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# Effects of fatty acid methyl esters proportion on combustion and emission characteristics of a biodiesel fueled diesel engine

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ABSTRACT

With the growing energy problems, scholars has focused on utilizing renewable biodiesel as a fossil fuel alternative. Four different typical biodiesels were employed to investigate the effects of fatty acid methyl esters proportion on combustion and emission characteristics of a biodiesel fueled diesel engine in terms of heat release rate, cylinder pressure, indicated power and formation of $NO_x$ emission. The corresponding computational fluid dynamic modeling was performed by KIVA4 coupled CHEMKIN II code, and a special chemical kinetics mechanism consisting of 106 species and 263 reactions was developed to simulate the combustion process since it contained methyl linoleate, a majority component in most biodiesel, thereby improved the accuracy of simulation. The simulation results indicated that chemical ignition delay time and kinetic viscosity of biodiesel played very important roles in combustion process. Higher saturation level could shorten chemical ignition delay time, but the higher saturation contents like C16:0 and C18:0 together with C18:1 (a single double bond methyl ester) would increase the kinetic viscosity, resulting in poor fuel–air mixing and evaporation process. Lower kinetic viscosity methyl esters like C18:2 and C18:3 was favorable for better fuel–air mixing and subsequent combustion, however, a higher $NO_x$ emission was discovered. Therefore, the relationship between saturation levels and combustion and emission characteristics of biodiesels is not simple and straightforward, the balance of five majority components is very important.



## 1. Introduction

Diesel engine is widely applied in various fields of power engineering for its higher efficiency compared to gasoline engine, but with the depletion of non-renewable crude oil, some renewable substitutes are attracting significant attentions. Meanwhile, the exhaust emissions from diesel engines like unburned nitrogen oxides ($NO_x$), hydrocarbon (HC), carbon monoxide (CO) and particulate matter (PM) were required to further reduce by the latest regulations in order to improve air quality [1]. These regulations also promoted the development of renewable substitutes. Among several feasible alternative resources, biodiesel was focused in the recent years because of its particular advantages. First of all, wide range of feedstocks could be used to produce biodiesel like various animal fats or vegetable oils [2]. Then, many studies have been conducted on the effects of biodiesel on life cycle environmental impacts, and biodiesel has been finally identified as an environmental-friendly fuel [3], for example, the sulfur content were lower with the increase of biodiesel in soybean biodiesel–diesel blends [4]. Next, biodiesel can be fueled in diesel engine due to its physicochemical characteristics close to traditional petroleum diesel [5]. Furthermore, although some factors may contribute to degradation of its quality, just like oxygen exposure, light exposure, metal contamination, et al., fortunately, some additives and technologies can mitigate these degradation [6]. Therefore, biodiesel can be extended in practice as a qualified alternative fuel, and many biodiesels manufactories were established in recent years, the production capacity of biorefineries had reached 300 million liters per year in Pennsylvania in 2011 [7].

Some experiments were conducted on the combustion and emission characteristics of biodiesel and its blends. The works conducted by Can [8] and Özener et al. [9] showed that the addition of biodiesel to conventional diesel could result in the decrease of torque and the increase of brake specific fuel consumption (BSFC), and similar phenomena could also be found in Refs. [10–12], due to the lower calorific value and shorter ignition delay of biodiesel. For improving the fuel properties, a recent work by Imdadul et al. [13] indicated that appropriate addition of pentanol

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**Table 1**
Engine specifications.

| Type | Light-duty 2KD-FTV Toyota engine |
|---|---|
| Bore × stroke (mm) | 92 × 93.8 |
| Swept volume (L) | 2.494 |
| Connecting rod (mm) | 158.5 |
| Compression ratio | 18.5 |
| Fuel injection holes | 6 |
| Nozzle radius | 45 nm |

to one biodiesel–diesel blends resulted in a reduced BSFC with higher brake thermal efficiency. On the other hand, the emissions studies on biodiesel [11,14–16] indicated that CO and unburned HC emissions were decreased significantly, while the $NO_x$ emissions were increased. It was suggested in Ref. [17] that the higher oxygen content of biodiesel and its blends contributed to an unburned HC and CO oxidation, thereby increasing region combustion temperature, so the $NO_x$ formation was increased and the HC, CO concentrations were reduced. Some other exhausts, such as mono- and polycyclic aromatic hydrocarbons were tested by Corrêa and Arbilla [18] and He et al. [19], results showed a mean reduction for mono- and polycyclic aromatic hydrocarbons with the addition of biodiesel.

The above results were from experiments. In the recent years, some detailed oxidization mechanisms of biodiesel or its surrogate were developed [20,21], but the size of detailed mechanisms are too large to simulate the biodiesel combustion process in computational fluid dynamics software, therefore, some methodologies were used to reduce these mechanisms [16,22,23], the reduced mechanism with responding numerical models could simulate the transient working process of diesel engines fueled by biodiesels under different conditions [24–28], effects of different biodiesel–diesel blends concentration, thermal–physical–chemical characteristics or various combustion chamber shapes on combustion and emission characteristics of biodiesel fueled engine were investigated. However, the detailed longitudinal analysis on biodiesels composed of varying fatty acid methyl esters (FAMEs) proportion is rarely addressed.

As we know, typical biodiesel fuels derived from vegetable oil or animal fat usually consists of five major long carbon chain FAMEs: methyl palmitate (MP, $C_{17}H_{34}O_2$, C16:0) and methyl stearate (MS, $C_{19}H_{38}O_2$, C18:0) as saturated FAMEs, methyl oleate (MO, $C_{19}H_{36}O_2$, C18:1), methyl linoleate (ML, $C_{19}H_{34}O_2$, C18:2) and methyl linolenate (MLE,$C_{17}H_{32}O_2$, C18:3) as unsaturated FAMEs [20], so the effect of FAMEs proportion on biodiesel working characteristics can't be ignored. Just as said in Ref. [15,17] that the $NO_x$ emissions level with the use of biodiesel can be correlated with the number of double bonds (unsaturation level). From this point of view, the purpose of this paper is to numerically investigate the combustion process of a diesel engine fueled with biodiesels composed of different FAMEs proportion.

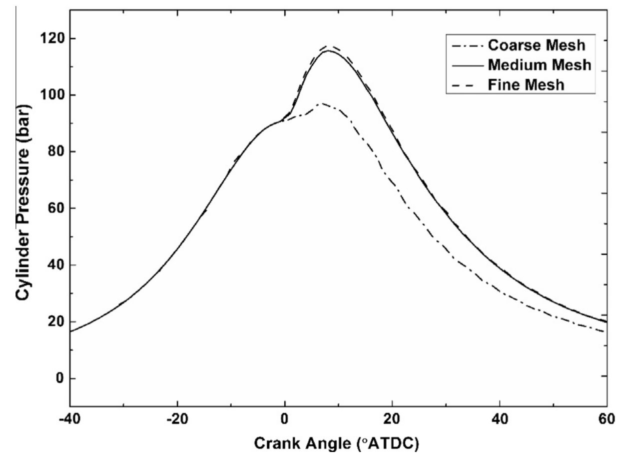


**Fig. 2.** Cylinder pressure comparison for grid independence test.

**Table 2**
Pure biodiesel compositions.

| Type | Percentage |
|---|---|
| Methyl palmitate | 10.13 |
| Methyl oleate | 53.34 |
| Methyl stearate | 8.34 |
| Methyl linoleate | 2.38 |
| Methyl eicosenoate | 7.63 |
| Methyl docosanoate | 1.58 |
| Methyl tetracosanoate | 1.38 |

**Table 3**
Operating conditions.

| Type | Biodiesel | | | | | |
|---|---|---|---|---|---|---|
| | B1 | | | B2 | | |
| Engine speed (rpm) | 2400 | | | 2400 | | |
| Load | 10% | 50% | 100% | 10% | 50% | 100% |
| Pressure at IVC (bar) | 1.33 | 1.64 | 1.87 | 1.33 | 1.62 | 1.85 |
| Fuel mass (kg/h) | 2.99 | 6.38 | 10.76 | 2.96 | 6.35 | 11.04 |
| Air flow rate (kg/h) | 231.23 | 269.43 | 292.03 | 232.32 | 272.06 | 292.11 |
| SOI (CAD ATDC) | −9.5 | −9.5 | −10.0 | −10 | −9.5 | −11 |
| EOI (CAD ATDC) | 2.0 | 4.0 | 4.0 | 1.5 | 3.5 | 4.5 |

In this paper, KIVA-4 combined with CHEMKIN II code was employed to simulate combustion process. The grid is firstly established according to a light-duty 2KD-FTV Toyota car engine, then validated by experimental results under the 10%, 50% and 100% load conditions at speed of 2400 rpm, finally, the combustion process of biodiesels composed by different FAMEs proportion were simulated and compared.

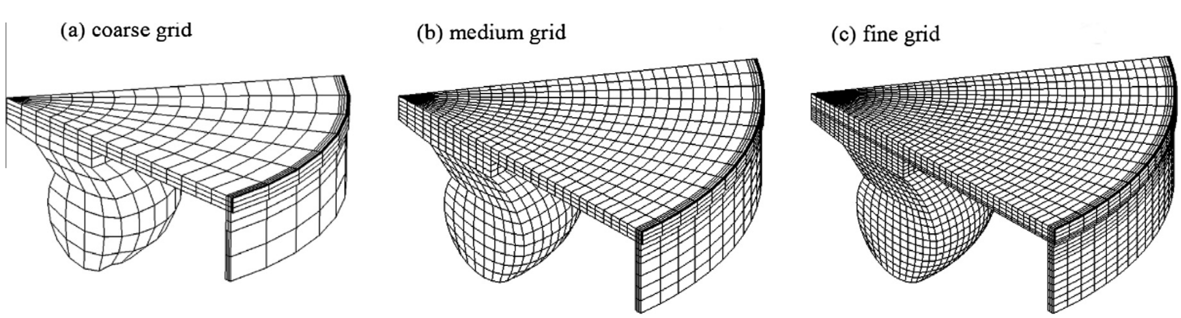


**Fig. 1.** The coarse, medium and fine 60° sector grid shown at top dead center.