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A Reduced Kinetic Model Approach to Quantifying Injector Spray Angle Influence on NG-Diesel Combustion

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Abstract

This study examines the influence of injector spray angle on combustion characteristics and emissions in an NG-diesel dual-fuel engine using computational fluid dynamics (CFD) with a reduced chemical kinetic model. The model, calibrated with experimental data, revealed that increasing the spray angle from 60° to 140° raised peak cylinder pressure and in-cylinder temperature, while changes beyond 140° were minimal. The optimal spray angle for combustion efficiency differed from that for maximum indicated work, underscoring the need for combined optimization of spray angle and combustion chamber design. Key findings include reductions in combustion duration, NOx, unburned methane, and carbon monoxide emissions up to a spray angle of 120°, with emissions stabilizing between 120° and 160°. The study identifies 120°–160° as the optimal spray angle range for balancing emissions and performance, offering valuable insights for developing more efficient and environmentally friendly dual-fuel engines.

Keywords: *Hydrogen substitution, Dual-fuel diesel engine, Combustion characteristics, NO_x emissions, Engine optimization*

1. Introduction

The search for cleaner alternative fuels is crucial to mitigate the fuel crisis and atmospheric pollution. Natural gas (NG) emerges as a promising candidate due to its low emissions, abundant reserves, and cost-effectiveness. Its superior combustion characteristics and emissions performance make it a viable option for energy conservation and emissions reduction .

NG's simple molecular structure results in significantly lower particulate emissions compared to diesel and gasoline. This, combined with its high-octane number, has made it a popular choice for heavy-duty engines. In NG-diesel dual fuel engines, NG is introduced into the intake manifold, while a small amount of diesel is injected near top dead center to ignite the mixture.

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Numerous experimental studies have investigated the combustion process and emissions characteristics of NG-diesel dual fuel engines. These studies have explored the effects of pilot fuel quantity, injection timing, and engine operating conditions on performance and emissions. However, these experimental studies often lack detailed insights into the in-cylinder combustion process.

Computational Fluid Dynamics (CFD) coupled with detailed chemical kinetics has emerged as a powerful tool to simulate and analyse the combustion process in NG-diesel dual fuel engines. Researchers have used this approach to investigate the effects of various parameters, such as injection timing, fuel composition, and combustion chamber geometry, on engine performance and emissions.

Despite these advancements, the impact of spray angle on the combustion and emissions characteristics of NG-diesel dual fuel engines remains relatively unexplored. This study aims to address this gap by using CFD coupled with detailed chemical kinetics to investigate the effects of spray angle on various aspects of engine performance, including thermodynamics, combustion, and emissions. The findings of this study will contribute to the optimization of NG-diesel dual fuel engines and the development of more efficient and environmentally friendly transportation systems.

2. CFD model and simulated engine

2.1 Engine bench test

This study utilized a six-cylinder, turbocharged diesel engine equipped with a common rail system. To accommodate dual fuel combustion, the engine's fuel supply system and electronic control unit (ECU) were modified. The engine specifications and test platform setup are outlined in Tables 1 and 2, and Figure 1.

A transient pressure sensor was installed in the cylinder head to record in-cylinder pressure. This data was processed by a combustion analyzer to determine heat release rates (HRRs) and combustion characteristics like start of combustion (SOC) and crank angle at 50% heat release (CA50).

A custom-developed ECU was designed to control both single-fuel (diesel) and dual-fuel (NG-diesel) modes. In dual-fuel mode, the ECU controlled diesel injection pulse width, start of injection (SOI), oil rail pressure, and CNG injection pulse width. Exhaust temperature and cylinder pressure were monitored to ensure optimal engine operation.

The study focused on two engine speeds (1000 rpm and 1500 rpm) and two loads (50% and 100% load), representing common operating conditions for heavy-duty engines. Before testing, the engine was warmed up in diesel-only mode until the coolant temperature reached 70-80°C. All tests were conducted at an ambient temperature of approximately 25°C, with intake gas temperature kept below 40°C.

In each test case, steady-state operation was achieved before recording in-cylinder pressure data for 200 consecutive engine cycles. Exhaust gas samples were analyzed to determine the concentrations of hydrocarbons (HC), carbon monoxide (CO), and nitrogen oxides (NOx).

Table 1. Specifications of the tested engine

Item	Content	Item	Content
Displacement (L)	9.726	Maximum torque (N·m)/Speed (rpm)	1550/(1200–1500)
Bore (mm)	126	Rated power (kW)/Speed (rpm)	247/1900
Stroke (mm)	130	Number of injector nozzle holes	8
Original compression ratio	17	Injector spray angle (°)	147
Connecting rod length (mm)	219		

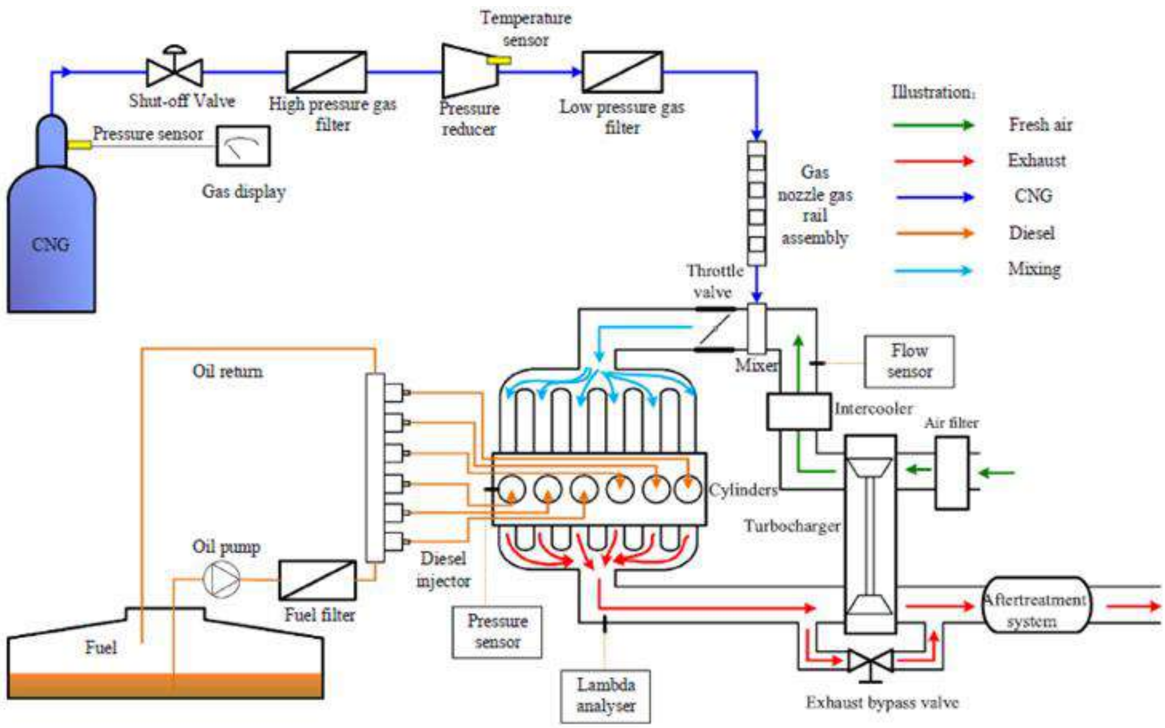

Fig. 1 Schematic diagram of experimental setup for NG-diesel dual fuel engine

Table 2. Specifications of main measuring instruments

Item	Content	Precession
Electric dynamometer	NIDY S22-2/0525-1BV-1	Torque:±0.5% F.S; Speed:±1 r/min
Dynamometer control system	PUMA OPEN1.4.1	±0.5% F.S
Air flowmeter	TOCEIL 20N125	±1%
Natural gas flowmeter	TOKYO KEISO TH-1800-CNG/TRX-700	±1%
Diesel flowmeter	TOCEIL CMFG010	0.12%
Temperature sensor	Thermojunction type	±0.5 °C
Pressure sensor	Piezo resistance type	±0.5% F.S
Emissions analyzer	AVL AMAi60	±0.5% F.S
Combustion analyzer	INDISET ADVANCED PLUS	/

2.2. Physical sub model test

In this research, the combustion processes and pollutant formation mechanisms in a natural gas (NG)-diesel dual-fuel engine were simulated using CONVERGE software, which incorporates a detailed chemical kinetics mechanism. The simulation utilized a series of numerical sub-models to effectively replicate the combustion dynamics.

To model turbulence, the Reynolds Averaged Navier-Stokes (RANS) approach was employed, specifically utilizing a modified rapid distortion renormalization group (RNG) $k-\varepsilon$ turbulence model created by Han and Reitz. This model is adept at calculating in-cylinder turbulent flows, considering the effects of gas density variations within the wall boundary layer and the Prandtl Number increases associated with turbulent flows. Notably, it also imposes lower requirements on the quality of the grid near the wall, which enhances computational efficiency.

For simulating the combustion process, the SAGE model—a detailed chemical kinetics solver within CONVERGE—was selected. This model encompasses a comprehensive chemical kinetics mechanism featuring 76 species and 464 reactions. In this context, n-heptane was utilized to represent diesel fuel, while methane was employed as a surrogate for natural gas. The pressure implicit with splitting of operators (PISO) algorithm was used for the numerical calculations, facilitating efficient computation.

The formation of nitrogen oxides (NOx) was modelled using an extended Zeldovich mechanism as proposed by Heywood. This mechanism consists of seven species and three reactions, enabling it to accurately predict NO formation across a broad range of equivalence ratios.

In the simulation, drop parcels were introduced at the injector location at a user-defined rate, representing clusters of identical droplets. These droplets underwent various processes from the moment of injection until vaporization. To model the breakup of the diesel spray, the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model was selected. This model is predicated on the physical properties governing the spray and mixing processes of diesel fuel. Within this framework, the Kelvin-Helmholtz mechanism is activated by high relative velocities and dense ambient conditions, primarily simulating the initial breakup of the spray. Conversely, the Rayleigh-Taylor mechanism operates during rapid deceleration of droplets, leading to the formation of surface waves at the droplet stagnation point, which is instrumental in simulating secondary breakup.

For the collision processes, the No Time Counter (NTC) method was utilized, drawing from techniques common in gas dynamics applied to Direct Simulation Monte Carlo (DSMC) calculations. This approach has demonstrated increased speed and accuracy compared to O'Rourke's model under certain conditions. The post-collision outcomes model, which incorporates both stretching separation and reflexive separation based on experimental findings related to hydrocarbon droplets, was also employed.

Given that the percentage energy substitution (PES) of diesel is lower, resulting in fewer diesel droplets colliding with solid surfaces, the Rebound/Slide model was deemed more appropriate for simulating interactions between spray droplets and solid boundaries. Additionally, the Frossling model was chosen to predict droplet evaporation, further enhancing the fidelity of the simulation.

This comprehensive approach to numerical simulation combines advanced turbulence modelling, detailed chemical kinetics, and well-established breakup and collision methodologies to accurately characterize the combustion processes and emissions in NG-diesel dual-fuel engines. The careful selection of models and techniques reflects an effort to capture the complex interactions that occur within the engine environment, ultimately contributing to a better understanding of combustion dynamics and pollutant formation. The findings from this study can inform future design improvements and optimization strategies for dual-fuel engine applications, addressing both efficiency and emissions reduction in line with contemporary energy challenges.

3. Results and discussion

To demonstrate the impact of spray angle on the combustion process and emissions of NG-diesel dual-fuel engines, a simulation was conducted where the amounts of methane and diesel fuel were kept constant while varying the spray angle at the same speed and load. The results were thoroughly analyzed, with crank angles CA10, CA50, and CA90 defined as the angles at which 10%, 50%, and 90% of combustion energy is released, respectively. The crank angle of CA10 is identified as the start of combustion (SOC), while the duration of combustion is defined between CA10 and CA90.

Figures displayed the in-cylinder pressure under various spray angles across four cases. It was observed that peak cylinder pressure occurred around a spray angle of 140°, rising with increasing angles from 60° to 140° but slightly declining when the angle reached 160°. Notably, when the spray angle was below 120°, the peak pressure was significantly lower than at 140°, indicating a substantial drop in combustion rate (HRR) at lower angles. As the spray angle exceeded 120°, the influence on HRR diminished.

Considering the engine's structural integrity, peak cylinder pressure must remain within a safe limit (e.g., 150 bar). To achieve this, the pilot diesel injection timing at full load may need to be delayed. Consequently, the timing of peak cylinder pressure in different cases reflected this adjustment. The sensitivity of peak cylinder pressure to spray angle was most pronounced at 100% load and 1000 rpm, where the maximum pressure variation reached 53 bar due to changes in spray angle.

Dynamic performance metrics such as combustion efficiency and indicated efficiency were also evaluated. The highest combustion efficiency was found at a spray angle of 120° in several cases; however, the indicated work at this angle was lower than at 140°. When the spray angle varied between 140° and 160°, both indicated and combustion efficiencies showed minimal variation, suggesting similar power performance within this range.

The heat release rate (HRR) was assessed for different spray angles, revealing that HRR peaked for angles greater than 100°. This behavior aligns with trends seen in spark ignition NG engines, attributable to a high percentage of energy substitution (PES) for NG, which minimizes the effect of spray fuel heat release on HRR. Additionally, at larger spray angles, the injected diesel fuel avoided wall collisions during the piston’s upward movement, enhancing diffusion and evaporation due to increased chamber space and temperature. Consequently, ignition sources became more plentiful, accelerating combustion and achieving a maximum HRR of 498 J/deg, substantially higher than the 5.0%/deg observed in spark ignition NG engines, thus improving thermal efficiency.

In contrast, when the spray angle dropped below 120°, HRR diminished significantly compared to 140°. The combustion process extended longer, even past 100° crank angle at higher RPMs. This extension resulted from two factors: the concentration of injected diesel at the chamber center slowed flame propagation, and the diesel fuel's tendency to collide with chamber walls at lower angles, decreasing evaporation rates and leading to a higher concentration of fuel on the wall surface.

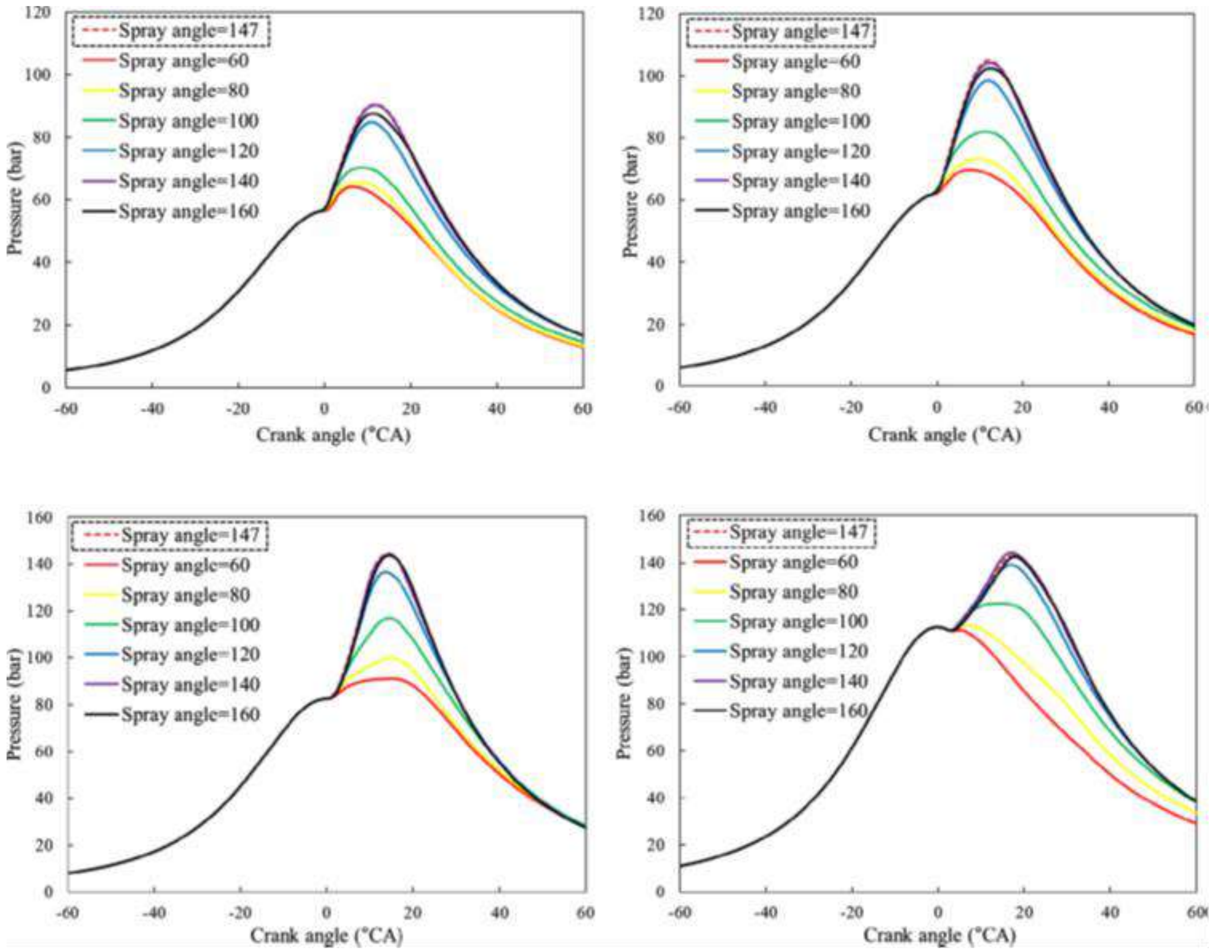

Fig. 2 The in-cylinder pressure with different spray angles in four cases

To further elucidate the effects of spray angle, several key combustion parameters were examined. As the spray angle increased from 60° to 120°, SOC decreased due to earlier wall collisions at lower angles. For spray angles above 80°, SOC variations became negligible, as wall collisions were minimal. At 120°, CA50 advanced and the duration between 10-50% combustion decreased, but remained stable above this angle.

Furthermore, CA90 advanced with increasing spray angle, while the durations of 50-90% and 10-90% combustion shortened—except in the case of 1000 rpm at 50% load. The steepest reductions occurred between spray angles of 60° and 120°, with lesser changes observed beyond this range, primarily because larger spray angles improved fuel evaporation and ignition source availability, leading to faster combustion.

To highlight the differences between operating conditions, temperature fields at CA50 and CA90 for 1000 rpm were illustrated. The temperature profiles indicated that at a spray angle of 60°, the combustion zone had a larger contact area with unburned methane compared to 100°, resulting in faster combustion and a shorter duration between CA50 and CA90 at the lower spray angle.

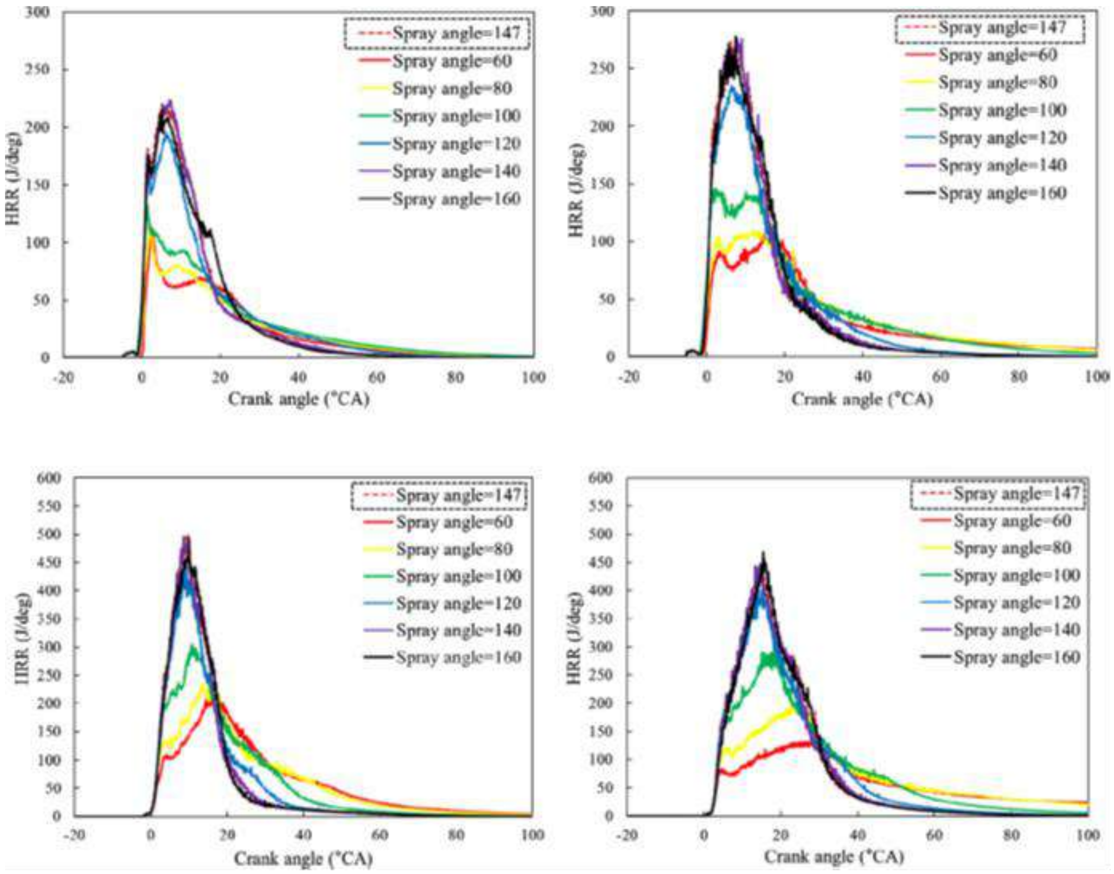

Fig. 3 The HRR at different spray angles in four cases

4. Conclusions

In this study, the impact of injector spray angle on the combustion characteristics and emissions of an NG-diesel dual-fuel engine was examined using computational fluid dynamics (CFD) coupled with a reduced chemical kinetic model. The CFD model was developed based on experimental data and calibrated across four typical operating conditions. By employing the reduced chemical kinetic model, the intermediate processes of combustion and emissions could be readily analyzed, helping to explain the variations observed in combustion and emissions parameters. The analysis of experimental data alongside simulation results led to several key conclusions.

Firstly, it was found that as the spray angle increased from 60° to 140°, the peak cylinder pressure also rose. However, when the spray angle was further increased to 160°, there was a slight decrease in peak pressure. Interestingly, the optimal spray angle for achieving the best combustion efficiency did not coincide with the angle that provided the highest indicated efficiency. This disparity highlights the necessity for a combined optimization of both spray angle and combustion chamber shape to achieve the best combustion efficiency and maximum indicated work simultaneously.

Secondly, the start of combustion (SOC), crank angle at 50% combustion (CA50), and the duration of combustion from 10% to 50% all decreased as the spray angle increased from 60° to 120°. Beyond this range, from 120° to 160°, these parameters exhibited only minor fluctuations. Notably, the greatest reductions in CA90, and the durations of 50–90% and 10–90% combustion were observed when the spray angle increased from 60° to 120°, with maximum reductions of 52.3°, 36.5°, and 49°, respectively. In contrast, the reductions when the spray angle increased from 120° to 160° were considerably smaller, at just 7.5°, 6.7°, and 7.5°, respectively. Additionally, the variation trends for these combustion parameters in Case 1 (1000 rpm and 50% load) differed from those observed in the other three cases.

Thirdly, as the spray angle increased from 60° to 140°, the average in-cylinder temperature also rose, and the duration during which the temperature exceeded 1800 K was prolonged. Consequently, NOx emissions increased with the spray angle, although differences in emissions were minimal when the spray angle ranged between 140° and 160°. In most cases, except for Case 3 (1000 rpm and 100% load), where unburned methane levels remained relatively constant, unburned methane emissions sharply decreased with increasing spray angle. In Case 1 (1000 rpm and 50% load), the maximum reduction rate reached 17,020 ppm as the spray angle changed from 60° to 120°. However, between 120° and 160°, unburned methane emissions stabilized and showed little change.

Moreover, carbon monoxide (CO) emissions declined as the spray angle increased from 60° to 120°, maintaining a lower emission level when the spray angle was between 120° and 160°. To achieve a balance among the emissions of NOx, unburned methane, and CO, the optimal spray angle was determined to be within the range of 120° to 160°.

This study provides valuable insights into the complex interactions between spray angle, combustion dynamics, and emissions characteristics in NG-diesel dual-fuel engines. The findings underscore the importance of optimizing spray angles to enhance performance while minimizing harmful emissions, contributing to the ongoing development of more efficient and environmentally friendly engine technologies.

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