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Direct injection of neat n-butanol for enabling clean low temperature combustion in a modern diesel engine

Ming Zheng [a,*], Tie Li [b], Xiaoye Han [a]

[a] Clean Combustion Engine Laboratory, Department of Mechanical, Automotive and Material Engineering, University of Windsor, Ontario, Canada
[b] State Key Laboratory of Ocean Engineering, Shanghai Jiao Tong University, Shanghai, China

HIGHLIGHTS

- A rarely studied fuel, n-butanol, is applied to replace diesel for clean combustion.
- Low temperature combustion is enabled via n-butanol high pressure direct injection.
- Emission benefits and control challenges of n-butanol combustion are identified.
- n-Butanol combustion offers ultralow NO_x and near-zero smoke emissions without EGR.
- Improved combustion control using multi-pulse injections with moderate EGR.

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ABSTRACT

This study investigates the effects of neat n-butanol replacing conventional diesel fuels to enable clean combustion on a modern common-rail diesel engine. Systematic engine experiments are conducted to examine the combustion characteristics and exhaust emissions in correlation to n-butanol's relatively high oxygen content and high volatility but low ignitability, and control strategies are thereafter developed for enabling clean and efficient combustion of neat n-butanol. Compared to its diesel counterpart, the single-shot injection of neat n-butanol offers substantially reduced NO_x emissions without the use of EGR and near-zero soot emissions, but the applicable injection timing window is narrower for n-butanol limited by high maximum rates of pressure rise and/or unstable combustion. EGR is effective to reduce the combustion roughness, but it further narrows the applicable injection timing window and deteriorates the HC and CO emissions. A control strategy that deploys multi-shot injections combined with moderate use of EGR is developed and applied to improve the combustion controllability and exhaust emissions while minimizing the penalties in the engine efficiency.

1. Introduction

Butanol can be produced from alcoholic fermentation of biomass feed stocks including edible materials such as corn, sugar cane, and molasses, as well as agricultural wastes such as wheat straw, corn stover and other celluloses. It is also reported that the crude glycerol, a by-product of biodiesel production during the transesterification processes, can be converted into the value-added biofuels comprised of mainly butanol [1,2]. As one of the next generation biofuels, butanol has attracted increasing attention for engine applications in recent years. There are two isomers (n-butanol and sec-butanol) of butanol with the straight carbon chain, and two other isomers (isobutanol and tert-butanol) with the branched carbon chain. Normal-butanol (n-butanol) with a straight carbon chain structure and a hydroxyl at the terminal carbon site is used in this study.

As a fuel, butanol has several advantages over ethanol for combustion engine applications. It is less corrosive and less prone to water contamination than ethanol, and thus minor or no modifications are required for the existing infrastructure for gasoline to be used for the butanol fuel distribution. The use of butanol replacing gasoline on spark ignition (SI) engines has been demonstrated in previous research without any engine modifications, such as in [3]. However, its lower octane number and lower latent heat of vaporization could be drawbacks of n-butanol as a fuel for SI engines, compared to ethanol. The lower latent heat of vaporization of n-butanol tends to reduce the charge density and thus decrease the engine power output, while the lower octane number leads to higher propensities to engine knock and reduced engine efficiency [4,5].

* Corresponding author.

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Nomenclature

ABE	acetone–butanol–ethanol
CA	crank angle
CA5	crank angle of 5% total heat release
CA50	crank angle of 50% total heat release
CA95	crank angle of 95% total heat release
CAI	California analytical instruments
CI	compression ignition
CO	carbon monoxide
DI	direct injection
DOC	diesel oxidation catalyst
$dp/d\theta_{max}$	maximum rate of pressure rise
EGR	exhaust gas recirculation
FPGA	field programmable gate array
FTIR	Fourier transform infrared spectroscopy
THC	total hydrocarbons
HCCI	homogeneous charge compression ignition
HCLD	heated chemiluminescence detector
HFID	heated flame ionization detector
HRR	heat release rate
ID	ignition delay
ID_{main}	ignition delay for the main injection
IMEP	indicated mean effective pressure
LTC	low temperature combustion
NDIR	non-dispersive infrared detector
NO_x	nitrogen oxides
PCCI	premixed charge compression ignition
PFI	port fuel injection
ppm	parts per million
p_{inj}	pressure of injection
p_{int}	pressure of intake
SI	spark ignition
SOI	start of injection
SOI_{main}	start of main injection
TDC	top dead centre

Higher fuel conversion efficiency is expected when n-butanol is used in the lean-burn and high compression ratio diesel engines instead of conventional SI engines. Compared to the majority of diesel fuels, n-butanol has certain preferred fuel properties for enabling low temperature combustion (LTC), including the relatively higher oxygen content and high volatility along with lower ignitability, which are deemed helpful to improve fuel–air mixing and reduce particulate emissions of diesel engines. Owing to its less hydrophilicity and higher miscibility with diesel fuel than ethanol, n-butanol is usually blended with diesel for engine tests in most studies [6–13]. Rakopoulos et al. conducted a series of experimental studies on the effects of n-butanol diesel blends on the performance and emissions of a heavy-duty diesel engine in either steady state operation [6,8] or during transient acceleration cycles [7]. Dogan [9] and Siwale et al. [13] evaluated the effects of n-butanol diesel blends on the combustion characteristics and exhaust emissions of a single-cylinder naturally aspirated diesel engine and a turbocharged four-cylinder automotive engine, respectively. These studies demonstrated that the soot emissions generally decreased remarkably with the increasing use of n-butanol in the blends, while nitrogen oxides (NO_x) decreased or slightly increased in different studies and under different engine operating conditions, but the increased NO_x emissions could be effectively suppressed by the use of exhaust gas recirculation (EGR).

Ballesteros et al. conducted carbonyls speciation of the exhaust gas from an automotive diesel engine fueled with diesel, bioethanol-diesel blends, and butanol-diesel blends [10]. The results indicated that the combustion of bio-alcohol blends produced higher carbonyl emissions than that of the pure diesel, and these carbonyl emissions could be effectively reduced through the diesel oxidation catalysts (DOC). Valentino et al. studied the performance and emissions of a high-speed turbocharged common-rail diesel engine fueled with blends of n-butanol and diesel under the premixed low temperature combustion mode [11], and simultaneous reduction of NO_x and soot emissions was obtained when the fuel injection was completed prior to the ignition event. This could be attributed to the prolonged ignition delay and improved fuel–air mixing before the start of combustion, which was achieved by appropriate control over the injection pressure, injection timing and intake oxygen concentration with the joint effect of increased resistance to auto-ignition and enhanced volatility of n-butanol blends than those of the pure diesel fuel. Merola et al. conducted an optical investigation on the spray and combustion processes of n-butanol diesel blends and, as shown by the test results, a minor increase in NO_x emissions but a significant reduction of soot emissions were observed in the spray flame of fuel blends compared to those of the pure diesel fuel [12]. Studies using n-butanol and bio-diesel blends showed similar results to those of n-butanol and diesel blends in terms of the engine performance and exhaust emissions [14,15]. Moreover, Lin et al. [16] and Chang et al. [17,18] investigated the water-containing butanol to simulate the hydrated n-butanol produced from the acetone–butanol–ethanol (ABE) fermentation and a simple distillation treatment. As emphasized in this work, the production of hydrated butanol rather than dehydrated butanol could substantially reduce the cost and energy consumption during the fuel refining processes. The results also indicated that the use of diesel blends with hydrated butanol (5–10%) did not require any modifications to the engine hardware while offering improved energy efficiency and reduced pollutant emissions.

Although the n-butanol blends with diesel and/or biodiesel have been extensively investigated as fuels for diesel or compression ignition (CI) engines, there are relatively limited publications on the use of neat n-butanol for CI engines. Chen et al. proposed a dual-fuel concept with port fuel injection (PFI) of n-butanol to prepare a premixed fuel–air mixture and direction injection of diesel fuel to ignite the mixture [19]. Han et al. [20] and He et al. [21], respectively, investigated the combustion characteristics and exhaust emissions for the compression ignition of the intake port injected neat n-butanol. All of these studies exhibited the potential of n-butanol for enabling efficient and clean combustion in CI engines. Particularly, preliminary tests of Han et al. [20] suggested that n-butanol delivered via high-pressure direct injection might be a more suitable fuel to enable clean combustion than diesel.

Detailed studies on the combustion characteristics of neat n-butanol using direct injection are rarely reported so far. Compared to the port fuel injection, the direction injection can provide more degrees of freedom for the control over the injection and the subsequent combustion process. In particular, the fueling strategies and fuel properties have significant impacts on engine operations in the low temperature combustion (LTC) mode, while optimization of the engine design (*e.g.* compression ratios) and/or operating parameters (*e.g.* EGR ratios) can be effective to enable LTC for simultaneous reduction of NO_x and particulate emissions, as reported in [22–32]. In terms of fuel properties, empirical results suggested that less ignitable fuels could assist to extend the LTC operation to higher engine loads, while the impact of fuel volatility was relatively minor [33–36]. In comparison to the majority of