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Effect of oxygenates addition on the flame characteristics and soot formation during combustion of single droplets of a petroleum diesel in air

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HIGHLIGHTS

- Effect of oxygenates on diesel droplet combustion and soot formation was studied.
- Oxygenates addition reduced soot emission, burning rate and flame temperature.
- Soot reduction correlated well with the oxygen content of the fuel mix.
- Ethanol was more effective than methyl oleate in reducing the soot emission.

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ABSTRACT

The effect of methyl oleate and ethanol addition on the combustion characteristics and soot emission of single droplets of diesel was studied by means of experimentation and kinetic modelling. The experiments were performed using a high-temperature tube furnace operating at 973 K and the soot intensity indicated by the soot *KL* factor, and flame temperature were simultaneously measured using a two-colour pyrometry technique and a colour CCD camera. A detailed chemical kinetic calculation was performed using CHEMKIN-Pro. The experimental results showed that adding methyl oleate to diesel significantly suppressed the soot formation. The burning rate and flame temperature of the droplets decreased with increasing methyl oleate addition up to 20 vol% and slowly increased again at methyl oleate addition exceeding 20 vol%. Ethanol addition up to 10 vol% in the diesel also led to less soot formation, lower flame temperature and burning rate. Kinetic modelling showed satisfactory agreement with the experimental results: the effectiveness of ethanol and methyl oleate in soot abatement was linear with the oxygen content in the fuel mixtures with ethanol being more effective than methyl oleate. The kinetic analysis also showed that ethanol utilised its oxygen atoms more efficiently than methyl oleate in suppressing the formation of soot precursors.

1. Introduction

Adding oxygenates into petroleum diesel fuel has been known to reduce particulate matter emissions in CI engines [1–3]. Among all oxygenated fuels reported in the literature, biodiesel and ethanol have emerged as strong candidates [2,3]. Both biodiesel and ethanol have lower tendencies than diesel to produce soot [4]. It has been widely reported in the literature that the additions of biodiesel and ethanol, respectively, into diesel reduced the total amount of particulate matter in the exhaust [4–10]. However, the working mechanisms of ethanol and biodiesel in diesel combustion processes and soot production process are not well understood [9,10].

Literature reports suggest that the overall oxygen content in an oxygenated fuel is the only parameter determining the capability of the fuel in suppressing soot emission [5,6]. Miyamoto et al. [5] found that oxygenated fuels, including di-n-butyl ether, ethylhexyl acetate, ethylene glycol mono-n-butyl ether, and diethylene glycol dimethyl ether, had the same effectiveness in reducing the Bosch Smoke number of the exhaust from a diesel engine when measured by the total oxygen mass fraction added into the base diesel [5]. Albeit interesting, this finding was challenged by many other diesel engine tests results, in which the molecular structure of the oxygenated compounds was also found to have some impacts on the soot emission [7–14]. Some engine experiments suggested that

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alcohols were more effective than ethers and esters in reducing soot [8,9]. Westbrook et al. [15] performed a detailed chemical kinetic simulation to investigate the effect of various oxygenated hydrocarbons on soot precursors in rich premixed homogeneous mixtures of *n*-heptane and oxygenates and found that all the oxygenated fuels tested reduced soot precursors but the extent of these reductions depended on the molecular structure of the oxygenates in the fuel mixtures [15]. However, experimental validation of the model simulation results would help understanding the mechanisms involved. The diverse experimental data from the widely varying diesel engine tests also makes it difficult to obtain the working mechanisms of biodiesel and ethanol in diesel combustion processes, particularly the kinetics involved in reducing the soot emission.

The present work investigated the potential of biodiesel and ethanol addition in petroleum diesel on the combustion characteristics and soot formation using droplets combustion experiments and whether the molecular structure of the oxygenated compounds have some impact in the soot formation. The single droplet experimentation approach has been adopted by many researchers to study the ignition and combustion characteristics of liquid fuels because of its simplicity and capability of providing fundamental perspectives into the combustion processes [16–22]. Detailed kinetic modelling was also carried out in order to understand the working mechanisms of the ethanol and biodiesel additions, respectively, in diesel soot precursor formation process.

2. Experimental

2.1. Materials

A commercial diesel (Caltex No. 2 diesel) and pure ethanol were used for the experimentation. A technical grade methyl oleate (70 vol% methyl oleate with 10 vol% methyl linoleate, 5 vol% methyl palmitate and 5 vol% methyl palmitoleate and other fatty acid methyl esters in balance) was used to represent biodiesel. Justifying the use of methyl oleate, it is a common component of most biodiesel fuels and the kinetic mechanisms of some methyl esters, which have similar chemical structure to methyl oleate, are available. This will make it possible to investigate the kinetic effect of the methyl ester group addition on diesel soot production process without the computational complexity of the actual biodiesel fuel. The thermochemical properties of the methyl oleate together with those of diesel and ethanol are listed in Table 1. For the convenience of discussion in this paper, the blends of biodiesel and diesel or ethanol and diesel are designated by their volume fractions. For instance, D90B10 means 90 vol% diesel and 10 vol% biodiesel and D90E10 means 90 vol% diesel and 10 vol% ethanol.

2.2. Experimental procedures

Single droplet combustion experiments of diesel and biodiesel were carried out using the experimental apparatus as schematically illustrated in Fig. 1. Briefly, the experimental rig consisted of a horizontal tube furnace (600 mm in length and 40 mm in diameter) with temperature control for providing a hot air environment, a droplet suspension system, a step motor for delivering the droplet into the furnace and a CCD camera for measuring flame temperature.

In a typical experiment, the tube furnace was heated to and maintained at 973 K, in which a droplet was ignited and combusted. The droplet was produced by a 10 μL micro-syringe and deposited on the tip of a silicon carbide fibre of 142 μm in diameter. A high speed CCD camera (Basler PIA-210gc) with exposure time of 20 ms was used to capture the images of the entire process from the moment when the droplet entered the furnace until it burned out. The video images taken on the colour CCD camera were subsequently analysed to obtain the flame temperature, soot intensity and burning rate of the burning droplet, following the procedures detailed in Section 2.3. To determine the burning rates from the changing droplet size during combustion, the burning droplet was backlit with a 50 W halogen lamp while being recorded on the CCD camera. A computer was used to operate the step motor and the CCD camera.

2.3. Data analyses

Using the optical images taken on the CCD camera, the soot intensity and the flame temperature were determined using the

Table 1
Major physical properties of diesel, ethanol and methyl oleate.

Fuels	Composition	Density (g ml^{-1})	Boiling point (K)	LHV (MJ kg^{-1})	Latent heat of vaporisation at boiling point (KJ kg^{-1})
Diesel	C10–C18	0.845	473–673	43.4	250
Ethanol	C_2H_6O	0.789	351	29.7	841
Methyl oleate	$C_{19}H_{36}O_2$	0.874	491	40.1	230

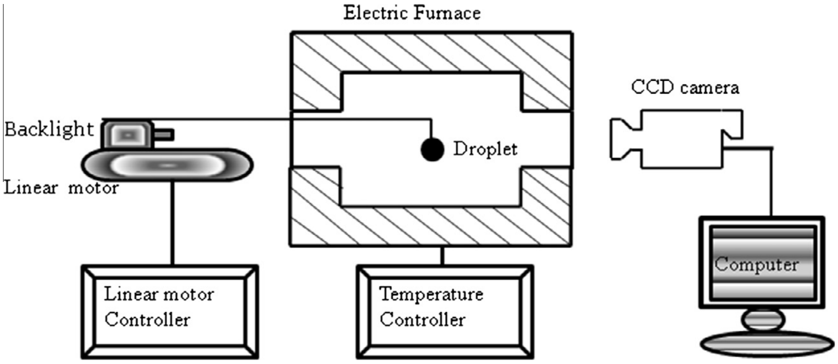

Fig. 1. A schematic diagram of the apparatus for the droplet combustion experiments.