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Optimization of combustion in diesel pilot ignition high-pressure direct-injection liquid ammonia

Dual Fuel / Gas / Diesel

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ABSTRACT

Ammonia is a potential zero-carbon alternative fuel for compression-combustion engines. The high pressure direct injection ammonia fuel combustion with eccentric configuration is an effective solution to achieve high ammonia substitution rate. However, the design of eccentric configuration fuel injection system and the matching scheme of fuel injection strategy have not yet formed a general criterion. In this study, a three-dimensional simulation model of the engine was constructed, and the effects of two key parameters, "offset"(distance between concentric and eccentric injectors) and "insert"(distance between cylinder head and eccentric injectors) on the ignition and combustion process under different loads were systematically studied by means of numerical simulation, and the injection strategy was optimized. The results show that small offset can increase the proportion of effective ignition of liquid ammonia plume, and then improve the combustion efficiency and thermal efficiency of the engine. When AD injection strategy is adopted at high load, the high overlap of liquid ammonia and diesel plume affects the development of diesel spray flame, and the combustion loss can reach 27.62%. By using ammonia two-stage injection (ADA) and optimizing the " insert " of diesel injector, the plume planes of liquid ammonia and diesel oil can be effectively staggered to improve the ignition and combustion process. The optimal scheme of the preferred injection system structure and injection strategy is as follows: when the offset=10 mm and the insert=6 mm, the optimal injection strategy with low load is DA, and the thermal efficiency can reach 49.68%. The optimal injection strategy for high loads is AD, which has a thermal efficiency of 50.75%. The second best option is: offset =10 mm, keep the other parameters of the fuel injection system unchanged, the best injection strategy is DA at low load, and the thermal efficiency can reach 50.12%. The optimal thermal efficiency of 49.93% can be obtained by using ADA strategy for high load.

1 INTRODUCTION

The reduction of engine carbon emissions and the achievement of national dual-carbon targets have driven the demand for novel alternative fuels in compression ignition (CI) engines [1]. Significant research has been conducted on low-carbon fuels such as natural gas [2] and methanol [3] for their application in internal combustion engines. Researchers are also investigating zero-carbon fuels like hydrogen and ammonia as a means to further reduce carbon emissions. While hydrogen presents promising potential, its high storage and transportation costs, as well as associated safety risks, pose significant challenges. In contrast, ammonia benefits from a mature production process, low preparation costs, and the ability to be easily stored as a liquid at 1.0 MPa under room temperature, with a relatively low risk of explosion during storage, transportation, and usage [4]. Furthermore, ammonia boasts a high energy density, approximately 1.6 times that of liquid hydrogen, making it an excellent hydrogen carrier.

Although ammonia combustion does not produce carbon emissions, challenges arise when using pure ammonia in CI engines due to its low flame speed, high auto-ignition temperature, high ignition energy requirement, and narrow combustion limits. Research by Gray et al. [5] indicates that achieving stable ignition of ammonia requires a high compression ratio, thus limiting its application in various engine configurations. To address these challenges, some studies propose the use of high-activity fuels to ignite low-activity ammonia in CI engines. This dual-fuel combustion mode can be categorized into low-pressure injection dual-fuel (LPDF) and high-pressure injection dual-fuel (HPDF), depending on the injection pressure of the low-activity fuel. In the LPDF mode, ammonia is mixed with air before the compression stroke, with the ammonia injector typically located in the intake manifold. A high-activity fuel is then injected into the cylinder during the latter part of the compression stroke to initiate combustion. Studies have shown that in the LPDF mode [6-7], ammonia combustion stability is relatively low under low load conditions, while at high loads, the pressure rise rate is high, leading to increased NO emissions. These factors limit the ammonia substitution rate and reduce the potential for lowering carbon emissions in dual-fuel combustion. Under the LPDF mode, ammonia forms a homogeneous mixture in the cylinder, but in regions near the chamber walls or narrow areas, the ammonia-air mixture may not burn completely. This incomplete combustion, caused by low reactivity and equivalence ratio imbalances, results in elevated HC and CO emissions. Moreover, intake manifold injection reduces the intake charge coefficient, leading to a decrease in engine power and increasing the risk

of ammonia mixture leakage during the scavenging process.

In research on the HPDF mode for ammonia, Frankl et al. [8] conducted numerical simulations and found that increasing the temperature of liquid ammonia could reduce ignition delay and accelerate the phase separation during combustion. Li et al. [9] compared the HPDF and LPDF modes for ammonia-diesel dual-fuel operation in a two-stroke low-speed marine engine, concluding that the maximum energy replacement by ammonia was approximately 80% in the LPDF mode, while it reached 97% in the HPDF mode. Additionally, the LPDF mode exhibited higher indicated thermal efficiency, whereas the HPDF mode resulted in lower NH₃, NO_x, and greenhouse gas emissions. Zhou et al. [10] also compared the engine performance of ammonia-diesel in both LPDF and HPDF modes, with both modes achieving indicated thermal efficiencies greater than 50%. Under optimal emission conditions in the HPDF mode, NO_x emissions were reduced by about 47%, while greenhouse gas emissions decreased by approximately 97%, with ammonia emissions being negligible compared to pure diesel mode. Zhang et al. [11] further studied the dual direct injection mode of ammonia-diesel in a low-speed two-stroke engine and demonstrated that adjusting the injection timing could alter ammonia ignition timing, allowing for precise control over the combustion process and improved fuel economy. Moreover, optimizing the injection timing for both diesel and ammonia fuels helped reduce NO_x emissions generated during ammonia combustion. Zhang et al. [12] also conducted numerical simulations of engine performance under the HPDF mode for ammonia-diesel, showing an 8.9% increase in IMEP and a 10.6% improvement in indicated thermal efficiency at an 80% ammonia substitution rate. Furthermore, the optimized HPDF strategy significantly reduced greenhouse gas emissions and NO_x emissions. By adjusting the injection timing and direction of liquid ammonia, better control over fuel combustion and pollutant formation was achieved, thereby minimizing unburned ammonia emissions under high ammonia fractions.

In summary, existing research indicates that the HPDF mode holds significant promise for reducing emissions and enhancing indicated thermal efficiency at high ammonia substitution rates. Generally, the injection systems used in the HPDF mode can be classified into two main categories: concentric dual-needle valve integrated injectors and separate multi-injector systems. Due to the complex structure, manufacturing challenges, and market limitations associated with concentric dual-needle valve integrated injectors, the

implementation of such a system remains challenging. In contrast, the separate multi-injector system, consisting of two or more commercially available high-pressure injectors, can be easily purchased from the market, requires no special structural design, and offers lower manufacturing costs [13]. Therefore, using a separate multi-injector system for implementing the HPDF mode with liquid ammonia presents a more cost-effective solution. It is important to note that, due to the different axial arrangements of the liquid ammonia and diesel injectors, the in-cylinder combustion process becomes more complex, and the combustion process is highly influenced by the injection of liquid ammonia. Previous studies on diesel-ignited high-pressure direct injection of liquid ammonia have focused primarily on macro parameters, such as injection strategies while leaving a significant gap in discussions regarding the design of liquid ammonia and diesel injectors. The design and optimization of injectors directly impact the injection process, which, in turn, influences the combustion characteristics in the HPDF mode. Moreover, research by Xiahou et al. [14]. The use of separate multi-injector systems in gasoline-diesel engines has demonstrated that varying the offset (the distance between concentric and eccentric injectors) significantly affects the in-cylinder combustion and ignition processes. By investigating the coupling of injection strategies and injector system structures to adjust the diesel ignition process, this study will contribute to the optimization of injectors and the development of combustion theory. Accordingly, this study proposes a collaborative optimization approach for injection strategies and system parameters under different operating conditions, based on numerical simulations. On one hand, adjusting the offset to alter the positioning of diesel-ignited liquid ammonia improves the utilization of the diesel ignition spray and ensures efficient ignition. An ideal offset value is proposed. On the other hand, the study analyzes the coordination mechanisms between different injector system designs and injection strategies under both low and high-load HPDF modes, exploring the principles for enhancing the quality of high-pressure direct injection ammonia ignition. This paper also presents a proposed injector system design. The findings of this research will contribute to the development of efficient ammonia combustion technologies for automotive engines and provide valuable data and theoretical support for future research on the optimization of separate multi-injector designs.

2 METHOD

2.1 3D Numerical Simulation Model

This study is based on a heavy-duty, single-cylinder test engine modified from the Yuchai K13 diesel engine, equipped with a dual direct injection (DI) system. A numerical engine model was developed (as shown in Figure 1), with the key parameters listed in Table 1. The combustion chamber of this test engine is equipped with a dual direct injection system, with the liquid ammonia injector placed centrally and the diesel injector located on the side. The numerical engine model utilizes the three-dimensional simulation software CONVERGE to simulate the combustion process. The Renormalization Group (RNG) $k-\epsilon$ model is employed to account for the effects of turbulence on the momentum, energy, and mass transport fields, which is widely used in engine modeling. This model takes into consideration key physical aspects of flame propagation under engine-like conditions, such as compressibility effects. The combustion process inside the cylinder is simulated using the SAGE chemical reaction kinetics model, which includes a mechanism for ammonia-diesel combustion consisting of 89 species and 422 reaction steps, with n-heptane used as a surrogate for diesel. This mechanism has been validated in engine combustion studies.

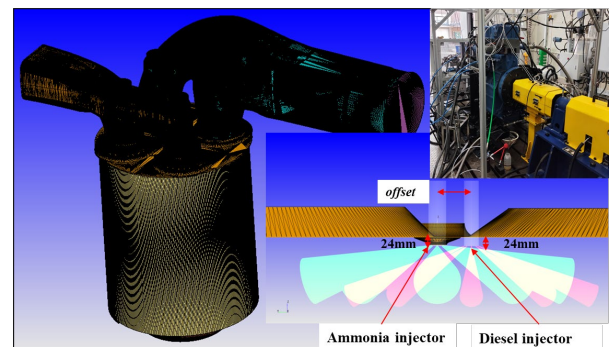


Figure 1. 3D numerical simulation model of engine

Table 1. Engine specifications

Parameter	Value
Bore (mm)	129
Stroke (mm)	155
Displacement (L)	2.0
Compression Ratio	16.5
Combustion Chamber	Omega-shaped (ω -type)
Intake Valve Closing	-159 CAD ATDC
Exhaust Valve Opening	128 CAD ATDC
Liquid Ammonia Injector	10 holes \times 0.22 mm \times 149°
Diesel Injector	10 holes \times 0.1 mm \times 135°

2.2 Spray Model and Engine Model Validation

Because combustion in the ammonia-diesel HPDF mode is controlled by the fuel-air mixing rate, the validation of ammonia spray is critical to

understanding the ammonia spray combustion process. Therefore, before conducting the numerical simulations of the engine, the model was validated based on the visual constant-volume ballistic test data for ammonia injection provided by Li et al. [10]. The selected operating conditions were as follows: injection pressure of 60 MPa, ammonia fuel temperature maintained at 350 K, and ammonia injected in its liquid state. The injector chosen for this study was a single-hole diesel injector with an injector diameter of 0.22 mm, and the injection pattern was an approximation of a square wave, generated from the data provided by Li et al. Detailed settings for the validation cases are listed in Table 2. A numerical simulation model was established using the RANS computational method, with the computational domain set as a three-dimensional cylinder, simulating the constant-volume environment in the actual experiment. The axial length was 108 mm, and the cylinder diameter was 108 mm. Liquid ammonia was used as the fuel, and in the calculations, the ammonia chemical reaction kinetics mechanism developed by Wang et al. [15] was employed, which consists of 84 species and 422 reaction steps.

Table 2. Parameter settings of spray experimental conditions

	Parameter	Value
Environmental Conditions	Ambient Temperature (K)	900
	Ambient Density (kg/m ³)	18
	Oxygen Content (%)	0
	Injector Diameter (mm)	0.22
Injection Parameters	Injection Pressure (MPa)	60
	Fuel Temperature(K)	350
	Injection Pulse Width (ms)	2.5

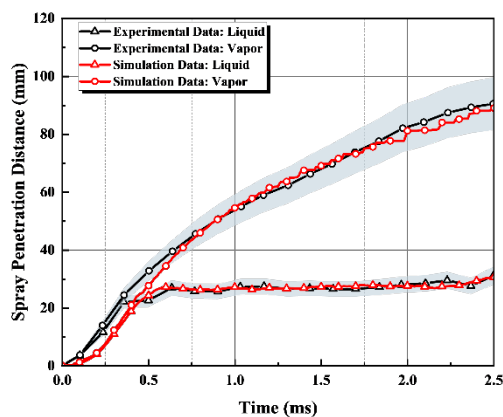


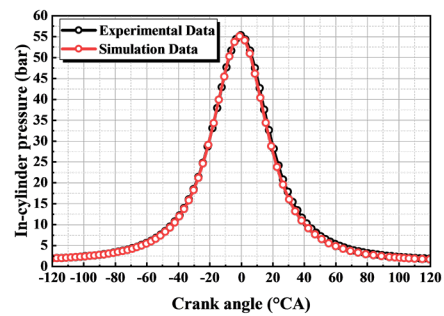
Figure 2. Liquid ammonia spray model verification

Figure 2 presents a comparison of experimental and simulated results for the spray's liquid and gas-phase penetration distances. The results show that the simulated spray penetration distance agrees

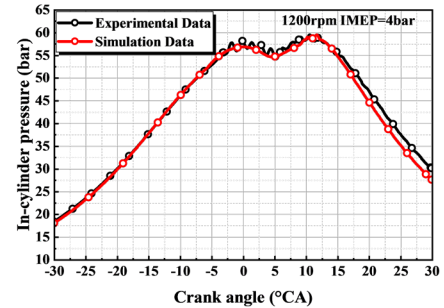
well with the experimental data, with an average error controlled within 10%. This validates the reliability of the high-pressure ammonia spray model.

Table 3. Verification conditions of engine experimental

Parameter	Value
Engine Speed	1200 rpm
Intake Pressure	1.18 bar
Intake Temperature	310 K
Exhaust Pressure	1.02 bar
Exhaust Temperature	454 K
Injection Pressure	800 bar
Diesel Pre-Injection Timing	-12°CA
Diesel Main Injection Timing	-2°CA
Diesel Pre-Injection Duration	2.736°CA
Diesel Main Injection Duration	6.12°CA



(a) Comparison of cold-state cylinder pressure data



(b) Comparison of cylinder pressure experimental and simulation results

Figure 3. Engine simulation model verification

To further validate the model's accuracy, simulations of the cold-start flow process under engine conditions of 1200 rpm and intake boosting were conducted. Figure 3(a) shows a comparison between the cylinder pressure data from the backdrop test and the simulated cylinder pressure data. The results indicate that the existing RANS-based engine model provides good predictive accuracy. Furthermore, the engine computational model was validated using actual thermodynamic test results. A low-load calibration condition with an IMEP of 4 bar was used to verify the numerical simulation results, with relevant engine operating parameters listed in Table 3. As shown in Figure

3(b), the current model can accurately predict the cylinder pressure during the engine's operating cycle. The relative error in the predicted maximum peak pressure is less than 0.3%, and the relative error in the predicted combustion duration is less than 10%.

2.3 Simulation Operating Conditions

In this study, the simulation conditions are shown in Table 4, where the "offset" is defined as the distance between the liquid ammonia injector and the diesel injector (i.e., the centrally positioned injector and the side-positioned injector). The engine speed is maintained at 1200 rpm, with a constant total fuel energy injection of 2000 J/cycle and 7000 J/cycle, corresponding to approximately 5 bar IMEP and 16 bar IMEP, respectively. The 5-bar IMEP condition is considered the low-load operating condition, and the 16-bar IMEP condition represents the high-load operating condition. Specifically, under the low-load condition, 10% of the total fuel energy is provided by diesel, which is injected directly by the side-positioned injector at -5°CA , while the remaining 90% of the total fuel energy, in the form of liquid ammonia, is injected into the cylinder at -3°CA . Under the high-load condition, 5% of the total fuel energy is provided by diesel, which is injected directly by the side-positioned injector at -10°CA , with the remaining 95% of the total fuel energy, in the form of liquid ammonia, injected into the cylinder at -6°CA . The injection strategy for both low- and high-load conditions is controlled similarly, with ammonia injection occurring after diesel injection, referred to as the DA injection strategy.

Table 4. Simulation conditions

Parameter	Value
Engine Speed	1200 rpm
IMEP	4 bar 14 bar
Ammonia substitution rate	90% 95%
Main Side injector	Ammonia diesel
Injection Pressure	600 bar 800 bar
Injection quantity(mg)	96.77/357.52 4.71/8.23
Injection duration($^{\circ}\text{CA}$)	9.5/42.1 1.256/2.673

3 RESULTS AND DISCUSSION

3.1 Effect of Offset on In-cylinder Combustion Process

3.1.1 Analysis of In-cylinder Combustion Process at Low Load

Figure 4 compares the in-cylinder pressure, heat release rate, combustion phase, and energy distribution under different offset distances and fixed injection settings ($\text{SOI}_D = -5^{\circ}\text{CA}$ and $\text{SOI}_A = -3^{\circ}\text{CA}$) at low-load conditions. Overall, the combustion process is characterized by two

stages: the first stage involves the ignition and combustion of the pilot diesel, while the second stage involves the heat release from the main fuel, liquid ammonia.

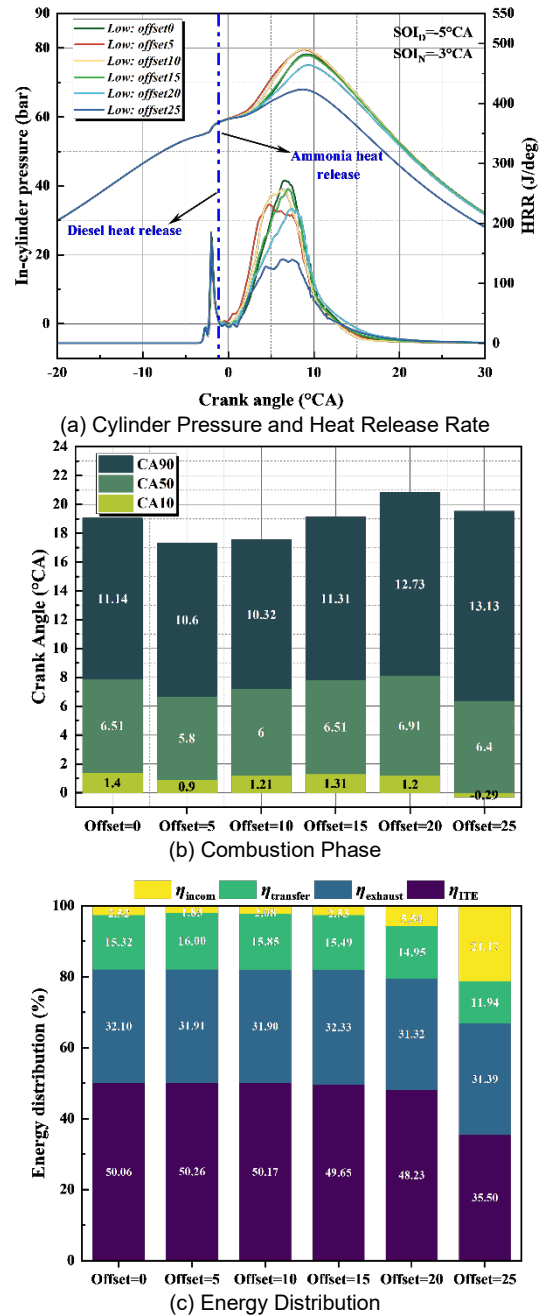


Figure 4. Combustion characteristics under low load with different offsets

As shown in Figure 4(a), with increasing offset, the cylinder pressure curve decreases. Additionally, as the offset increases, the initial heat release rate of liquid ammonia decreases, and the peak of the maximum heat release rate first rises slightly before significantly decreasing. With increasing offset, both CA50 and CA90 are delayed, resulting in an overall increase in the combustion duration, as shown in Figure 4(b). Figure 4(c) demonstrates that

when the offset is ≤ 10 mm, the in-cylinder combustion loss is minimal, staying below 3%. However, when the offset is between 15 mm and 25 mm, the combustion loss increases rapidly, reaching up to 21.17% at an offset of 25 mm. For offsets ≤ 15 mm, the heat release rate of liquid ammonia is faster, CA50 occurs earlier, the combustion is more homogeneous, and the combustion efficiency is higher, resulting in an indicated thermal efficiency of approximately 50%. The maximum indicated thermal efficiency of 50.26% is observed at an offset of 5 mm. Further increases in offset lead to a significant reduction in the early heat release rate of liquid ammonia, causing delays in CA50 and deterioration in combustion efficiency, which results in a decrease in indicated thermal efficiency. The fundamental reason for these phenomena is the variation in the number and areas of liquid ammonia fuel bundles ignited by the diesel fuel bundles under different offset conditions. A detailed analysis of this cause will be provided in the subsequent sections.

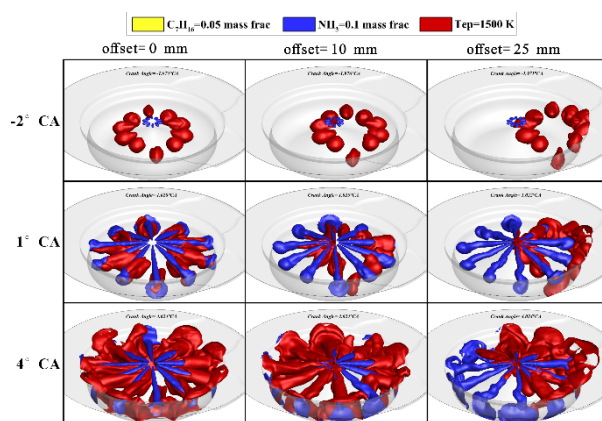


Figure 5. Ignition and combustion process under low load with different offsets

Figure 5 compares the ignition and combustion processes in the cylinder under low-load conditions with an injection strategy of SOID = -5°CA and SOIA = -3°CA , for different offset settings. When the offset is 0, the initial flame of the pilot diesel is symmetrically distributed within the cylinder. However, when the offset is non-zero, the initial flame of the pilot diesel forms on one side of the cylinder, exhibiting an asymmetric distribution. As the offset increases, the degree of bias in the diesel flame also increases. The bias of the ignition injector results in a more complex interaction between the pilot diesel flame and the liquid ammonia fuel bundle. Specifically, a portion of the liquid ammonia fuel bundle can directly contact the pilot flame generated by the diesel and ignite immediately, while the remaining fuel bundles require ignition via the high-temperature flame or gases from adjacent fuel bundles. Notably, liquid ammonia fuel bundles located farther from the

ignition injector may not be effectively ignited. At a crank angle of -2°CA (the initial moment of the diesel flame appearing in the cylinder), the initial diesel flame deviates from the center of the cylinder, impacting the injected liquid ammonia fuel bundles as the offset increases. When the offset is ≤ 15 mm, all liquid ammonia fuel bundles are ignited by the diesel pilot flame. However, when the offset is between 15 mm and 25 mm, as the offset increases, the proportion of liquid ammonia fuel bundles on the side away from the diesel flame that is directly ignited decreases. The unburned liquid ammonia fuel bundles may wet the cylinder walls or enter the squish zone, leading to more difficult combustion in later stages. This is the fundamental reason why increased offset leads to a reduction in combustion efficiency and indicated thermal efficiency.

3.1.2 Analysis of In-cylinder Combustion Process at High Load

Figure 6 compares the in-cylinder pressure, heat release rate, combustion phase, and energy distribution under high-load conditions with different offset distances and fixed injection settings (SOID = -10°CA and SOIA = -6°CA). Overall, the combustion process is similar to that under low-load conditions, consisting of two stages. The difference is that, at high loads, the injection duration of liquid ammonia is significantly longer, approximately four times that under low-load conditions. As shown in Figure 6(a), when the offset is ≤ 20 mm, the cylinder pressure curve decreases with increasing offset, and the initial heat release rate of liquid ammonia decreases as well. However, when the offset exceeds 20 mm, the initial heat release rate of liquid ammonia increases with further increases in offset. When the offset is ≤ 5 mm, CA10, CA50, and CA90 advance as the offset increases, resulting in a shorter overall combustion duration. When the offset is between 5 mm and 20 mm, CA50 and CA90 are delayed, and the overall combustion duration becomes longer. When the offset exceeds 20 mm, CA50 and CA90 are slightly advanced, leading to a shorter overall combustion duration, as shown in Figure 6(b). Figure 6(c) shows that when the offset is ≤ 10 mm, the in-cylinder combustion loss is small, remaining below 0.3%. When the offset is between 10 mm and 20 mm, combustion losses increase as the offset increases, reaching 1.49% at an offset of 20 mm. When the offset exceeds 20 mm, combustion losses decrease, resulting in a slight increase in indicated thermal efficiency. Furthermore, the overall indicated thermal efficiency at high load is lower than that at low load, approximately 47%. Although combustion efficiency is higher at high loads, the extended injection duration of liquid ammonia leads to a longer combustion period,

which is the primary reason for the decrease in indicated thermal efficiency. When the offset is ≤ 10 mm, the early heat release rate of liquid ammonia is faster, CA50 advances, the combustion is more homogeneous, and the combustion efficiency is high. The maximum indicated thermal efficiency of 47.71% is achieved at an offset of 5 mm.

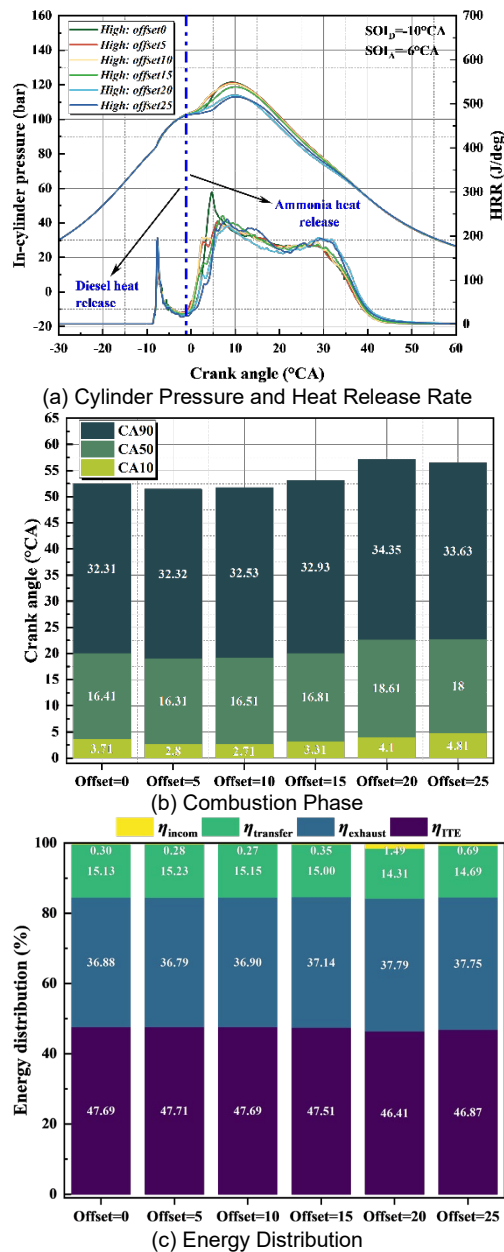


Figure 6. Combustion characteristics under high load with different offsets

As the offset increases further, the early heat release rate of liquid ammonia decreases significantly, resulting in delayed CA50 and deteriorated combustion efficiency, leading to a reduction in indicated thermal efficiency. Figure 7 compares the ignition and combustion processes in the cylinder under high-load conditions with an

injection strategy of $SOID = -10^\circ CA$ and $SOIA = -6^\circ CA$, for different offset settings. As shown in Figure 7, the ignition and combustion processes are similar to those at low load. When the offset is ≤ 15 mm, all liquid ammonia fuel bundles are ignited by the diesel pilot flame. When the offset is between 15 mm and 25 mm, as the offset increases, the proportion of liquid ammonia fuel bundles on the side away from the diesel flame that is directly ignited decreases. However, due to the extended injection duration of liquid ammonia at high load, compared to the low-load case shown in Figure 4, the in-cylinder liquid ammonia approaches near-complete combustion.

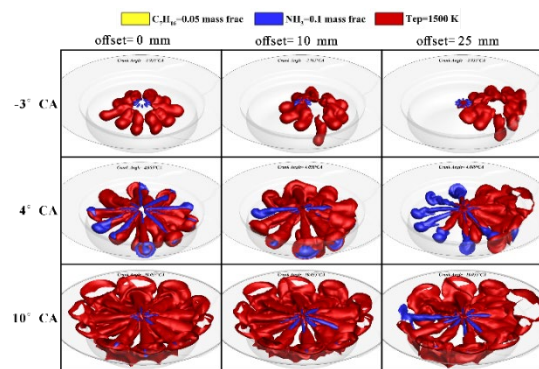


Figure 7. Ignition and combustion process under high load with different offsets

In summary, for both low and high-load conditions, a small offset is beneficial for improving combustion efficiency, which in turn enhances the indicated thermal efficiency. To achieve a combustion process in the cylinder that is closer to coaxial injection, the ideal range for the offset should be between 5 mm and 15 mm. Due to spatial constraints during engine injector layout, achieving an offset of 5 mm is difficult. After comprehensive consideration, an offset of 10 mm is selected as the optimal offset distance. Therefore, subsequent research will be based on an offset of 10 mm. Additionally, since the combustion duration at a high load is constrained by the injection duration of liquid ammonia, an excessively long injection duration hinders the improvement of indicated thermal efficiency at a high load. Therefore, the subsequent work will focus on addressing the solutions to enhance the indicated thermal efficiency at high load.

3.2 Collaborative Optimization of Injection Strategy and Injection System Parameters

3.2.1 Influence of Injection Strategy and Injection System Parameters under High-Load Conditions

At high load conditions, the excessively long injection duration of liquid ammonia leads to a

reduction in indicated thermal efficiency. Therefore, it is necessary to optimize the injection duration of liquid ammonia. However, the current limitations on liquid ammonia injection pressure and the limited improvement in indicated thermal efficiency by increasing injection pressure are important constraints. Additionally, the current liquid ammonia injector has 10 injection holes. Further increasing the number of injection holes may result in a too-close spacing between adjacent fuel sprays, reducing the amount of air entrained by the liquid ammonia, which is unfavorable for forming a combustible mixture. Therefore, in this section, we aim to address the engine performance degradation caused by the excessively long injection duration of liquid ammonia from the perspective of injection strategy. We propose two control strategies: ammonia pre-injection prior to diesel injection (AD) and two-stage injection of liquid ammonia (ADA), as shown in Figure 8.

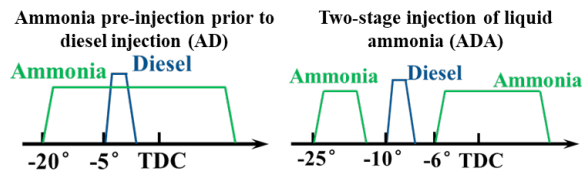
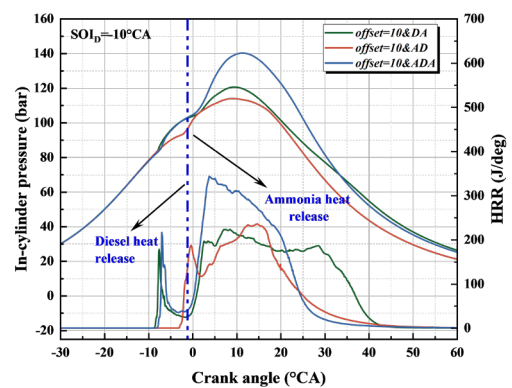


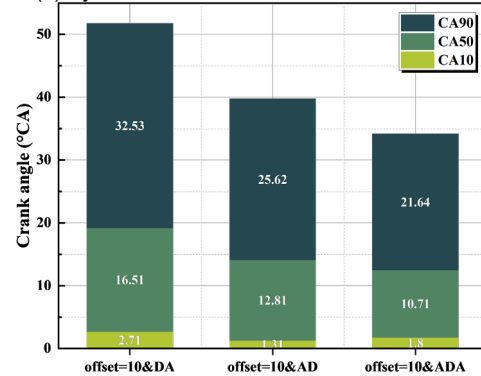
Figure 8 Optimized injection strategy under high load

Figure 9 compares the in-cylinder pressure, heat release rate, combustion phase, and energy distribution under high load conditions for the AD, DA, and ADA injection strategies with an offset of 10 mm. As shown in Figure 9(a), the cylinder pressure and heat release rate curves for the ADA strategy are higher than those for DA and AD. This is because the ADA strategy premixes some liquid ammonia in the cylinder early on. After the diesel fuel is injected into the cylinder to form the initial flame, the premixed liquid ammonia combusts together with the diesel. Compared to DA, both CA50 and CA90 are advanced in ADA and AD, which shortens the overall combustion duration. Among these strategies, ADA results in the greatest reduction in combustion duration, shortening by 34.01% compared to the DA injection strategy, as shown in Figure 9(b). From Figure 9(c), it can be observed that the combustion loss in the cylinder for ADA and DA is relatively small and both are below 2%, while AD has a combustion loss of up to 27.62%, resulting in an indicated thermal efficiency of only 36.10% for AD. Additionally, the indicated thermal efficiency for ADA reaches 49.93%, which is a 4.70% increase compared to DA. This improvement is due to the advanced CA50, shortened combustion duration, enhanced combustion volumetric efficiency, and reduced exhaust losses, leading to a higher indicated

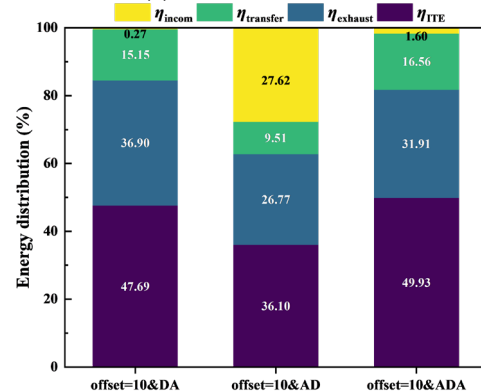
thermal efficiency. Figure 10 shows the ignition and combustion processes in the cylinder under the AD strategy with an offset of 10 mm. Under the AD injection strategy, after the diesel is injected into the cylinder, it is pushed toward one side of the cylinder due to the influence of the liquid ammonia spray. The interaction between the fuel sprays causes the initially injected liquid ammonia to obstruct the development of the diesel spray flame. As a result, some of the liquid ammonia sprays are not directly ignited, especially those farther from the ignition injector. Therefore, the main reason for the low combustion efficiency under the AD strategy is the high overlap of the fuel spray paths of liquid ammonia and diesel, where the obstruction of the diesel spray flame leads to fewer liquid ammonia sprays being effectively ignited.



(a) Cylinder Pressure and Heat Release Rate



(b) Combustion Phase



(c) Energy Distribution

Figure 9. Combustion characteristics of different injection strategies under high loads

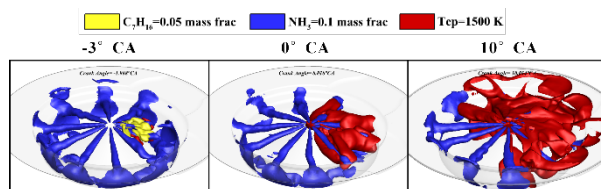


Figure 10. Ignition and combustion process under high load with AD

At high load conditions, the key factor affecting AD combustion performance is the improvement of combustion efficiency. The inherently low combustion efficiency is due to the poor interaction between the liquid ammonia and diesel fuel sprays. Therefore, to avoid the interference caused by the high overlap of the spray paths between liquid ammonia and diesel, a strategy is proposed to adjust the injector insert, termed "insert," to stagger the planes of the liquid ammonia and diesel plume and prevent the interference with the diesel spray flame. Given that liquid ammonia is the main fuel and its injection quantity is relatively large, the amount of air entrainment directly impacts the ability of liquid ammonia to form an ideal combustible mixture. As a result, the strategy does not consider lowering the injector for the main fuel (liquid ammonia).

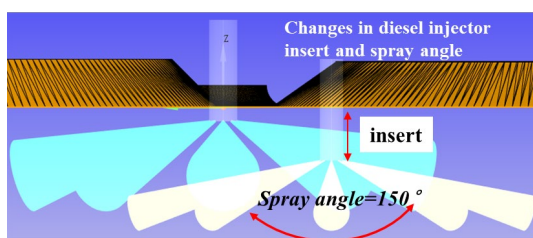


Figure 11. Optimization diagram of diesel injector insert

Figure 11 illustrates the schematic of the diesel injector insert. During the process of lowering the diesel injector, to ensure that the liquid ammonia spray contacts the pilot flame formed by the diesel fuel, the injection angle must be simultaneously adjusted to 150°. Figure 12 compares the in-cylinder pressure, heat release rate, combustion phase, and energy distribution under high load conditions with different penetration depths and fixed injection settings (SOID = -20°CA and SOIA = -5°CA). Overall, the combustion process is divided into two stages: the first stage involves the release of heat from the pilot diesel flame and a portion of the premixed liquid ammonia, and the second stage involves the heat release from the remaining liquid ammonia. As shown in Figure 12(a), by changing the diesel injector layout, as the insert increases, the cylinder pressure curve first increases and then decreases, and the second-

stage heat release rate for liquid ammonia first increases and then decreases. As the penetration depth increases, when the insert ≤ 6 mm, CA50 and CA90 advance, shortening the overall combustion duration. When the insert is between 6 mm and 8 mm, CA50 and CA90 are delayed, and the overall combustion duration lengthens, as shown in Figure 12(b).

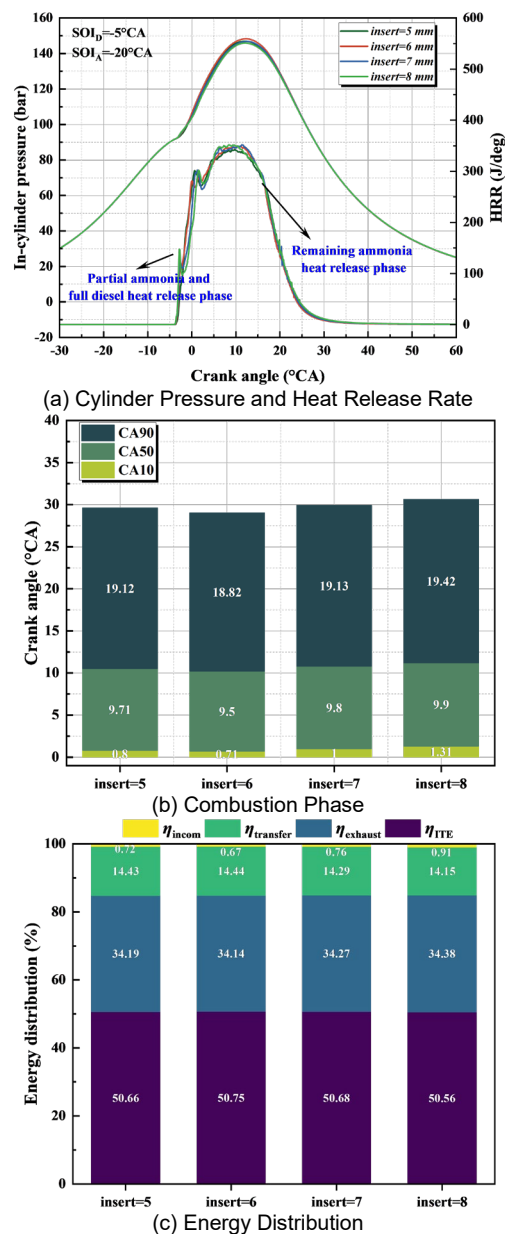


Figure 12. Combustion characteristics of diesel injectors with different inserts

As shown in Figure 12(c), the combustion losses in the cylinder are relatively small and all less than 2%. When the insert exceeds 6 mm, the combustion losses increase slightly. At an insert of 6 mm, the combustion loss is minimized at 0.67%. By changing the diesel injector layout, the second-stage heat release rate of liquid ammonia is faster, CA50 advances, combustion volumetric efficiency

increases, and combustion efficiency improves. As a result, the indicated thermal efficiency reaches approximately 50%. At insert= 6 mm, the maximum indicated thermal efficiency of 50.22% is achieved. Further increases in insert result in a reduced heat release rate in the second stage, causing CA50 to be delayed, and the combustion efficiency deteriorates, leading to a decrease in the indicated thermal efficiency.

3.2.2 Optimal Injection System and Injection Strategy

The optimization of both the injection system structure and the injection strategy can improve the interaction between the liquid ammonia and diesel plume, effectively mitigating the issue of reduced combustion efficiency at high loads due to interference of the liquid ammonia spray with the diesel fuel flame. The optimal solution for the coordinated optimization of the injection system structure and injection strategy is as follows: Offset =10 mm and insert=6 mm, the best injection strategy for low load is DA, which achieves a thermal efficiency of 49.68%. For high load, the optimal injection strategy is AD, which effectively reduces the overlap between the fuel sprays and achieves a thermal efficiency of 50.75%. The second-best coordinated optimization solution is: offset=10 mm and maintaining the original injection system structure, the best injection strategy for low load is DA, which achieves a thermal efficiency of 50.26%. For high loads, the ADA strategy yields the best thermal efficiency of 49.93%.

4 CONCLUSIONS

(1) As the offset increases, the proportion of the liquid ammonia spray on the side away from the diesel that is directly ignited decreases, leading to reduced combustion efficiency, an increase in combustion duration, and a decrease in engine thermal efficiency. Smaller offsets are beneficial for improving combustion efficiency and, in turn, enhancing thermal efficiency. To achieve a combustion process closer to coaxial injection, the ideal range for the offset should be: $5 \text{ mm} \leq \text{offset} \leq 15 \text{ mm}$.

(2) With offset =10 mm, and without changing other aspects of the injection system design, the optimal injection strategy for low load is DA, which achieves a thermal efficiency of up to 50%. However, at high loads, the excessive liquid ammonia injection duration leads to prolonged combustion duration when using the DA strategy, resulting in reduced thermal efficiency. The AD strategy, due to the high overlap between the diesel and liquid ammonia sprays, causes combustion deterioration. The ADA strategy provides the best thermal efficiency of 49.7%.

(3) Increasing the insert of the diesel injector can avoid the issue of high overlap between the diesel and liquid ammonia plume at high loads. A moderate increase in the diesel injector intrusion, combined with the AD injection strategy, can achieve the optimal indicated thermal efficiency of 50.75% at high load, while the thermal efficiency at low load is slightly lower than that achieved with the original injector intrusion and the DA injection strategy.

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