Energy 107 (2016) 305–320

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Impact of chemical structure of individual fatty acid esters on combustion and emission characteristics of diesel engine

Lei Zhu [a,*], C.S. Cheung [b], Zhen Huang [a]

[a] Key Laboratory for Power Machinery and Engineering of M.O.E, Shanghai Jiao Tong University, Shanghai, PR China
[b] Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong Special Administrative Region

A R T I C L E I N F O

Article history:
Received 16 February 2015
Received in revised form
10 February 2016
Accepted 6 April 2016
Available online 29 April 2016

Keywords:
Fatty acid ester
Molecular structure
NO_x
Soot
Particle size distribution

A B S T R A C T

The effects of fatty acid chain length, number of double bonds and alcohol moiety chain length on combustion and emission characteristics were investigated. With the increase of carbon chain length of methyl ester, HC (hydrocarbon), CO and smoke emissions increase. The particle number concentration of nucleation mode decrease and accumulation mode increases with carbon chain length. The diameter of primary particle increases with carbon chain length. The double bonds of methyl ester are strongly correlated with CO, HC, nucleation mode and accumulation mode particles. The BSFC of unsaturated methyl ester is slightly higher. With increase of alcohol moiety chain length, the start of combustion is advanced, leading to lower premixed combustion, and thus resulting in the higher HC, CO and smoke and lower NO_x emissions. Ethyl ester generates lower number concentration in nucleation mode, while it has higher number concentration in accumulation mode. The primary particle size of ethyl ester is larger than that of methyl ester. These results indicate that molecular structure of ester has great influence in combustion and emission characteristics. The composition of biodiesel could be modified and optimized during production process through new techniques or various feedstocks in order to improve combustion and emission of biodiesel.

1. Introduction

In recent years, in order to reduce the reliance on fossil diesel fuel for various applications, there is increasing interest in investigating the potential application of alternative fuels, such as biodiesel or alcohol, to diesel engines [1]. Biodiesel is an alternative diesel fuel consisting of alkyl monoesters of fatty acids derived from vegetable oil, animal fats or waste cooking oil through the transesterification reaction. Due to its similar physical properties to diesel fuel, neat biodiesel or its blends with diesel fuel can be used on diesel engines directly [2]. Many studies have reported that the application of biodiesel in diesel engines could reduce the HC (hydrocarbon), carbon monoxide (CO) and PM (particulate matter) emissions, while increase nitrogen oxides (NO_x) emission, when compared with using diesel fuel [3–6]. All these changes in gaseous emissions are attributed to the effect of oxygen in the ester group (−COOH) in improving combustion. While the reduction of PM emissions is not only attributed to oxygen content in fuel, but also to the lack of aromatics in biofuel molecule.

The typical biodiesel components are saturated and unsaturated fatty acid methyl esters or ethyl esters with 12–20 carbon atoms in the carbon chain. However, the compositions vary with the feedstocks. Differences in molecular structure influence the physical and chemical properties of a biodiesel, and hence affect the combustion and emission characteristics during in-cylinder combustion process. The molecular structure of a biodiesel can be characterized by the fatty acid chain length, the degree of unsaturation and the alcohol chain length.

Various studies have been conducted to investigate the relationship between chemical–physical properties of a biodiesel and its molecular structure. Both moieties, the fatty acid and alcohol had considerable influence on fuel properties [7]. Cetane number, heat of combustion, melting point, and viscosity of neat fatty compounds increase with the increase of chain length and decrease with unsaturation. Fatty acid profile of biodiesel corresponds to that of its feedstock. Most common feedstocks possess fatty acid profiles consisting mainly of five C16 to C18 fatty acids, namely, palmitic, stearic, oleic, linoleic and linolenic acids [8].

* Corresponding author. School of Mechanical Engineering, Shanghai Jiao Tong University, Shanghai, PR China. Tel./fax: +86 3420 5949.
E-mail addresses: tonyzhulei@gmail.com, tonyzhulei@sjtu.edu.cn (L. Zhu).

http://dx.doi.org/10.1016/j.energy.2016.04.030
0360-5442/

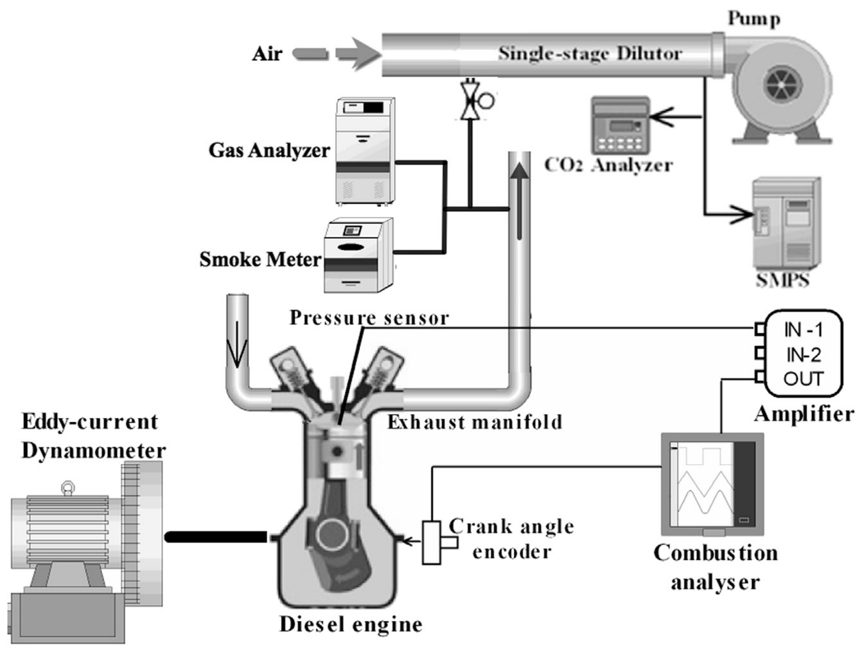

Fig. 1. Schematic diagram of experimental system.

Several investigations have been conducted on the influence of biodiesel components on the combustion and emissions characteristics. Jha et al. [9] evaluated the effect of unsaturation level and hydrocarbon chain length on the temperature of open flames. They found that the presence of saturated components and lower carbon chain length components led to higher flame temperatures. Puhan and Nagarajan [10] investigated the effect of biodiesel unsaturated fatty acid on the combustion characteristics and emissions of a single cylinder direct injection diesel engine. They concluded that (a) a biodiesel fuel with more unsaturated fatty acid composition has higher density but lower viscosity; (b) a biodiesel with more unsaturated fatty acid components has lower cetane number, higher activation energy and longer ignition delay period; (c) a biodiesel with more unsaturated biodiesel fuels emits higher HC, CO and smoke emissions; (d) more NO was observed in case of highly unsaturated biodiesel fuel due to longer ignition delay and advanced fuel injection timing; (e) higher gas pressure, higher exhaust gas temperature and higher heat release rate were observed in case of highly unsaturated biodiesel. Lapuerta et al. [11] concluded that as the biodiesel fuel became more unsaturated, NO_x emissions increased by 10% and particle mass emissions decreased by 20%. Salamanca et al. [12] investigated the variations in the chemical composition and morphology of soot induced by the unsaturation degree of biodiesel and a biodiesel blend. They found that with an increase in degree of unsaturation in biodiesel, there is increase in smoke opacity, PM, volatile matter content of PM and aliphatic content of PM. However, these studies focused on influence of methyl ester distribution with different types of biodiesel, not on influence of molecular structure with different individual fatty acid ester.

There are very few investigations on the effects of ester molecular structure on engine combustion and emission. Schönborn et al. [13] conducted a series of experiments on a single-cylinder research engine, investigating the influence of the molecular structure on the combustion behavior of eight fatty acid alkyl ester molecules from C12 to C22 and four biodiesel fuels under diesel engine conditions. Experiments were conducted at the same indicated mean effective pressure but no details on the engine load were mentioned. They concluded that (a) increasing fatty acid chain length, increasing saturation and an increase in chain length of the alcohol moiety decrease the ignition delay and thus decrease the fraction of premixed combustion; (b) molecules with shorter fatty acid chains produce more NO_x in diesel combustion because of the longer ignition delay of the shorter chain fatty acid molecules; (c) the number of double bonds present in the fatty acid moiety of the molecules was strongly correlated with the emission of accumulation mode soot particles; and (d) the specific particulate number concentration of nucleation mode particles correlates well with the boiling points of the individual fatty acid methyl ester molecules. Pourkhesalian et al. [14] investigated the influence of fuel molecular structure on the volatility and oxidative potential of biodiesel particulate matter. They observed that more saturated fuels with shorter carbon chain lengths result in lower particle mass but produce particles that are more volatile and also have higher levels of reactive oxygen species. However, these investigations were conducted at a single engine load and with emphasize on NO_x and PM emissions. Moreover, there is lack of comparison on the diameter of primary soot particles formed during combustion of individual fatty acid ester.

The present study further investigates the effects of fatty acid chain length, number of double bonds and alcohol chain length on combustion and emission characteristics of a four cylinders diesel engine. HC, CO, NO_x, smoke opacity, particle size distribution, and diameter of primary soot particle of five individual fatty acid esters

Table 1
Engine specifications.

Model	Cummins 4BTA
Type	In-line 4-cylinder
Suction type	Turbo intercooler
Maximum power	88 kW/2800 rev/min
Maximum torque	380 Nm/1600 rev/min
Bore × stroke	102 mm × 120 mm
Displacement	3920/cc
Compression ratio	17.5:1
Injection pump type	In-line Bosch P7100