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## Effect of Premixed n-Butanol Ratio on the Initial Stage of Combustion in a Light-Duty Butanol/Diesel Dual-Fuel Engine

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Received: 23 June 2020; Accepted: 13 August 2020; Published: 19 August 2020



**Abstract:** The impact of premixed n-butanol mixture on the heat release rate was investigated based on a modified light-duty diesel engine. The results show that reactivity stratification is formed in the cylinder through n-butanol port fuel injection (PFI) and diesel direct injection (DI). The initial heat release rate of the diesel/butanol dual-fuel combustion is restrained due to the low ignitability of butanol and the high volatility. Because of the auto-ignition of diesel, premixed n-butanol undergoes a high-temperature reaction, which has an active influence on the heat releasing of diesel/butanol dual-fuel combustion. With the increase of the amount of premixed n-butanol injected, the heat release rate in the initial combustion period has a critical value. When the n-butanol injection quantity is less than 13 mg/cycle, the initial heat release rate of dual-fuel combustion is lower than the pure diesel combustion because the lean premixed n-butanol/air mixture limits the flame propagation. When the fuel injection rate of n-butanol is higher than 13 mg/cycle, the heat release rate is accelerated, leading to obvious flame propagation.

**Keywords:** n-butanol; reactivity stratification; initial combustion period; high-temperature reaction; flammability limit

### 1. Introduction

In traditional diffusion combustion, the non-uniform distribution of the temperature and the mixing-controlled propagation of the diffusion flame [1,2] leads to the formation of large amounts of soot and NOx [3]. In order to make the diesel engine adapt the stringent limits on exhaust emissions, both domestic and foreign researchers are committed to exploring a cleaner and higher-efficiency combustion regime, such as the low temperature combustion (LTC) [4]. The ignition delay period of diesel is increased [5] by applying the technologies like exhaust gas recirculation (EGR), high injection pressure, or intake valve variable timing [6–8]. Longer ignition delay period gives the diesel a longer time to mix. The bulk fuel in the cylinder could be dramatically eliminated [9]. But when fuel/air mixture becomes richer, more EGR is needed to keep the self-ignition of the air-fuel mixture at a suitable time. The advanced ignition of the diesel will hinder the further application of LTC in commercial engines due to its uncontrollable burning rate and high combustion noise [10,11].

Therefore, in order to break through the obstacle of the advanced combustion mode, dual-fuel injection mode by using high-ignitable fuel to ignite low-ignitable fuel is considered as a potential method to achieve LTC [12,13]. This mode is able to control the heat releasing in-cylinder according to different loads by adjusting the composition of the mixture [14,15]. Low-ignitable fuels (such as



gasoline, natural gas, methanol, ethanol, n-butanol) are delivered into the inlet manifold, which forms a homogeneous mixture charge in the combustion chamber [16]. High-ignitable fuel (such as diesel) is injected into the cylinder directly which forms reactivity stratification with the homogeneous mixture. The self-ignition first occurs in a high-ignitable area and then spreads to the premixed mixture area in the combustion chamber [17–19]. In the dual-fuel injection mode, the chemical activity of the mixture can realize a real-time adjustment by changing the fuel distribution [20,21]. Besides, combining with EGR, the dual-fuel injection mode can control the main combustion phase and combustion duration at high-load conditions [22–26].

Recently, Sage et al. [27] researched the effect of active stratification in the cylinder on the heat release rate on a visualization dual-fuel engine. The result showed that the flame first appeared in the rich n-heptane layer (downstream from the injector in the combustion chamber) and then another auto-ignition process occurred in the region of the low reactivity layer (central part of the combustion chamber). The combustion events proceed in particular sequences, which keeps the maximum cylinder pressure rise rate at a low level. Chen et al. [28] investigated the effects of port fuel injection (PFI) of butanol and EGR on combustion characteristics of a dual-fuel compression ignition engine. Their results demonstrated that when EGR rate is above 45%, the longer ignition delay and longer combustion duration are achieved with increased butanol concentration, which also accompanied by a lower peak cylinder pressure and peak heat release rate. Han et al. [29] studied the combined combustion with butanol port injection and diesel in-cylinder direct injection in a diesel engine experimentally and reported that when the engine was operating at high loads (IMEP = 1 MPa), the proportion of diffusion combustion with the rising of the butanol/diesel injection ratio and excellent combustion and economy performance could be achieved by adjusting butanol/diesel injection ratio.

In summary, in a dual-fuel engine, the key point to realize about the LTC at high loads is that the main combustion phase and heat release rate are controlled by the reactivity of the charge in the cylinder. The objective of the present study is to construct an evaluation index system for analyzing the influence of premixed n-butanol on the heat release rate of dual-fuel combustion. The evaluation index system includes two aspects, which include the time spent on reaching the given value of accumulated heat and the accumulated heat release amount in a specific time interval.

#### 2. Description of Experiments

The schematic of the experimental setup in this study is shown in Figure 1. The engine specifications are given in Table 1.



Figure 1. Schematic of the experimental setup.

Engine Type	4 Valves, Water-Cooled
Bore $\times$ stroke	93 × 102 mm
Intake methods	Naturally aspirate
Displacement	2.77 L
Compression ratio	17.5:1
Direct-injection system	High pressure common-rail (120 MPa)
Port-injection system	Low-pressure common rail (5 MPa)

Table 1. Engine specifications.

The experiments were performed without EGR. The n-butanol supply system included a common rail fuel injection circuit and four GDI injectors. In this experiment, butanol was used as the port injection fuel. Compared with other alcohol fuels such as methanol and ethanol, butanol has a higher viscosity. In order to overcome the higher viscosity of butanol, a GDI injector was used in the experiment, which was beneficial to improve the atomization effect of butanol. An accumulator which was connected to the nitrogen vessel provided a constant 5 MPa pressure for the butanol common rail. The specifications of the GDI injector are provided in Table 2.

Table 2. N-butanol injector specifications.

Injector Type	Bosch GDI
Fuel	High purity (99% +) n-butanol
Numbers of holes	6
Supply pressure	5 MPa
Nominal orifice diameter	150µm

BOSCH high-pressure common rail system was used for diesel direct injection and the injector specifications are given in Table 3. The fuel injection was controlled by the ECU (Electronic Control Unit).

Table 3. Diesel injector specifications.

Injector Type	DEFI1.4	
Fuel	0#Diesel	
Numbers of holes	6	
Supply pressure	120 MPa	
Nozzle flow	600 mL/min	

The cylinder pressure was measured by a pressure sensor (Kistler 6125 C) connected to a Kistler 5064 C charge amplifier and data acquisition system. The pressure data was recorded every 0.5 °CA (crank angle), and analyzed by a real-time combustion analyzer.

#### 2.1. Tested Fuels

The properties of the tested fuels can be seen in Table 4.

Fuel	Diesel	n-Butanol
Formula	CH <sub>1.89</sub>	C <sub>4</sub> H <sub>9</sub> OH
Density $\cong 20 ^{\circ}\text{C}  (\text{kg/m}^3)$	846	810
Cetane number	50~53	~25
Octane number	~25	~87
Lower heating value (MJ/kg)	42.5	36.1
Oxygen (% weight)	0	21.6
Boiling temperature (°C)	229~337	117.4
Flash point (°C)	73.3	35
Auto-ignition temperature $\cong$ 1 bar abs (°C)	254~285	355
Latent heat of evaporation (KJ/kg)	250	585
Flammability limits (excess air coefficient)		0.45~3.33

Table 4. Properties of tested fuels.

#### 2.2. Experimental Methods

After the engine was warmed up until the lubrication oil and coolant fluid temperature were 85 °C, the engine speed was set to 2000 rpm in traditional diesel combustion mode for background data. Then the port injector was used to inject low reactivity fuel (n-butanol). Meanwhile, the diesel injection quantity and injection timing were maintained constantly. The diesel and n-butanol injection quantity in each case are shown in Figure 2.



Figure 2. Fuel injection energy per cycle in each case.

The combustion parameters of n-butanol are shown in Table 5. The maximum pressure rise rate (PRR) was maintained under 1.0 MPa/°CA. The engine operating parameters are shown in Table 6.

n-Butanol Injection Quantity (mg/cyc)	Combustion Efficiency (%)	IMEP (MPa)
0	97.2	0.36
6	89.8	0.46
8	96.7	0.54
13	96.9	0.65
17	91.2	0.70

 Table 5. combustion parameters of n-butanol.

Table 6. Engine operation conditions.

Item	Parameters
Speed	2000 rpm
Intake pressure (P <sub>intake</sub> )	0.1 MPa
Intake temperature (T <sub>intake</sub> )	$30 \pm 1$ °C
Diesel quantity per cycle (Md) mg/cycle	13.2
Start of injection (SOI)	-8 °CA(crank angle) ATDC (after top dead center)
n-butanol injection quantity per cycle (Mb) mg/cycle	6, 8, 13, 17
Maximum pressure rise rate	<1.0 MPa/°CA

### 2.3. Parameters Definition

- (1) Crank angles at 10%, 30% and 50% cumulative heat release are defined as  $\theta_{CA10}$ ,  $\theta_{CA30}$  and  $\theta_{CA50}$ , respectively.
- (2) In this study, the apparent heat release rate is calculated using Equation (1).

$$HRR = \frac{1}{(\gamma - 1)} \times \left[ \gamma P \frac{dV}{d\theta} + V \frac{dp}{d\theta} \right]$$
(1)

where  $\gamma$  is the ratio of specific heats for the cylinder charge, *p* is the measured cylinder pressure (pa), *V* is the cylinder volume (m<sup>3</sup>),  $\theta$  is the crank angle (°/CA).

(3) Based on the crank angle  $\alpha$  (1.5 °CA, 2.4 °CA, 3.4 °CA) corresponding to the 10%, 30%, 50% of the total heat release in pure diesel combustion, the accumulated heat release rate starting from SOI to  $\alpha$  is calculated by Equation (2). Furthermore, those three angles (1.5 °CA, 2.4 °CA, 3.4 °CA) divide the initial period of the heat release curve into three intervals, as shown in Figure 3.



Figure 3. Heat release rate during the combustion initial stage.

In Equation (2), HRR is the heat release rate (J/°CA),  $\alpha$  is the crank angle corresponding to the 10%, 30%, 50% of total heat release ( $\alpha_1 = 1.5$  °CA,  $\alpha_2 = 2.4$  °CA,  $\alpha_3 = 3.4$  °CA)

$$\sum Q_{\alpha} = \int_{SOI}^{\alpha} HRR \cdot d\theta \tag{2}$$

#### 3. Results and Discussion

# 3.1. Effect of Premixed n-Butanol on Heat Release Rate during the Three Time Intervals at the Combustion Initial Period

Figure 4 shows the cylinder pressures and heat release rates of n-butanol/diesel dual-fuel combustion with five different concentrations of premixed n-butanol mixture. As the n-butanol injection quantity increases, the maximum cylinder pressure and maximum heat release rate are gradually increasing and the combustion phase is retarded.



Figure 4. Cylinder pressure and heat release rate in each n-butanol concentration.

According to the definition of the parameters, the curves are divided into three intervals as is shown in Figure 3.

When  $\theta \in (0, 1.5)$  °CA and Mb  $\leq 13$  m/cycle, the heat release rate curve shows a descending trend with increasing n-butanol injection quantity. However, if n-butanol injection quantity is 17 mg/cycle, the upward trend of the heat release curve becomes steeper and the value is still lower than that of the pure diesel mode. Two reasons may account for this phenomenon: on the one hand, due to the high latent heat of evaporation of n-butanol, it absorbs more heat in the cylinder, which results in a lower pressure and temperature. On the other hand, the low cetane number and high octane number enhance the n-butanol as an inert substance, which inhibits the auto-ignition probability of premixed n-butanol mixture.

During the period when  $\theta \in (1.5, 2.4)$  °CA and Mb  $\leq 13$  mg/cycle, the rising slope of the heat release rate curve is increased and is higher than that of the pure diesel combustion with increasing n-butanol injection quantity. It shows a trend that the effect of the premixed n-butanol fuel on diesel fuel heat release will experience a transition stage when the n-butanol injection quantity is changed. It can be seen from Figure 5 that most experiment conditions with different n-butanol injection quantity), indicating that the combustion process of n-butanol/air mixture is mainly premixed combustion. Although the premixed n-butanol/air mixture is not rich enough to spread the flame, the high temperature reaction zone with premixed n-butanol/air mixture keep becoming larger as the in-cylinder instantaneous temperature increases. Besides, as concentrations of premixed n-butanol increases, the flame propagation goes faster, which accelerates the heat releasing and offset the impact of suppression to the heat release [30,31].



Figure 5. The excess air ratio of premixed n-butanol corresponding to the n-butanol injection quantity.

During the period when  $\theta \in (2.4, 3.4)$  °CA, the rising slope of heat release rate curves under cases fueled with n-butanol become steeper comparing to the case only fueled with pure diesel. It reveals that the premixed combustion and diffusion combustion process may both exist in n-butanol/diesel dual-fuel combustion. High reactivity ingredients are produced after a longer period of high temperature reaction, which promotes the entire dual-fuel combustion process tends to active stage. This phenomenon is more obvious under the case that the n-butanol injection quantity is 17 mg/cycle. According to the discussion above, the premixed n-butanol restrain the heat release in cylinder at the initial period of the combustion process. When  $\theta \in (2.4, 3.4)$  °CA, the premixed n-butanol mixture may promote the heat release of dual-fuel combustion process.

## 3.2. The Effect of the Premixed n-Butanol Mixture on the Heat Release Rate at the Initial Period of Dual-Fuel Combustion

 $\theta_{CA10}$ ,  $\theta_{CA30}$ ,  $\theta_{CA50}$  at different n-butanol concentrations are shown in Figure 6. In Figure 6, all the three  $\theta_{CA10}$ ,  $\theta_{CA30}$ ,  $\theta_{CA50}$  curves show a tendency that firstly increases, afterwards decreases, while the highest value appears at the n-butanol injection quantity at 13 mg/cycle. Due to the reactivity, stratification is formed through this dual-fuel injection mode, the time spent on specific accumulated heat release rate is firstly increased and then decreased with the increase of concentrations of the premixed n-butanol, which reveals that the initial period of the dual-fuel combustion is sensitive to the concentrations of the premixed n-butanol. Moreover, a critical value in the concentration of premixed n-butanol may exist. When the n-butanol injection quantity is lower than the critical value, the propagation of the flame will be restricted due to the high octane number and low cetane number of the premixed n-butanol. When n-butanol injection quantity is higher than the critical value, the auto-ignition flame caused by diesel combustion can spread fast and lead to ignition of the premixed n-butanol. The premixed n-butanol plays a catalytic role in influencing the heat release rate of the dual-fuel combustion.



**Figure 6.**  $\theta_{CA10}$ ,  $\theta_{CA30}$ ,  $\theta_{CA50}$  at different n-butanol concentrations.

The accumulated heat release rate starting from SOI to  $\alpha$  under conditions with dual-fuel combustion are calculated. According to Figure 7, the three  $\sum Q_{\alpha 1}$ ,  $\sum Q_{\alpha 2}$ ,  $\sum Q_{\alpha 3}$  decrease as the injected n-butanol increases until 13 mg/cycle and increase as the injected n-butanol increases.



**Figure 7.**  $\sum Q_{\alpha 1_{i}} \sum Q_{\alpha 2_{i}} \sum Q_{\alpha 3}$  at different n-butanol concentration.

It can be seen that, under the conditions that  $Mb \le 13$  mg/cycle, adding n-butanol can suppress the initial heat release from dual-fuel combustion, which results in the reduction in the accumulated heat release within a specific time interval at the early stage of engine heat release. Under the conditions that Mb > 13 mg/cycle, adding n-butanol can help to increase initial heat release of dual-fuel combustion. In addition, when n-butanol injection quantity is 17 mg/cycle, the engine's maximum pressure rise rate is the highest (about 1 MPa/°CA) compared with other cases, which is because of the higher heat release rate. It may cause the pre-ignition of the premixed n-butanol/air mixture [23,32]. This can also be revealed in Figure 5 that, when  $Mb \le 13$  mg/cycle, the excess air coefficient is higher than the flammability limit, so the heat release rate decreases as the injected butanol increases. When Mb > 13 mg/cycle, the excess air coefficient is lower than the flammability limit, leading to obvious flame propagation.

### 3.3. The Pressure Rise Rate under Different Premixed n-Butanol Mixture Concentrations

As is shown in Figure 8, the maximum pressure rise rate is increased with the increasing concentrations of premixed n-butanol. Even at initial period of the combustion, the premixed n-butanol mixture can suppress the heat release of the diesel. However, due to the probable increase in the high temperature reaction products when more n-butanol been injected, the acceleration of the heat releasing rate will be amplified.



Figure 8. The maximum pressure rise rate in different n-butanol concentration.

Figure 9 shows the crank angle corresponding to the maximum pressure rise rate under the different concentrations of premixed n-butanol. The maximum pressure rise rate appears when the piston moves downward. When  $Mb \le 8$  mg/cycle, the crank angle corresponding to the maximum pressure rise rate will be more retarded with the increase of the n-butanol injection quantity. With the increase of the n-butanol injection quantity, the suppression effect on the heat release rate of the dual-fuel combustion may be amplified. Moreover, when Mb > 8 mg/cycle, the crank angle corresponding to the maximum pressure rise rate fixes at 4 °CA ATDC (after top dead center). It indicates that there may be a balanced relationship between the amount of the fuel and the maximum pressure rise rate. The more fuel is injected, the more time it will take for the n-butanol/diesel dual-fuel combustion to become faster.



**Figure 9.** The crank angle corresponding to the maximum pressure rise rate in different n-butanol concentration.

#### 4. Conclusions

- (1) The reactivity stratification caused by dual-fuel injection is formed in the combustion chamber, the suppression and stimulation effect of low reactivity zone on the heat releasing may exist simultaneously. During the period when  $\theta \in (0, 1.5)$  °CA, the suppression to the heat release plays a major role. During the period when  $\theta \in (1.5, 2.4)$  °CA, the suppression and stimulation effect of n-butanol premixed mixture on heat releasing are balanced. During the period when  $\theta \in (2.4, 3.4)$  °CA, the enhancement of premixed n-butanol on the heat release rate plays a major role.
- (2) When  $Mb \le 13$  mg/cycle, the higher the premixed n-butanol concentration is, the more suppressed the heat release is. When Mb > 13 mg/cycle, the auto-ignition in the premixed n-butanol mixture is able to accelerate the heat release of the n-butanol/diesel dual-fuel combustion.
- (3) When the excess air coefficient of premixed n-butanol mixture reaches the flammability limit, auto-ignition phenomenon may happen in the premixed n-butanol mixture and spread faster, which results in a higher pressure rise rate.
- (4) There may be a balanced relationship between the amount of the fuel and the heat release rate. The more fuel is injected, the more time it will take for the n-butanol/diesel dual-fuel combustion to become faster.

**Author Contributions:** Conceptualization, W.T., H.Z. and Z.H.; Data curation, W.T., H.Z. and L.W.; Formal analysis, W.T., H.Z. and L.W.; Methodology, W.T., H.Z. and Z.H.; Resources, W.Y.; Writing—original draft, W.T.; Writing—review & editing, L.W. and W.Y. All authors have read and agreed to the published version of the manuscript.

**Funding:** The research is sponsored by the National Natural Science Found of China through its project of 51776177 and Chun Hui project of Z2015083.

Conflicts of Interest: The authors declare no conflict of interest.

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