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Modeling soot formation in diesel-biodiesel flames

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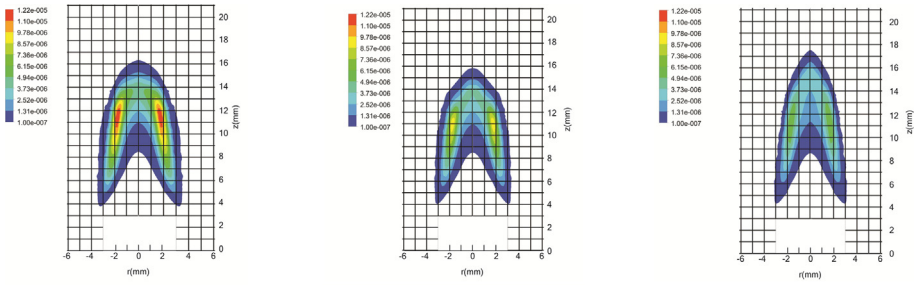
HIGHLIGHTS

- A new phenomenological soot model is proposed for diesel-biodiesel blends.
- The model takes into account the main soot-reducing factors of biodiesel blending.
- The model is solved for the standard smoke point lamp using CFD.
- The model computations are in very good agreement with published experimental results.

GRAPHICAL ABSTRACT



Computational soot volume fraction reduction in the smoke point lamp with the proposed phenomenological soot model from diesel B0 (left) to B20 diesel-biodiesel blend (middle) and B60 diesel-biodiesel blend (right)

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ABSTRACT

We propose a modified phenomenological model for soot formation that occurs during the combustion process of diesel-biodiesel blends. The diesel-biodiesel blend is represented by three generic fuel groups: aromatic, aliphatic, and ester fuels, such that the aromatic content of the diesel fuel and the oxygen content of the biodiesel fuel are considered quantitatively. The soot formation is evaluated for specific selected blends. The different oxidative reactivity between soot particles originating from diesel and biodiesel is accounted for via their oxidation rates. The use of the present phenomenological soot model is demonstrated by its implementation in a computational fluid dynamics (CFD) commercial code for the case of the standard smoke point lamp. Very good agreement was achieved between model predictions and experimental results in terms of maximal soot volume fraction (SVF) and its decrease when switching from plain diesel to a diesel-biodiesel blend.

1. Introduction

Today, particulate emission from diesel engines constitutes a major environmental problem. In June 2012, the World Health Organization classified diesel engine exhaust as carcinogenic [1]. In 2014, the European Environment Agency reported that at present, particulate matter (PM) and ground level ozone are Europe's most problematic pollutants for human health [2]. Our research focuses on biodiesel blending as a means of decreasing diesel particulate emissions.

Abbreviations: 1-MNa, 1-methylnaphthalene; B0, plain diesel; B20, diesel-biodiesel blend containing 20% biodiesel by liquid volume; B60, diesel-biodiesel blend containing 60% biodiesel by liquid volume; B100, biodiesel; CFD, computational fluid dynamics; Coag, coagulation; coll, collision; EEA, European Environment Agency; F&J, Fenimore and Jones model; HAB, height above burner; IDEA, Integrated Diesel European Action; LII, laser-induced incandescence; MD, methyl decanoate; NSC, Nagle and Strickland-Constable model; Nuc, nucleation; oxid, oxidation; P, soot particle; PAHs, polycyclic aromatic hydrocarbons; PM, particulate matter; PR, soot precursor; ppm, parts per million; Sur, surface growth; SVF, soot volume fraction; UDFs, user-defined functions; WHO, World Health Organization.

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Soot is a particulate carbonaceous matter with a characteristic lattice structure. It is formed during high temperature pyrolysis or combustion of hydrocarbons. It consists mainly of carbon and small amounts of other elements, such as hydrogen and oxygen [3]. Diesel engine exhaust gases are among the main sources of soot [4], and the main component of diesel particulates is soot on which organic compounds adsorb or condense [5].

Small particulates formed during combustion and suspended in the atmosphere have adverse health effects. The soluble organic fraction of diesel particulates includes compounds that may cause health and environmental hazards [5]. In particular, the association of polycyclic aromatic hydrocarbon (PAHs) with particulates has been suggested as a cause for particulates' hazardous health effects [6]. In addition, particulates play a significant role in the radiative balance of the atmosphere, thereby contributing to global warming, depending on their size, concentration, and optical properties [3].

Models of soot formation can be classified into three major groups: empirical, detailed, and phenomenological. The empirical models are based on correlations of soot emissions versus system parameters and combustion conditions and are usually very specific to fuel type, composition, and combustion chamber structure. The detailed models attempt to meticulously describe soot formation by means of hundreds or even thousands of chemical equations while using dozens to hundreds of chemical species and their respective rate equations. The phenomenological models assume that the formation of soot particles can be represented by only a small number of global processes with their respective rate equations. While phenomenological models are based on physical and chemical processes of soot formation, their moderate level of complexity constitutes a significant advantage for understanding these complex processes and their application in CFD codes.

While Kennedy [7] thoroughly reviewed earlier models of soot formation and oxidation, the following survey will focus on later models of soot formation and oxidation relevant to the present study. In a series of studies, Foster, Reitz, and their colleagues developed a 9-step phenomenological model and studied soot formation in diesel engines [8–13]. Their latest nine-step model [13] assumed the formation of growth species (acetylene) as a direct product of fuel pyrolysis and subsequent formation of a precursor from the growth species while neglecting the direct formation of a precursor from the fuel. This model included particle nucleation from soot precursors, coagulation, particle surface growth by growth species, particle oxidation by O_2 and OH, growth species oxidation, and precursor oxidation. The most fundamental weakness of their recent model is its inability to predict differences in soot formation for different fuels [14]. In particular, their model does not account for the effects of the aromatic content of the fuel on soot formation. While PAH deposition on the particle surface was included in a previous model presented by Kazakov and Foster [9], this feature was neglected in a later model [13]. Brookes and Moss [15] proposed a soot model based on calculations of methane turbulent jet diffusion flames. The Moss-Brookes model is available in the ANSYS FLUENT software. In this model, acetylene serves as both a precursor and a growth species. The reactions include soot particle nucleation from acetylene, surface growth of soot particles by acetylene, soot particle oxidation by OH radicals, and soot particle coagulation. Two conservation equations are solved: one for the soot mass, and one for the soot particle number.

Hall et al. [16] suggested a soot model in which the following processes were included: nucleation, acetylene-assisted soot particle surface growth, oxidation by OH radical, oxidation by O_2, and coagulation. The nucleation rate of Hall et al. [16] was expressed as the sum of formation rates of two-ring and three-ring aromatic species, $C_{10}H_7$, and $C_{14}H_{10}$, respectively. These formation rates were calculated from the concentrations of acetylene, benzene, phenyl radical (C_6H_5), and hydrogen.

Jay et al. [17] and Knop et al. [18] suggested a phenomenological soot model for diesel engines based on alkane fuel. They added reactions of acetylene formation from ethylene and acetylene oxidation to the four-step alkane oxidation model of Hautman et al. [19]. In their model, where PAH served as a precursor, they included its formation from acetylene, nucleation by the collision of two PAHs, acetylene-assisted particle surface growth, PAH-assisted particle growth, coagulation, PAH oxidation, and particle oxidation by O_2 and OH.

While the above phenomenological models were all based on a single model fuel, blending plain diesel and biodiesel can be used to reduce soot emissions from diesel engines. The blended biodiesel affects the formation and oxidation rates of the soot particles and thereby reduces the soot volume fraction. In addition, model fuel blending makes it possible to account for two major soot-reducing factors: the absence of aromatic compounds in the biodiesel and its oxygen content. The former is achieved by incorporating the aromatic model fuel into the model fuel blend, whereas the latter is obtained by incorporating the ester model fuel into it. The previous phenomenological models were unable to address the fuel blending effects, in particular of diesel and biodiesel fuels, on soot formation, oxidation, and emission. Here we propose to modify the single fuel model by blending three generic representative fuels, i.e., 1-methylnaphthalene (aromatic), n-decane (aliphatic), and methyl decanoate (ester) fuels. Each of these fuels represents a different generic group typically contained in diesel-biodiesel blends. The diesel fuel is represented by a blend of aromatic and aliphatic model fuels. The biodiesel fuel is represented by the ester model fuel. When biodiesel is added to the diesel blend, the ester fuel concentration increases at the expense of the aromatic fuel concentration, which decreases. The oxygen content in the fuel blend increases with the ester fuel concentration increase. The aromatic content of the fuel blend decreases with the decrease in aromatic fuel concentration.

In this study, a new phenomenological model of soot formation was developed for diesel-biodiesel blends. To the best of our knowledge, the proposed phenomenological soot model is the first phenomenological model for diesel-biodiesel blends and the first phenomenological model that takes into account diesel aromatic content. This model takes into consideration the main factors for soot emission reduction when using biodiesel or diesel-biodiesel blends. The proposed fuel blend makes it possible to consider the diesel aromatic content and the biodiesel oxygen content quantitatively. The different oxidative reactivity between soot particles that originate from diesel and biodiesel is taken into account in their oxidation rates. The present phenomenological soot model was implemented in CFD calculations for the standard smoke point lamp. The results were compared with previously published experimental results. The main factors for soot emission reduction when using biodiesel or diesel-biodiesel blends are described in Section 2. The proposed phenomenological soot model is described in Section 3. The CFD methodology is described in Section 4. Section 5 includes the literature soot measurements, the present respective computational results, and their comparison. Finally, the conclusions of the study are presented in Section 6.

2. The effects of biodiesel on soot formation and oxidation

Biodiesel is a general name for mixtures of long chain esters, generally methyl or ethyl esters, used as fuels in diesel engines. Biodiesel is produced by transesterification, usually of vegetable oils, with short chain aliphatic alcohols, usually methanol or ethanol. Most researchers agree that diesel engine particulate matter