashing one. This implies that it is still difficult to capture spray local features across all regimes using a spark ignition technique, particularly when using a novel fuel like ammonia. However, upon examining the five places, trend-wise projections suggest that the exterior locations, as seen in the simulation, had bigger droplets.

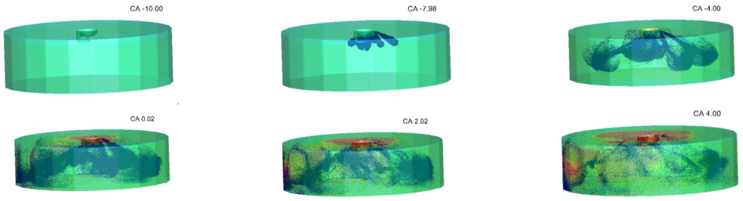

Fig. 4 Spray development (y-axis direction)

CONCLUSION

This study used CFD modeling to examine the impact of spark discharge from direct ammonia injection into RCEM on combustion and performance. Using several ignition strategies for ammonia direct injection, the simulation was created to determine its viability.

The in-cylinder temperature and flow field have an impact on flame formation. A positive feedback loop is formed when the CR rises and the in-cylinder temperature progressively rises as well, intensifying the combustion. An ammonia spark ignition engine's ignition stability can be improved, and the in-cylinder combustion time shortened by increasing the CR.

Fuel NOx generation is increased by the rise in CR, which also raises the in-cylinder pressure and temperature. The improved ignition strategy creates circumstances for fuel NOx formation by prolonging the high in-cylinder temperature. Reducing NOx emissions can be achieved by after-treatment.

Future research will focus on expanding the combustion parameters of an ignition strategy to increase fuel economy and exhaust emissions, as well as examining the ammonia injection location to achieve the highest combustion efficiency.

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