

A Numerical Study of the Effects of FAME Blends on Diesel Combustion and Emissions Characteristics Using a 3-D CFD Code Combined with Detailed Kinetics and Phenomenological Soot Formation Models

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ABSTRACT

The objective of the present research is to analyze the effects of using oxygenated fuels (FAMES) on diesel engine combustion and emission (NO_x and soot). We studied methyl oleate (MO), which is an oxygenated fuel representative of major constituents of many types of biodiesels. Engine tests and numerical simulations were performed for 100% MO (MO100), 40% MO blended with JIS#2 diesel (MO40) and JIS#2 diesel (D100). The effects of MO on diesel combustion and emission characteristics were studied under engine operating conditions typically encountered in passenger car diesel engines, focusing on important parameters such as pilot injection, injection pressure and exhaust gas recirculation (EGR) rate.

We used a diesel engine complying with the EURO4 emissions regulation, having a displacement of 2.2 L for passenger car applications. In engine tests comparing MO with diesel fuel, no effect on engine combustion pressure was observed for all conditions tested. However, combustion was enhanced by using MO under low temperature and high EGR rate (high equivalence ratio) conditions. Using MO, soot emission was significantly reduced without a concomitant increase in NO_x emission, but the apparent brake specific fuel consumption (BSFC) was worsened. However, the brake specific energy consumption (BSEC), defined on an energy basis, did not change significantly between the tested fuels. In addition, CO and THC emissions were reduced by using MO. These effects were due to the enhancement of low temperature reactions with oxygenated fuels like MO.

We also conducted a 3-D numerical study using the KIVA-3V code with modified chemical and physical models. To predict soot emission, a model dealing with the formation of precursors including polycyclic aromatic hydrocarbons (PAHs) was coupled with a detailed phenomenological particle formation model, taking into account soot nucleation from the precursors, surface growth/oxidation and particle coagulation. We adopted an engine condition of 25% load and 1500 rpm because it is typically encountered in the NEDC mode.

The calculated in-cylinder pressure traces and heat release rates (HRRs) for all the fuels were in close agreement with the measured engine data and the results on soot emission also agree with analyzed data. Further, the numerical results suggested that the oxygenated fuel did not greatly affect soot oxidation rates and rates of oxidation by OH radicals. Instead, soot nucleation from the precursors and surface growth were found to be major factors influencing soot emission for the oxygenated fuel.

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INTRODUCTION

Global warming and fossil depletion issues are of increasing concern in the transportation sector. To help alleviate these problems, diesel engines with high-efficiency

and low fuel-consumption are being introduced in the worldwide market. However, the exhaust from diesel engines contains high particulate matter (PM). Biodiesel fuel (BDF) has attracted considerable interest over the last few decades as a potential substitute for fossil fuels. In addition to being a

Table 1. Components of BDFs

Material	Fatty acid methyl ester %									
	Caprylic acid methyl ester	Methyl decanoate	Methyl laurate	Methyl myristate	Methyl palmitate	Methyl stearate	Methyl oleate	Methyl linoleate	Methyl Linolenate	Others
	C ₉ H ₁₈ O ₂	C ₁₁ H ₂₂ O ₂	C ₁₃ H ₂₆ O ₂	C ₁₅ H ₃₀ O ₂	C ₁₇ H ₃₄ O ₂	C ₁₉ H ₃₈ O ₂	C ₁₉ H ₃₆ O ₂	C ₁₉ H ₃₄ O ₂	C ₁₉ H ₃₂ O ₂	C>21
Soybean					11	5	25	52	7	
Rapeseed					4	2	62	20	8	1
Palm				1	45	6	38	9		
Jatropha					15	12	71	2		
Coconut	8	8	45	18	10	2	8	2		
Cooking oil					10	3	42	35	5	

renewable fuel derived from vegetable oil, BDF has the advantage that it can be used as a blend with diesel fuel without the need for changing engine design parameters. Furthermore, BDF is useful to reduce CO₂ emissions through the life cycle, as well as to significantly reduce PM emissions [1, 2, 3].

In recent years, numerous researchers have reported an increase in NO_x emissions from diesel engines fueled with BDF, and several biodiesel combustion kinetics models have been developed [4, 5, 6, 7, 8] to explain this behavior. These models could be used to simulate in-cylinder combustion processes coupled with mixing and chemical processes in order to determine optimal engine control and design parameters to reduce NO_x emissions with blended BDFs. However, few of these models have been validated sufficiently against test data on combustion and emissions, specifically on PM emissions in recently developed diesel engines.

The objective of the present research is to analyze the effects of using BDF on diesel engine combustion and emission by employing both engine tests and numerical simulation. BDF consists of several fatty acid methyl esters (FAMES), e.g., methyl palmitate (C₁₇H₃₄O₂), methyl oleate (C₁₉H₃₆O₂), methyl linoleate (C₁₉H₃₄O₂) and so forth. We chose methyl oleate (MO) as a test fuel representative of major constituents of many types of BDFs (as shown in Table 1[9]) and compared different fuel compositions, i.e., 100%

MO (MO100), 40% MO blended with JIS#2 diesel (MO40) and JIS#2 diesel (D100).

The engine tested in this study was equipped with an ECU, allowing not only exhaust gas recirculation (EGR) and injection pressure control but also pilot injection combustion. Although the effects on diesel combustion have been investigated under similar conditions [10, 11, 12, 13, 14], in the present study, we attempted to explain FAME combustion processes with the aim of optimizing engine operating parameters to ensure high thermal efficiency together with reduced emissions.

In a previous study, we used a zero-dimensional reaction model adopting in CHEMKIN-Pro to identify factors affecting engine combustion and emissions [15]. The results obtained with the numerical model suggested that the ignition delay with D100, MO40 and MO100 was almost similar at low equivalence ratios. By contrast, when equivalence ratio (ϕ) increased, the ignition delay decreased specifically in the low temperature range with MO. Further, MO100 resulted in emission of soot at high temperatures, whereas the blended fuel resulted in emission of soot at lower temperatures similar to ordinary diesel fuel. However, NO_x emission did not vary significantly between diesel fuel and biodiesel.

In the present study, we used the 3-D CFD code based on the reaction model described previously to investigate the effect of MO on engine combustion processes. We also employed a phenomenological soot formation model to identify the soot generation mechanism with MO.

EXPERIMENTAL SETUP

Test Engine

The engine used in the present study was a production turbocharged 2.2 L DI diesel engine designed for passenger cars, complying with the Euro 4 regulation. The main specifications of the engine are shown in Table 2.

Table 2. Engine specifications

Item	Specifications
Engine type	Water-cooled, 4-stroke-cycle, DI diesel engine
Valve train	DOHC 4 valves
Cylinder	L4
Bore x Stroke mm	85.0 x 97.1
Displacement cc	2204
Compression ratio	16.7
Fuel supply	Common-rail (Max.160 MPa) Nozzle cone angle 153° Φ 0.133mm×6 holes
EGR system	HP-Hot-EGR / HP-Cooled-EGR
Boost control	VNT turbocharger
Swirl control	Continuously variable (Swirl ratio: 1.2-4.4)
Max. power kW/rpm	103/4000
Max. torque Nm/rpm	340/2000

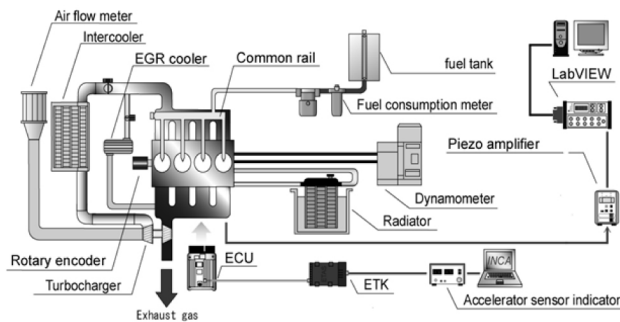


Figure 1. Experimental setup

The engine and measuring apparatus were configured as shown in Figure 1. Fuel consumption was measured using an FX-1100 gravity flow sensor developed by ONO SOKKI.

Exhaust gases were sampled at the engine outlet before the DOC using a MEXA 1500DEGR, while an AVL 415SE smoke meter was used to measure filter smoke number with

conversion to soot emission (g/kWh). The intake gas composition was also recorded to calculate the EGR rate.

Fuels

The following fuel compositions were used:

D100: standard ultra low sulfur diesel fuel compliant with JIS#2 (sulfur < 10 ppm).

MO100: 100% methyl oleate (C₁₉H₃₆O₂), which is representative of major constituents of many types of BDFs.

MO40: 40% mass blend of MO100 with D100.

The properties of the tested fuels are listed in Table 3.

Table 3. Composition and properties of fuels

Item		D100	MO100	MO40
Density (@ 15°C) g/cm ³		0.8318	0.8740	0.8487
Viscosity (@30°C) mm ² /s		3.212	4.041	4.041*
CHO mass %	C	86.0	76.9	82.4
	H	13.7	12.1	13.2
	O	0.0	10.8	4.4
Aromatic vol. %		18.8	0.0	11.3
Lower heating value kJ/kg		42970	36980	40574
Flash point °C		73.5	174.0	-
Sulfur mass ppm		6	0	3.6
Cetane number		58.3	66.1	61.4

This viscosity value marked with * is an estimated value based on reference [16]. The other values for MO40 were calculated from D100 and MO100 values as shown in Equation (1).

$$Q_m = \sum_i \sum_j y_i y_j Q_{ij} \quad (1)$$

where, Q_m is the property of the blend, Q_{ij} is the mean property, and y_i and y_j are the volumetric ratios of each pure component.

Although binary interactions between D100 and MO100 would be considered ideally, these were considered negligible [17].

EXPERIMENTAL RESULTS

Experimental Conditions

To analyze the effects of using MO on diesel engine combustion and emission characteristics, we set the engine at a speed of 1500 rpm and load of 25% as the base condition

typically encountered in NEDC and JC08 modes. Details of the base conditions are listed in Table 3. In the engine tests, the EGR rate and injection pressure was varied to evaluate the combustion reactions of MO. For all conditions, the 50% mass fraction of burned fuel (MFB50) was kept at the same crank angle by adjusting injection timing to enable fair comparison between the different fuels. The detailed base condition is shown in Table 4. D100 and MO40 fuels were used for the engine experiments. For all EGR conditions, the cooled EGR gas was mixed with fresh air upstream of the intake pipe.

Table 4. Engine base operating conditions

Engine speed rpm		1500
Torque Nm		72
BMEP kPa		411
Load rate %		25
EGR ratio %		36
Swirl ratio		3.4
Boost pressure kPa		12
Injection pressure MPa		73
Injection quantity	pilot mg/str.	1.69
	main mg/str.	13.2
Injection timing	pilot deg.ATDC	-11
	main deg.ATDC	-4.0
MFB50 deg.ATDC		10.3

Experimental Results

Pilot injection

Pilot injection, originally utilized to prevent diesel engine noise and vibration by reducing ignition delay with diesel fuel, has been investigated in many studies [18, 19, 20]. In the present study, we measured in-cylinder pressure, heat release rate (HRR) and emissions using MO40 as a typical biodiesel fuel to analyze the effects on combustion process.

The results showed no significant differences in the main combustion characteristics between MO40 and D100, as shown in Figure.2 (a). However, the combustion phase with pilot injection was advanced by using MO40 due to enhancement of the combustion reactions in the low temperature range, as shown in Figure.2 (b). The ignition delay was shorter with MO than diesel at low temperatures and for high equivalence ratios, as calculated in [15]. NOx emission was reduced by using MO40 as shown in Figure.2 (c), owing to the increased combustion at low temperatures. Further, the local equivalence ratio was increased by using

MO40, resulting decreases in the total hydrocarbons, CO and soot emissions as shown in Figure.2 (c). The combustion efficiency was also improved by using MO40, and thus the brake specific energy consumption (BSEC) with MO40 was better than with D100. However, the brake specific fuel consumption (BSFC) with MO40 was worse than with D100 because MO40 had a lower heating value, as shown in Figure.2 (c).

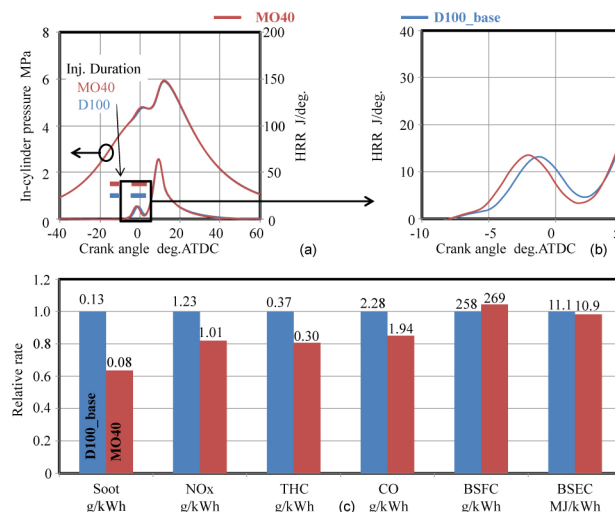


Figure 2. Results for pilot injection: (a) injection duration, in-cylinder pressure and heat release rate for each fuel, (b) effect on the heat release rate of using the different fuels showing differences in the combustion phase between MO40 and D100, (c) emissions and consumption results

High Pressure Injection

High pressure injection can enhance the atomization and evaporation of spray as well as reduce soot emission [12-13]. In this study, we increased the injection pressure to 160 MPa, and examined the effects of using MO40 on combustion and emission characteristics.

Because of the enhancement of atomization and evaporation of the spray for high pressure injection, the injection timing was shortened and the mixture timing for fuel and air was lengthened [13]. This meant that premixed combustion was observed for both fuels. Thus, the maximum in-cylinder pressure and maximum rate of pressure rise were higher than with pilot injection for both fuels as shown in Figure.3 (a). On the other hand, combustion in low temperature range was enhanced, but there was slight the decrease in main combustion with MO40, as shown in Figure.3 (b). Owing to the increased mixture timing, soot emission was reduced. However, NOx emission was increased for both fuels but was significantly increased for MO40, as shown in Figure.3 (c).