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Study on the Effect of High Ammonia Energy Ratio on the Performance of Caterpillar 3400 Diesel Engine

Dong Tang*, Ruixiao Tian

School of Automotive and Traffic Engineering, Jiangsu University, 212013, Zhenjiang, China

*Email: dtang@ujs.edu.cn

Abstract

Ammonia is considered as an ideal alternative engine fuel because of its absence of carbon atoms, as well as its high ignition energy, high octane number, and its application in high compression ratio engines. Taking a Caterpillar 3400 diesel engine as the research object, the engine combustion chamber simulation model is established in CONVERGE, and the simulation results are compared and verified. On this basis, the influence law of ammonia energy ratio on the performance of dual-fuel engine is investigated, and the results show that when the ammonia energy ratio is increased from 50% to 90, ammonia fuel dominates the exotherm, the flame propagation in the cylinder becomes slower, and the exotherm in the premixed combustion region decreases, retarding the crankshaft angle of CA10, CA50 and CA90. Blending of ammonia in the diesel engine improves the combustion CE before 90% ammonia energy ratio. but when the ammonia energy ratio reaches 90%, the CE decreases. at 80% ammonia energy ratio, the CO and CO_2 emissions are 2.42 g/kW·h and 18.70 g/kW·h, respectively, and the N_2O emission is 0.22 g/kW·h, and the greenhouse gases such as GHGs and nitrogen oxides achieve the optimum emission level.

Keywords

Diesel; Dual Fuel; Ammonia Energy Ratio; The Numerical Simulation.

1. Introduction

Nowadays, the world is developing rapidly and people's quality of life has improved significantly. However, the rapid development of society has led to a massive consumption of energy, which in turn has led to pressing problems such as the energy crisis, the greenhouse effect and environmental pollution. To address these challenges, countries are actively restructuring their energy mix and advocating the use of clean and renewable energy sources. Ammonia (NH_3), as a zero-carbon fuel, has no greenhouse gas components or harmful pollutants in the combustion products of hydrogen fuels from the perspective of fuel components. Compared to hydrocarbon fuels, ammonia has a higher auto-ignition temperature (924 K) and ignition limit (16.1%-25%) [1], which makes ammonia combustion require higher ignition temperatures; secondly, ammonia laminar flame propagation is slower (6-8 cm/s), and its complete combustion requires a longer period of time, which results in a higher risk of deterioration of ammonia combustion under in-cylinder combustion conditions of engines. To improve the in-cylinder combustion of ammonia, ammonia can be ignited by introducing more chemically active fuels, such as natural gas, hydrogen, and diesel [2].

In recent years, the basic research on the combustion and pollutant generation characteristics of ammonia and different combustion fuels has been widely reported. Rocha et al. [3] investigated the ignition characteristics of ammonia/hydrogen combination combustion with different hydrogen ratios and premixed flame propagation characteristics, and found that the ignition delay period was

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shortened and the flame speed was significantly increased with the increase of hydrogen ratio. Tang et al [4] investigated the flammability limits of ammonia blends formed by blending hydrogen and methane, respectively, and found that hydrogen was more advantageous than methane in improving the ammonia reactivity. Cellek [5] investigated the NOx generation pattern of composite combustion with different proportions of ammonia with hydrogen, methane, and propane under lean combustion conditions, and the results showed that compared with the combustion of pure components of each combustion fuel, the blending of the fuel with the appropriate proportion of ammonia could help to reduce NOx emissions under lean combustion conditions. The results show that, compared with the pure component combustion of each combustion fuel, blending a suitable proportion of ammonia into the fuel for compound combustion can help reduce the NOx emission under lean combustion conditions. As for the composite combustion of ammonia and large molecule carbon-based fuels, the research teams from Shanghai Jiaotong University, Huazhong University of Science and Technology and Dalian University of Technology [6-10] carried out the studies on the ignition characteristics of ammonia/n-heptane and ammonia/diesel fuel composite combustion, in which the ammonia composite combustion process with a larger proportion of carbon-based fuel assistants has a shorter ignition delay, and with the increase of the proportion of ammonia in fuel, the ignition characteristics of the negative temperature coefficient zone of the n-alkanes are typical of the n-alkane combustion process. The typical ignition characteristics of n-alkanes in the negative temperature coefficient region gradually disappeared as the proportion of ammonia in the fuel increased.

As a widely used fuel in the field of internal combustion engines, diesel fuel has the advantages of combustibility and the related mature fuel supply technology, which meets the demand for highly reactive combustion fuels for ammonia fuels in practical combustion equipment. The ammonia/diesel dual-fuel combustion mode is the most widely used combustion mode for ammonia fuels, as it does not require significant modifications to the existing internal combustion engine structure [11]. Reiter et al. [12] carried out an experimental study on the combustion and pollutant generation characteristics of the dual-fuel mode of ammonia/diesel under constant engine power conditions, and the results showed that when the ratio of the ammonia energy is 40-60%, the best engine fuel economy can be achieved the best engine fuel economy; when the ammonia energy ratio is less than or equal to 40%, the NO emission of ammonia/diesel composite combustion is lower than that of pure diesel combustion mode NO emission. Liu et al [13] investigated the effect of ammonia substitution rate on the combustion characteristics of an ammonia/diesel dual fuel engine, and the results showed that the tendency of diesel fuel to undergo premixed combustion increased with the increase of ammonia substitution rate, while diffusion combustion was weakened, which led to an increase in the area in the combustion chamber where the flame could not propagate, which in turn intensified the unburnt ammonia emission and decreased the thermal efficiency, and the increase of ammonia substitution rate led to an N_2O emission increase. Jin et al [14] carried out a numerical simulation study of the ammonia/diesel composite combustion process in a compression-ignition engine, and found that the use of a large ammonia energy substitution ratio will lead to a serious decrease in the engine indicated thermal efficiency and a sharp increase in the unburned ammonia emissions. Chen et al [15] carried out a special study on the emission characteristics of an ammonia/diesel dual fuel engine, and the results showed that, with the increase in the ammonia energy ratio, the N_2O emissions do not vary monotonically, but show a trend of decreasing and then increasing, and there is a trade-off relationship between total NO and N_2O emissions and NOX emissions. Amin et al [16] found that NOx emissions decreased by 58.8% for ammonia energy fractions ranging from 0 to 40%, but unburned NH_3 and N_2O emissions increased. From these studies, it is seen that there are fewer studies in the ammonia/diesel composite combustion model regarding the achievement of efficient and clean combustion under the condition of large ammonia energy ratio, so a lot of research work needs to be carried out on these issues as a means of finding the means of achieving efficient and clean combustion under the condition of large ammonia energy ratio and the emission characteristics of N_2O, NO, etc., are finalised, on the basis of the tests conducted by Yousefi et al [17].

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2. Research Methodology

2.1 Research Target

The study is based on a Caterpillar 3400 four-stroke supercharged water-cooled diesel engine. As shown in Tab. 1, the original engine has a compression ratio of 16.25, a bore and stroke of 137.2 and 165.1 mm, respectively, and a single-cylinder diesel engine. The engine was modified to be suitable for ammonia/diesel dual fuel engine combustion as shown in Fig. 1, where the ammonia fuel was introduced into the cylinder through the intake manifold while the diesel fuel was injected directly.

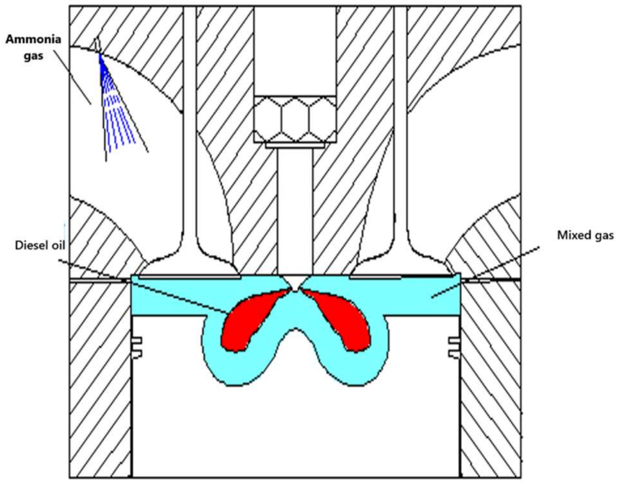

Fig. 1 Schematic diagram of ammonia/diesel dual-fuel engine

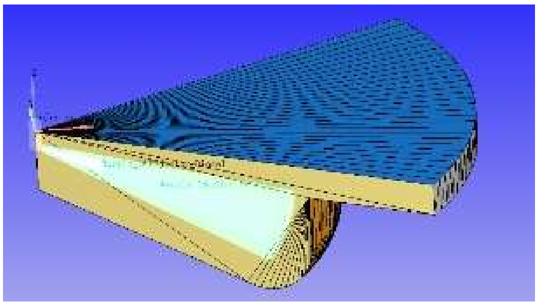

Fig. 2 Engine combustion chamber model

The calculation process is from inlet valve closed (-169.7 °CA) to exhaust valve open (145.3 °CA). Because the number of nozzles is 6 and uniformly distributed in a circle, in order to reduce the calculation time, a sector of 1/6 of the circumference of the combustion chamber is selected as the combustion chamber model, as shown in Fig. 2.

2.2 Computational Models and Conditions

Numerical simulations were performed using CONVERGE v3.0 software. In order to predict the amount of combustion and pollutants, the chemical reaction kinetic mechanism of NH_3/n-heptane was combined with a CFD solver, and the simplified mechanism proposed by Xu [18] was chosen as the ammonia/diesel combustion chemical reaction mechanism, which contains 69 components and 389 steps of reaction. As shown in Tab. 2, the initial temperature in the cylinder is 350 K, the initial pressure is 1.3 bar, the diesel injection start time is -24° CA, and the flow coefficient Cd is 0.597.

Turbulent flow generated in the engine, evaporation of spray, fragmentation, heat transfer, etc. are physical phenomena, so the physical phenomena are constructed into corresponding physical models. The turbulence model is the RNG k-ε model of the vortex viscosity model [19]. The heat transfer

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between the gas and the wall is considered through the wall function heat transfer model, and the Han-Reitz model [20] is chosen as the heat transfer model. The Frossling [21] model is used to simulate the conversion of liquid oil droplets into gaseous evaporation process. The use of RANS in conjunction with the detailed chemical kinetics SAGE [22] model allowed for accurate prediction of most combustion processes. The following demonstrates the chemical reaction mechanism of SAGE, see equation (1).

$$\sum_{m=1}^{M} V'_{m,r} X_m \Leftrightarrow \sum_{m=1}^{M} V''_{m,r} X_m \qquad r=1,2, \quad R \tag{1}$$

Where $V'_{m,r}$ denotes the stoichiometric coefficient of the reactant; $V''_{m,r}$ denotes the stoichiometric coefficient of the product; $X''_{m,r}$ denotes the chemical symbol for substance m; and r denotes the total number of reactions.

Due to the presence of nitrogen atoms in ammonia, NOx emissions were investigated separately for NO, NO_2, and N_2O. NO_2 emissions are small and the production and decomposition of NO and N_2O were mainly investigated. The emission model chosen for thermal NOx [23] is an extension of the Zel´dovich mechanism, see equation (2).

$$\begin{aligned} O + N_2 &\Leftrightarrow NO + N \\ N + O_2 &\Leftrightarrow NO + O \\ N + OH &\Leftrightarrow NO + H \end{aligned} \tag{2}$$

Tab. 1 Engine technical parameters

Technical Parameter	Index
Engine type	Caterpillar 3400
Speed	910 r/min
Connecting rod length	261.62 mm
Compression ratio	16.25
Number of cylinders	1
Displacement	2.44 L
Bore × Stroke	137.2 × 165.1 mm
Number of spray holes	6
EVC	348.3 °ATDC
EVO	145.3 °ATDC
IVC	−169.7 °ATDC
IVO	−358.3 °ATDC

The ammonia energy ratio is calculated as in equation (3), and analysing the ammonia energy percentage helps to assess the effect of ammonia fuel on engine performance.

$$\text{Ammonia energy ratio (\%)} = \frac{m_{NH_3} LHV_{NH_3}}{m_{NH_3} LHV_{NH_3} + m_{diesel} LHV_{diesel}} \times 100\% \tag{3}$$

Where: m_{NH_3} and m_{diesel} are the mass of ammonia and the mass of diesel, kg, LHV_{NH_3} and LHV_{diesel} are the low calorific values of diesel and ammonia, MJ/kg.

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Tab. 2 Simulated initial and boundary conditions

Factor	Settings
SOI	-24 °CA
Duration of Diesel Injection	12 °CA
Mass of Diesel	11.5 mg/cycle
Mass of NH_3	97.9 mg/cycle
IVC Temperature	350 K
IVC Pressure	1.3 bar
Equivalence ratio	0.35

2.3 Grid-independent Analysis

In the simulation and calculation process, the mesh has a large influence on the model. In order to select a suitable base mesh, 4mm, 5mm and 6mm were used as the base mesh size respectively. The base mesh is classified as a coarse mesh, and regions such as nozzle and piston are encrypted with 3 levels of fixed encryption, while other regions are encrypted with 3 levels of adaptive encryption according to the temperature and velocity gradient, and the number of meshes finally reaches 2000000. From Fig. 3, it can be seen that the simulation results converge when the base grid size is reduced to 4mm, so 4mm is chosen as the base grid size.

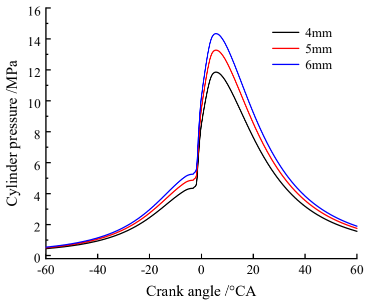

Fig. 3 Cylinder pressure for different base grid sizes

2.4 Model Validation

The model was validated against the experimental data of Yousefi et al. at 40% ammonia energy ratio for a dual fuel engine. It can be seen from Fig. 4 that the simulated cylinder pressure values and exergy rate values are in good agreement with the experimental results before and after combustion, and the error is within 5%, so the computational model has some accuracy.

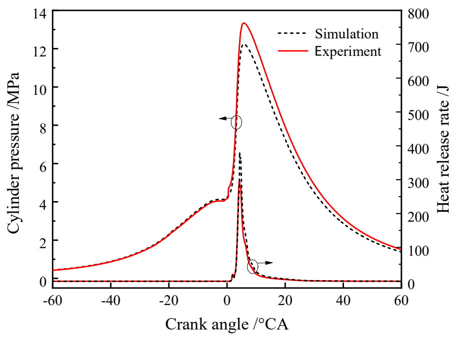

Fig. 4 Simulated and experimented cylinder pressure and heat release rate at 40% ammonia energy ratio

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3. Results and Analysis

3.1 Effect of Energy Ratio on Combustion Process

An ammonia energy ratio of 50% ~ 90% was selected for the study, and the cylinder pressure and exothermic rate during combustion of the dual-fuel engine with different ammonia energy ratios were calculated by simulation, as shown in Fig. 5 and as shown in Fig. 6.

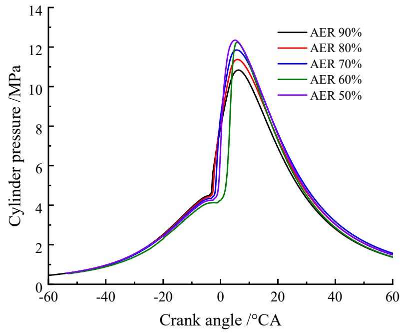

Fig. 5 Cylinder pressure at different ammonia energy ratios

Overall, as the ammonia energy ratio increases, the in-cylinder pressure of the engine decreases, which is due to the lower cylinder pressure resulting from the lower percentage of diesel fuel and the slower flame propagation rate of ammonia. The peak cylinder pressure remained essentially constant at ammonia energy ratios of 50 and 60 per cent. However, with the increase of ammonia energy ratio, the combustion of NH_3/diesel after the upper stopping point, the in-cylinder pressure decreased significantly down to as low as 0.32 MPa. At this time, the lesser amount of diesel resulted in poor spontaneous combustion, and therefore the peak exothermic rate in the premixed combustion region decreased and the main combustion duration was prolonged.

Fig. 7 shows the variation of CA10, CA50 and CA90 for different ammonia energy ratios. Where CA10 represents the start of combustion with a cumulative heat release of 10%, and the combustion duration is the crankshaft angle experienced by the cumulative heat release from CA10-CA90. When the ammonia energy ratio increases, the ammonia fuel dominates the heat release, the flame propagation in the cylinder slows down, and the heat release rate in the premixed combustion region decreases, thus delaying the crankshaft angle of CA10, CA50, and CA90.

Fig. 8 shows the CE curves for different ammonia energy ratios in the dual-fuel combustion mode, and the CE indicates how much chemical energy in the fuel is converted into heat energy. As the ammonia energy ratio increases, the CE shows an increasing and then decreasing trend, reaching 98.87% at an ammonia energy ratio of 80%, and decreasing to 86.65% at an ammonia energy ratio of 90%, a decrease of 12%, which can be attributed to the misfire during the combustion process and the slowing down of the combustion rate of the ammonia-air mixture.

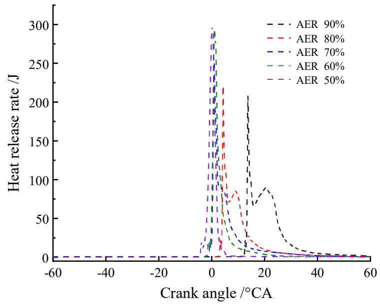

Fig. 6 Heat release rate at different ammonia energy ratios

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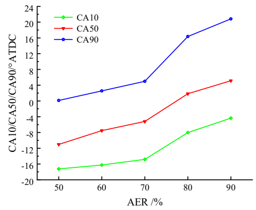

Fig. 7 CA10, CA50 and CA90 at different ammonia ratios.

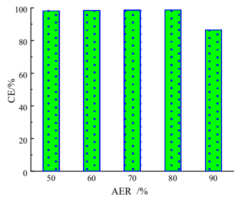

Fig. 8 CE at different ammonia ratios

3.2 Effect of Energy Ratio on Emissivity

Figure 10 shows the emission of each pollutant at different ammonia energy ratios. When the ammonia energy ratio increases from 50 per cent to 80 per cent, the change in HC emission is insignificant. However, when the ammonia energy ratio exceeds this point, the HC emission increases significantly. The HC emission at 90% ammonia energy ratio is 18.41 g/kW·h, which can be attributed to the incomplete combustion process. When the ammonia energy ratio increased, the emission of unburnt NH3 increased. When the ammonia energy ratio is increased from 50% to 80%, the unburned NH3 emission is only 0.54 g/kW·h. When the ammonia energy ratio is increased to 90%, the unburned NH3 emission reaches 1.83 g/kW·h. This is due to the fact that ammonia consumes ammonia more slowly because of the decreasing flame propagation speed. As a result, the unburned NH3 emissions are increasing.

Incomplete combustion of hydrocarbon and ammonia fuels pollutes the environment, with N_2O producing more than 300 times the greenhouse effect of CO_2. As can be seen in Figure 12, both CO and CO_2 decrease with the increase of ammonia energy ratio. When the ammonia energy ratio is 50%, the diesel injection is the largest, and the CO and CO_2 emission levels are the highest, reaching 13.63 g/kW·h and 37.25 g/kW·h, respectively; when the ammonia energy ratio is 90%, the diesel injection is the smallest, and the CO and CO_2 emission levels are the lowest, which are only 0.88 g/kW·h and 10.22 g/kW·h. 80% of the ammonia energy ratio has a CO and CO_2 emission level of 2.42% and 2.42% respectively. CO_2 emissions were 2.42 g/kW·h and 18.70 g/kW·h, respectively, which were at a lower level.

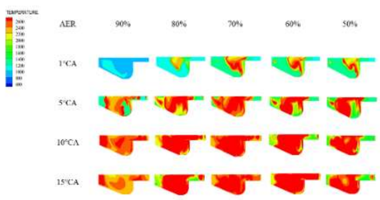

Fig. 9 Temperature cloud for different ammonia energy ratios

Although ammonia combustion does not produce CO, CO_2 type greenhouse gas emissions. However, the use of ammonia fuels releases N_2O, a by-product usually associated with the combustion of

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nitrogen-containing fuels. The reactions in equations (4) and (5) can be referred to as reaction pathways [24].

$$NH + NO \rightarrow N_2O + H \tag{4}$$

$$NH_2 + NO_2 \rightarrow N_2O + H \tag{5}$$

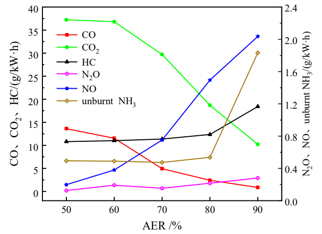

Fig. 10 CO, CO_2, HC, NO_2, NO and unburnt NH_3 emissions for different ammonia energy ratios

Both NO and N_2O emissions increased with increasing ammonia energy ratio. When the ammonia energy ratio was increasing, the local temperature in the cylinder was increasing, which increased the production of thermophilic NO, and therefore the NO emissions were increasing. When the ammonia energy ratio increased from 50% to 70%, however, the N_2O GHG emissions decreased slightly. From the temperature cloud in the cylinder in Fig. 9, it can be seen that the high-temperature region accounts for the largest proportion when the ammonia energy ratio is 70%. As a result, the thermal decomposition reaction of N_2O is intensified and the level of N_2O GHG emission decreases slightly. When the ammonia energy ratio exceeds 70%, the N_2O emission gradually increases again. This is because the flame temperature decreases with the increase of ammonia energy ratio. As a result, the oxidation of the intermediate products of ammonia is incomplete, resulting in the generation of a large amount of N_2O. When the ammonia energy ratio is 80%, the N_2O emission is 0.22 g/kW·h even though it is in a slight upward trend, which is comparable to the N_2O emission at 70% ammonia energy ratio and is also at a lower emission level. At an ammonia energy ratio of 90 per cent, N_2O emissions gradually increase because of incomplete combustion.

4. Conclusion

(1) With the increase of ammonia energy ratio, the combustion stage is delayed, the peak pressure in the cylinder decreases, and reaches a minimum of 0.32 MPa at 80% ammonia energy ratio. At high ammonia energy ratio, the flame propagation speed in the cylinder slows down, and the exothermic rate of premixed combustion region also decreases, and the combustion duration is prolonged. The CE shows a trend of increasing and then decreasing, and reaches 98.87% at the ammonia energy ratio of 80%.

(2) GHG and NOx emissions are optimal at 80% ammonia energy ratio. HC emissions do not change significantly from 50% to 80% ammonia energy ratio. 80% ammonia energy ratio, CO and CO2 emissions are 2.42 g/kW·h and 18.70 g/kW·h, respectively, which are both at a low level. NO emissions increase with the increase of ammonia energy ratio. When the ammonia energy ratio is 80%, it is also at a lower emission level.

(3) From the comprehensive indexes and characteristics of engine combustion, power and emission, the overall characteristics of the engine are best when the ammonia energy ratio is 80%.

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