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Development of a diesel/biodiesel/alcohol (up to n-pentanol) combined mechanism based on reaction pathways analysis methodology

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HIGHLIGHTS

- A combined reduced combustion mechanism of diesel/biodiesel/alcohol was developed.
- Well validated against the ignition delay times, flame speeds and spray combustion.
- Addition of biodiesel retards ignition time of diesel in low temperature high pressure regime.
- Butanol and pentanol blends have similar ignition delay times with the base fuel.
- Adding biodiesel or C1–C5 alcohols (up to 20%) would not change flame speeds of diesel significantly.

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ABSTRACT

Recently, diesel/biodiesel/alcohol blend fuels have attracted tremendous attention as a potential alternative fuel in internal combustion engines, because of their beneficial effects on pollution emission and engine performance. However, there are few chemical mechanisms to forecast combustion characteristics of the ternary blends, especially for those blending with long-chain alcohols, such as butanol and pentanol. The objective of this paper is to develop a combined reduced combustion mechanism for the combustion simulation of diesel/biodiesel/alcohol (up to n-pentanol). This new combined mechanism, consisting of 229 species and 902 elementary reactions, was constructed by integrating two separated reduced mechanisms; one is the PRF-alcohols' mechanism (Liu et al., 2016), and another is the biodiesel mechanism (Luo et al., 2012). The new combined mechanism reproduced well predictions of fuel ignition and flame speed compared with those obtained using the original ones. Extensive validations were performed against various experimental data for 0-D homogenous systems, 1-D freely propagating premixed flames and 3-D spray combustion flames. The proposed combined mechanism was shown to be versatile and robust, successfully integrating the biodiesel reaction mechanism and the long-chain alcohol reaction mechanisms into a single reaction scheme. Coupling with advanced simulation technology, it could be a powerful numerical tool in the design and optimization of new generation engines which are fueled with clean alternative fuels, especially when concerning long-chain alcohols. In addition, the effects of adding biodiesel and different kinds of alcohols on fundamental combustion characteristics of diesel/biodiesel/alcohol blend fuels were investigated using the proposed combined mechanism.

1. Introduction

As an energy conversion device with high thermal efficiency, high stability and using flexibility, diesel engines have been widely used in many fields for more than a century. However, the wide application of diesel engines results in a heavy dependence on fossil fuels, and causes a large quantity of harmful emissions, including greenhouse gases (especially CO_2) and other pollutant chemicals. Nowadays, biofuels are gaining more and more attentions worldwide as alternatives or supplements to fossil fuels in the engine. As derived from biological raw materials, biofuels have many advantages, such as renewable, biodegradable and mostly environment-friendly [1]. In addition, they are also called carbon-neutral fuels which are produced largely from atmospheric carbon dioxide and sunlight [2]. Thus the wide application of biofuels would help to control greenhouse gases emissions.

Among those biofuels, biodiesel has been considered as the one with most potential for large-scale applications worldwide [3]. Biodiesel is a renewable and eco-friendly biofuel, which transformed from various

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feedstocks such as plant seeds, microalgae, biological oil and fat via transesterification [4]. Compared with fossil diesel, biodiesel has similar cetane number and better lubricity. A number of researches have focused on the effect of fueling biodiesel or diesel/biodiesel blends on the performance and emission of diesel engine, and found the application of biodiesel could achieve a substantial reduction of unburned hydrocarbon (UHC), carbon monoxide (CO) [5] and soot [6]. However, the poor volatility and high viscosity of biodiesel restrict its substitution ratio in engines. An et al. [7] reported a tangible drop in thermal efficiency of a diesel engine when biodiesel blend ratio exceeds 50%. Woo et al. [8] suggested that although increasing the biodiesel concentration in biodiesel-diesel blends could achieve the synchronous reduction of smoke/NO_x emissions, the biodiesel concentration still should not exceed 10% to avoid the unacceptable brake specific fuel consumption. Lahane et al. [9] recommended 15% biodiesel as the optimum blend in biodiesel-diesel fuel, due to a low level of NOx emission and no wall impingement.

In the last decade, researchers have shown great interest in the utilization of alcohols as a supplement for diesel/biodiesel blends to reduce the concentration of fossil fuel. Short-chain bio-alcohols, such as methanol [10] and ethanol [11] from renewable sources. Short-chain alcohols have been investigated widely owing to their more mature production technology. Their high volatility, low viscosity and high oxygen content also could improve fuel spray combustion and bring down emissions [12]. However, some disadvantages, such as high latent heat of vaporization, low heating value low cetane number, prevent their large proportion applications in diesel engines.

In order to solve such problems, more attentions have been paid to use long-chain bio-alcohols, such as butanol and pentanol, as main alternative fuels in diesel engines [13]. Compared with short-chain alcohols, long-chain alcohol has many advantages over short-chain one, such as higher cetane number and calorific value, lower latent heat of evaporation [14]. Moreover, long-chain alcohol presents better blend stability and could be injected directly to the combustion chamber by blending with diesel or biodiesel at any ratios [15]. Among these long-chain alcohols, n-pentanol is regarded as the most potential next-generation alternative biofuel with its excellent physicochemical property [16]. Recent works focused on the spray combustion characteristics of n-pentanol blends have revealed that addition of n-pentanol could effectively improve air-fuel mixing [17] and reduce soot formation in diesel flames [18] and biodiesel flames [19]. A few experimental researches have been carried out to investigate the influence of using long-chain bio-alcohols in diesel/biodiesel/alcohol blend on diesel engines. Li et al. [20] investigated the effects of adding n-pentanol to diesel/biodiesel blend on the combustion and emission of a diesel engine, and the concentrations of n-pentanol and biodiesel in test fuels both reached 30%. They found these ternary blends were able to reduce soot, carbon monoxide and unburnt total hydrocarbons emissions while maintained higher indicated thermal efficiency. Imdadul et al. [21] compared the performance, emission, and combustion characteristics of a diesel engine fueling different proportion of n-pentanol treated diesel/biodiesel blends under different speed conditions, and concluded that blending 20% n-pentanol could optimize engine performance and emission without any engine modification. They [22] also compared the diesel engine performance and exhaust emission which respectively fueled by n-butanol and n-pentanol treated diesel/biodiesel blends, and found n-pentanol blends showed better overall performance and emission than n-butanol blends. However, a contrary conclusion was drawn by Yilmaz et al. [23]. They have observed that addition of n-pentanol would cause a significant increase of CO, HC and NO_x emissions, which attributed to the higher latent heat of evaporation and higher oxygen content of n-pentanol.

Besides the experimental investigations, it is necessary to construct chemical mechanisms for the oxidation of biofuels, which could provide further insight into the combustion processes of biofuels. Moreover, those detailed in-cylinder processes, including fuel oxidation and emission formation, can be obtained easily by coupling the chemical mechanism calculation and accurate 3D computational fluid dynamics (CFD) simulation; that will be great help to achieve the collaborative optimization between fuel properties and the combustion system, then obtain the optimum performance of engines. However, restricted to the current computational ability, those chemical mechanisms used in CFD studies have to be simplified from (more realistic) detailed mechanisms.

Practical diesel and biodiesel are composed of hundreds of compounds, and it is very difficult to consider the actual oxidation evolution of all these components during CFD simulation. Thus, a common approach is to use simplified surrogate components with reduced mechanisms to represent the combustion behavior of practical fuels. In literatures, n-heptane [24], n-decane [25] and primary reference fuels (PRF, combining n-heptane and iso-octane) [26] were several typical surrogates representing diesel oxidation mechanism, while some low carbon methyl esters and their normal alkanes blends were chose to substitute for biodiesel. For example, a combined reduced mechanism consisting of methyl butanoate (MB) and n-heptane blends were developed by Brakora et al. [27]. However, MB does not adequately characterize the combustion behaviors of large methyl esters, such as the negative temperature coefficient behavior and related low-temperature phenomena [28]. Brakora et al. [29] later developed a new biodiesel surrogate mechanism involving methyl decanoate (MD), methyl-9-decenoate (MD9D) and n-heptane components, and proved to be more reliable accuracy in predicting important combustion characteristics of biodiesel. Similar works were also reported by Luo et al. [30], Cheng et al. [31] and An et al. [32]. Recently, Liu et al. [33] and E et al. [34] proposed a skeletal four-component biodiesel surrogate mechanism, including MD, MD5D, n-decane and methyl linoleate. The mechanism was shown to be accurate to predict the effect of varying fatty acid methyl ester proportion on biodiesel ignition and combustion.

However, compared with those abundant surrogate mechanisms that substitute for practical diesel and biodiesel, the surrogate mechanisms considering the addition of alcohol are still scarce, particularly when long-chain alcohols blended in. Mohan et al. [35] developed a novel coupled biodiesel surrogate and PRF oxidation skeletal mechanism based on decoupling methodology, which used for simulating combustion behaviors of diesel/biodiesel blends. The mechanism included oxidation sub-mechanisms of MD, MD9D n-heptane and iso-octane, and was well validated with shock-tube ignition delay time, laminar flame speed and 3D engine simulations. Wang et al. [36] proposed a reduced chemical reaction mechanism for modeling the combustion process and soot emissions for diesel and n-butanol blends. The proposed mechanism consists of 76 species and 349 reactions, and was validated with experiments in shock tubes, constant volume chambers and testbed engine data. Then they [37] developed a reduced chemical kinetic mechanism for the combustion simulation of engines fueled with n-butanol/biodiesel blends. This mechanism was constructed by combining a n-butanol mechanism reduced from the detailed mechanism of Sarathy et al. [38] with a reduced biodiesel mechanism obtained from their previous work [39]. A reduced PRF/alcohol mechanism with 108 species and 435 reactions was proposed by Wang et al. [40], and they have verified the effectiveness of this mechanism in homogeneous charge compression ignition engine predictions. Later, Liu et al. [41] constructed a combined reduced PRF-alcohols (up to n-pentanol) combustion mechanism with the addition of the reduced mechanism of n-pentanol. Coupled with the toluene-polycyclic aromatic hydrocarbons sub-mechanism, this mechanism was used to investigate the effect of fueling diesel/alcohol blend fuels on the combustion and soot formation characteristics in a direct injection diesel engine, and some useful conclusions have been drawn.

Unfortunately, there are few chemical mechanisms to forecast combustion characteristics of diesel/biodiesel/alcohol blend fuels. The only combined chemical mechanism of these ternary blends was proposed by Alviso et al. [42] recently; they developed and validated a combined chemical mechanism of diesel/biodiesel/ethanol ternary