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# Impacts of Acetone–Butanol–Ethanol (ABE) ratio on spray and combustion characteristics of ABE–diesel blends

Han Wu [a,b], Karthik Nithyanandan [b], Jiaxiang Zhang [c], Yilu Lin [d], Timothy H. Lee [b], Chia-fon F. Lee [b,*], Chunhua Zhang [a]

[a] *School of Automobile, Chang'an University, Xi'an 710064, China*
[b] *Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA*
[c] *State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China*
[d] *Center for Combustion Energy and State Key Laboratory of Automotive Safety and Energy, Tsinghua University, Beijing 100084, China*

## HIGHLIGHTS

- Spray and combustion characteristics of ABE–diesel blends were studied.
- Volatility and latent heat show competitive effects on spray performance.
- There exists a critical ABE ratio between 20% and 50% spray characteristics.
- Soot reduction potential of blends significantly increase with ABE ratio.
- Among tested blends, ABE50 can maintain diesel combustion characteristics.

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## ABSTRACT

Acetone–Butanol–Ethanol (ABE), the intermediate product while producing bio-butanol, has been proposed to be used as an alternative fuel directly to reduce the butanol recovery/separation costs. It is important to understand how the ABE ratio influences the combustion process because of the large differences in physical and chemical properties between the ABE components and diesel. Therefore, a wide range of ratios of ABE (0%, 20%, 50%, and 80% in volume referred to as D100, ABE20, ABE50 and ABE80 respectively) were blended with diesel and combusted in a constant volume chamber under various ambient temperatures (1200 K, 1000 K, and 800 K) and various ambient oxygen concentrations (21%, 16%, and 11%). Mie scattering images of the liquid spray and broadband flame luminosity images were captured by a high speed camera coupled with a copper vapor laser beam as light source. The results show that ABE20 exhibits spray characteristics similar to those of D100 while ABE50 exhibits spray characteristics similar to those of ABE80. However, the sprays of ABE50 and ABE80 are much shorter and narrower compared to those of D100 and ABE20. It is predicted that there exists a critical ratio between 20% and 50% for ABE, beyond which the spray characteristics of the blend will be dominated by ABE. The intermediate ABE blend, ABE50 achieves a shorter ignition delay (slightly longer than that of D100) and combustion duration compared to those of ABE20 and ABE80 because of its improved spray performance and relatively low latent heat and high cetane number. The natural flame luminosity is found to be reduced significantly with an increasing ABE ratio due to the fuel-borne oxygen that accelerates soot oxidation along with longer flame lift-off length that effectively decreases the equivalence ratio in the combustion region. Overall, ABE50 is the blend that displays combustion characteristics similar to neat diesel while achieving a shorter combustion duration and lower natural flame luminosity. Thus, ABE50 could potentially increase thermal efficiency and decrease soot emissions when applied in diesel engines.



## 1. Introduction

Bio-butanol has been considered as a promising alternative fuel for transportation due to its advantageous physical and chemical

* Corresponding author. Tel.: +1 217 3335879; fax: +1 217 2446534.
*E-mail address:* cflee@illinois.edu (C.-f.F. Lee).

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properties [1–3]. With the use of butanol blended with diesel, it was reported that soot emissions could be reduced significantly, while carbon monoxide (CO) and hydrocarbon (HCs) emissions, and NOx emissions were reduced or slightly increased under various operating conditions [1,4].

Acetone–Butanol–Ethanol (ABE) fermentation is the typical method used to produce bio-butanol from renewable feedstock. It was first developed in the UK in 1912 and commercial production quickly spread around the globe during the first and second world wars [5], but lost competitiveness by the 1960s [6]. As a relatively mature process, several species of clostridium bacteria have been found to be capable of metabolizing different sugars, amino and organic acids, polyalcohols and other organic compounds to butanol together with acetone and ethanol under anaerobic conditions. After the fermentation, ABE concentration in the broth is relatively low e.g., less than 25 g/L, due to the large content of water [7]. Thus, the desired product, butanol, needs to be recovered and purified in downstream processing. It is these high recovery and purification costs that make the ABE fermentation process problematic; separating butanol from the fermentation broth by the traditional method, i.e., direct distillation, requires 18.4 MJ/kg, which is approximately 54% of butanol's combustion heat value [8]. In order to get high purity butanol, the byproducts, acetone and ethanol, also need to be removed completely from the solvent. Since acetone and ethanol also contain energy, and given that ethanol has been widely used as an alternative fuel for spark ignition engines, there exists a possible solution to use acetone and ethanol together with butanol as a transportation fuel. In this way, the downstream recovery process can be simplified and the separation costs can be reduced.

Some ABE fermentation researchers have tried to use biodiesel as an extractant during the fermentation process to obtain ABE–biodiesel blends directly. They found that with biodiesel added in the broth during the fermentation process, the fermentation could achieve a higher productivity of ABE [9]; In addition, the biodiesel–ABE mixture was comparable to that of no. 2 diesel fuel in terms of fuel characteristics, but superior in cetane number [10]. This technique definitely can be counted as one of the potential methods to consume ABE as an alternative fuel because of the accessibility of biodiesel [11] and the enhanced fuel properties. In addition, Chang et al [12] found that with acetone and ethanol blended with butanol (prepared in lab; acetone, butanol, ethanol – volumetric ratio of 5:14:1), the ABE mixture was fully miscible with diesel, and more importantly, the tested ABE mixtures containing up to 5% water by volume could mix with diesel without separation at room temperature. These findings gave way to further studies into both the ABE fermentation process and its applications in internal combustion engines. Kraemer et al. [13] designed an extraction–distillation downstream process with mesitylene as a solvent by means of a computer-aided molecular design, with a bio-butanol production rate of 40,000 tons/annually. The process includes one step of extraction followed by three steps of distillation. Fortunately, after the first distillation the ABE mixture with less than 0.38% water by weight could be obtained. As mentioned earlier, this level of purity is sufficient for full miscibility with diesel. It is known that solvent selectivities are typically inversely related to the solvent capacities. Therefore, a low-cost and high-productivity downstream process could be developed by optimizing the strategy specifically for ABE while considering its tolerance of water.

In addition, the ABE fuel properties can be adjusted to suit internal combustion engine requirements by changing the ratio of the ABE components through fermentation. The typical ratio of acetone, butanol and ethanol is 3:6:1 during the formation process [14], but this is adjustable to some extent. Modification of bacterial strains at the genetic level is the common method for researchers to optimize production components. At the same time, fermentation products and the ratio of their formation also vary with the fermentation conditions such as pH, temperature, nutrients [7].

Due to the advantages and feasibility of ABE as detailed above, a few studies on ABE combustion have been carried out recently. Nithyanandan et al. [15] from the authors' group, tested ABE–gasoline blends on a spark-ignited engine, and found that the addition of less than 40 vol.% ABE did not change the combustion characteristics significantly, but improved efficiency slightly. Van Geem et al. [16] generated a detailed mechanism containing around 350 species and more than 10,000 reactions for the pyrolysis and oxidation of ABE based on a mechanism of hydrocarbon fuels, which showed good agreement with observed experimental data. Chang et al. [12] carried out the study of ABE–diesel and water–ABE–diesel blends on a diesel engine. They reported that with the use of the ABE and diesel blends, both particulate matter (PM) and total toxicity equivalency of polycyclic aromatic hydrocarbons (PAHs) could be reduced significantly, but NOx emission would increase when using a 20 vol.%. ABE and 80 vol.% diesel blend. However, the undesired NOx increase could be further eliminated by using a solution containing 0.5 vol.%. water. By using ABE–diesel blends, the brake thermal efficiency was found to increase by up to 8.56%. In their later study [17], ABE–biodiesel–diesel blends were tested on a diesel engine. The results show that, with the use of ABE–biodiesel–diesel blends, PM and NOx could be simultaneously reduced by 4.30–30.7% and 10.9–63.1% respectively compared to regular diesel. This solves the high NOx emission problem for biodiesel and biodiesel–diesel blends applied in diesel engines. In the authors' group, more fundamental studies were carried out on an optical constant volume chamber. Zhou et al. [18] studied the combustion characteristics of Acetone–Butanol–Ethanol (ABE) and diesel blends under different ambient temperatures and oxygen concentrations. It was found that the longer flame lift-off length exhibited by ABE–diesel blends allowed more air entrainment in upstream of the spray jet which enhanced air–fuel mixing. ABE20 (20 vol.% ABE and 80 vol.% diesel) achieved close-to-zero natural luminosity and higher efficiency combustion at low ambient temperature compared to neat diesel fuel. But it was also found that under lower ambient temperature the ABE–diesel blends show a significantly longer ignition delay than neat diesel fuel. In author's previous work [19], the spray and combustion characteristics of neat ABE and neat butanol were compared. It was found that neat ABE and neat butanol have similar characteristics in terms of spray and combustion performance, but ABE showed a higher potential on soot emission reduction. In another study, the authors [20,21] studied the influence of ABE components on the combustion process. The results showed that the ratio of the acetone in ABE significantly influenced the combustion characteristics of blends. With more acetone in the blend, the combustion phasing was advanced under lower ambient temperature conditions, and performed very similar to neat diesel due to the higher volatility caused by extra acetone. The overall physical and chemical properties of ABE itself are quite different from those of neat diesel (seen in Table 1). In this regard, it is worthwhile to understand how the ABE content influences the combustion process of blends.

Similar to the authors' previous studies mentioned above, the experiments in this study were also carried out in an optical constant volume chamber coupled with a high speed camera and a copper-vapor laser beam. Based on the spray, broadband natural flame images and combustion pressure, the influence of the ABE ratio on the spray and combustion characteristics of blends were analyzed in a fundamental way. During the experiment, a wide range of ABE percentages, i.e., 20%, 50%, and 80% (by volume) were chosen to cover low, moderate and high ABE ratios in ABE–diesel blends. Different oxygen concentrations ranging from 21% to 11% combined with various ambient temperatures ranging from