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# Comparative analysis of soot formation processes of diesel and ABE (Acetone-Butanol-Ethanol) based on CFD coupling with phenomenological soot model

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## HIGHLIGHTS

- The soot generation processes of ABE and diesel were compared.
- The reason why ABE has less soot than diesel is explained.
- At 800 K and 21% oxygen concentration, soot mass peak of ABE is 1/12 of diesel's.
- As oxygen concentration decreases to 16%, soot mass peak of ABE increases by 25%.

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## ABSTRACT

The improved nine-step phenomenological soot model of diesel and ten-step phenomenological soot model of ABE (Acetone-Butanol-Ethanol) which had been confirmed in previous studies were implemented into KIVA-3V Release 2 code, and then multi-dimensional computational fluid dynamics (CFD) simulations were conducted to investigate the combustion characteristics and soot formation process of diesel and ABE in constant volume chamber at different temperatures (800 K and 1000 K) and oxygen concentrations (21% and 16%). The comparative results of their soot formation processes and intermediate products indicate that, in the combustion process, the soot mass of ABE and diesel presents in the form of parabolic curve with time change, the soot generation tendency of ABE is lower than diesel, and the initial temperature and oxygen concentration have little effect on the relative relations of their soot and intermediate products mass. At the oxygen concentration of 21%, when initial temperature decreases from 1000 K to 800 K, the soot mass peak values of diesel and ABE reduce by 40% and 83%, respectively. At the initial temperature of 800 K, the relative relations of their soot number and OH free radical keep unchanged; nevertheless, the mass of ABE's $C_2H_2$ and precursor exceeds that of diesel's in the early stage of combustion. At the initial temperature of 1000 K, when oxygen concentration decreases from 21% to 16%, the soot mass peak values of diesel and ABE increase by 20% and 25%, respectively. At the same time, the $C_2H_2$, precursor and soot number increase in diesel but decrease in ABE.

## 1. Introduction

Because internal combustion (IC) engine is one of the largest consumers for fuel and also one of the largest pollutant emission sources, almost all countries have regarded that IC engine has been an important object for energy saving and emission reduction [1–4]. In order to protect environment, many countries have developed increasingly stringent emission regulations to restrain the emissions of IC engine. Soot, as one of the main emissions in diesel engine, not only has bad effects on people's respiratory system [5], but also is one of the main reasons for the atmospheric haze. For this reason, many researches have made unremitting efforts for reducing the soot emission from IC engine [6,7]. For example, the studies of soot formation process gave many possible methods and the researches of biodiesel provided some better fuels to reduce soot emission [8–11]. Generally speaking, knowing the

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*Abbreviations:* ABE, Acetone-Butanol-Ethanol; CFD, computational fluid dynamics; IC, internal combustion; RNG, renormalization group; ASOI, after start of injection; PCCI, premixed charge compression ignition; EGR, exhaust gas recirculation.

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intermediate products can be used to find justification to phenomena that are observed experimentally and to know those intermediate products allows to make simulations and more precise chemical models that diminish the uncertainty, so we could better understand soot formation process which is beneficial for reducing the soot emission.

Diesel is a traditional fuel for automobile engine, and many soot models of diesel have been proposed in the previous studies [12–17]. Nevertheless, due to the complexity of the chemical reaction kinetics, the details of how soot particles and their precursors are formed have not been clearly understood. So, many researchers have introduced soot formation mechanism with phenomenological soot models which describe the complex process of soot formation and oxidation in terms of several global steps that are particularly advantageous for practical combustion simulations. Fusco et al. [18] described the formation process of soot in diesel engine by eight-step phenomenological soot model. Because Fusco's soot model has fewer steps and includes those agreements of soot formation mechanism, it was developed by many researchers [19–23]. Tao et al. [21] proposed a nine-step phenomenological soot model, and the validations of the model were conducted over a wide range of engine conditions from conventional to PCCI-like (premixed charge compression ignition) combustion and the results revealed that the nine-step model is not only computationally efficient but also fundamentally reliable and robust. These phenomenological soot models have provided simple ways to understand the soot formation process and possible methods to reduce the soot emission of IC engine.

Due to the better emission characteristics, oxygenated fuels have raised concerns in recent years [24,25]. Miyamoto et al. [26] concluded that soot reduction is related to the oxygen content of the fuel regardless of the type of fuel. Iannuzzi et al. [27] investigated different oxygenated fuels in a constant volume chamber with large optical access and the results highlighted nearly smokeless combustion for pure oxygenated fuels and a non-linear soot emission reduction with increasing oxygen content in the blend. As an oxygenated fuel, Acetone-Butanol-Ethanol (ABE) is regarded as a potential alternative fuel for IC engine. n-Butanol is of particular interest as a renewable biofuel as it is less hydrophilic, and possesses higher energy content, higher cetane number, higher viscosity, lower vapor pressure, higher flash point and higher miscibility than ethanol, making it more preferable than ethanol for blending with diesel fuel [28]. ABE is one of the major methods to produce butanol using biomass. The direct use of ABE could save enormous expenses for separating n-butanol from ABE. Zhou et al. [29] conducted an experimental investigation of ABE-diesel blend combustion in a constant volume chamber. They found that at low ambient temperature of 800 K and ambient oxygen concentration of 11%, ABE20 (the mass fraction of ABE is 20%) presented close-to-zero soot luminosity with better combustion efficiency compared to D100 (the mass fraction of diesel is 100%), and considered ABE as a very promising alternative fuel to be directly used in diesel engines especially under low temperature combustion conditions. To research the combustion characteristics of ABE-diesel blends, Wu et al. [30–32] measured soot distribution and soot mass of spray combustion of ABE and diesel by forward illumination light extinction technology, and compared the spray and combustion characteristics of neat ABE, n-butanol and diesel in a constant volume chamber. Yet, all of Wu's studies about ABE have demonstrated that ABE has less soot emission than diesel by experiment data. In the meantime, Zhao et al. [33,34] proposed two kinds of phenomenological soot model for ABE mixtures based on the soot model structure raised by Tao et al. [21] and the proposed model showed good agreement with experimental data qualitatively, and then predicted the soot formation process of ABE with different oxygen concentrations.

The previous studies about the phenomenological soot models of diesel have provided effective methods for understanding soot formation process and predicting soot emission. And many experiments have demonstrated that oxygenated fuels have less soot emission than diesel [35,36]. However, to the authors' knowledge, it is the first time to illustrate the depth difference of the soot formation process between diesel and ABE through phenomenological soot model. Through comparing the soot formation processes of diesel and ABE, one can have a clearer understanding of ABE as a clean alternative of ABE compared with diesel can be further revealed. Meanwhile, the formation mechanism of soot in ABE mixtures is still not clear, and thus people do not know how to improve the emission performance of engine fueled with ABE. Hence, further study is still necessary to extend this research field. As a continuing study, the comparative analysis of soot mass and intermediate products between diesel and ABE has been conducted at different initial temperatures and oxygen concentrations by using the phenomenological soot model.

## 2. Simulation models

### *2.1. Phenomenological soot model*

The improved nine-step phenomenological soot model of diesel and ten-step phenomenological soot model of ABE are chosen from our previous work, their reaction processes are shown in Tables 1 and 2, respectively, and these two models have been validated in the research [33,37].

### *2.2. Experimental processes and simulation processes*

The optically accessible constant volume chamber test system has been introduced in the previous study [33]. The test was started by filling the chamber with the premixed mixture which included acetylene, oxygen and nitrogen. The mixture was then ignited by a spark to create a high-temperature/pressure environment inside the chamber, and slowly cools down due to the heat loss. The spray injection and camera were triggered simultaneously when the pressure reached the desired test conditions. The initial temperature and initial oxygen concentration of the gas at the time of injection in the chamber could be controlled as desired by adjusting the injection timing and partial pressure [30]. The test conditions are shown in Table 3. And the ABE solution is prepared with a volume fraction of 3:6:1 (acetone/butanol/ethanol), which is a typical composition of the product of ABE fermentation.

As the injection nozzle was located in the central axis of cylinder near cylinder head and six nozzle holes distributed symmetrically, the cylinder model was simplified as a 60° fan-shaped area which was symmetric by the center of single fuel spray. In this way, the speed of calculation could be improved. Mesh was generated by ICEM-CFD software and it was presented in Fig. 1. The KIVA-3V Release 2 code was used as the simulation tool to solve the mass, momentum and energy conservation equations for main species. The renormalization group (RNG) $k-\varepsilon$ model [41] was used to simulate the low Mach-number turbulent effect on transportation and flow field. The "blob" model [42] was used for simulating the fuel parcel injection dynamics, while the Kelvin–Helmholtz and Rayleigh–Taylor models [43,44] were used for simulation of spray atomization and droplet breakup. For the combustion process, the "Shell" ignition model [45] was used for simulating the auto-ignition process related to low-temperature reactions. For different fuels, the "Shell" model specifies different values for the kinetic parameter of the crucial reaction, leading to the production of the branching agent. Basic parameters of the simulated constant volume chamber are listed in Table 4.