Comparative assessment of n-butanol addition in CTL on performance and exhaust emissions of a CI engine

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Abstract

Coal to liquid (CTL) is a diesel alternative fuel based on Fischer-Tropsch (FT) process, which has shown promising application value. Besides, as an oxygenated biofuel with high oxygen content and volatility, n-butanol can be blended with hydrocarbon fuels to improve engine performance. This study aims to investigate the effects of CTL/n-butanol blends on the performance of the compression-ignition (CI) engine, and to reveal the influence of combustion boundary conditions such as n-butanol blending ratio, the start of injection (SOI), and exhaust gas recirculation (EGR) on the combustion and emissions characteristics. The results show that blending n-butanol with CTL is beneficial to improve the fuel-gas mixture distribution in the cylinder, and the premixed combustion ratio (PCR) increases by 13.66% as the energy ratio of n-butanol increases to 30% (B30)

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compared with the pure CTL. CTL/n-butanol blends make particulate emission tend to be shifted towards nucleation mode and the particulate mass emission significantly reduced, especially the particulate mass of B30 reduce by 68.6%; meanwhile, the NOx emission shows an upward trend. Compared with n-butanol blended, adjusting the SOI impacts NOx emissions significantly, while its influence on the indicated thermal efficiency (ITE) and particulate emissions is relatively slight. Moreover, through the synergistic control of n-butanol addition and EGR, the trade-off relationship between NOx and particles is mitigated.

Highlights:

- CTL facilitates lower the PCR and results in increased particle emissions.
- N-butanol blended suppresses the particle emissions from the combustion of CTL.
- N-butanol blended promotes the shifting of particles towards the nucleation mode.
- The trade-off relationship between NOx and particle is mitigated by using EGR and n-butanol.

Keywords: Coal to liquid; N-butanol; Combustion process; Particulate mode; Pollutant emissions

Abbreviations

CTL	Coal to liquid	BTDC	Before top dead center
FT	Fischer-Tropsch	PCR	Premixed combustion ratio
CN	Cetane number	ITE	Indicated thermal efficiency
CI	Compression-ignition	CD	Combustion duration
ESC	European stationary cycle	CA	Crank angle
ID	Ignition delay	CA50	Gravity of heat release

HRR	Heat release rate	NMP	Nucleation mode particle
EGR	Exhaust gas recirculation	AMP	Accumulation mode particle
SOI	Start of injection	TDC	Top dead center
ECU	Electronic control unit	SHC	Specific heat capacity
IMEP	Indicated mean effective pressure	CMD	Count median diameter

1. Introduction

For a long time, fossil energy has played a pivotal role in various fields, such as industry, agriculture, and transportation [1, 2]. According to the U.S. Energy Department, the global energy demand has grown since the Industrial Revolution, and more than a billion barrels of oil per day will be consumed by 2035 [3, 4]. The world is facing severe energy problems, so the search for alternative energy sources and the efficient use of energy have become a worldwide challenge [5]. At the same time, the increasingly serious environmental pollution and global carbon emissions have also attracted attention from all walks of life [6, 7]. Obviously, the transportation field consumes a large amount of fuel (greater than 25% of total) and is also the primary source of environmental pollution problems. For the automotive industry, which is required to meet the regulations of fuel consumption and pollutant emission [8, 9], and it is essential to develop energy diversification strategies based on the local resource endowment.

In recent years, numerous researches have been conducted on alternative fuels for automobiles. Natural gas, hydrogen, biomass fuels, synthetic fuels, etc., have shown good potential as alternative fuels for gasoline and diesel engines [10-13]. With coal as the primary raw material in many countries such as China, coal to liquid (CTL) is a high-quality and clean alternative fuel produced by chemical processing and synthesis technology [14]. A lot of research has been done on CTL in

the field of economy and technology, and a more comprehensive evaluation of CTL technology has been made from the aspects of resource consumption, economic cost, and environmental pollution [15, 16]. With the progress in coal catalytic conversion technology and emission reduction technology, the resource utilization rate of coal liquefaction technology has been upgraded, the carbon emissions of that have been greatly reduced, and the economic cost of CTL has reached a level comparable to that of the petroleum-based fuels [17, 18]. In addition, because the direct use of coal would lower energy utilization efficiency and cause considerable emissions that account for the main source of air pollution, the efficient and clean use of coal resources through synthetic technology is also of strategic significance [19]. The core reaction of CTL production is the Fischer-Tropsch (FT) synthesis reaction, and the CTL produced by FT synthesis is mainly composed of saturated alkane [20]. CTL has the characteristics of high cetane number (CN), low sulfur, low nitrogen, and low aromatic content, so CTL is a high-quality diesel alternative fuel [21]. Besides, CTL can be intermixed with conventional petroleum-based fuels in any ratio, making it compatible with the existing automotive technology systems and having broad application prospects in internal combustion engines [22, 23]. Song C et al. studied the effects of FT diesel on compression-ignition (CI) engines under the European stationary cycle (ESC) and constant speed/varying load test conditions, and the results show that burning FT diesel is beneficial to reduce engine pollutant emissions [24]. Research by Dai YL et al. showed that when burning CTL liquefied by FT method, the ignition delay (ID) is shorter, the peak heat release of the premixed combustion is lower, and the use of CTL can effectively reduce the soot emissions [25].

In addition, oxygen fuels such as biodiesel, alcohols, esters, ethers, etc., have also become research hotspots due to their potential for high-efficient and clean combustion [26-28]. In particular,

74 butanol can be produced through the fermentation of agricultural waste and other biomass [29].
75 Compared with low-carbon alcohols such as methanol and ethanol, butanol has the characteristics
76 of high calorific value, high CN, high density, high viscosity, and good lubricity. At the same time,
77 it has better miscibility with alkane fuels. As an additive, butanol has excellent potential for
78 application in the CI engine [30-32]. Since the butanol molecule contains oxygen atoms, blending
79 butanol with diesel helps to increase the oxygen content of the fuel so that it can reduce the emissions
80 such as particles from CI engines [33-35]. Many research teams used butanol as an additive to blend
81 with diesel, biodiesel, etc., to explore the potential of achieving high-efficiency and clean
82 combustion for internal combustion engines by improving fuel characteristics [36-38]. Rajesh
83 Kumar B et al. studied the effects of butanol/diesel blends on the combustion and emission
84 characteristics of CI engines in a low-temperature premixed combustion mode, showing that butanol
85 blended resulted in a longer ID and a higher premixed heat release rate (HRR), and combining with
86 exhaust gas recirculation (EGR) technology can simultaneously reduce the NOx and smoke
87 emissions of the engine [39]. Chen Z et al. found that the combination of high butanol/diesel
88 blending ratio and medium EGR ratio has the potential to achieve extremely low NOx and soot
89 emissions while maintaining a high level of thermal efficiency [40]. Huang et al. investigated the
90 particle emission characteristics of diesel/n-butanol under different EGR conditions, the results
91 showed that the addition of n-butanol to the fuel makes both the soot emissions and the average
92 geometric size of particles decrease for EGR ratios smaller than 20%, while the total particle number
93 concentration of D70B30 compared to D100 reduces by 74.7% at large EGR ratios [41].
94 In order to solve the problems of the short ID and the insufficient premixed combustion of
95 burning pure CTL in the CI engine, the method of blending n-butanol with CTL was adopted to

change the physicochemical properties of the fuel to explore the effects of the CTL/n-butanol blends on the combustion and emissions characteristics of a CI engine. The combustion boundary conditions such as the n-butanol blending ratio, the start of injection (SOI), and the EGR ratio were adjusted to reveal the potential of CTL/n-butanol blends to reduce pollutant emissions, especially particulate emissions.

2. Experimental system and test procedure

2.1 Experimental engine and apparatus

The experimental engine is a single-cylinder CI engine modified from a four-cylinder four-valve high-pressure common-rail diesel engine, and the main specifications of the engine are shown in Table 1. In order to flexibly control the SOI and the intake charge, the second cylinder of the experimental engine is equipped with an independent direct-injection system and intake/exhaust system, while the other three cylinders are not supplied with fuel. The open electronic control unit (ECU) is used to control the direct-injection system, and the ECU-NI2106 can achieve flexible control of the SOI and the injection mass. In addition, the intake/exhaust system consists of a two-stage simulated supercharge system and an EGR system. The two-stage simulated supercharge system uses an air compressor as the intake air source, and a two-stage pressure surge chamber stabilizes the high-pressure air from the compressor. The intake pressure of the engine is flexibly adjusted between 0 MPa and 0.3 MPa (gauge pressure) by a pressure sensor and a flow-limiting valve. The EGR system stabilizes the pressure of the exhaust surge chamber by adjusting the opening of the exhaust backpressure valve and then controls the EGR ratio (up to 30%) by adjusting the EGR valve.

Table 1. Engine specifications

Category	Properties
Geometric compression ratio	17.1
Cylinder diameter / mm	95.4
Piston stroke / mm	104.9
Connecting rod length / mm	162
The number of nozzles holes	7
Injector orifice diameter / mm	0.12
Oil jet cone angle / (°)	12
Swirl number	0.97
The shape of combustion chamber	ω

The measurement and control equipment used in the engine test platform mainly includes the eddy current dynamometer, the in-cylinder pressure transducer, the fuel flow meter, the airflow meter, the fast NOx analyzer, the fast HC analyzer, the fast CO&CO_2 analyzer, the electron particle spectrometer. The cylinder pressure is collected by a combustion analyzer at 0.1° CA intervals and averaged over 50 cycles at each operating point to eliminate measurement errors. The schematic diagram of the experimental setup is shown in **Fig. 1**, and the main parameters of the equipment are shown in **Table 2**.

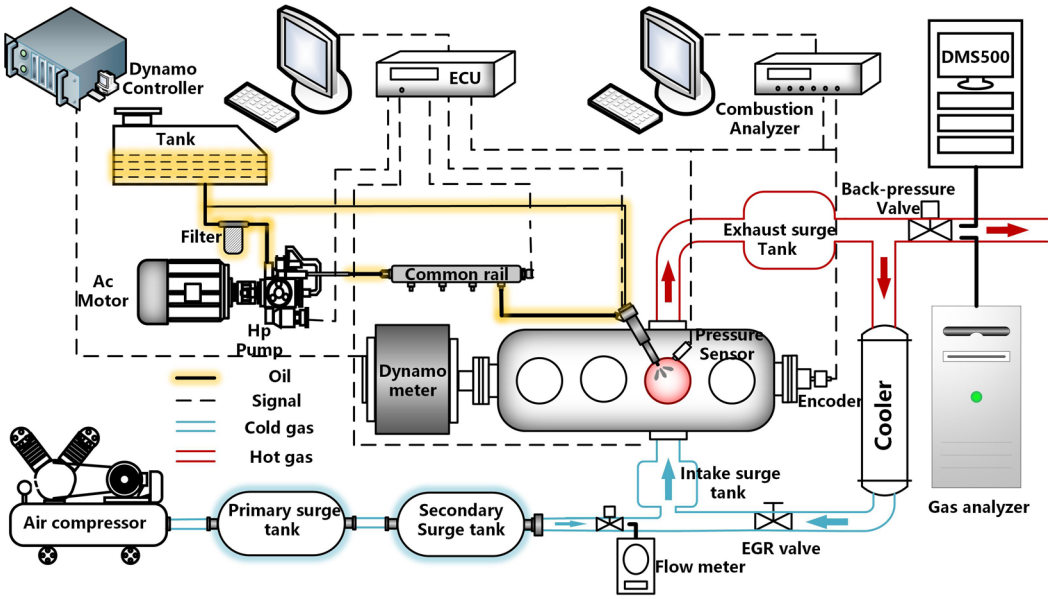


Fig. 1 Schematic diagram of experimental setup

125 **Table 2.** Main equipment

Category	Measuring instruments	Manufacturer	Accuracy
Dynamometer	CW260	CAMA	Torque: ± 0.5 NM Speed: ± 2 r/min
Rotary encoder	S4001	Bangman	—
Fuel flow meter	FX-100	ONO-SOKKI	± 0.12%
Air flow meter	20R100	TOCEL	± 1%
Cylinder pressure	6052C	Kistler	± 1%
CO&CO_2	NDIR500	Cambustion	< 2% FS/hour
HC	HFR500	Cambustion	< 1% FS/hour
NOx	CLD500	Cambustion	< 5 ppm/hour
Particle	DMS500	Cambustion	—

126 *2.2 Methodology and test conditions*

127 The basic fuels used in the experiment are low sulfur diesel, CTL, and n-butanol. The main
128 physicochemical properties of the basic fuels are shown in **Table 3,** the basic parameters are
129 measured at 25℃. In addition, this study adopts CTL/n-butanol blended fuels defined as BXX, of
130 which the XX represents the calorific value percentage of n-butanol. For example, the blended fuel
131 composed of 70% CTL and 30% n-butanol (by calorific value) is defined as B30. Moreover, the
132 engine operating conditions are shown in **Table 4**. The engine worked at the maximum torque speed
133 of 1400 r/min, and the load rate was about 50% (the indicated mean effective pressure (IMEP) was
134 about 0.85 MPa). When comparing between different fuels, the calorific values of CTL and its
135 blends were kept the same as the calorific value of diesel (1438 J/cycle), so n-butanol ratio of the
136 blended fuels were set to 10%, 20%, and 30% based on energy ratio. In the experiments, SOI was
137 selected from 5°CA before top dead center (BTDC) to 13 °CA BTDC with the step of 2 °CA, and
138 the EGR ratio was selected from 0% to 30% with the step of 10%. Moreover, the EGR ratio was
139 defined as the ratio of the CO_2 content in the intake and that in the exhaust of the engine, and the
140 CO_2 content was measured by the exhaust gas analyzer. In addition, when adjusting the EGR ratio
141 during the experiment, the pure air flow rate (35 kg/h) into the intake remained unchanged, and the
142 EGR ratio was adjusted by controlling the mass of introduced exhaust gas.

143 The DMS500 measures the particle size/number distribution in an engine exhaust. However,
144 particle mass has been long established as a metric for legislative measurements of particle
145 emissions from engines, but particle mass and particle number measurements do not demonstrate a
146 direct correlation. Therefore, given a size/number distribution, it is desirable to calculate in real-
147 time a mass concentration, so the conversion equation is as follows:

148 $$Mass(\mu g) = \text{Density Factor} \cdot Dp^{power\ factor}$$

149 For Diesel engine agglomerates, research shows that the DMS500 mass calculation gives good

150 agreement with gravimetric techniques using a density factor of $2.2 \cdot 10^{-15}$ and a power factor of 2.65.

151 **Table 3.** Main properties of tested fuels

Fuel property	CTL	N-butanol	Diesel	B10	B20	B30
Density under 25℃/ ($kg \cdot m^{-3}$)	757.0	805.5	840.0	763.1	768.9	774.3
Cetane number (CN)	75.4	25	52.9	69.4	63.6	58.1
Low calorific value / ($MJ \cdot kg^{-1}$)	43.07	33.19	42.69	41.89	40.76	39.68
Total Aromatics / %	≤ 0.8	0	≤ 3.6	≤ 0.7	≤ 0.6	≤ 0.5
Latent heat of vaporization / ($kJ \cdot kg^{-1}$)	~	626	270	~	~	~
Sulfur content / 10^{-6}	0.38	0	3.7	0.33	0.29	0.25
Oxygen mass fraction / %	0	21.62	0	2.57	5.05	7.41
Viscosity under 25℃ / ($mm^2 \cdot s^{-1}$)	2.14	3.64	4.27	2.32	2.49	2.65
Theoretical air-fuel ratio	14.96	11.2	14.3	14.5	14.1	13.7

152 **Table 4**. Engine operating conditions

Category	Properties
Engine speed	1400 r/min
IMEP	About 0.85 MPa
Injection pressure	100 MPa
SOI	5 - 13 °CA BTDC

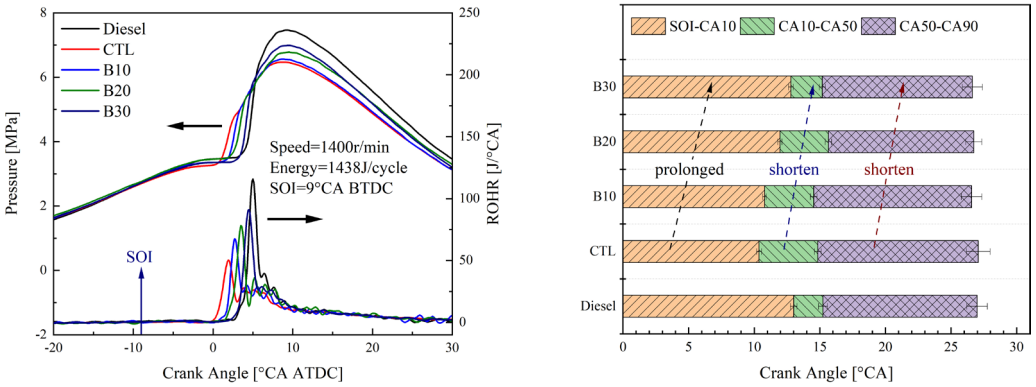
EGR ratio	0 - 30%
Inlet air temperature	25 ± 1°C
Cooling water temperature	80 ± 1°C

3. Results and discussions

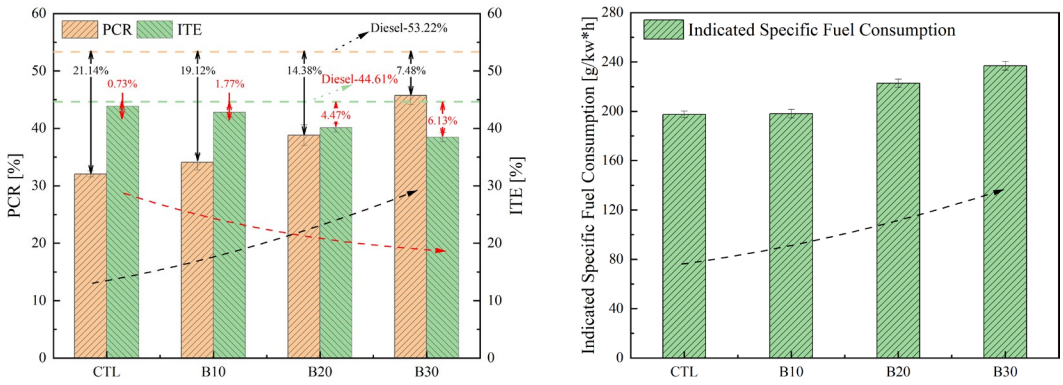
3.1 Effects of CTL/n-butanol blends on combustion and emissions characteristics of the CI engine

Compared with conventional diesel, CTL has higher CN, lower sulfur and aromatic content, so it can be used to improve the combustion and emission performance of the CI engine. However, applying pure CTL still has the problems of the slow combustion speed caused by the short ID. Aiming at the problems of CTL combustion, n-butanol is blended into CTL to explore the way to achieve the high-efficient and clean combustion of the CI engine.

3.1.1 The effects of burning CTL/n-butanol blends on the combustion process



(a) Cylinder pressure and HRR (b) Combustion phasing



(c) PCR and ITE (d) ISFC

Fig. 2 Comparison of the cylinder pressure, the HRR, the combustion characteristics, and ISFC in the cases of burning diesel, CTL, and CTL/n-butanol blends

In order to investigate the effects of blending n-butanol with CTL on the combustion process of the CI engine, a comparative analysis of the combustion characteristics of diesel, CTL, and CTL/n-butanol blends is carried out. **Fig. 2** shows the comparison of the cylinder pressure, the HRR, and the combustion characteristics of diesel, CTL, and CTL/n-butanol blends. In this study part, the SOI is fixed at 9°CA BTDC and, the EGR ratio is set to 0%. In **Fig. 2(b)**, the SOI-CA10 represents the ID, and CA10-CA90 represents the combustion duration (CD). The CAXX represents the crank angle (CA) at which the accumulated heat release reaches XX% of the entire cycle heat release, and the HRR referred to in this article is the apparent heat release rate. This paper defines the premixed combustion ratio (PCR) as the ratio of the cumulative heat release of the premixed combustion endpoint (the crank angle corresponding to the minimum value of the heat release acceleration) to the total cumulative heat release. It can be seen from **Fig. 2** that due to the higher CN and reactivity meaning better ignitability, the CTL combustion has a shorter ID and a smaller PCR than those of diesel, leading to the reduced peak value of HRR and cylinder pressure as well as the advanced combustion phasing using CA50 as indicator. The HRR curves also show that applying CTL makes

175 the boundary between premixed and diffusion combustion more apparent, and the duration of
176 diffusion combustion is significantly prolonged. Since premixed combustion speed is faster than
177 that of diffusion combustion, the smaller PCR of CTL leads to a longer CD. The extended CD will
178 reduce the propensity for constant volume combustion, leading to a decrease in the ITE. On the
179 other hand, the inadequate premixed combustion is not conducive to the inhibition of particle
180 generation.

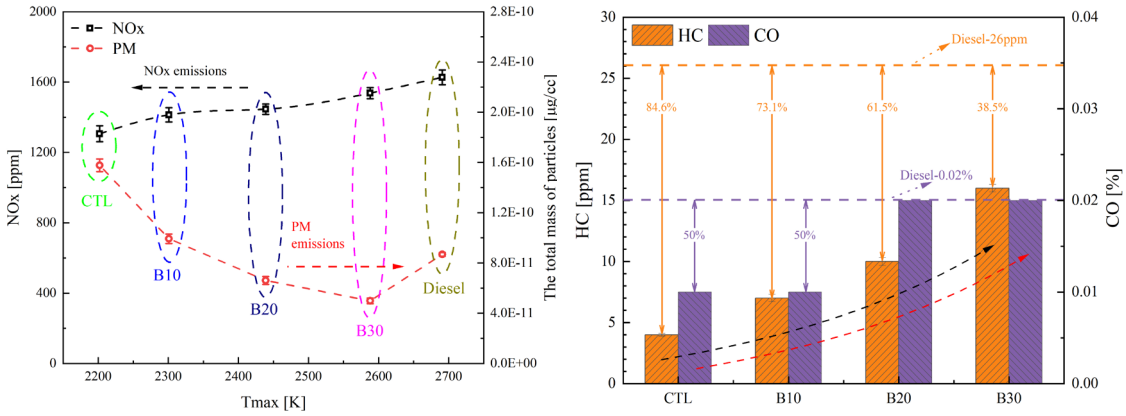
181 In the interest of solving the problems of inadequate premixed combustion of burning pure
182 CTL, n-butanol is blended with the CTL to reduce the reactivity of the in-cylinder fuel/air mixture
183 and improve the homogeneity of the mixture. As illustrated in **Fig. 2**, the fuel reactivity decreases
184 after adding n-butanol, resulting in a prolonged ID. Moreover, the addition of n-butanol with greater
185 volatility is more conducive to forming the homogeneous mixture, so the PCR is significantly
186 improved after the use of CTL/n-butanol blends. Compared with the pure CTL, the PCR of B10,
187 B20, and B30 fuels increase by 2%, 6.76%, and 13.66%, respectively. At the same time, it can be
188 observed from **Fig. 2(a)** that the high PCR causes an increase in the peak value of HRR and cylinder
189 pressure. With the increase in the proportion of n-butanol from **Fig. 2(b)**, the reduced ignition
190 performance and a larger latent heat of vaporization during the early atomization and vaporization
191 process of the n-butanol have more noticeable effects on extending the ID, and the CA50 is
192 postponed making the overall combustion phase more behind. From the perspective of the chemical
193 reaction mechanism, alkanes produce a large number of OH radicals in the low-temperature reaction
194 stage, and part of the OH radicals will be occupied and consumed by n-butanol. At this time, alkanes
195 and n-butanol are in a competitive relationship to grab OH radicals, but the critical reaction is the
196 dehydrogenation reaction between n-butanol and OH radicals suppressing ignition. Thereby, the

low-temperature ignition of the fuel is suppressed [42]. This phenomenon is more obvious with the increase in the proportion of n-butanol. Moreover, due to the addition of n-butanol, the PCR increased significantly, which considerably shortens the post-burning (CA50-CA90) duration reducing CD.

In general, increasing PCR contributes to the enhanced propensity for constant volume combustion to increase the ITE. However, it can be noticed from **Fig. 2(c)** that although blending n-butanol with CTL can effectively increase the PCR, the ITE of the engine decreases instead. The reason is that n-butanol has a higher latent heat of vaporization, which leads to a reduction of the cyclic heat release, and the addition of n-butanol also causes the combustion phasing to be delayed. The two reasons above harm the ITE corresponding to the fuel consumption rate from **Fig. 2(d)**. What can be seen is that the indicated specific fuel consumption (ISFC) of CTL, B10, B20 and B30 are 197.4141g/kw*h, 198.1227g/kw*h, 222.7769g/kw*h and 236.9085g/kw*h, so fuel consumption rate has increased as the proportion of n-butanol increases.

3.1.2 The effects of burning CTL/n-butanol blends on the emissions

Blending n-butanol with CTL is beneficial to improving the homogeneity of fuel/air mixture and increasing the PCR, and the oxygen-containing molecular structure of n-butanol is helpful to reducing pollutant emissions. Accordingly, the emissions characteristics of diesel, CTL, and CTL/n-butanol blends are analyzed in this section.



(a) NOx and particles (b) HC and CO

Fig. 3 Influence of diesel, CTL, and CTL/n-butanol blends on engine emissions

Due to the trade-off relationship between NOx and particulate emissions, the emission control of CI engines has always been a difficulty focused by researchers. The influence of diesel, CTL, and CTL/n-butanol blends on NOx and particles is shown in Fig. 3(a). Since the maximum combustion temperature is significantly affected by the premixed combustion, the order of the maximum combustion temperature of different fuels is that CTL < B10 < B20 < B30 < diesel. The in-cylinder high-temperature environment promotes NOx formation, so the NOx emissions of the engine increase with the increase in the n-butanol blending ratio. However, all of the NOx emissions of CTL/n-butanol are lower than that of diesel. The particles are more prone to be generated in the environment of high-temperature and fuel-rich, which is more likely to appear during the process of diffusion combustion [43]. Fig. 3(a) shows that blending n-butanol with the CTL effectively suppresses the particulate emissions. The higher peak combustion temperature will promote the initial generation of particulate matter in the local oxygen-lean area, but there is an obvious effect on reducing particulate emissions by CTL/n-butanol blends. The addition of n-butanol into CTL can prolong the ID and improve the concentration distribution of the fuel-gas mixture before ignition. Besides, the n-butanol molecule has the property of oxygen containing, which is propitious to reduce

the local fuel-rich region in the combustion process. At the microscopic level, n-butanol contains OH radicals, which can be formed directly from n-butanol molecules by the cracking of the C-O bonds, while the alkane fuels need first to break C-H bonds to form active H ions and then combine with the O atoms in the air to form OH radicals. The OH radicals can effectively inhibit the generation of the soot precursor. Therefore, as the n-butanol blending ratio increases, the particulate emissions are reduced. Taken together, blending n-butanol with CTL mitigates the trade-off relationship between NOx and particulate emissions relative to diesel combustion. Accordingly, the NOx and particulate emissions obtained by using B30 fuel are reduced by 11.12% and 23.9%, respectively, compared to those of diesel fuel.

Fig. 3(b) presents the influence of diesel, CTL, and CTL/n-butanol blends on HC and CO emissions. As shown in **Fig. 3(b)**, the HC emissions gradually increase as the n-butanol blending ratio increases, but the B30 fuel still has lower HC emissions than diesel. This phenomenon is related to the change in the ID. The longer ID makes fuel adhere more easily to the cylinder wall, and the fuel distributing on the cylinder wall cannot be fully oxidized in the combustion process, resulting in higher HC emissions. Another reason for the lower HC emissions of CTL and CTL/n-butanol blends is that the low distillation temperature and high volatility of CTL lead to a reduction in the fuel-rich region of the cylinder, which also helps to suppress unburned HC emissions. **Fig. 3(b)** also illustrates that CO emissions rise with the increase of the n-butanol blending ratio but remain within the lower level.

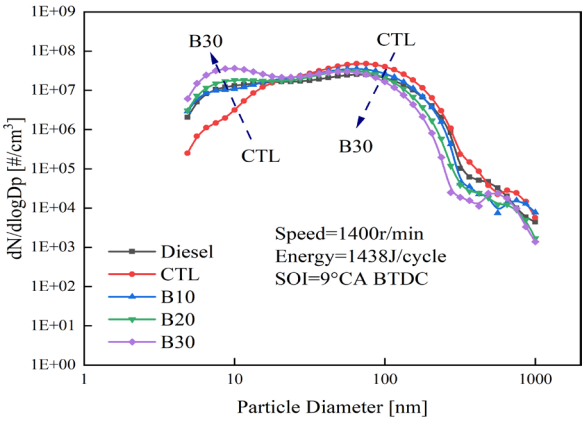
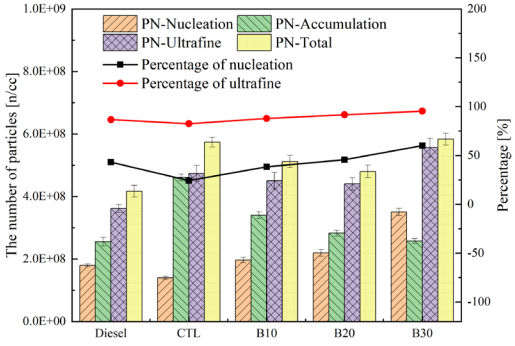


Fig. 4 Influence of diesel, CTL, and CTL/n-butanol blends on particle size distribution

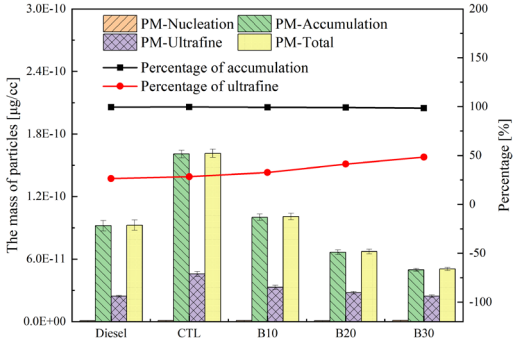
Since the particles in CI engines are complex in composition and cover a wide range of sizes, the particle size distributions of diesel, CTL, and CTL/n-butanol blends are extracted as shown in **Fig. 4**. The particles with a diameter smaller than 35 nm are defined as the nucleation mode particle (NMP), and the particles with a diameter larger than 35 nm are defined as the accumulation mode particle (AMP). It can be seen from **Fig. 4** that, with 35 nm as the demarcation point, the change rules of NMP and AMP present an opposite trend. The reason is that the formation mechanisms of different mode particles are discrepant. The NMP is mainly formed by the unburned HC during the exhaust dilution and cooling, and the AMP is mainly generated by the aggregation of carbonaceous particles produced by the dehydrocyclization of fuel in the region of high-temperature and fuel-rich [44]. The combustion of CTL undergoes a larger proportion of diffusion combustion, so there are more high-temperature and hypoxic regions in the combustion process. At the same time, the HC emissions are lower when burning CTL. Thus, compared with diesel, fueling CTL in the CI engine can significantly reduce the number of NMP, while the peak number of AMP significantly rises. As the blending of n-butanol with CTL can improve the concentration distribution of fuel/air mixture and its molecule contains oxygenated radicals, it can be found from **Fig. 4** that n-butanol blended

264 can help to suppress the higher AMP emission caused by the CTL combustion and promote the

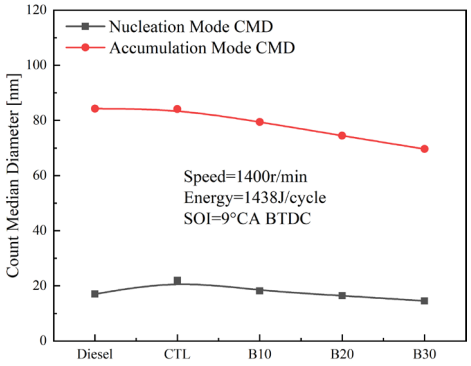
265 shifting of particles towards NMP.



(a) Particulate number



(b) Particulate mass



(c) CMD

Fig. 5 Influence of diesel, CTL, and CTL/n-butanol blends on different mode particles and CMD

266 The earlier emission regulations only restricted the mass emission of particles, but in recent

267 years, the emission regulations have added limitations on the number emission of particles [45].

268 Therefore, number emissions, and mass emissions and CMD of different mode particles of diesel,

269 CTL, and CTL/n-butanol blends are further extracted, as shown in **Fig. 5**. The figure indicates that

270 the ultrafine particles (the particles with a diameter smaller than 100 nm) account for most of the

271 total particulate number (over 80% in all conditions), while the AMP mass is in the majority of the

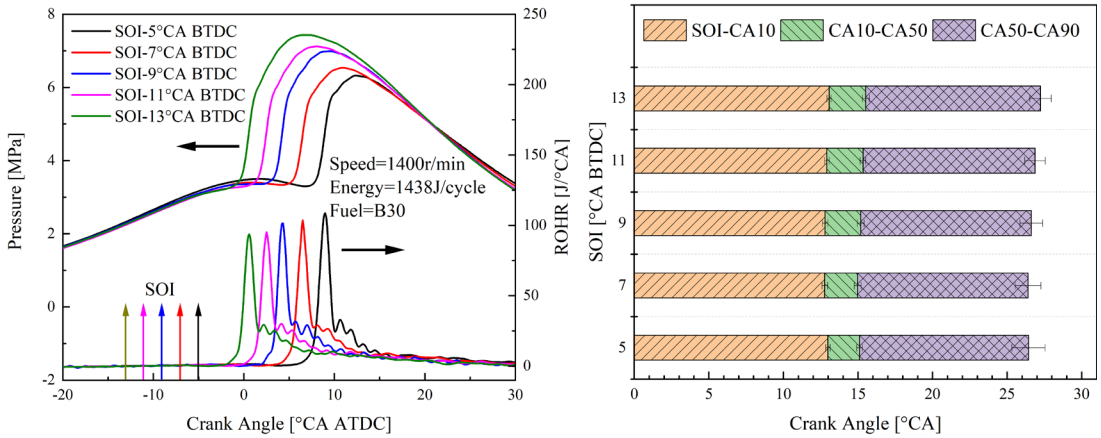
272 total particulate mass (over 98% in all conditions). As depicted in **Fig. 5(a)**, compared with diesel,

when fueling CTL in the CI engine, the number of NMP decreases by 22.2%, the number of AMP increases by 80.7%, and the total particulate number and mass increases by 37.7% and 74.5%, respectively. The CTL/n-butanol blends effectively reduce the emission of AMP but lead to an increase in the number and proportion of NMP. Since the mass of AMP accounts for the majority of the total particulate mass, blending n-butanol with CTL can effectively reduce the particulate mass emissions. Compared to the total particulate mass emissions of the pure CTL, those of the B10, B20, and B30 fuel were reduced by 37.8%, 58.3%, and 68.6%, respectively. However, since the particulate number of the NMP and AMP shows an opposite trend with an increase in the n-butanol blending ratio, the total particle number emissions are not significantly affected by the addition of n-butanol. At the same time, the particulate size characteristics of the above test fuels can also be reflected in the changing trend of CMD in **Fig. 5(c).** It can be seen from the figure that, although the above conclusions indicate that CTL particulate matter emissions are relatively high, ultrafine particles account for a relatively large proportion for CTL, making its accumulation mode CMD the same as diesel. Moreover, with the addition of n-butanol in the CTL, both nucleation mode CMD and accumulation mode CMD decrease significantly with n-butanol ratio increasing. In particular, the decline of accumulation mode CMD is evident compared with pure hydrocarbon fuels such as diesel and CTL, demonstrating that the addition of n-butanol has a noticeable effect on inhibiting the AMP produced by CTL. For example, the degree of reduction of accumulation mode CMD of B30 reaches 17.37% compared with pure CTL.

3.2 Effects of fuel injection strategy on the combustion and emissions of the CTL/n-butanol blends engine

In order to obtain a suitable fuel injection strategy for the CTL/n-butanol blends engine, the

effects of fuel injection conditions on the combustion process and primary emissions of the engine fueled the CTL/n-butanol blends are investigated in this section.



(a) Cylinder pressure and HRR (b) Combustion phasing

Fig. 6 Influence of SOI on the combustion process when burning B30 fuel

Fig. 6 shows the influence of SOI on the combustion process when burning B30 fuel. What can be observed from **Fig. 6** is that, as the SOI advances, the ID remains almost constant, so the ignition timing is advanced, and the combustion process is closer to the top dead center (TDC). Since the cylinder volume decreases as the piston gets closer to the TDC, the maximum cylinder pressure increases with the advance of the SOI. However, as the SOI advances, the HRR curves move forward while the shapes remain approximately the same. Since the higher temperature and pressure near the TDC facilitate the combustion process, early injection slightly shortens the CD.

Since the addition of n-butanol and SOI both have a significant influence on the combustion process of the engine and thus on the ITE, the influence of the injection strategy on the ITE of the engine fueled CTL/n-butanol blends is shown in **Fig. 7**. The early injection will cause the combustion process to approach the TDC, which is conducive to improving the propensity for constant volume combustion. Hence, the figure presents that the advanced injection contributes to

enhancing the ITE. However, blending n-butanol with CTL causes a decrease in ITE due to the high latent heat of vaporization and the postponed combustion. Among them, the effect of n-butanol blended on ITE is more significant than adjusting the SOI. The ITE is increased by about 2% after advancing the SOI from 5 °CA BTDC to 13 °CA BTDC for all fuels. At the same SOI, the ITE is reduced by about 5% after increasing the n-butanol blending ratio from 0% to 30%. It indicates that the SOI needs to be advanced by about 6 °CA to recover the ITE degradation caused by the 10% n-butanol addition.

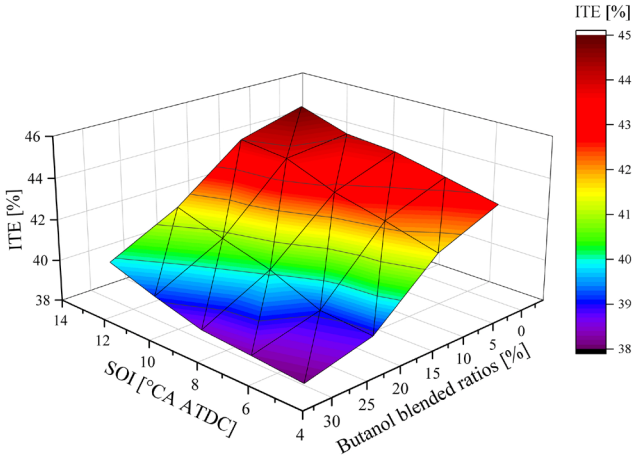
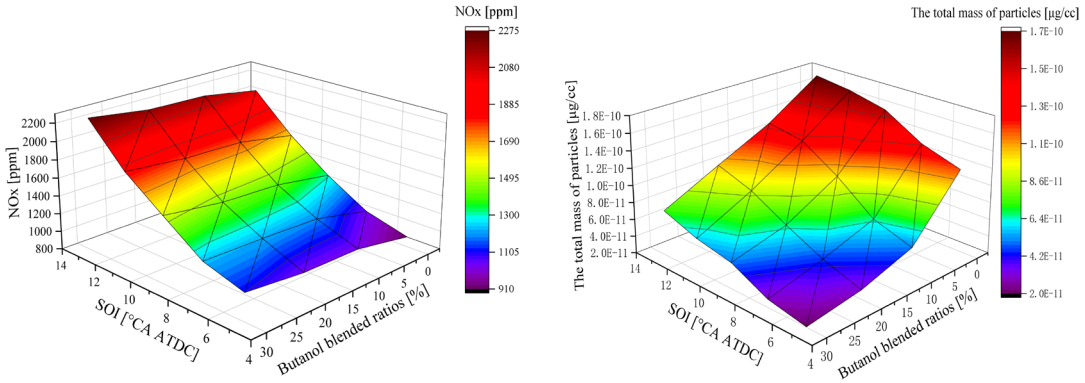


Fig. 7 Influence of injection strategy on the ITE of the CTL/n-butanol blends engine



(a) NOx emissions (b) Particulate emissions

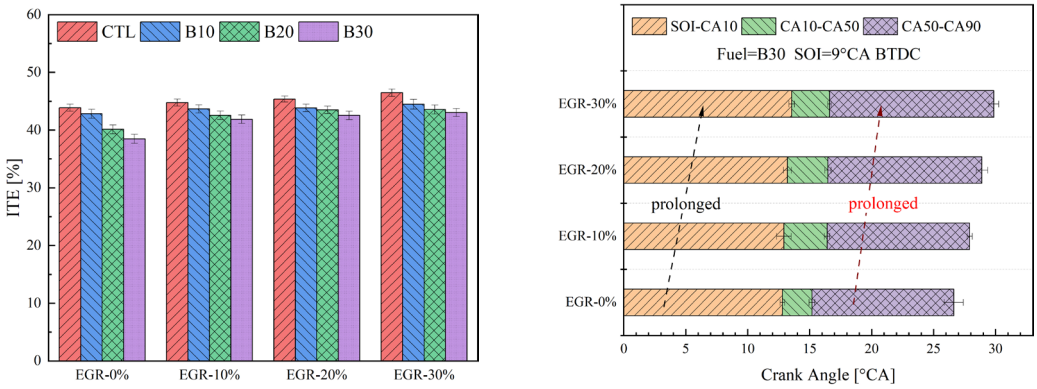
Fig. 8 Influence of injection strategy on the emissions of the CTL/n-butanol blends engine

Fig. 8 demonstrates the influence of injection strategy on the NOx and particulate emissions

317 of the CTL/n-butanol blends. As can be observed from **Fig. 8(a)**, the advanced injection or
318 increasing the n-butanol blending ratio can both lead to an increase in NOx emissions, and the
319 influence of SOI on NOx emissions is far more significant than that of n-butanol addition. The NOx
320 emissions are increased by about 1150 ppm after advancing the SOI from 5 °CA BTDC to 13 °CA
321 BTDC for all fuels. At the same SOI, the NOx emissions are increased by about 210 ppm after
322 increasing the n-butanol blending ratio from 0% to 30%. The reason is that the advanced injection
323 and the n-butanol addition both make the combustion process close to the TDC, which leads to a
324 rising combustion temperature and promote the generation of NOx emissions, but the influence of
325 the change in SOI is much greater than that of blending n-butanol. As shown in Fig. 8(b), the addition
326 of n-butanol significantly reduces particulate emissions, while the higher temperature brought by
327 advanced SOI leads to an increase in particulate emissions, and the effect of blending n-butanol on
328 particulate emissions is more obvious. Consequently, the particulate emission of CTL increases by
329 49.5% after advancing the SOI from 5 °CA BTDC to 13 °CA BTDC. At the SOI of 5 °CA BTDC,
330 the particulate emission is reduced by 82.7% after the n-butanol proportion is increased from 0% to
331 30%.

332 *3.3 Effects of EGR on ITE and emissions of the CTL/n-butanol blends engine*

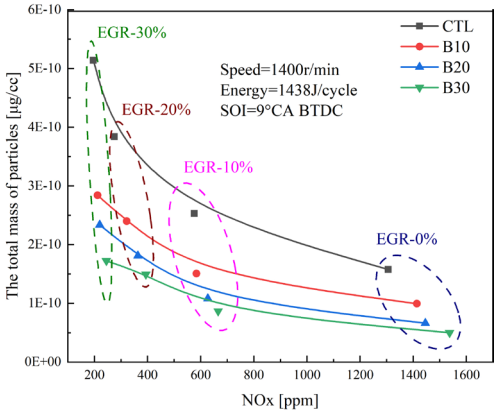
333 In order to control the increased NOx emissions caused by the addition of n-butanol, the
334 introduction of EGR was adopted to control NOx emissions. The potential for high-efficient and
335 clean combustion through the synergistic control of EGR and the addition of n-butanol is explored.



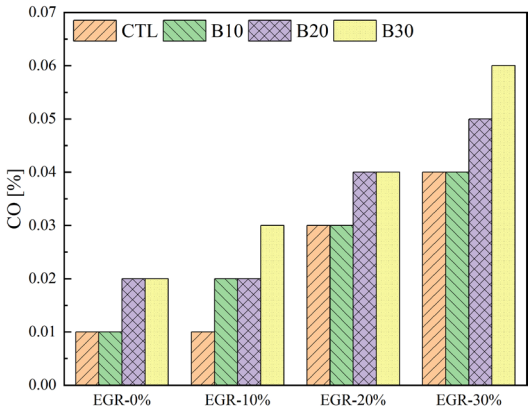
(a) ITE (b) Combustion phasing

Fig. 9 Influence of EGR on the ITE and combustion phasing of the CTL/n-butanol blends engine

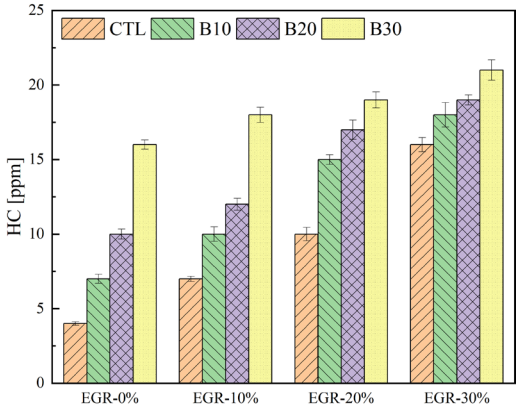
Fig. 9 presents the influence of EGR on ITE and combustion phasing, respectively. As shown in **Fig. 9(a)**, the ITE is reduced with the increase of n-butanol proportion at all EGR ratios. Since the EGR ratio is adjusted by introducing the exhaust flow while keeping the flow of intake air constant through the simulated supercharge system in this experiment, the high EGR ratio increases intake pressure and charge. The high intake pressure and the heat introduced by the EGR bring extra work, so an increasing EGR ratio will result in a slightly higher ITE. However, the three-atomic molecules (H_2O, CO_2) contained in the EGR have a higher specific heat capacity (SHC) than the two-atomic molecules (O_2, N_2) in the air, so the introduction of EGR can effectively reduce the in-cylinder combustion temperature. **Fig. 9(b)** shows the combustion phasing of B30 under different EGR ratios. It can be found that with the EGR ratio increasing, the ID increases slightly, but the lag of CA50 is even more significant. The introduction of EGR reduces the oxygen concentration in the cylinder, further reducing the reaction activity and temperature of the mixture, so the combustion at middle and later stages (CA10-CA90) is slowed down, resulting in a more extended CD.



(a) NOx and particulate emissions



(b) CO



(c) HC

Fig. 10 Influence of EGR on the emissions of the CTL/n-butanol blends engine

Fig. 10 suggests that the influence of EGR on emissions of the CTL/n-butanol blends engine. **Fig. 10(a)** illustrates that the introduction of EGR significantly reduces the high NOx emissions associated with the addition of n-butanol. Simultaneously, due to the enhanced tolerance of particulate emissions to EGR by blending CTL with n-butanol, the introduction of EGR would not lead to an excessive increase in particulate emissions. Therefore, the trade-off relationship between NOx and particulate emissions can be mitigated through the synergistic control of EGR and the addition of n-butanol. Among them, the NOx and particulate emissions of using B30 at 10% EGR are reduced by 45.1% and 49%, respectively, compared to those of using pure CTL with no EGR introduced. **Figs. 10(b)** and **(c)** show the CO and HC emissions of the test fuels at different EGR

ratios, respectively. At a fixed EGR ratio, the changing trend of CO and HC emission results for different test fuels is the same as in section 3.1.2. It can be seen from **Fig. 10(b)** that CO emissions increase as more EGR introducing, and this phenomenon is more obvious for CTL/n-butanol blends. The main reasons are that the addition of n-butanol causes the combustion duration to be longer, and the combustion phasing is too backward. Especially when the n-butanol proportion becomes larger, the combustion efficiency is reduced, leading the CO emissions to be relatively high. It also can be seen from **Fig. 10(c)** that although the HC emissions become higher with the n-butanol proportion rising, the HC increasing degree of the blends is much smaller than that of the pure CTL with an enlarged EGR ratio. For example, when the EGR ratio changes from 0% to 30%, the HC increasing degree of B30 is 31.25% while the CTL reaches 300%, indicating that the addition of n-butanol can improve the tolerance of HC emissions to the EGR ratio.

4. Conclusions

In this paper, the effects of the CTL/n-butanol blends on the combustion and emissions of the CI engine are investigated on a modified engine with flexible and adjustable control parameters, and the potential for reducing pollutant emissions from CTL/n-butanol blends by adjusting combustion boundary conditions is explored. The main findings can be summarized as follows:

(1) Compared to conventional diesel, CTL has higher reactivity which means better ignitability helping to shorten the ID. The PCR of CTL is smaller than that of diesel, and the boundary between the premixed and the diffusion combustion is more apparent. Accordingly, applying CTL can reduce NOx emissions but has higher particulate mass emissions.

(2) The improved concentration distribution of fuel/air mixture brought by the addition of n-butanol and the oxygen-containing property of n-butanol contributes to suppressing the high

particulate emissions caused by pure CTL combustion and promoting the shifting of particles towards nucleation mode, thus effectively reducing the total particulate mass emissions. At the same time, blending n-butanol with the CTL increases the PCR and the maximum combustion temperature, which results in higher NOx emissions, although it is still lower than the condition of pure diesel combustion.

(3) Adjusting the SOI mainly affects the combustion phase but slightly changes the ID and the shapes of HRR curves. Compared with the addition of n-butanol, adjusting the SOI has a marked effect on NOx emissions while has a minor influence on the ITE and particulate emissions.

(4) The introduction of EGR can significantly reduce the increased NOx emissions caused by the addition of n-butanol, and the tolerance of particulate emissions and HC to EGR is improved after blending n-butanol with CTL. Through the coordinated control of EGR and the addition of n-butanol, the trade-off relationship between NOx and particulate emissions can be mitigated.

Notes

The authors declare no competing financial interest.

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