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Development and validation of a new reduced diesel-*n*-butanol blends mechanism for engine applications

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ABSTRACT

A reduced *n*-heptane-toluene-*n*-butanol-polycyclic aromatic hydrocarbon (PAH) combustion mechanism was developed for a blended fuel of *n*-butanol and diesel, including 101 species and 531 reactions. A sensitivity analysis was conducted for the optimization of the mechanism. The optimized mechanism was widely validated with ignition delays, laminar flame speeds, species concentrations in premixed flame and counterflow flame, and homogeneous charge compression ignition (HCCI) engine combustion. According to the validation results, the optimized mechanism shows favorable predictions, especially on the important species related to the PAH formation. Moreover, the reduced mechanism was coupled with computational fluid dynamic (CFD) to conduct direct injection compression ignition (DICI) engine tests within a wide range of exhaust gas recirculation (EGR) ratio and also shows favorable prediction results. Therefore, the proposed mechanism can be used to simulate the combustion of diesel or *n*-butanol-diesel blends in multi-dimensional CFD modeling. Besides, the main formation pathways of benzene (A_1), a precursor of soot, were analyzed in a single-zone HCCI engine model. Results show that, in addition to the traditional pathways of '$C_4 + C_2$' and '$C_3 + C_3$', toluene was quite crucial to produce A_1. The counterflow flame validation tests also demonstrated the importance of the addition of toluene to the PAH and soot formation. In the early combustion period, C_6H_5OH significantly contributed to the formation of A_1, while toluene directly produced a large amount of $C_6H_5CH_2$ and thus promoted the formation of A_1. In the middle combustion period, $OC_6H_4CH_3$ played an important role in the formation of A_1, while toluene made less contribution.

1. Introduction

Internal combustion engine (ICE) is still the most widely used power unit all over the world, especially in automotive industry. With ever-increasing automobile ownership, energy storage and environmental pollution have become more and more serious issues. To achieve high efficiency and clean combustion in ICEs, it is urgent to seek new alternate fuels and meanwhile adopt some advanced combustion modes. Compared to fossil fuels, biofuels show remarkable advantages in renewability and emission and have aroused great attention [1–3].

Currently, the commonly used biofuels mainly include biodiesel, alcohols, and ethers [4–6]. Alcohol fuels are generally liquid under normal pressure and temperature and thus easy to store and transport; owing to the existence of oxygen atoms, soot emission is significantly reduced during the combustion of alcohol fuels [7–9]. Moreover, alcohol fuels are characterized by a high octane number and latent heat of vaporization that improve the complete combustion of the fuels in a cylinder. Methanol, ethanol, and *n*-butanol are currently widely used, because of their simple production process and low preparation cost. All these advantages promoted further applications of alcohol fuels.

Methanol and ethanol are two types of most widely used alcohol fuels. Ethanol shows outstanding superiorities in high cetane number and low toxicity and thus has long been considered as one of the most promising alternate fuels for gasoline engine. Compared to methanol and ethanol, *n*-butanol has a higher low-heating value, indicating that the addition of *n*-butanol can make the blended fuel maintain a high energy density while slightly affecting the power. Additionally, *n*-butanol has a lower volatility that can help to reduce the vapor lock in engine oil pathway; compared to methanol and ethanol, *n*-butanol also shows a significantly higher cetane number and lower latent heat of vaporization, improving the engine's starting and ignition performances under cold-starting or low-load conditions. Both methanol and ethanol are quite soluble in water, but *n*-butanol is slightly soluble in water, i.e., *n*-butanol is not easily polluted by water. Besides, the viscosity of *n*-butanol is closer to diesel than methanol and ethanol. Because of all these advantages, *n*-butanol has become a highly competitive alternative oxygenated biofuel and also an additive that can be used in ICEs. In the past several years, extensive studies have been conducted on the

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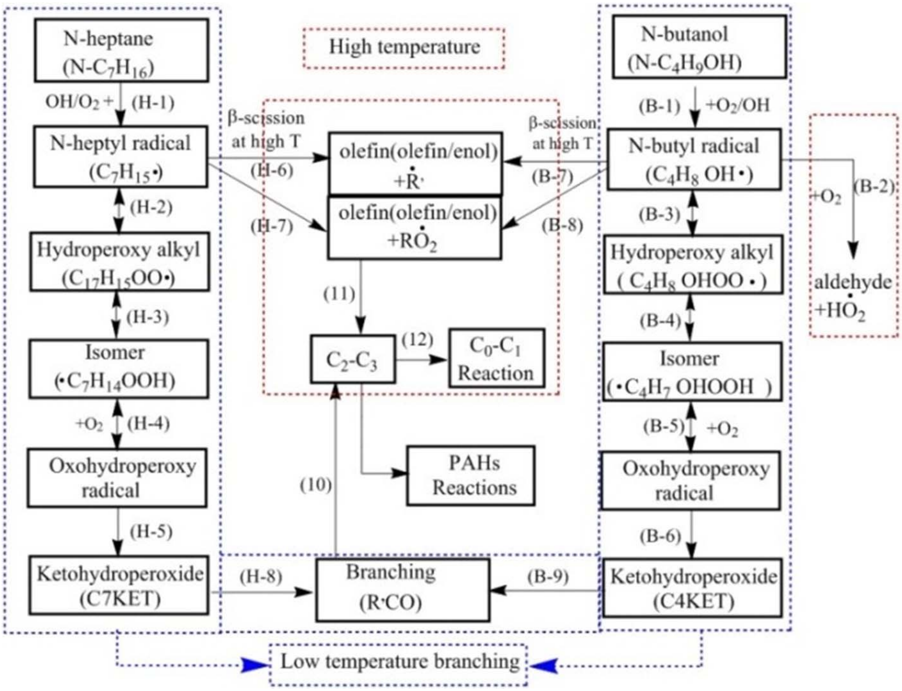

Fig. 1. Main reaction pathways for the combustion of *n*-heptane and *n*-butanol (R represents C_5 or C_2 radical).

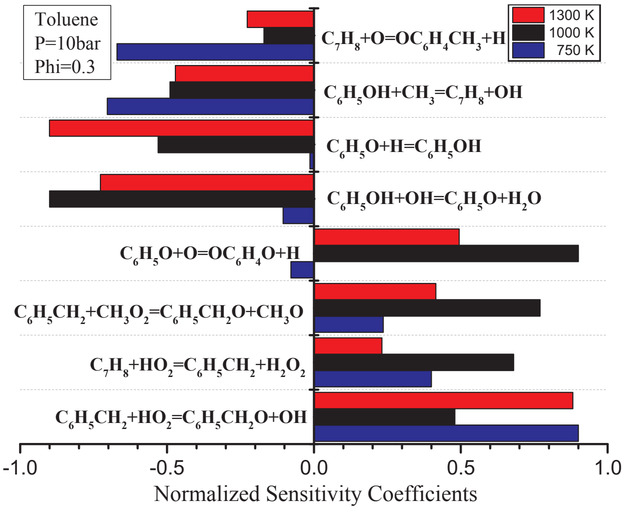

Fig. 2. Sensitivity analyses of ignition delay for toluene.

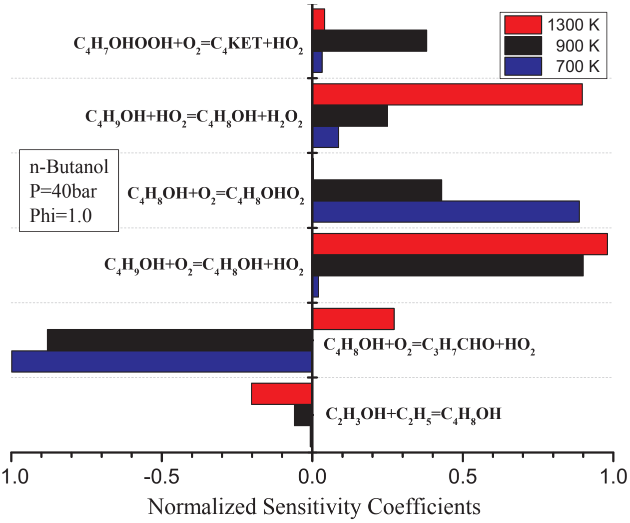

Fig. 3. Sensitivity analyses of ignition delay for *n*-butanol.

applications of *n*-butanol in engines [10–17].

At present, the combustion characteristics of butanol have been extensively studied, mainly focusing on fundamental research on pyrolysis, premixed laminar flames, ignition delays, and chemical kinetic models [18–27]. Sarathy et al. [27] developed a detailed kinetic model for the four isomers of butanol. The model was composed of 426 species and 2335 reactions and included the detailed high-temperature and low-temperature pathways of four different isomers of butanol; it was well validated by the species concentrations of premixed flame, laminar flame speed, ignition delay, and jet stirred reactor (JSR) performance. Wang et al. [28] simplified the abovementioned detailed mechanism of *n*-butanol and combined this mechanism with a reduced *n*-heptane-PAH mechanism to construct an *n*-heptane-*n*-butanol-PAH combustion mechanism for a blended fuel of *n*-butanol and diesel, which was extensively validated by the results of ignition delay, species concentrations of premixed flame, and engine test and showed favorable prediction results. Considering that the aromatic hydrocarbons present in diesel may affect soot formation, Zhou et al. [29] added the related reactions of toluene to the reduced mechanism of Wang et al. [28] for *n*-butanol/diesel blends; moreover, they coupled the mechanism to CFD and investigated the effects of the mixing proportion of *n*-butanol and exhaust gas recirculation (EGR) rate on the formation of soot precursors during the low-temperature combustion (LTC) of *n*-butanol and diesel. According to their results, with the increase in the mixing proportion of *n*-butanol, the formation of soot precursors, namely, benzene (A_1), naphthalene (A_2), phenanthrene (A_3), and pyrene (A_4) was delayed; when the mixing proportion of *n*-butanol exceeded 20%, the effect on the formation of soot precursors A_1, A_2, A_3, and A_4 weakened; with the increase in the EGR rate, the formation of soot precursors was also delayed. However, the established kinetic mechanism of *n*-heptane-toluene-*n*-butanol-PAH lacked extensive experimental validations and did not completely consider the low-temperature reaction pathways of toluene.

This study first developed a new reduced *n*-heptane-toluene-*n*-butanol-PAH combustion mechanism for diesel/*n*-butanol blends and made some optimizations through sensitivity analysis. Then, the