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The influence of various oxygenated functional groups in carbonyl and ether compounds on compression ignition and exhaust gas emissions

Eлина Koivisto^{a,*}, Nicos Ladommatos^a, Martin Gold^b

^a Department of Mechanical Engineering, University College London, Torrington Place, London WC1E 7JE, United Kingdom

^b BP plc, Fuels and Lubricants Research, Technology Centre, Whitechurch Hill, Pangbourne, Reading RG8 7QR, United Kingdom

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ABSTRACT

This study relates to the development of future biofuels and it reports the effects of fuel molecular structure of various oxygenated compounds on compression auto ignition and exhaust emissions. The experimental study was conducted on a single cylinder compression ignition research engine. Ethers and various carbonyl compounds were investigated, including ketones, carboxylic acids and methyl esters. The results for these compounds were also compared to those for alcohol and alkane combustion obtained in a previous study. It was found that oxygen-bearing functional groups within various C8–C16 fuel molecules have a significant influence on the ignition delay and on engine in-cylinder temperatures. Carbonyl compounds had longer ignition delays compared to the corresponding alkanes, whereas ether compounds decreased the ignition delay. It is suggested that these observations relate to the changes in the relative ease of hydrogen abstraction and the ability of a fuel peroxy radical to undergo isomerization during the low-temperature combustion chemistry preceding ignition. In addition, it was observed that, both moving a carbonyl group closer to the centre of the carbon chain of a molecule and adding a double bond to a carboxylic acid increased the ignition delay. Oxygen in the fuel molecule, excluding carboxylic acids, was observed to increase the NO_x emissions and decrease the mass of particulates in the exhaust gas.

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1. Introduction

There is a growing interest in renewable transportation fuels. To enable faster transition away from fossil fuels, new sustainable transportation fuels should be compatible with existing engines at least in the short to medium term. The development of future bio-fuels, as well as synthetic fossil fuels, provides new opportunities for the development of sustainable fuel molecules which burn more cleanly and efficiently, than conventional fuels blended from fractionally distilled crude oil streams. The natural raw materials available for the development of sustainable fuels offer opportunities for a wide range of new biofuel molecules. Therefore, the types of molecules which could provide this desirable performance in compression ignition engines are increasingly the focus of global fuel research. Oxygenated fuel molecules are particularly attractive for bio-fuel production, due to their lower carbon emissions and potentially increased security of supply. Currently commercially

available biofuels include alcohol–fossil diesel fuel blends and biodiesel containing methyl esters as its main component [1,2].

Fuel molecular structure affects the combustion process mainly through ignition delay, which results from the low temperature (600–1000 K) ignition reactions of the fuel molecules [3]. Whilst the general kinetic steps of low temperature oxidation are relatively well understood for some of the hydrocarbons present in fossil fuels, the low temperature oxidation of oxygenated fuel molecules present in biofuels is not yet fully understood. In the case of oxygenated fuel molecules, the combustion chemistry is altered compared to non-oxygenated hydrocarbon combustion, due to the higher electronegativity of an oxygen atom compared to that of a carbon or a hydrogen atom [4]. In turn, the changes in the ignition delay caused by the high electronegativity of oxygen atoms affect the formation of exhaust gas emissions [5,6].

Several researchers have investigated the low temperature ignition and combustion chemistry and emission formation of different oxygenated fuel molecules, both by means of modelling and experimentally in shock tubes, rapid compression machines (RCM) and in compression ignition (CI) engines [4,7–10]. However, comparison of results from these studies is difficult due to differences in the apparatus used and experimental

* Corresponding author. Tel.: +44 (0)20 7679 3907; fax: +44 (0)20 7679 0180.

E-mail addresses: elina.koivisto.11@ucl.ac.uk, elina.koivisto3@gmail.com (E. Koivisto).

conditions. Additionally, the research has mainly focused on first generation biofuels, such as alcohols, methyl esters and ethers with little research being conducted on other potential fuel molecules, such as ketones [11]. Therefore, further fundamental engine studies are required, so as to inform the selection of new biofuel molecules for development and large scale production.

The aim of the present study is to investigate systematically in a single cylinder CI research engine the auto ignition behaviour and emission formation of a wide range of oxygen-bearing fuel molecules, including ketone, carboxylic acid, methyl ester and ether molecules. The paper makes an assessment for these molecules of their combustion characteristics and exhaust pollutant emissions. The assessment includes the impact of altering the position of the carbonyl group in a molecule and the level of carboxylic acid unsaturation. A comparison is then made of the results from these molecules and those of the several alcohol molecules from a previous companion study [12]. It is suggested in the paper that two key aspects to understanding how molecular structure affects ignition delay are the relative difficulty of hydrogen abstraction from the fuel molecule and the subsequent ability of the fuel peroxy radical to isomerize through hydrogen transfer [13,14]. Therefore, the assessment of the ignition delays of various molecules reported in this paper was made in context of this hypothesis. Taken together, the results reported here provide a broad picture of the combustion and exhaust emissions of almost 50 oxygenated molecules which could potentially be produced from renewable energy sources.

2. Experimental methods

2.1. Engine

The experimental investigations were conducted using a naturally aspirated, direct injection, single cylinder compression ignition research engine. The engine specification is shown in Table 1. The dynamic in-cylinder pressure was measured every 0.2 crank angle degrees (CAD) using a piezoelectric high pressure transducer (Kistler 6056AU38) located in the engine glow plug adapter. The in-cylinder pressure was pegged each combustion cycle at bottom dead centre using a piezoresistive pressure transducer (Druck PTX 7517-3257), which in turn was located in the engine intake manifold 160 mm upstream of the intake valves. A charge amplifier (Kistler 5011) was used to amplify the signal from the Kistler pressure transducer.

In order to test fuel samples in as small quantities as 120 ml an ultralow volume fuel system was used. This was necessary due to the high purchase cost of some of the fuel molecules investigated. The fuel system was originally designed by Schönborn et al. [15] and later modified by Hellier et al. [16].

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

Table 1
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
Number of valves	4
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 μ s accuracy (EMTRONIX EC-GEN 500)
High pressure fuel system	160 MPa common rail (BOCH CRS2)

premixed air–fuel mixture combusted. To calculate this fuel flow rate, the spill from the injector was continuously measured using a precision mass balance and the high pressure fuel flow rate supplied to the injector itself was measured using a flow measurement system designed for this purpose. A more detailed description of the flow measurement system can be found in Ref. [12].

2.2. Exhaust emissions analysis

The engine exhaust gas was sampled unfiltered 180 mm downstream of the exhaust valves. The sample was fed via heated lines (80 °C) to two analysers. The first analyser, MEXA 9100HEGR system, was used to determine the dry concentrations of nitrogen oxides (NO_x), carbon dioxide (CO₂), carbon monoxide (CO), oxygen (O₂) and wet concentration of unburned hydrocarbons. The second analyser, a differential mobility spectrometer Cambustion DMS 500, was used to measure the total particulate mass and particle number per unit volume of exhaust gas, as well as the exhaust particle size distribution from 10 to 1000 nm. The particulate density was assumed to be 1.77 g/cm³ [17].

2.3. Test conditions

All combustion experiments were conducted at engine speed of 1200 rpm, 600 bar injection pressure, 4 bar indicated mean effective pressure (IMEP) and a fixed engine injection timing of 7.5 CAD before top dead centre (TDC). Each test day was started and ended with a reference diesel fuel test to detect any day to day drift or longer term change in the experimental equipment and instrumentation. From this data it was possible to calculate for diesel fuel the long term mean value, standard deviation and the standard error of the mean value for NO_x as follows: 921 ppm, 29.4 ppm and 5.76 ppm, respectively. The corresponding values for the mass of particulates in the exhaust gas were 0.0563 μ g/cm³, 0.00779 μ g/cm³ and 0.00179 μ g/cm³, respectively, and for the number of particulates 57.1 * 10⁶ units/cm³, 8.99 * 10⁶ units/cm³ and 1.74 * 10⁶ units/cm³ respectively. This data, therefore, provided a measure of the test-to-test repeatability of the emissions over several dozens of tests.

The fuel temperature during most of the combustion experiments was 305 ± 3 K. For fuel molecules with melting points above this temperature, the fuel was heated to 343 ± 3 K (Appendix 1). To determine the effect of fuel heating on combustion and emissions results, several molecules were tested at both temperatures of 305 K and 343 K (nonanoic acid, methyl octanoate and methyl nonanoate). The 38 K rise in temperature was observed to cause only a small decrease in ignition delay (0.20, 0.28, 0.20 CAD, respectively). These changes in ignition delay were deemed insignificant compared to the shaft encoder resolution of 0.2 CAD, and the 0.1 CAD test-to-test standard deviation of ignition delay with reference diesel fuel. Nonetheless, the fuel test temperatures are mentioned in the results section where applicable.

2.4. Fuel molecules investigated

Altogether, 46 oxygen bearing molecules were investigated having eight to 16 carbon atoms each and incorporating the following functional groups; hydroxyl (ROH), carbonyl (RR'CO), carboxyl (RCOOH), ester (RCOOR') and ether (ROR'). Additionally, seven alkanes and two alkenes were tested to provide reference data for comparison with the oxygenated molecules. The molecular structures and physical properties of the alkanes, alkenes and alcohols are presented in [12] and the molecular structure of the ketones, carboxylic acids, esters and ethers are presented in Fig. 1. Appendix 1 lists the physical properties of the ketones, carboxylic acids, esters and ethers [18–23].

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