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Numerical modeling of acetone–butanol–ethanol and diesel blends droplet evaporation process

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HIGHLIGHTS

- Droplet evaporation model of acetone–butanol–ethanol (ABE) and diesel blends.
- ABE local boiling points quickly being exceeded causes internal gasification.
- Increasing mass fraction of ABE or ambient temperature shorten droplet lifetime.
- ABE Mass fraction and ambient temperature affect performance of internal gasification.

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ABSTRACT

To investigate the evaporation characteristics of acetone–butanol–ethanol (ABE) and diesel blends, a multi-component evaporation model for ABE–diesel blend droplet coupled with six components to represent diesel and Universal Functional Activity Coefficient (UNIFAC) method has been built and validated with droplet fiber-suspension evaporation experimental results. The evaporation characteristics of ABE–diesel blend as well as the effects of ABE mass fraction and ambient temperature are analyzed. The results show that ABE–diesel blend droplets evaporate faster than diesel, the addition of ABE affects the early stage of evaporation process, especially at high temperature, which lead to the occurrence of internal gasification observed in experiments. With increasing the ABE mass fraction, the evaporation rate increases, and the internal gasification is more prone to occur later but preform more intensively. The droplet lifetime decreases non-linearly with the increasing ambient temperature, and the evaporation of low volatile components are enhanced significantly. Meanwhile, the increasing ambient temperature leads to the performance of internal gasification faster and more intense.

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1. Introduction

Increasing concerns over energy crisis and environmental preservation pushes the research on clean alternative fuels for internal combustion engines. Among various renewable fuels, butanol is considered to be a promising alternative fuel due to its excellent fuel properties. Compared to methanol and ethanol, butanol is less hydrophilic, has a higher cetane number and heat value, a lower vapor pressure, and a much greater miscibility with diesel [1]. The application of butanol as a supplementary compression ignition engine fuel could promote air–fuel mixing, increase the combustion efficiency, reduce the peak combustion temperature, and thus lead to lower exhaust emissions. The previous studies have reported that butanol–diesel blends showed the satisfied exhaust emissions and engine performance [2–5].

Butanol is mainly produced by acetone–butanol–ethanol (ABE) fermentation from biomass feedstock. The fermentation products contain acetone, butanol and ethanol with the volumetric ratio of approximately 3:6:1. Based on the production data of an average industrial ABE plant in 2008 in China, the production cost of ABE was about $1440/ton [6]. However, the separation of butanol from dilute fermentation broth requires high cost and extra energy consumption [7], which reduces the economic value of butanol as a renewable fuel. In addition, acetone, ethanol and butanol are oxygenated compound. If ABE could be directly used for spray combustion, the separation cost would be eliminated. It is in this respect that the related investigations of ABE as a renewable fuel have been conducted. Lee et al. [8,9] investigated the ABE–diesel blends and water-containing-ABE–diesel blends in both diesel engine generator and diesel engine dynamometer. They found that the ABE–diesel blends even with small amount of water (0.5–1.0 vol.%) were stable in the stability tests. The water-containing-ABE–diesel blend could overcome the trade-off between

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particulate matter (PM) and nitrogen oxides (NOx), such as ABE20W0.5 (a diesel emulsion with 20 vol.% ABE-solution and 0.5 vol.% water). Meanwhile, ABE20W0.5 showed better break thermal efficiency. That might be caused by micro-explosions, which enhanced the atomization of fuel spray and allowed more complete combustion. In another work, the combustion performance and emissions of water-containing-ABE–biodiesel–diesel blend were investigated [10]. In order to study the fundamental combustion and emissions characteristics, Zhou et al. conducted a series of investigation about the spray combustion characteristics of ABE and diesel blends in a constant volume chamber under both conventional diesel combustion and low temperature combustion conditions [11–15]. The general results showed that ABE–diesel blends had longer ignition delay and soot lift-off length compared with pure diesel. The ABE–diesel blends presented better combustion performance and lower soot emission especially at low temperature combustion conditions. In addition, the authors indicated the drastically different volatilities of components in ABE–diesel blends that greatly favored the occurrence of micro-explosion might result in better atomization and air–fuel mixing, which partially explained the superior combustion performance of ABE–diesel blends at low temperature combustion conditions.

Based on the above analysis, it is clear that ABE–diesel blends is a type of multi-component fuel with drastically different volatilities, which may produce micro-explosions in the evaporation process and thus promote combustion performance. Motivated in this regard, the droplet evaporation characteristics of ABE–diesel blends were investigated in our previous study [16]. The results showed that the ABE–diesel blends evaporated faster than diesel, and its evaporation characteristics varied with ambient temperature. At high temperature, the droplets exhibited the expansion and shrinkage phenomena due to bubble formation and rupture. Strong puffing was observed during the ABE–diesel blends evaporation process at 823 K. The macroscopic droplet evaporation behavior of ABE–diesel blends at different ambient temperature (423–823 K) has been observed in the previous study. Hence, as a continuing study, it is necessary to deeply understand the observed droplet behavior. Developing a validated multi-component droplet evaporation model capable of comprehensively describing the evaporation process of ABE–diesel blends fuel droplets in high temperature environment is main objective of the present study.

The case of a single droplet evaporation is a classical heat and mass transfer problem that has been studied in several books, reports and papers [17]. Fuels are usually characterized by a single surrogate component in most evaporation models. However, single component evaporation models are insufficient to predict complex evaporation behavior of real multi-component fuels. Studies has been performed to represent heat and mass transfer for multi-component droplet evaporation. Brenn et al. [18] developed a theoretical multi-component droplet evaporation model based on the model by Abramzon and Sirignano [19]. The numerical results were in excellent agreement with single droplet evaporation in an acoustic levitator. Zhang and Law [20] employed the conduction–diffusion limit model to study the gasification mechanism of a stagnant droplet in still air. And calculations were performed using realistic and temperature-dependent physical properties. Dirbude et al. [21] established a simple single droplet infinite conductivity model to study the evaporation characteristics of rapeseed and sunflower methyl esters. Sazhin and his group have reported a series of studies on multi-component droplet evaporation [22–25]. They have developed effective conduction–diffusion multi-component model for two-component and several components. Ra and Reitz [26] developed a discrete multi-component vaporization model to predict the evaporation of gasoline and diesel fuel droplets at different temperatures and pressures. Since the choice of the component or components (in the case of a multi-component droplet) inside of the droplet is crucial in determining the evaporation rate and droplet lifetime history They utilized six hydrocarbon components to model the properties and composition of a typical diesel fuel presented by Butts [27]. In present study, the six components are used to represent diesel fuel.

As the polarity of ABE is highly different from hydrocarbons. The ABE–diesel blends are highly non-ideal. Raoult' law for ideal behavior is deemed unacceptable for present study, and activity coefficient is introduced to correct for non-ideal behavior in droplet evaporation model. Several studies have adopted activity coefficient to simulate the relatively high polarity fuel evaporation characteristics, e.g., Brenn et al. [18], Sazhin et al. [22], Banerjee [28] and Hallet et al. [29] are examples.

Given the drastically different volatilities of ABE–diesel blends, the phenomena of internal gasification should be considered. Internal gasification occurs due to the heating of the entrapped components of higher volatilities beyond their local boiling point resulting in obvious fluctuation in the droplet size. Sirignano and Wu [30] indicated that the local boiling point of each component in a multi-component droplet was higher than its boiling point in pure form, and it was exponentially correlated with local component concentration. Saha et al. [31] investigated the evaporation characteristics of pure and blended biodiesel droplets, and analyzed the possibility of internal gasification of biodiesel and diesel blends by comparing the local boing point with the droplet center temperature.

The purpose of this study is to analyze the evaporation characteristics of ABE–diesel blends droplets in high temperature environment. A multi-component droplet evaporation model of ABE–diesel blend is developed, which takes into account all key processes, including the distribution of the temperature and diffusion of liquid components inside the droplet and the activity coefficient for non-ideal behavior. The model is validated by the droplet fiber suspension technique experiments of diesel, ABE and ABE–diesel blend. In addition, the effects of ambient temperature and mass fraction of ABE in blends on droplet evaporation behavior are also analyzed.

2. Models

2.1. Assumptions

The evaporation model is set up based on the following assumptions: (1) the system is one dimensional and spherically symmetric; (2) the droplet surface temperature is uniform but varies with time, which allows the calculation separation for the gas and liquid phases; (3) the gas phase surrounding the droplet is in a quasi-steady state; (4) both liquid and gaseous phases at the droplet surface are at thermodynamic equilibrium; (5) the surrounding gas mixture is insoluble in the liquid droplet, which leads to one way diffusion, or the so-called Stefan flow; (6) both liquid and gaseous phases at the droplet surface are at thermodynamic equilibrium.

2.2. Gas phase

Gas phase model is aimed at the heat and mass transfer during the process liquid turns into gas, containing the mass evaporation rate and its related calculation parameters. The mass evaporation rare of an N-component mixture droplet is calculated as followed:

$$\dot{m}_{\mathrm{d}} = \sum_{i=1}^{n} \dot{m}_i = \begin{cases} -2\pi r_{\mathrm{s}} \sum_{i=1}^{n} \rho_{i,g} D_{i,g} Sh_i^* \ln(1 + B_{M,i}) \\ -2\pi r_{\mathrm{s}} \sum_{i=1}^{n} k_{i,g} Nu_i^* \ln(1 + B_{T,i}) / c_{p,iv} \end{cases} \quad (1)$$

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