Simulation Research on Ammonia-Hydrogen Mixed Combustion Engine

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Abstract. To achieve low carbon emissions throughout the entire lifecycle, including preparation, storage, transportation, and use, hydrogen(H_2) and ammonia(NH_3) energy represent effective solutions to address significant challenges in energy development. Hydrogen stands out as a promising carbon-free energy carrier due to its calorific value, which is roughly three times that of gasoline or diesel. However, hydrogen's high flammability, high diffusivity, and low liquefaction temperature limit its broad application in engines. Ammonia, on the other hand, serves as a hydrogen-rich energy carrier with a volumetric energy density three times that of hydrogen, offering a viable solution to mitigate the drawbacks of hydrogen energy in engines. Nevertheless, ammonia's laminar flame speed is relatively slow, about one-fifth that of gasoline, and it is not easy to ignite. Combining ammonia and hydrogen in combustion can address issues related to the challenging control of hydrogen combustion and the difficulty of igniting ammonia. The application of ammonia-hydrogen mixed combustion in vehicles involves using ammonia cracking as the hydrogen supply source, which circumvents the problem of hydrogen storage. Utilizing low-carbon and zero-carbon fuels remains the sole path to achieving environmentally friendly and sustainable transportation development. This article focuses on the ammonia-hydrogen mixed combustion model integrated into vehicle engines and explores engine thermal efficiency and emissions across various ammonia-to-hydrogen ratios.

Keywords: Ammonia engine; hydrogen; zero carbon; sustainability.

1. Introduction

With the rapid development of the world economy, the world's coal, oil and other fossil energy consumption is too fast. Fig. 1 shows the proportion of various primary energy consumption in 2022. Obviously, the use of fossil fuels still accounts for a large proportion. At the same time, with the extensive use of fossil fuels, greenhouse gas emissions continue to rise significantly, and the greenhouse effect becomes increasingly serious [1]. Humanity is faced with the increasing demand for fossil energy and the greenhouse effect caused by the extensive use of fossil energy. In order to resolve this contradiction, humans have been actively exploring new energy sources to replace fossil energy and control greenhouse gas emissions, which means using cleaner fuels to replace coal in traditional thermal power and oil in the power industry.

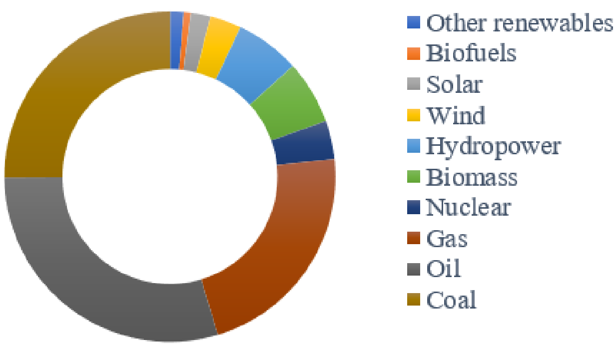

Fig. 1 Global direct primary energy consumption, 2022 [2,3]

H_2 and NH_3 are effective ways to break through major bottlenecks in the development of zero-carbon emissions and low energy throughout the energy life cycle [4]. However, hydrogen is flammable, explosive and difficult to liquefy, making its transportation, storage and use very difficult. Converting hydrogen into an "energy carrier" with high energy density and easy transportation and storage is an effective solution [5]. NH_3 can not only be used as a hydrogen energy carrier, but it is also a directly usable zero-carbon fuel. It can also be produced through renewable energy and has low carbon emissions during the entire life cycle of "preparation-storage-transportation-use" [6]. In 2017, the Global Ammonia Energy Alliance proposed the new concept of Ammonia=Hydrogen 2.0, predicting that "ammonia will be the winner of green energy in the future." In 2021, the U.S. Department of Energy and the Japanese government both released ammonia energy strategies, pointing out that NH_3 is a true zero-carbon fuel with high energy density and can be widely used in energy power equipment and systems [7]. However, high ignition energy and low combustion rate are two major technical bottlenecks in the development of ammonia engines. Compared with traditional hydrocarbon fuels, ammonia has low reactivity and high auto-ignition temperature. Its minimum ignition energy is more than 60 times that of gasoline, and its laminar flame speed is about 1/5 that of gasoline.

Ammonia-hydrogen mixed fuel can effectively solve the above problems. "Ammonia-hydrogen fusion" is conducive to meeting the technical challenges of single hydrogen energy utilization in transportation, storage, on-board, safety, cost and other aspects. The utilization technology of NH_3 as a hydrogen energy carrier is the current and future international cutting-edge scientific and technological innovation. The purpose of this study is to conduct theoretical exploration and simulation experiments on the NH_3-H_2 mixed combustion model and compare the effects of different NH_3-H_2 mixing ratios on the combustion characteristics, emissions and thermal efficiency of the engine cylinder. This study theoretically explores the changing trends of engine representation characteristics with respect to variables through simulation experiments, thereby providing theoretical support for practical experiments.

2. Simulation Model Setup

A four-stroke single-cylinder engine modified from the ammonia-diesel dual-fuel (ADDF) engine model in literature was used for simulation experiments [8]. In this research model, the NH_3-H_2 mixture enters the air passage from the injector in the intake port and forms a mixed gas with air in the air passage, then enters the cylinder and is ignited by the spark plug.

2.1. Engine Apparatus

Table 1. Engine specifications

Parameter	Description
Cylinder diameter /mm	83.1
Piston stroke /mm	92
Connecting rod length /mm	145.1
Rotating speed /rpm	2000
Compression ratio	12:1
Type of aspiration	Nature aspiration
Intake valve open timing (Crank angle)	-364
Intake valve close timing (Crank angle)	-97
Exhaust valve open timing (Crank angle)	128
Exhaust valve close timing (Crank angle)	420

The simulated engine has a compression ratio of 12:1 and a constant speed of 2000 rpm. Other parameters of the test engine are listed in Table 1. Fig. 2 is a three-dimensional diagram of the model.

The model is an ignition engine, which mainly consists of an intake port, an exhaust port, a valve, a cylinder wall, a piston, a spark plug, and a fuel injector arranged on the intake port.

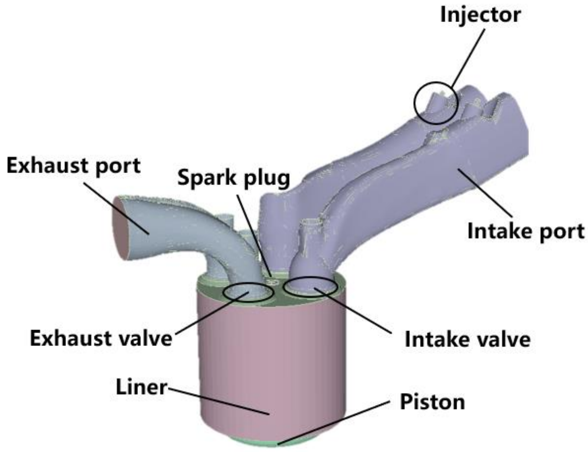

Fig. 2 Ammonia hydrogen engine model (Photo/Picture credit: Original)

2.2. Reaction Mechanism

Typically, comprehensive chemical reaction mechanisms feature hundreds of species and chemical processes, combinations of simulation algorithms, and complex combustion chemical kinetics. The reaction mechanism used in the model based on NH_3-H_2 mixed combustion in this project includes 560 substances and more chemical processes, including NH_3-H_2 combustion, NOx formation and other mechanisms. It plays a very important role in analyzing kinetic processes and determining the reaction paths of important components. Among them, the reaction rate constant of each elementary reaction is expressed in the form of Arrhenius, that is

$$k_f = AT^b \exp\left(-\frac{E_a}{R_u T}\right) \tag{1}$$

In the formula (1), A is the frequency factor, which is a constant; b is the temperature index; E_a is the activation energy. This study adopted the H_2/NH_3-related reaction mechanism developed by Shrestha et al., which has been verified in terms of IDT, LFS and species concentration [9].

2.3. Simulation Boundary Parameters

This study is based on CONVERGE 2.3 software to study the effects of different proportions of NH_3-H_2 fuel on emissions and thermal efficiency. The measured data of References 6 and 7 in Table 2 are used as the boundaries of the engine model, and multiple experiments are conducted with the molar ratio of the NH_3-H_2 mixture injected into the inlet as a variable. The experimental data were processed using MATLAB programming and Ensight software.

Table 2. Engine specifications [10]

Part	T(K)	P(MPa)
Cylinder	800	0.101325
Intake port	363	0.101325
Exhaust port	800	0.101325
Injector	373	0.6

3. Results and Discussion

This study presents experimental results on the effect of the NH_3-H_2 mixture ratio on in-cylinder combustion. In order to study the performance of this engine, the changes in the effective pressure and pressure rise rate in the cylinder were first evaluated. The mixture ratio was analyzed to evaluate engine thermal efficiency as well as NOx emission characteristics to assist in the discussion.

3.1. Engine Performance

As shown in Fig. 3, with the increase of the proportion of hydrogen energy, the maximum pressure in the cylinder also gradually increases, and the maximum pressure point gradually moves to near the top dead center of the piston, which means that the combustion process in the cylinder is closer to constant volume process. At the same time, as the proportion of hydrogen increases, the combustion delay period in the cylinder continues to shorten, and the slow combustion period continues to increase, which means that the fast combustion period of the internal combustion engine becomes shorter and shorter, the flame diffusion speed accelerates, and the combustion becomes more intense.

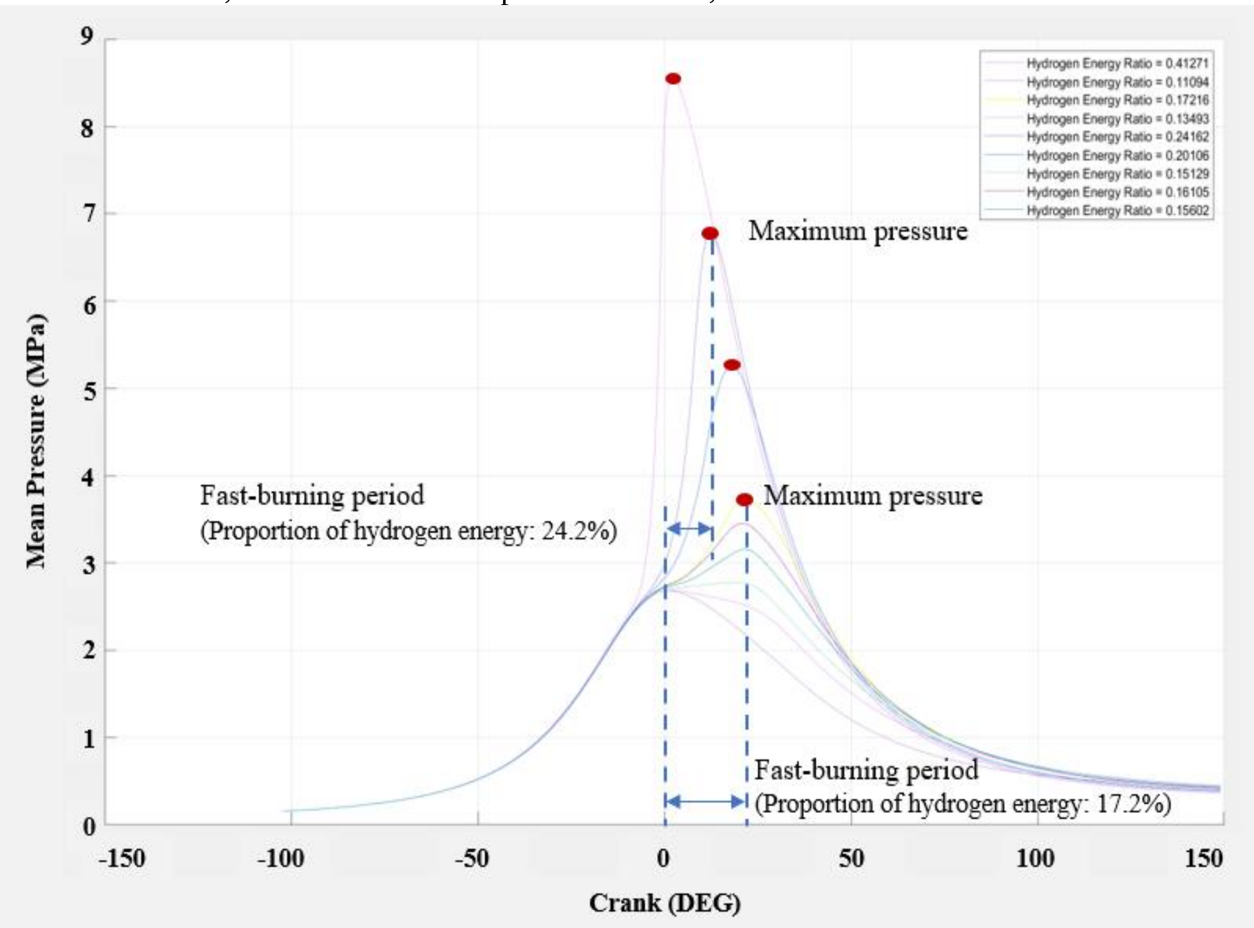

Fig. 3 Effect of NH_3-H_2 mixture ratio on cylinder pressure (Photo/Picture credit: Original)

3.2. Combustion Analysis

Normally, when the pressure rise rate reaches a certain value, usually 5 times that of normal combustion, as shown in Fig. 4(a), the engine will detonate at this time. Knocking is usually caused by rapid temperature rise, as shown in Fig. 4(b), or by spontaneous combustion at the end of the mixture inside the cylinder caused by high temperature. At this time, the engine will make a loud operating noise, and the engine structure may also be damaged. Therefore, in this model, the proportion of hydrogen energy should be reduced as much as possible to avoid strong detonation.

H_2O_2 is an important oxide that reflects the mixed combustion of ammonia and hydrogen. It is also an indicator of high-temperature combustion and the overall chemical process rate. As shown in Fig. 5, the distribution of H_2O_2 in the cylinder at the CA10 time of the engine is shown under knocking and normal combustion conditions. The red area in Fig. 5 represents the area with a higher concentration of H_2O_2, which means that a violent combustion reaction is taking place in this area. In panel a, due to the higher temperature of the cylinder wall, the final mixture spontaneously ignites, thereby causing a knock.

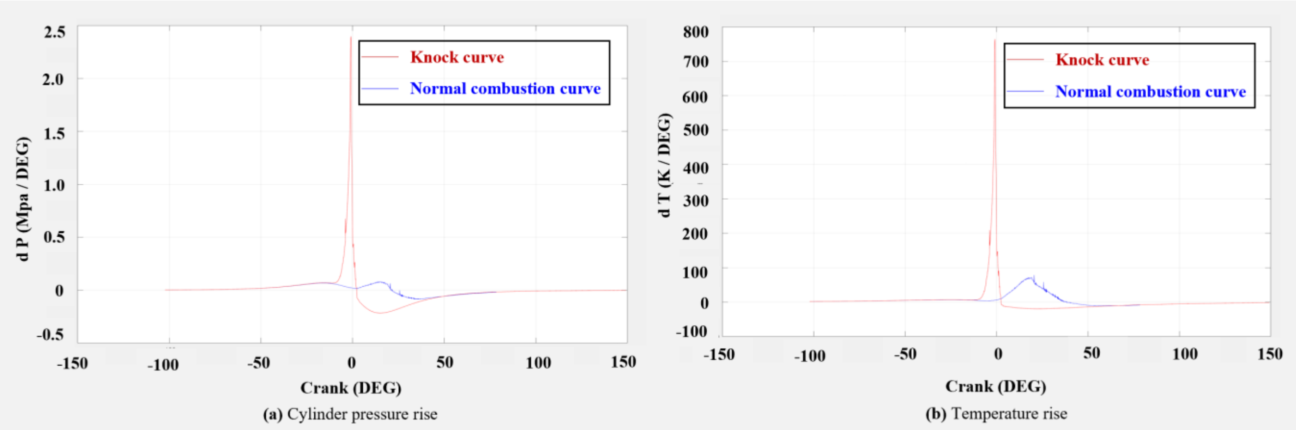

Fig. 4 Effect of NH_3-H_2 mixed fuel ratio on (a) cylinder pressure rise and (b) temperature rise (Photo/Picture credit: Original)

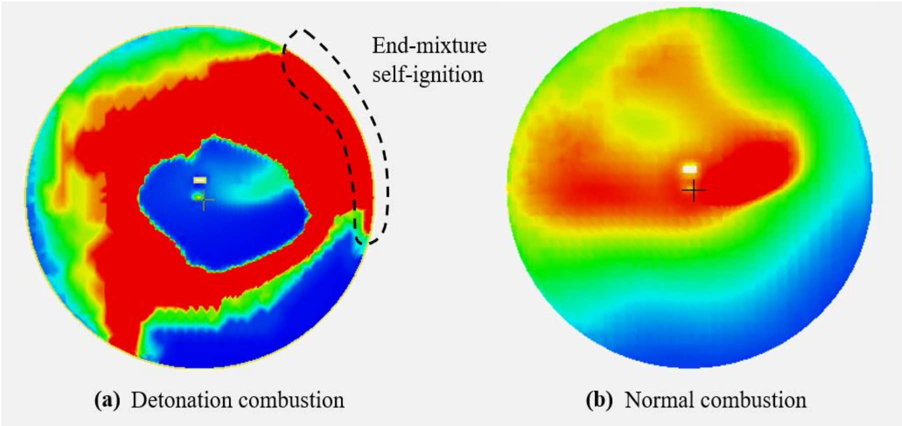

Fig. 5 H_2O_2 distribution in the cylinder when the crankshaft angle is 10° (Photo/Picture credit: Original)

3.3. Effects of Ammonia-Hydrogen Mixed Combustion Ratio on Thermal Efficiency and Emissions

Nitrogen oxides are the main emissions in the mixed combustion of ammonia and hydrogen, and large accumulations of these emissions often cause disasters such as acid rain. Through simulation experiments, it is found that with the increase of the proportion of hydrogen, the combustion temperature in the cylinder increases, which promotes the oxidation reaction of nitrogen and produces more nitrogen oxides, as shown in Fig. 6. Therefore, in this case, the generation of thermal nitrogen oxides is much greater than that of fuel-type nitrogen oxides, which shows that the greater the proportion of hydrogen, the lower the NO_x emissions are, and the opposite is true. This occurs simply because a high proportion of hydrogen causes the combustion chamber temperature to remain in a temperature range suitable for the formation of nitrogen oxides for a long time.

Through Fig. 7, when the energy provided by hydrogen accounts for less than 17% of the total energy, the NH_3-H_2 mixed fuel will hardly burn. This is a manifestation of the difficulty of ammonia catching fire. When the hydrogen energy supply increases to about 40%, the thermal efficiency increases rapidly and reaches the maximum value. Reach 45%. When the thermal efficiency gradually reaches the maximum, the emission of NO_x does not increase rapidly and is within the acceptable range. In addition, as the proportion of hydrogen energy supply increases, the combustion center gradually advances, and the combustion duration shortens, in line with expectations. When the proportion of hydrogen energy exceeds 30%, nitrogen oxide emissions will increase sharply as the proportion of hydrogen energy increases. As shown in Fig. 8, when the thermal efficiency gradually reaches the maximum value, as the proportion of hydrogen energy increases, the emission of nitrogen oxides does not increase rapidly and is still within the acceptable range.

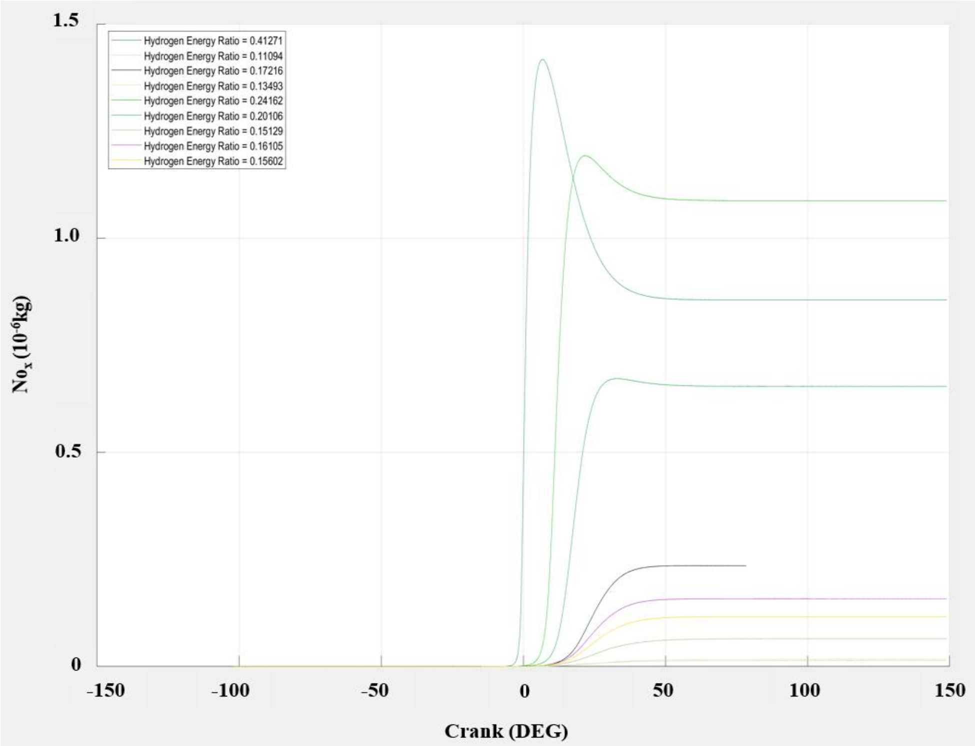

Fig. 6 Effect of NH_3-H_2 mixed fuel ratio on cylinder NO_x emissions (Photo/Picture credit: Original)

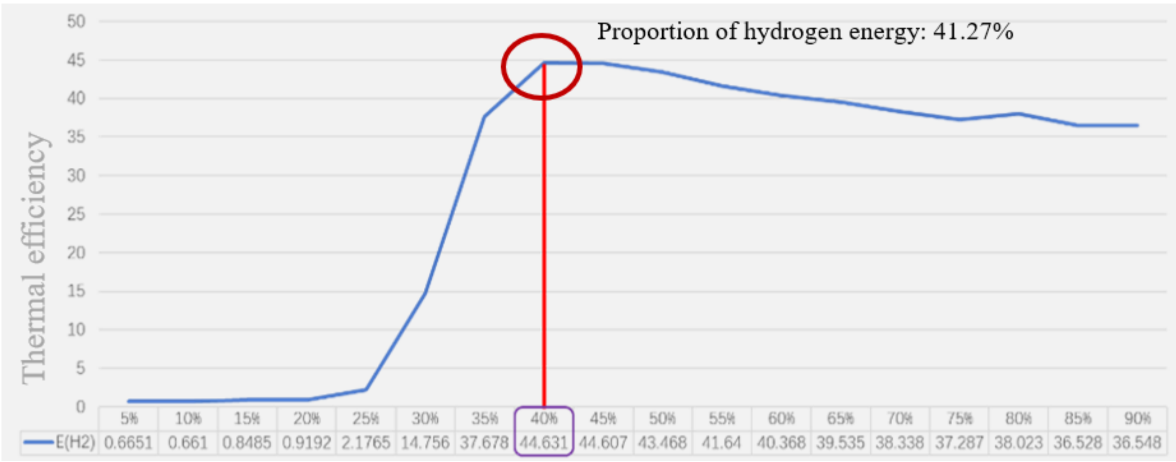

Fig. 7 The relationship between thermal efficiency and hydrogen energy supply ratio (Photo/Picture credit: Original)

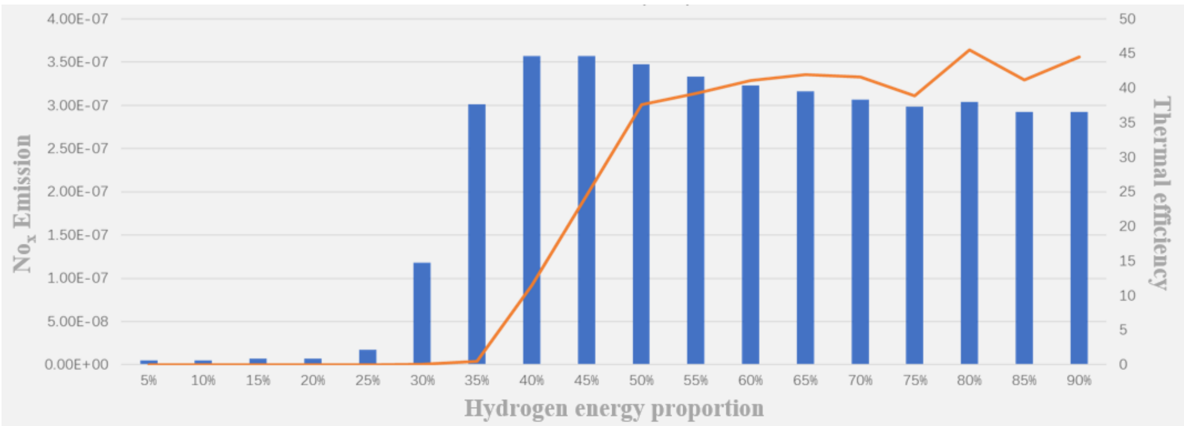

Fig. 8 The relationship between NO_x emissions and the proportion of hydrogen energy supply (Photo/Picture credit: Original)

4. Conclusions

This study is based on an improved NH_3-H_2 mixed combustion engine and uses Converge software to study the theoretical impact of using different NH_3-H_2 mixture ratios as engine fuel on various engine performances. Research shows that the minimum proportion of hydrogen energy that can allow the mixture to burn normally is about 17%. When the proportion of hydrogen energy reaches about 40%, the engine has the highest thermal efficiency. In simulation experiments, nitrogen oxide emissions were always within a reasonable range.

Since this study is only based on pure theory, there will inevitably be numerical differences in experimental results between simulation experiments and actual experiments. However, the reason why simulation experiments are used for analysis is to obtain the trend relationship between variables and results so as to use the simulation results to guide the actual experiments and use the actual experimental results to test the simulation theory. Existing diesel engines usually need to replace nine parts to be converted into hydrogen-ammonia fuel internal combustion engines, which will give the diesel engine industry a new lease of life in the carbon-neutral era. As a zero-carbon fuel, the mainstream production methods of ammonia and hydrogen still rely on the thermal decomposition of fossil fuels. Producing 1kg of hydrogen or ammonia results in 2.81 kg ~ 4.22 kg of carbon dioxide emissions. Although hydrogen or ammonia can also be produced in combination with a variety of renewable energy sources, such as solar, wind, and hydropower production methods, their costs need to be reduced.

But the reason why hydrogen ammonia fuel is launched is because the market depends on demand. As long as this new technology is demonstrated to the public, it can attract more attention to the alternative fuel field. After raising investment, the production technology of this upstream segment of raw materials can be further improved and iterated, thus driving the development of the entire industry and technology.

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