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Numerical study of soot particles from low temperature combustion of engine fueled with diesel fuel and unsaturation biodiesel fuels

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HIGHLIGHTS

- Engine combustion was numerical studied with a quad-component biodiesel mechanism.
- Less soot exhausted from biodiesel fuel engine combustion than that fueled with diesel fuel.
- Biodiesel fuel with higher fraction of unsaturated FAMEs produces more soot precursor.

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ABSTRACT

In this study, numerical analysis of fuel structures on engine soot particles' mass and size were done by CFD combustion modelling using diesel and different levels of unsaturated biodiesel fuels through the KIVA4-CHEMKIN platform. The proposed numerical approach, with a quad-component skeletal mechanism of biodiesel blend surrogates along with a multi-step phenomenological soot particle model, could capture the soot particle characteristics of test fuels with acceptable accuracy under engine combustion conditions. The reduction of exhaust soot from biodiesel combustion, compared to diesel fuel, was attributed to the suppressed soot precursors formation and lower number of particles in total. However, it was concluded that the biodiesel fuel with a higher fraction of unsaturated FAMEs (more double carbon bonds C═C) contributed more to the formation of soot precursors, thus producing a higher amount of soot particles in mass and numbers as a consequence of accelerated soot particle nucleation and soot surface growth.

1. Introduction

Over the past decades, regulators throughout the world have taken major steps to mitigate the negative health impacts on humans caused by cars, buses, trucks, non-road diesel engines, as well as other transportation-related pollutants. This drives the formulation of the next generation of fuels, filters as well as advanced emissions control technologies and strategies, which will cause the black smoke of an old diesel bus or truck a thing of the past. All of these great progresses have occurred as result of the increasing understanding of the strong link between Particulate Matter (PM) emissions from diesel-fueled vehicles to fatal human health impacts, including increased asthma emergencies, cancer, heart and lung diseases, and premature death.

The particulates are composed primarily of agglomerated solid carbonaceous material (i.e. soot), liquid phase hydrocarbons and a small portion of adsorbed sulphates. Primary particles are formed during the early stages of soot formation from molecular precursors like polycyclic aromatic hydrocarbons (PAHs) after fuel decomposition, and can grow via two mechanisms, either by collision coagulation (physical process) or by surface growth (chemical process). The smaller the particles are (smaller than 2.5 μm in diameter), the greater the impact on human health. They are not major factors towards overall PM mass, but these fine particles contribute the most to the overall Particle Numbers [1]. The control strategies of PM mainly fall into three general categories. They are fuel based strategies (e.g., changing fuel properties and introducing alternative biodiesel fuel [2,3]); engine-based strategies (e.g., optimized combustion clean combustion [4,5]); and strategies focused on emissions abatement before they leave the tailpipe (known as after treatment technologies like diesel particulate filters [6]).

To achieve the goal of formulating the fuel of the future, intensive investigation were carried out on new surrogate fuels that could be easily produced within the techno-economic constraints of a refinery and that have the potential to reduce pollutant emissions when being added to fossil-derived fuels. Now, biodiesel has been considered as a promising fuel to substitute diesel fuel because it is renewable,

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biodegradable, lower in sulfur and aromatics, higher flash point and higher in cetane number, which can fill the gap of energy shortage while maintaining the engine's efficiency [7,8]. Normally, biodiesel refers to a mixture of long carbon chain fatty acids methyl esters (FAMEs) consisting of saturated and unsaturated compounds obtained by transesterification of the triglycerides contained in vegetable oils and animals fats. With the diversity of the feedstock that is being used, the concentrations of types of methyl esters in biodiesels are different from each other, leading to the diversity of chemical and thermo-physical properties for biodiesel surrogates, thus in turn result in the differences on biodiesel's performance, combustion and emission characteristics [9].

The previous findings concluded that the chemical compositions of emitted particulate matter (PM) were much more sensitive to the degree of unsaturation of the methyl esters present in biodiesel. Salamanca et al. [10] found that linseed biodiesel fuel would produce more particulate matter and hydrocarbons than Palm biodiesel fuel due to its higher level of unsaturated composition, hence favoring the soot precursor formation during the combustion process. Similar results had also been noted by Sarathy et al. [11] through both experimental and numerical tests on combustion of Methyl Butanoate and Methyl Crotonate in the opposed-flow diffusion flame and jet stirred reactor. It was found that the burning of unsaturated FAME produced greater sooting tendency than the saturated FAME due to the presence of C═C bound in MC.

Most studies showed significant PM reduction using neat biodiesel fuel or diesel–biodiesel blend fuels compared to pure diesel fuel [2,3,12–14]. These variations are mainly attributed to the suppressed formation of soot precursors along with enhanced soot oxidation due to the oxygen content as well as the absence of sulfur and aromatic in biodiesel fuels. Meanwhile, it was found by Wang et al. [15] that the soot precursor, acetylene, generated in the biodiesel pyrolysis was proportional to the concentration of unsaturated fatty acid methyl ester (the number of C═C double bonds). In addition, the double bonds of methyl ester were strongly correlated with gaseous emissions like CO and HC, which further influenced the formation of soot particles both in nucleation mode and in accumulation mode [16].

Given that the biodiesel fuel decomposition is much more complex than its counterpart like diesel fuel, as well as the impact of unsaturation degree of biodiesels on physical properties (cetane number, heat of combustion and viscosity), it is necessary to investigate the combustion characteristics of varied FAME fuels to figure out the impacts of fuel structure on soot particle characteristics in order to achieve ultra-low emissions footprint. In our previous studies [17–19], a skeletal quad-component biodiesel combustion mechanism comprising methyl decenoate, methyl-5-decenoate, *n*-decane and methyl linoleate was proposed and the feasibility of this new model had been widely tested against ignition delay and in-cylinder heat release based on available experiments. Good performances of the effects of fatty acid methyl esters proportion on combustion and NOx emission characteristics were also discovered. In this study, numerical analysis of fuel structures on soot particles was given by CFD modelling of combustion using different levels of unsaturated fuel in engine operating conditions. Comparison of the combustion with soot particles between biodiesel and diesel was driven by our quad-component skeletal mechanism of biodiesel blend surrogates [17] along with a multi-step phenomenon soot particle model [20]. Furthermore, the influence of fuel structures on soot particles mass and size was conducted from the perspective of chemical and physical properties among test fuels by tracking the overall soot formation process.

2. Numerical approach

2.1. Biodiesel reaction mechanism

Derived from animal fat or vegetable oil, the typical biodiesel fuels usually contain five long carbon chain FAMEs as the major components: Methyl Palmitate ($C_{17}H_{34}O_2$, $C_{16:0}$) and Methyl Stearate ($C_{19}H_{38}O_2$, $C_{18:0}$) as saturated FAMEs; Methyl Oleate ($C_{19}H_{36}O_2$, $C_{18:1}$), Methyl Linoleate ($C_{19}H_{34}O_2$, $C_{18:2}$) and Methyl Linolenate ($C_{17}H_{32}O_2$, $C_{18:3}$) as unsaturated FAMEs [9]. The quad-component skeletal mechanism of biodiesel fuel used in this study was derived by Liu et al. [17], which including four components as the surrogate fuel: Methyl Decanoate (MD), Methyl-5-Decenoate (MD5D), ML and *n*-decane. The first species MD is designed to stand for the saturated FAMEs, while MD5D and ML are unsaturated FAMEs that contain C─C double bonds, and *n*-decane is added to balance input energy as well as ratio of C/H/O. The reaction mechanism of the multi-component biodiesel fuel, consists of 160 species and 263 reactions, was integrated into KIVA4-CHEMKIN II code for the corresponding computational fluid dynamic numerical study of engine combustion.

In this study, Rapeseed biodiesel and Sunflower biodiesel were chosen to test against the reference diesel fuel on the same engine operating since these two kinds of biodiesel fuels have different unsaturation levels and. According to our previous findings [19], the chemical ignition delay time and kinetic viscosity of biodiesel fuel are sensitive to the unsaturation levels as well as the double bond contents, but the relationship between saturation levels and combustion features are still not straightforward. Therefore, Table 1 gives the physical properties of the test fuel including diesel and the biodiesel fuels in this study. Biodiesels have higher densities and viscosities but lower heating values and sulfur content compared to the diesel fuel. Moreover, according to the weight proportion of fatty acid methyl esters in the two biodiesel fuels in Table 2, the unsaturation level of Rapeseed biodiesel is higher than that of Sunflower biodiesel; as a consequence, the cetane number, heat of combustion, and viscosity of neat fatty compounds increase with the increase of chain length and decrease with unsaturation level [16]. The obvious feature of physical and chemical properties of diesel and biodiesel fuel will in turn result in the differences on engine's performance, combustion and emission characteristics

2.2. Numerical models

In this study, numerical modelling was conducted using the KIVA4 platform coupled with CHEMKIN II code. FORTRAN programming had been done to improve the fuel evaporation model and cavitation induced spray break up model in our previous studies. The Taylor Breakup model which is the original sub-model for breakup process has been replaced with the Kelvin–Helmholtz and Rayleigh–Taylor with cavitation induced spray break up model [21,22] and RNG (Re-Normalization Group) k–Ɛ model [23] is selected for turbulence.

The thermo-physical proprieties such as latent heat of vaporization, liquid density, viscosity, surface tension, vapor pressure and thermal conductivities of methyl esters like $C_{16:0}$, $C_{18:1}$ and $C_{18:2}$ were calculated using the methodologies introduced by Ref. [24], and these methyl esters are taken as MD, MD5D and ML, respectively. What's moreover,

Table 1
Physical properties of the test fuel in this study.

	Density (kg/m^3)	Viscosity at 40 °C (cSt)	Sulfur content (ppm)	Cetane Number	Heating value (MJ/kg)	Oxygen content (wt%)
Diesel (ULSD)	827	2.47	26	50	43.3	0
Rapeseed bio-diesel	882	4.48	1.5	51–59	37.4	10.84
Sunflower bio-diesel	860	4.72	2.4	61.2	39.6	10.49