



Systematic study of the effect of the hydroxyl functional group in alcohol molecules on compression ignition and exhaust gas emissions



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HIGHLIGHTS

- The effect of a hydroxyl group on combustion was investigated.
- Adding a hydroxyl group to an alkane increased ignition delay and NO_x emissions.
- Moving hydroxyl group towards the centre of carbon chain increased ignition delay.
- These effects were attributed to the high electronegativity of oxygen atom.
- Unsaturation and branching in alcohols increased the ignition delay.

ARTICLE INFO

Article history:

Received 14 January 2015

Received in revised form 11 March 2015

Accepted 17 March 2015

Available online 28 March 2015

Keywords:

Oxygenated biofuels
Fuel molecular structure
Alcohol
Diesel ignition delay
Fuel effect on NO_x
Particulate emissions

ABSTRACT

This paper presents the results of experiments conducted in a single cylinder compression ignition research engine to investigate the combustion performance of various alcohol fuel molecules. Alcohols of C8–C16 chain lengths were tested and the results of these experiments were compared with those for corresponding hydrocarbon molecules. Alcohols had higher ignition delays than the various hydrocarbons tested. This is believed to be due to the increased difficulty of both hydrogen abstraction and isomerization, caused by the higher electronegativity of the oxygen atoms in alcohols compared to carbon atoms. Additionally, the location of the hydroxyl group was found to affect ignition delay; molecules in which the hydroxyl group was closer to the centre of the carbon chain were observed to have longer ignition delays. In addition, both higher degree of unsaturation and methyl branching were shown to increase the ignition delay of alcohols, as was expected. Due to higher ignition delays, alcohol combustion resulted in higher in-cylinder temperatures than those corresponding to hydrocarbon combustion, giving rise to greater NO_x emissions. In the case of exhaust particulate matter, a shift was observed for alcohols towards a greater number of nucleation particles, in comparison to corresponding alkane molecules.

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Introduction

The development of new sustainable transportation fuels is required in order to meet the World's growing demand for energy, improve the security of fuel supply, and reduce the rate of global warming. Alcohol molecules produced from renewable sources are potential sustainable fuels for compression ignition engines. Today, ethanol diesel blends are commercially available and several alcohols from methanol to hexanol have been studied, with particular focus on C4 alcohols [1]. Increasing the length of alcohol carbon chain generally improves the ignition qualities of the

alcohol molecule, which makes higher alcohols more attractive biofuels than lower alcohols. Currently, however, the low production levels of higher bio-alcohols prevents their utilization on commercial scale [2]. Therefore, a better understanding of both the ignition chemistry and formation of exhaust gas emissions of higher alcohols is required in order to inform the development of their production processes, for example through metabolic engineering.

The low temperature chemistry (600–1000 K) leading to auto ignition is well established for hydrocarbons, which are the main component of fossil diesel fuels. However, the low temperature kinetics of alcohol ignition is less well understood. The differences in ignition delay between hydrocarbons and alcohols are mainly caused by the higher electronegativity of an oxygen atom in the alcohol molecule compared to that of a carbon or hydrogen atom

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in the corresponding hydrocarbon molecule. This higher electronegativity of the oxygen atom affects the bond strengths of the fuel molecule and hence changes the kinetic combustion mechanisms. Additionally, the difference in molecular structure affects the formation of exhaust gas emissions, partially through a lengthening of the ignition delay. [1] Several authors have experimentally investigated the combustion of higher alcohols [3–5] and discussed their ignition delay times [6–9], but a significantly low number of engine studies have been conducted on this subject [10–15]. Furthermore, the engine studies of higher alcohols generally investigate the combustion of alcohol–diesel blends instead of the combustion of higher alcohol molecules.

This paper discusses the results of experiments conducted in a single cylinder compression ignition research engine using several different higher alcohol molecules. Seventeen alcohol molecules, which could potentially be used in compression ignition engines as biofuels, were investigated. These alcohol molecules included primary alcohols with carbon chain length of eight to 16 carbon atoms, alcohols with the hydroxyl functional group in different positions within the molecule and unsaturated alcohols and branched alcohols. Ignition delays observed in the combustion engine experiments are compared to the low temperature ignition mechanisms found in published literature. Hydrogen abstraction from the fuel molecule and the following isomerization after fuel radical oxidation have been shown to be the two main initial reactions with significant effect on the duration of ignition delay [16,17]. Therefore, the comparison between ignition delays of different fuel molecules was carried out by discussing the rates of these two reactions. Corresponding alkanes and alkenes were also tested to provide reference data for comparison with the ignition and emissions data of alcohols. The analysis of exhaust gas emission focuses on NO_x and particulate matter. The results of this study may be used in the development of future biofuels by identifying alcohol molecular structures with desirable ignition properties and combustion profiles and which could lead to lower pollutant exhaust emissions.

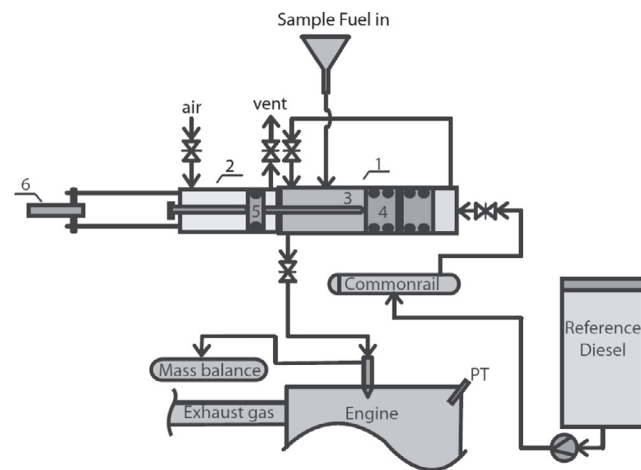
1. Experimental methods

1.1. Engine

A naturally aspirated, direct injection compression ignition engine was used (Fig. 1). The engine cylinder pressure was continuously measured at every 0.2 crank angle degrees (CAD) using a piezoelectric transducer (Kistler 6056AU38) located in an engine glow plug adapter and connected to a charge amplifier (Kistler 5011). The cylinder gas pressure measured by the piezoelectric transducer required a reference absolute pressure and this was provided once per engine cycle at the bottom dead centre (induction stroke) by a piezoresistive pressure transducer (Druck PTX 7517-3257) located in the engine intake manifold 160 mm upstream of the intake valve. A shaft encoder, having a resolution of 0.2 CAD, was used to trigger the data acquisition system (DAQ) by means of a reference signal at top dead centre (TDC). The DAQ also clocked the sampling of the cylinder gas pressure at every 0.2 CAD. One hundred consecutive engine cycles were recorded for subsequent heat release rate analysis. The experimental set-up for combustion studies is shown Fig. 1.

Some of the investigated fuel molecules were only available in small quantities (<200 ml) due to their high purchase cost. Therefore, an ultralow volume fuel system, which allows comprehensive testing with fuel samples as small as 120 ml, was used (item labelled 1 in Fig. 1). The fuel system was originally designed by Schönborn et al. [18] and later modified by Hellier et al. [19].

Additionally, knowledge of the fuel flow rate consumed by the engine was required for analysis to allow the calculation of the



Engine specification	
Engine model	Ford Duratorq
Stroke (mm)	86
Bore (mm)	86
Displacement (cc)	499.56
Compression ratio	18.2 : 1
Piston bowl design	ω - bowl
Maximum cylinder pressure (MPa)	15
Coolant water temperature (K)	353
Engine oil temperature (K)	353
Injector type	6-hole (DELPHI DF1 1.3)
Injector control	1 μs accuracy (EMTRONIX EC-GEN 500)
High pressure fuel system	160MPa common rail (BOCH CRS2)

Fig. 1. Experimental set-up for combustion studies. (1) the ultralow volume fuel system; (2) the flow measurement system; (3) rod; (4) pistons in the ultralow volume fuel system; (5) piston in the flow measurement system; (6) ultrasonic proximity sensor.

fraction of premixed air–fuel mixture combusted. This required two separate fuel flow measurements; first, the high pressure fuel flow rate supplied to the fuel injector itself and secondly, the low pressure fuel spill flow rate from the fuel injector. The slip flow, comprising of about 45% of the fuel flow rate to the injector, was subtracted from the flow rate to the injector so as to give the net fuel rate injected into the engine combustion chamber. In order to measure the flow rate to the injector a flow measurement system was designed and implemented (labelled 2 in Fig. 1). At the beginning of an experiment, the sample fuel was transferred to the low volume fuel system by means of a funnel and the flow measurement system piston was pushed to the right with high pressure air, so as to allow the rod (labelled 3 in Fig. 1) attached to the piston of the flow measuring system to come into contact with the fuel system's two pistons (labelled 4 in Fig. 1). This arrangement is shown in Fig. 1. During an experiment, common rail diesel fuel pressure pushed the fuel system pistons (labelled 4 in Fig. 1) to the left, thereby creating the necessary injection pressure for the fuel sample. These pistons (labelled 4 in Fig. 1) also pushed the flow measurement system piston (labelled 5 in Fig. 1) to the left and this movement was recorded by the ultrasonic proximity sensor (labelled 6 in Fig. 1), which allowed calculation of volumetric sample fuel flow rate to the injector. The injector spill was measured with a precision mass balance, so that the net flow rate of the fuel sample to the engine combustion chamber could be established.

1.2. Exhaust gas emissions analysis

The exhaust gas from combustion experiments was sampled unfiltered 180 mm downstream of the exhaust valve and the gas

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