



Full Length Article

Effect of acetone–butanol–ethanol addition to diesel on the soot reactivity

Jianfei Luo, Yongming Zhang, Jinjun Wang, Qixing Zhang*

State Key Laboratory of Fire Science, University of Science and Technology of China, Hefei, Anhui 230026, PR China

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ABSTRACT

The ability of acetone–butanol–ethanol (ABE) to reduce pollutant emissions has been validated in recent studies. In this study, the effect of addition of ABE (up to 30% by volume) to diesel on the soot oxidation reactivity was investigated to further evaluate the feasibility of increasing the particulate filter regeneration rate. The oxidation activities of soot samples were compared using the average activation energies calculated from the thermal gravimetric curves. It was found that the average activation energies of the ABE–diesel–blends–derived soot are lower than that of diesel–derived soot. The variations in the physical and chemical properties of the soot samples were investigated to determine the parameters that improve the soot oxidation reactivity. Several experimental diagnostic techniques, such as Fourier transform infrared spectroscopy, elemental analysis, X-ray diffraction, and high-resolution transmission electron microscopy, were used to investigate the changes in the functional groups, atomic O/C and H/C ratios, nanocrystallite parameters, and soot nanostructures. With increasing concentration of ABE in diesel, the size of the primary particles, nanocrystallite length, and amount of aromatic C=C functional groups in the soot decrease, while the nanocrystallites tortuosity, amount of oxygenated functional groups, and atomic O/C and H/C ratios increase. The changes of these parameters prove the higher reactivity of ABE–diesel–blends–derived soot.

1. Introduction

Soot particles are the product formed in the fuel-rich zones of combustion, and they are composed of polycyclic aromatic hydrocarbons (PAHs) and aliphatic chains [1]. They are the second biggest contributor to the global warming effect [2]. Furthermore, air polluted by soot particles can cause cancer, asthma, and cardiac disease [3]. Therefore, it is important to understand the soot formation process [4,5], physicochemical properties of soot [6–18], and develop technologies to reduce soot emissions [19].

Removal of soot particles from exhaust gas has been a research hot spot for several decades. Installing particulate filters in exhaust system is the simplest and easiest method. However, the blockage caused by filters affects the working pressure in the engine. To overcome this problem, soot oxidation removal in the presence of catalysts has been proposed. An intrinsically more reactive soot will make regeneration of catalytic filters less problematic [20–22]. This is also limited by the high price of catalysts. Therefore, lots of researchers have searched for the inexpensive catalysts and investigated implanting catalysts or addition to fuels to make the produced soot more active [23–26]. Adding biomass fuels to diesel and gasoline has attracted increasing attention, because cheap biomass fuels are beneficial for reduction of pollutant emissions and enhancing the soot oxidation activity.

The most commonly used biomass fuels are biodiesel, alcohols (e.g., methanol, ethanol, and butanol), dimethyl ether, and 2, 5-dimethylfuran (DMF). However, the costs of the raw materials and esterification technology used in production of biodiesel are expensive [27,28]. The strong water absorption capacities, high volatilities, high nitrogen oxide (NO_x) emissions, and low heating values of methanol and ethanol restrict their application [29,30]. Similarly, application of dimethyl ether is limited because of its low boiling point, low viscosity, and limited source [31]. DMF and butanol are considered to be potential biomass fuels because of their high heating values, abundance, and low water absorbencies [32–36]. It has been found that the particulates matter (PM) can be reduced by 80% with addition of 40 vol% DMF [37]. Similarly, PM, NO_x, and CO emissions simultaneously decrease with addition of butanol [32]. Their abilities to improve the soot oxidation reactivity have also been demonstrated [38,39].

Acetone–butanol–ethanol (ABE), the intermediate product in the bio-butanol production process using biological fermentation and purification technology [40], has recently attracted a lot of attention as a promising alternative fuel. Application of ABE fuel is because the heat required to separate bio-butanol from ABE solution through fractionation and distillation technology is about 50% of the butanol energy density [41]. Several researchers have investigated the emission behavior of ABE blends. Chang et al. [42,43] found that the PM emission

* Corresponding author.

E-mail address: qixing@ustc.edu.cn (Q. Zhang).

factors are reduced by between 17.8% and 50.4% when diesel is blended with 10–30 vol% ABE, and it can successfully avoid the trade-off puzzle between PM and NO_x emissions. In our previous work [44], we evaluated the sooting tendency of ABE–diesel blends using the Threshold Sooting Index (TSI). We found that the normalized TSI value exponentially decreases with increasing blending ratio. Along with studies of the PM emissions, experimental and theoretical studies of the combustion characteristics of ABE and ABE–diesel blends have also been performed. VanGeem [45] established a reaction mechanism model containing 350 species and 1000 reactions to simulate oxidation and pyrolysis of ABE. Yang et al. [46] measured the detailed chemical structures of ABE in laminar premixed flame using molecular beam mass spectrometry with the synchrotron vacuum ultraviolet technology, and evidenced their ABE kinetic chemical reaction model. Zhao et al. [47] developed a phenomenological soot model to calculate the soot behavior in an engine based on the KIVA-3 V Release 2 code, and the trends of the predicted soot behavior with various oxygen concentrations were in agreement with measurements. Zhou et al. [48] and Wu et al. [49–51] investigated the flame behavior of ABE–diesel blends burned in an engine model under different temperatures and oxygen concentrations. They found that ABE has similar spray combustion performance to diesel, the flame lift-off height of ABE–diesel blends is longer than that of regular diesel, and a higher content of acetone in ABE can reduce the ignition delay time.

ABE inherits the excellent properties of butanol, which has a strong ability to reduce soot emissions. However, no studies have investigated the variation in the soot oxidation reactivity upon addition of ABE to diesel. This is closely related to the utilization efficiency of the diesel particulate filters. Thus, the aim of this present study is to evaluate the effect of ABE addition to diesel on the soot oxidation reactivity. Soot samples were collected from the ABE–diesel blend diffusion flame. The soot reactivity was quantified using the activation energy. The variations in the types of functional groups, elemental composition, PAHs nanocrystallite parameters, and soot nanostructures were analyzed to explain the change in the soot reactivity.

2. Experimental details

The ABE solution was prepared by mixing 30 vol% acetone, 60 vol% butanol, and 10 vol% ethanol. The purities of reagents were 99.7%. Their properties can be seen in [44]. Diesel blends with 0, 10, 20, and 30 vol% ABE are referred as D, ABE10, ABE20, and ABE30, respectively.

A wick-fed burner was used to produce a stable diffusion flame. The burner consists of a fuel reservoir, a wick tube, a wick sheath, and a height adjustment system as shown in [44]. This apparatus performs combustion of liquid fuels without a specialized device to gasify the liquid fuel. The sooting tendency of fuels can be obtained by investigating the relationship between the flame height and the fuel consumption rate. The flame height and fuel uptake rate were altered by changing the length of the exposed wick.

A 47 mm filter assembly with a polytetrafluoroethylene (PTFE) membrane (Millipore, Ireland) was used to collect the soot particles. PTFE can significantly reduce absorption of volatile organic carbon in the flow. A sampling tube with a 0.3 mm orifice was placed on the top of the flame to reduce the exposure time in air [38]. The filter assembly was connected to a diaphragm vacuum pump. All of the samples were stored in a refrigerator. In the process of soot collection, no changes of the flame height and fuel consumption rate were observed after igniting the wick, so the initial combustion conditions for each blend were maintained and the reproducibility of the collected samples is guaranteed.

A synchronous thermal analyzer (STA 449 F1 Jupiter) were used to determine the oxidation activities of the soot samples. The samples were heated from 25 to 400 °C in N₂ to decompose the volatile organic compounds, and then non-isothermally heated from 400 to 700 °C in air

at a heating rates of 3, 5, or 7 °C/min. Thermogravimetric analysis (TGA) were performed with the NETZSCH Kinetics Neo software.

The soot oxidation reactivity is dependent on the physical and chemical properties of the soot, such as the content distribution of chemical elements, functional groups, nanocrystallite parameters, and soot nanostructures. Thus, several characterization experiments were performed to obtain these parameters.

CHNS elemental analysis (Vario EL cube) was performed to determine the distribution of C and H elements in the soot. Because soot particles only contain C, H, and O atoms, the O content can be calculated from the CHNS results [52].

Fourier transform infrared (FTIR) spectroscopy was performed to investigate the functional groups in the soot, using a Nicolet 8700 FTIR spectrometer (Thermo Nicolet Corporation). Analytical samples were prepared by compressing mixtures consisting of 10 mg analytical KBr and 0.02 mg soot particles. Each sample was scanned in the range of 400–4000 cm⁻¹ with a resolution of 2 cm⁻¹.

X-ray diffraction (XRD) was performed with a Panalytical X'Pert Pro powder X-ray diffractometer using Cu K α radiation ($\lambda = 0.154$ nm) to evaluate the crystallite parameters of the soot samples. The scan step size and scan speed were 0.02° and 240 s/step, respectively, in the scan range 10–60°.

High-resolution transmission electron microscopy (HRTEM) images of the soot samples were recorded to investigate the variation in the soot nanostructures. The HRTEM images were obtained using a Talos F200X transmission electron microscope (Field Emission Inc.) with an energy-filtered camera. The soot samples were prepared by ultrasonically dispersing the soot particles in ethanol for 10 min and then applying a drop of the suspensions to Lacey carbon-coated copper grids.

3. Results and discussion

3.1. Smoke point

Selection of the fixed flame height is crucial so that sufficient soot particles can be collected and the flame is not affected. Flame heights near the smoke point were considered. Higher flame heights were not used to avoid introduction of a pulsating flame. Lower flame heights were not considered because of the low yield of soot particles. The smoke points of D, ABE10, ABE20, and ABE30 are 21.8, 24.9, 27.8, and 30 mm, respectively [44]. Therefore, the fixed sampling height was set to 30 mm.

3.2. TGA

Fig. 1 shows the variation of soot conversion (α) with temperature (T) at different heating rates. Soot conversion is defined as $\alpha = \Delta M_T / \Delta M_L$, where ΔM_T is the difference between the initial soot mass and the soot mass at T . ΔM_L is the difference between the initial soot mass and the remaining soot mass. The remaining soot mass was zero for all of the soot samples. The trends of conversion curves are basically consistent for the different heating rates, and the curve shifts to higher temperature with increasing the heating rate. The temperatures corresponding to 1%, 50%, and 90% conversion are regarded as the initiation oxidation temperature (T_i), fast oxidation temperature (T_{max}), and oxidation burnout temperature (T_{end}), respectively. They were used to compare the soot reactivity, and their values are listed in Table 1. These characteristic temperatures of diesel-derived soot are higher than those of ABE for the same heating rate, which indicates that oxidation reaction of diesel-derived soot is more difficult.

To further quantitatively investigate the oxidation reactivity of the soot samples, the activation energies required for soot oxidation by O₂ were calculated using the Friedman method [53], which is an iso-conversional method. The activation energy was obtained by plotting the conversion rate against $1/T$. The conversion rate in TGA is defined as

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