

Impacts of ester's carbon chain length and concentration on sooting propensities and soot oxidative reactivity: Application to Diesel and Biodiesel surrogates

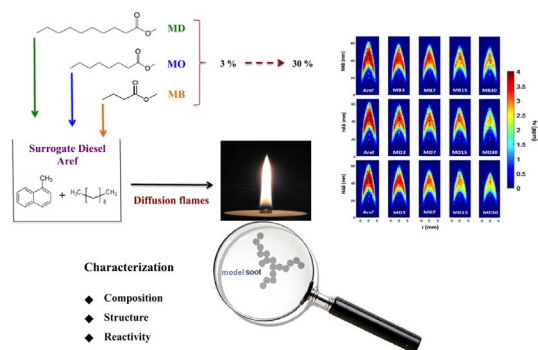
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GRAPHICAL ABSTRACT



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ABSTRACT

This study is devoted to the evaluation of the impact of both esters' carbon chain length and concentration on sooting propensities of Diesel and Biodiesel surrogates. Soot particles were produced using a steady atmospheric axis-symmetric co-flow diffusion flame burner. Concentrations ranging from 3 to 30% (on molar basis) of methylbutanoate (MB), methyl octanoate (MO) or methyldecanoate (MD) were added to a surrogate Diesel made up of a binary mixture of 70% n-decane and 30% α -methyl naphthalene (α -MN). For every considered mixture, the sooting propensity was measured in terms of Yield Sooting Index (YSI) in a methane diffusion flame doped with 3.5% vapor of the mixture. Maps of soot volume fraction in the flame were extracted using a light extinction method (LEM). Soot samples produced along the combustion of surrogate Diesel and Biodiesel fuels were then collected and characterized using physico-chemical techniques, i.e. elemental analysis (CHONS), Thermogravimetric Analysis (TGA), Raman spectroscopy, and Temperature Programmed Oxidation (TPO).

Results evidenced that ester functions contained in Biodiesel surrogates reduce soot production. This decrease was more pronounced when the concentration of the oxygenated additive investigated was higher. However, it has been surprisingly determined that YSI decreases when the aliphatic carbon chain of the ester additive is longer. On the other hand, physico-chemical characterizations of the generated model soot revealed that oxygen and soluble organic fraction (SOF) content decreases when the amount of biodiesel surrogate in the fuel in-

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creases. Nevertheless, no important dissimilarities have been registered in the graphitic structures of the different soot. Finally, the behavior towards oxidation reactivity indicated that the Biodiesel-derived soot were less reactive than the Diesel-derived one.

1. Introduction

As the world energy demand continues to increase, the use of alternative sources of energy that are renewable, sustainable, reliable and ecological has been rapidly expanding in order to meet this growing request [1,2]. Among these bioresources, Biodiesel is a major compound used as a liquid biofuel in transportation [3,4]. It consists of a mixture of highly saturated long carbon chain of alkyl esters ($\approx C_{12}$ – C_{22}) obtained by the conversion of triglycerides contained in vegetable or animal fats with methanol or ethanol [5]. The chemical reaction is called transesterification, which generally occurs in the presence of catalysts [6]. In compression ignition engines, Biodiesel is mostly used blended with conventional Diesel. However, it can completely substitute Diesel fuel for some heavy-duty vehicles that run exclusively on pure Biodiesel “B100” [7]. Due to the complex composition of biodiesel fuels, surrogate model-fuel mixtures, composed of model organic molecules, are generally used in comparative studies between Diesel and Biodiesel. Surrogate model-fuel mixtures have a well known chemical composition leading to a better identification of the different factors that govern Biodiesel combustion process in Diesel engines and affect pollutant emissions [8,9]. Among these toxic emissions that have been proven to be harmful for biosphere, climate, and public health, are particle matters (PM), and more specifically soot particles generally emitted from automobile exhaust following an incomplete combustion of Diesel and Biodiesel blends in the cylinders [10,11]. Nevertheless, Biodiesel fuel contains oxygen and displays chemical and structural properties that can significantly affect combustion processes, therefore ultimate releases such as soot. According to numerous studies, conducted either in laboratory flame conditions [12–17] or in Diesel engine ones [18–20], these dissimilarities that include aromatic and oxygen contents, functional groups, unsaturation, branching, and carbon number, lead to a decrease of soot formation. It has also been reported that the structure of alkyl ester additives influences soot emission [21–25]. Therefore, studies have shown that thermal decomposition and oxidation mechanisms are key factors during soot formation in the flame, hence they need to be taken into account when assessing predictive detailed kinetic models for surrogate fuels incorporating methyl esters [26–29]. This knowledge is especially crucial in the case of biodiesel surrogates in order to simulate the pyrolysis process that occurs in the combustion chamber of a Diesel engine in which soot are produced at first then potentially oxidized at the flame front. Hence, it was shown that the first step of fuel molecule decomposition leads to the formation of CO and CO_2 through either unimolecular reactions or bimolecular H-abstraction reactions [30]. Thus, authors have measured CO_2 and CO yields during the pyrolysis of the biodiesel surrogates and afterwards used the CO_2/CO ratio as a consistent indicator to evaluate the efficiency of the oxygenate compound addition in reducing soot precursors and consequently soot formation [27,5,31–33]. Indeed, the pyrolysis of methyl ester leads to a decrease in the CO_2/CO ratio, which evidences a higher tendency of the Biofuel to reduce soot emissions.

On the opposite, there is a lack of information on the physical and chemical properties of soot particles generated from the incomplete combustion of surrogate Biodiesel in the post flame region. Zhang and Boehman [34] studied the oxidation behavior of soot generated from the combustion of methyl 2-butenate and n-pentane in a laminar co-flow diffusion flame burner. These authors noticed that the fuel-bound oxygen contained in fatty acid esters with the same number of carbon atoms does not affect soot oxidative reactivity. Barrientos et al. [35] extended this previous work and investigated the effect of carbon chain

length and unsaturation degree of ester structures on soot properties and oxidative reactivity. Their results showed that there is an impact of ester composition on soot properties and oxidative reactivity in contrast with Zhang and Boehman's conclusion [34]. Barrientos et al. [35] found that shorter alkyl chain length slightly decrease sooting tendencies and generate less ordered soot structure leading to a higher oxidative reactivity. Furthermore, Omidvarborna et al. [36] investigated the characteristics of soot particles collected from the combustion of large and pure fatty acids (C_{12} – C_{18}), representative of biodiesel blends, in a laboratory combustion chamber. These authors reported that the amount of soot particles emitted is inversely proportional to the portion of Biodiesel in the blend. In addition, particles emitted from Biodiesel combustion were smaller and more reactive than the ones obtained by Diesel blend combustion. However, all these works focused on the characteristics of soot generated from the combustion of pure compounds of Biodiesel surrogate. Recently, Abboud et al. [17] formulated a representative mixture of surrogate Biodiesel, adding different concentrations of methyldecanoate to a binary surrogate Diesel blend. The result showed that the oxygenated additive reduces the sooting tendency. Likewise, these authors noticed a decrease in size and oxidative reactivity of Biodiesel-derived soot when increasing the alkyl ester compound content.

The aim of the present study is to assess the impact of ester carbon chain length on the characteristics and reactivity of model surrogate soot. Blends of surrogate Biodiesel containing different kinds of methyl ester structures were investigated in a laminar co-flow diffusion flame burner operating under well-controlled conditions. Sooting propensities of selected surrogates were first measured in term of yield sooting index (YSI). Model surrogate soot were collected and sampled in order to examine the potential correlation between carbon chain length of alkyl esters and soot properties and oxidative reactivity. To this end, physico-chemical characterizations of soot samples were conducted using elemental analysis of soot particles (CHONS), thermogravimetric analysis (TGA), Raman spectroscopy, and temperature-programmed oxidation (TPO).

2. Evaluation of sooting propensities

2.1. Experimental approach

In the present study, the experimental procedure that enables the quantification of the sooting tendencies is identical to the one outlined in our previous work [17]. The setup allowing for the generation of diffusion flames above an atmospheric axisymmetric laminar co-flow burner has been extensively used by numerous studies [37–42] and have proven to provide appropriate understanding of soot production mechanisms in this kind of flame configuration [43,44]. This setup is here briefly reminded. As shown in Fig. 1, the stream mixture consisting of a carrier gas (CH_4 ; > 99.995% stated purities) and vapors of the surrogate to be investigated flows through a vertical axial brass duct which has an 11 mm inner diameter. The co-flowing oxidizer stream consisting of filtered laboratory compressed air is introduced into a concentric brass cylinder of 102 mm of inner diameter via four bent tubes. Mass flow controllers adjust all flow rates. Table 1 shows the experimental parameters that were kept constant along the present study.

The yield sooting index (YSI) introduced by McEnally and Pfefferle [45] is defined as a linear function of the maximum soot volume fraction ($f_{v,max}$) measured directly in the methane diffusion flames doped with fuel vapors, as follows:

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