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Modeling study of oxygenated fuels on diesel combustion: Effects of oxygen concentration, cetane number and C/H ratio

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ABSTRACT

The present modeling study aims to gain better insights on the effects of oxygenated fuels on the diesel oxidation and emission formation processes under realistic engine operating conditions. To do that, various blend fuels formulated from diesel, biodiesel, ethanol and DMC fuels were obtained with different oxygen concentrations, cetane numbers and C/H ratios. Simulations were conducted using the coupled KIVA–CHEMKIN code on a light duty diesel engine at a fixed engine speed of 2400 rpm under full load conditions. Constructed numerical simulation models integrated with detailed chemical kinetics were validated against the experimental results with reliable accuracies. Simulation results revealed that as the overall oxygen concentration of the blend fuel increased, significant beneficial effects were shown with reduced NO_x, CO and soot emissions. Particularly, with the increase of oxygen concentration, the peak CO concentration and its final emission level were found to be remarkably reduced due to the fuel borne oxygen, reduced carbon influx as well as the possibility accelerated CO oxidation rate. More tangible reductions were shown on the soot emissions probably because the C–O bond in the oxygenated blend fuels had played an important role in inhibiting the carbon atoms from soot formation. Furthermore, as oxygenated fuels were added, the peak concentration of the soot precursor C_2H_2 species and small hydrocarbon intermediates such as C_2H_4 and C_2H_6 were also significantly reduced. In general, it was found that compared to the effects of physical properties such as cetane number and C/H ratio of the blend fuel, the overall oxygen concentration seemed to be the major factor dominating the emissions and major intermediate species formation processes.

1. Introduction

Among the various types of internal combustion (IC) engines, diesel engine plays a dominant role in the field of transportation due to its superior fuel economy. It has a higher thermal efficiency as compared to gasoline or turbine engines due to its high compression ratio and low exhaust losses. However, despite many merits of diesel engine, it still suffers from the inherently high particulate matter (PM) and nitrogen oxides (NO_x) emissions, which has posed great challenges to the engine manufacturers. To meet the ever-increasingly strengthened emission regulations, many research activities have been devoted to combustion optimization, aiming to significantly reduce the PM and NO_x emissions. Besides the many techniques that have been developed and utilized such as high injection pressure, exhaust gas recirculation, water induction, or selective catalytic reduction, the use of oxygenated fuels such as biodiesel has been identified as one of the promising solutions to modify fuel compositions in the form of additives, significantly optimizing the combustion process and reducing the PM emissions.

Biodiesel derived from vegetable oils or animal fats can serve as a reliable, long-term alternative energy source. It shows similar physical properties as conventional diesel which provides the ease of application in modern diesel engines even in its neat form. Previous studies have demonstrated that as an oxygenated fuel, biodiesel produces cleaner combustion with reduced carbon monoxide (CO), unburned hydro-carbon (HC) and PM emissions [1–5]. However, it has also been identified that the large kinematic viscosity of biodiesel is one of the major drawbacks that limits its spray and atomization processes, eventually deteriorating its performance and emissions especially during cold weather applications. As a practical solution, some researchers [6–14] have been suggesting the partial replacement of diesel with biodiesel blended with small proportion of low viscosity oxygenated fuels, rather than solely replacing fossil diesel with biodiesel. The technical merits of a properly designed ternary fuel of diesel, biodiesel blended with a low viscosity oxygenated fuel are: (i) it can alter the physical properties of the blend fuel to regain the desired viscosity, volatility and

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cetane number, (ii) it can increase the optimum biodiesel blend ratio and stability especially under cold temperature environments and (iii) it could significantly reduce the PM emissions through increasing the overall oxygen content. For example, Wang et al. [6] constructed various pairs of blend fuels consisting of diesel, biodiesel blended with ethanol or dimethyl carbonate (DMC) to explore their potential on PM reductions. It was proposed that an oxygenated blend fuel formulated from 50% biodiesel, 15% DMC and 35% diesel was able to meet the China 4th Stage Standard (equivalent to Euro IV) for heavy duty diesel engines without the use of exhaust aftertreatment devices. Tüccar et al. [7] experimentally investigated the effects of diesel–biodiesel–butanol blend fuels on the performance and emissions of a diesel engine. It was discerned that the measured physical properties such as density, viscosity, cetane number and pour point of the diesel–biodiesel–butanol mixture were very comparable to those of diesel fuel. The engine testing results further revealed that although butanol addition caused slight reductions on the engine brake power and output torque, the CO, NO_x and smoke opacity values were significantly improved. A similar study was also conducted by Zhang and Balasubramanian [8] who focused on the effects of butanol addition on diesel/biodiesel blend fuel's engine performance, $PM_{2.5}$ and carbon concentrations, particle number concentrations and size distribution as well as particle-phase PAHs emissions. It was reported that when butanol was added by up to 10% to B20 blend (20 vol% PME (Palm Methyl Ester) and 80 vol% diesel), the ternary fuels showed a slight increase in the thermal efficiency under medium and high engine loads. Compared to B20, the addition of butanol further reduced the $PM_{2.5}$ concentrations by 1.9–5.5%, 4.3–18.7% and 6.9–25.0%, respectively from low to high engine loads, out of which most reductions were attributed to the reduction of element carbon (EC) reductions. Furthermore, the addition of butanol could also effectively reduce the particle number concentrations, particle geometric mean diameter and total particle-phase PAHs emissions comparing to diesel/biodiesel blend fuels. In addition to the above experimental investigations concerning the use of ethanol–biodiesel–diesel or butanol–biodiesel–diesel fuel blends, there are also some modeling studies analyzing the effects of oxygenated fuel addition on diesel combustion. In the earlier studies, Zannis et al. [15] numerically simulated and compared the effects of oxygen addition on diesel combustion by increasing the partial pressure of oxygen in the intake air and by oxygenating the fuel. The comparison results showed that both techniques produced increased cylinder pressure and reduced soot formation, with the fuel oxygenation being more effective. However, the drawback is that both techniques increased NO_x emissions, with the fuel oxygenation being more detrimental. Later, Chen et al. [16] numerically examined the effects of oxygenated fuel addition on premixed n-heptane flames. Three types of fuels including methanol, dimethoxymethane (DMM), and dimethyl carbonate (DMC) were investigated, and the mole fraction profiles of major and intermediate species were predicted and validated against experimental results. It was found that as oxygenated fuels were added, mole fractions of most C_1–C_5 hydrocarbon intermediates were reduced by 10–30% while that of benzene decreased apparently. A similar work was also performed by Xu et al. [17] who experimentally and numerically studied the effects of methanol and ethanol addition on a laminar premixed low-pressure n-heptane/toluene flame. The same carbon flux and equivalence ratio were maintained for all tested flames, and the mole fraction profiles of major species including most aromatic species were computed and validated against measured results. It was identified that with the addition of alcohols, massive HO_2 and OH radicals were induced in the intermediate temperature regions and the rate of toluene consumption through hydrogen abstraction increased. For this reason and together with the partial replacement of toluene with alcohols, the toluene consumption rate decreased significantly in the high-temperature zones, thereby significantly inhibiting the formation of polycyclic aromatic hydrocarbons (PAHs).

Following the above experimental and modeling studies, the objective of this work is to gain better insights on the effects of oxygenated fuels on diesel combustion under realistic engine operating conditions. Various blend fuels are constructed for diesel, biodiesel blended with ethanol or DMC fuels, and the compositions for each blend fuel are specially formulated to characterize the oxygenated fuels with different oxygen concentrations so that the effects of oxygen concentration, cetane number and C/H ratio can be extensively evaluated by investigating the impacts on major exhaust emissions of CO, NO_x and soot, as well as by determining the major factors responsible for these observed changes.

2. Numerical approaches

2.1. Numerical models

The effects of oxygenated fuels on diesel combustion were numerically simulated using the coupled KIVA–CHEMKIN code which was developed based on the multi-dimensional CFD simulation software KIVA4 and CHEMKIN II code [18–20]. It is a specially developed framework for the transient analysis of two or three dimensional, chemically reactive flows and sprays inside the combustion chamber, with detailed chemistries. It employs the finite volume scheme to solve the conservation of mass, momentum and energy equations, and uses the CHEMKIN package code to formulate and solve the complex gas phase chemical kinetics. It comprises many mathematical models to account for the liquid fuel spray, breakup, collision and coalescence, and evaporation processes, with the RNG k–ε model to characterize the turbulent properties of the flow. Different from the original KIVA4 code, the Kelvin–Helmholtz and Rayleigh–Taylor (KH–RT) hybrid breakup model was integrated to replace the original Taylor Analogy Breakup (TAB) model for better spray simulation accuracies. Detailed mathematical models can be found in [18,21]. The computational mesh was constructed based on the piston bowl geometry of a four-cylinder, turbocharged, direct injection diesel engine, and some major specifications of the test engine is shown in Table 1. To take advantage of the symmetric distributions of the injector nozzle holes (6 holes), numerical calculations were performed using a 60 degrees polar sector mesh with the piston crevice region included as shown in Fig. 1. Mesh independence test has been conducted in our previous works [22] and will not be discussed here.

2.2. Kinematic mechanism

A multi-component fuel skeletal mechanism developed by us in [23] was employed to emulate the ternary fuel oxidation of diesel, biodiesel blended with ethanol or DMC. A brief description on the development process is provided here. It starts with the generation of a reduced reaction mechanism which could treat both ethanol and DMC oxidation reactions using the directed relation graph with error propagation and sensitivity analysis (DRGEPSA) method

Table 1
Engine specifications.

Engine type	Four stroke, DI, water cooled
Number of cylinders	4
Bore × stroke	92 × 93.8 mm
Connecting rod	158.5 mm
Compression ratio	18.5:1
Rated power	75 kW at 3600 rpm
Fuel injection system	Common rail, Denso