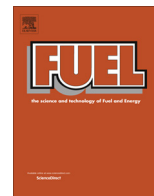




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A 'smart' fuel of photochemically-controlled reactivity

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HIGHLIGHTS

- A photochemically-controlled 'smart' fuel of variable ignition delay was developed.
- The ignition timing of the fuel with air can be controlled photochemically.
- Ignition timing control was simulated for an HCCI engine.
- Ignition delays were calculated at various temperatures and pressures.

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ABSTRACT

A 'smart' fuel whose molecular structure can be adapted via irradiation with light was calculated to provide control over ignition timing in a Homogeneous Charge Compression Ignition (HCCI) engine. The fuel consisted of isopropanol that was partially reacted into propane peroxide during a photochemical reaction with air, prior to combustion. The ensuing combustion of fuel with air in the engine, was simulated using zero-dimensional homogeneous gas phase chemical kinetic calculations. The calculations indicated that ignition timing could be controlled via the preliminary photochemical reaction. This was attributed to the presence of varying proportions of propane peroxide molecules within the fuel, which were responsible for the formation of methyl peroxy radicals early during the engine cycle. The methyl peroxy radicals increased the formation of hydrogen peroxide and hydroxy radicals during the induction period, which accelerated the decomposition reactions of the fuel, and triggered the high-temperature ignition of the fuel and air mixture.

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1. Introduction

Homogeneous Charge Compression Ignition (HCCI) combustion and the partially stratified Reactivity Controlled Compression Ignition (RCCI) combustion, are promising technologies for conversion of the next generation fuels into power. They combine high engine efficiency with low pollutant emissions by igniting a premixed charge of fuel and air by compression [1–4]. State-of-the-art experiments have shown that in RCCI, the fuel consumption can be reduced by about 20% compared to modern diesel engines. The gross indicated thermal efficiency of this type of combustion engine has been reported to reach 55–60% for light-duty automotive scale engines, which is comparable to the most modern large-scale combined-cycle electric power stations available today [1]. In HCCI and RCCI, the autoignition timing of a homogeneous charge of fuel and air can be controlled by varying the autoignition quality of the fuel, and in the case of RCCI by stratifying the fuel

and air mixture of different reactivities [5]. This results in a relatively fast and efficient, combustion process around the point of maximum compression, i.e. at top-dead-centre (TDC) of the piston. Exhaust gas recirculation (EGR) can be used to moderate the rate of combustion to avoid engine knock. Variation of the ignition quality of the fuel is necessary if ignition is to be achieved around TDC at different operating conditions of the engine, in terms of load, speed and operating temperature [6]. The state-of-the-art approach to achieving this is to have two fuels of different ignition quality on-board a vehicle, and to blend these in varying proportions so as to obtain the appropriate ignition delay for optimal engine operation [1,5,7]. This has the disadvantage that a vehicle employing dual-fuel ignition control requires two fuel tanks, and that operation ceases as soon as one of the tanks is depleted. The requirement for two different fuels is considered a sufficiently serious issue by vehicle manufacturers, to prevent commercialisation of dual-fuel combustion techniques in passenger vehicles [8]. In HCCI and RCCI combustion, the time of ignition of the fuel air charge is dependent on the chemical species present in the reactant mixture, consisting of air and fuel.

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A number of studies have shown that the species composition can be used to control ignition timing. Flynn et al. [9], Foucher et al. [10], and Masurir et al. [11,12] demonstrated that transforming the oxygen present in the air into ozone decreases the ignition delay of the reactants and can be used as a means of controlling ignition in HCCI engines. Yao et al. [13] proposed that methanol fuel could be dehydrated to dimethyl ether on-board an engine, to provide a second fuel of differing ignition quality using a single fuel supply of methanol. It has been demonstrated that ozone can also be used to partly alter the molecular structure of the fuel into peroxides prior to combustion, as a means of controlling ignition timing [14]. In addition, photochemical reactions have been shown to be effective in reducing ignition delays of reactant mixtures. This has predominantly been achieved by decomposing molecular oxygen into atomic oxygen [15,16].

The chemical kinetic calculations described herein propose a method of controlling the point of ignition through controlling the molecular structure of the fuel by photochemically reacting a variable proportion of the fuel with air under the irradiation of ultra-violet (UV) light, prior to its introduction into the combustion chamber.

The fuel used for these simulations consists of isopropanol, which is a potentially renewable fuel that can be produced from cellulosic biomass via initial hydrolysis and subsequent fermentation [17], or via metabolic pathways in bacteria [18]. It has been documented in the literature that isopropanol reacts into peroxides in a photochemical reaction of sunlight and air [19]. This concentration of isopropanol peroxides has been reported to be able to reach high concentrations in excess of 25,000 ppm. The production of peroxide in a simple glass flask left in sunlight was reported at a rate of about 1750 ppm per 48 h of irradiation with sunlight [19]. The aim of the present study is to investigate the possibility of using this photochemical reaction of isopropanol with air to control its reactivity in an ensuing combustion reaction, in particular its ignition timing in an HCCI engine.

2. Approach and method

In this study, ignition timing of smart fuel controlled by light irradiation prior to the combustion process was simulated in an HCCI engine. The fuel consisted of isopropanol, which was reacted with air into propane peroxides in varying fractions, via the photochemical reaction described by Redemann [19]. Redemann verified the

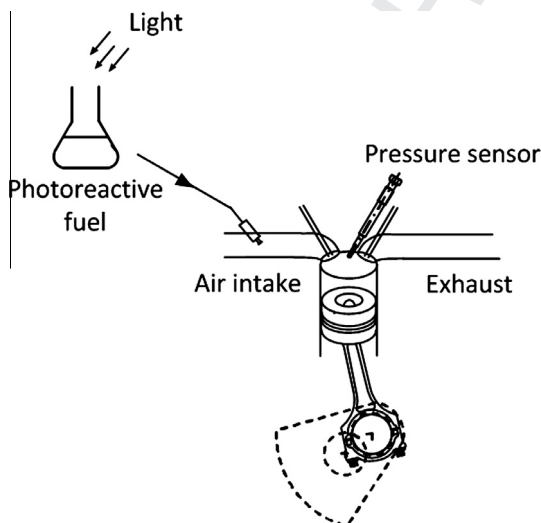


Fig. 1. Illustration of ignition control in an RCCI engine via a photochemical smart fuel.

formation of peroxides using different wet-chemistry tests, and quantitative the concentration using iodometric titration. It is also known from literature, that the presence of peroxides in fuels can shorten its ignition delay, and has been shown to be effective in controlling ignition timing in HCCI combustion [20,14,21]. An illustration of the approach used to control ignition timing by adjusting the fuel molecular structure by photochemical reaction is shown in Fig. 1.

The ignition and combustion of the charge in an RCCI engine was simulated numerically, using a single-zone piston-cylinder reactor model and detailed chemical kinetics. The simulations were performed using the Cantera 2.1.2 software tools in the Python 3.3.5 programming language. The thermodynamic engine process was simulated according to slider-crank equations and was programmed in Python. The influence of progressively changing the fuel composition was investigated under different HCCI engine loads, speeds, EGR rates, as well as for constant pressure conditions typical of gas turbine combustors.

2.1. Reactant composition and chemical kinetic mechanism

The reactants used in the simulations consisted of isopropanol and air. A variable proportion of the isopropanol (C_3H_8O) was replaced with propane peroxides ($C_3H_8O_2$) [19]. Air was modelled as consisting of molar fractions of 21% O_2 and 79% N_2 . Recirculated exhaust gases (EGR) were simplified as complete combustion products of the equivalence ratio at which the engine was operating, i.e. CO_2 , H_2O , O_2 and N_2 . This is a reasonable assumption if external cooled EGR after an oxidation catalyst is used. All gas-phase chemical reactions were modelled using the chemical kinetic mechanism of Frassoldati et al. [22] for low and high-temperature combustion kinetics. This detailed chemical kinetic mechanism comprises 484 species and 19,341 reactions.

2.2. Engine model

The engine was simulated as a single-cylinder of a light-duty automotive engine of 17:1 compression ratio with 499.56 cc swept volume. The cylinder was simulated as having a diameter of 86 mm a stroke of 86 mm, and a connecting-rod length of 160 mm. The reactant gases were simulated as having an inlet temperature of 384 K, and an inlet pressure of 102 kPa at the start of compression, representing naturally aspirated conditions and heat addition from the engine during the induction and charge preparation process. The start of the compression stroke was defined as 0° crank angle (CA), and TDC as 180° CA.

All simulations employed a single-zone reactor model assumed to have a homogeneous distribution of temperature, pressure, reactant species and product species. This simulation is thus representative of an ideal and fully homogeneous HCCI combustion case, and does not consider stratification effects, spray formation, evaporation and charge cooling effects that would naturally be present in RCCI combustion. The reactants were assumed to be homogeneously premixed when the piston was located at bottom-dead-centre (BDC). Although such a single-zone model is a simplification of the engine process, it has been proven to be adequate in predicting ignition timing trends of HCCI combustion [21].

Heat transfer from the reactants to the combustion chamber walls during the engine cycle was simulated using the semi-empirical model of Woschni for a four-stroke four-valve quiescent diesel engine as $h_c = 3.26B^{-0.2} p^{0.8} T^{-0.55} w$, where h_c is the heat transfer coefficient, B is the cylinder bore, p is the cylinder pressure, T is the global cylinder temperature, and w is taken as the instantaneous piston velocity [23,24]. Heat transfer was assumed to simply cause a reduction in the global gas temperature, with no thermal stratification.

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