



Full Length Article

Impacts of oxygenated compounds concentration on sooting propensities and soot oxidative reactivity: Application to Diesel and Biodiesel surrogates



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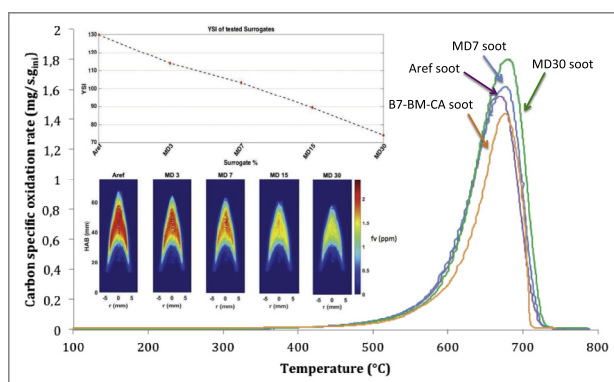
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HIGHLIGHTS

- Adding oxygenated compounds on a surrogate Diesel decreases the sooting tendencies of fuels.
- « Biosoot » present smaller particle size distribution and more ordered graphite-like structures.
- “Bio-soot” are less reactive than Diesel soot in terms of oxidation.
- Soot derived from a co-flow axisymmetric burner are well correlated with “Real-soot” generated on a Diesel engine.

GRAPHICAL ABSTRACT



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ABSTRACT

The aim of this paper is to evaluate the effect of oxygenated compounds concentration on sooting propensities of surrogate Diesel and Biodiesel, and to investigate the oxidative reactivity of soot obtained by combustion of these surrogates using an atmospheric axis-symmetric co-flow diffusion flame burner. For this end, concentrations from 3 to 30% (in mole%) of methyl decanoate (MD) are added to a surrogate Diesel made up of a binary mixture of 70% of *n*-decane and 30% of α -methyl-naphthalene (α -MN). The sooting propensities of these mixtures are here measured in terms of Yield Sooting Indices (YSIs) in methane diffusion flames doped with 35,000 ppm vapors of tested surrogate. Data of soot volume fraction were extracted using light extinction method (LEM). Additionally, soot generated from the combustion of the model Diesel and Biodiesel fuels was then collected, sampled and characterized using physico-chemical techniques. Addition of MD was found to reduce sooting tendencies. This decrease is more pronounced when the concentration of oxygenate additives increases. On the other side, the oxidative reactivity of soot generated from the diffusion flame burner was found to decrease by increasing Biodiesel percentage. Furthermore, soot generated from the combustion of surrogate Diesel and Biodiesel showed different behaviors. Biodiesel-derived soots were smaller and less reactive than Diesel-derived soots. These last displayed less ordered graphite-like structures and higher amorphous carbon concentration.

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1. Introduction

Biofuel sector is gaining more and more ground as it's emerged as one of the best contributors for the reduction of greenhouse gases (GHG) emissions. In fact these products are attained from natural sources and are well known for their renewability and the ability to represent a carbon dioxide-cycle during their combustion through photosynthetic ways [1]. Biodiesel is a synthetic Diesel-like fuel produced from transesterification of triglycerides contained in vegetable or animal fats [2]. It can be used blended or not with conventional Diesel [2,3]. The impact of the combustion of Biodiesel and Biodiesel blends in Diesel engines in terms of emissions, especially particulate matter (PM) has been paid special attention for the past few years [4–7]. Soot represents a significant component of the PM emitted by engines [8]. These emissions contribute to smog and are suspected to affect local climate [9]. Furthermore, the harmfulness of soot particles on human health is mainly attributed to adsorbed species. In fact, soot particles may contain many chemical species: heavy metals, inorganic compounds as well as organic species such as polycyclic aromatic hydrocarbons (PAHs) [10,11]. The latter are classified as carcinogenic, mutagenic or toxic for the reproduction (CMR) by the International Agency for research on Cancer (IARC) [12].

The mechanisms governing soot formation and oxidation in Diesel engines during fuel combustion are complex processes and hard to evaluate. Thence, to a better understanding of fundamental chemical and physical factors leading to soot production, laboratory scale laminar non-premixed flames were used. Studies on academic diffusion flames tended to evaluate the sooting tendencies of various model fuels using Smoke Point as index to assess soot propensity [13–15]. All the previous results on the impact of oxygenated additives on sooting tendencies of surrogate fuels showed that the sooting tendency monotonically decreases with increasing oxygenate concentration in the fuel mixture. Three main factors have been identified: the dilution effect of the base fuel by adding oxygenated additives [16,17], the reduction of the mole fractions of key intermediates that play an important role in the formation of soot precursors [18] and the formation of oxidant radicals that enhances soot oxidation rather than soot formation [19].

Furthermore, McEnally and Pefferle [20] measured the sooting tendencies of 186 oxygenated hydrocarbons in terms of Yield Sooting Index (YSI). These authors found that direct chemical effects associated with the structure of additives mainly govern the measured trends. At a given carbon number, the YSI increases in the following order: ethers < primary alcohols \approx *n*-alkanes < secondary alcohols. They also found that the molecular structure of ester compounds plays a key role and has more effect on soot suppression compared to the carbonyl compounds with a single oxygen atom like alcohols and ethers.

The structure, the composition and the morphology of soot depend largely on their origin and the conditions of production. This fact has triggered a debate in order to highlight which of these factors most contribute and affect soot reactivity. Many studies have correlated soot characteristics and reactivity with the internal structure (nanostructure) of its primary particles, which depends, among others, on the type and origin of fuel [21,22]. As an illustration, Vander Wal and Tomasek [23] showed that soot nanostructure depends first of all on the synthesis conditions like temperature, time and the nature of the fuel. They also evoked the dependence of reactivity on the relative number and accessibility of potential reactive carbon edge sites.

Other studies emphasized the role of the composition of tested fuels, more specifically the impact of oxygenate additives on soot

formation and reactivity. For instance, Soeong and Boehman [19] suggested that the earlier soot is formed in a given flame, the less reactive it will be when it escapes from the flame tip. They also found that surface oxygen content is proportional to soot oxidative reactivity and may be the governing factor for increased oxidation reactivity of oxygenated soot. On the other hand, Ghiassi et al. [24] studied the impact of *n*-butanol addition at different mole fractions (10%/30%/60%) on a Diesel surrogate, i.e. *n*-dodecane. By quantifying soot stability during oxidation process, they found that the oxidation reactivity increases with increasing alcohol percentage up to 30%. After this they noticed a decrease of activity at 60% *n*-butanol even though that the amount of soot produced was less. They attributed this non-monotony of reactivity to dissimilar nanostructure. In fact soot derived from 30% *n*-butanol has shorter carbon segments on the other hand the one derived from 60% has higher amount of layer planes with high curvature. This latter nanostructure was suggested to be less active than the first one.

Barrientos et al. [25] studied soot samples generated from the combustion of various methyl esters, *n*-alkanes, Biodiesel and Diesel fuels in laminar co-flow diffusion flames via thermogravimetric analysis (TGA) and Raman spectroscopy. It was found that ester compounds contained in Biodiesel have an impact on soot oxidative reactivity and soot characteristics. Along the combustion of shorter alkyl chains of methyl esters, soot particles generated exhibit higher soot reactivity and lower structural ordered. The authors also found that the impact of fuel-bound oxygen on the reactivity of soot becomes less significant as the carbon chain length increases.

Similar studies were performed in the case of real soot produced on test bench. Song et al. [26] studied the reactivity of soot derived from the combustion of neat Biodiesel (B100), ultra-low sulfur Diesel (ULSD), Fischer-Tropsch synthetic Diesel fuel (FT100) and ULSD blended with 20% Biodiesel. In order to explain the high reactivity found in B100 derived soot, the authors speculate that B100 derived soot undergoes a unique oxidation process called "internal burning" leading to a total destruction of the core and eventual formation of graphene layer structures. It was also discussed that not only the initial nanostructure determine the reactivity of soot but also the degree of internal structure change during oxidation has a strong influence as well. In other study [27] it was found that the abundance on the soot surface of oxygen functional groups could enhance soot reactivity. This incorporation of oxygen due to the use of Biodiesel may be more crucial than the initial structure and pore size distribution of soot particles in terms of soot oxidative reactivity. In addition to the high oxygen content, López-Suarez et al. [28] attributed the higher reactivity of B100 soot to the presence of metallic impurities which can play a catalytic role.

In the present work Diesel and Biodiesel surrogates are incorporated into the fuel stream burning in a laminar co-flow diffusion flame. The burner used especially allows the conditions to be strictly controlled. Thus, the impact of various oxygenated compounds like esters on both sooting tendencies and soot oxidative reactivity can be assessed. The sooting tendency of selected surrogates was measured in term of the yield sooting indices (YSIs) in methane diffusion flames doped with the vapors of tested fuels. The structure and the oxidative reactivity of soot samples generated from the combustion of these surrogates are investigated using temperature-programmed oxidation (TPO), thermogravimetric analysis (TGA) and Raman spectroscopy. The results are contrasted with those featuring the reactivity of soot generated by a real Diesel engine.

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