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Research article

# 1-hexene autoignition control by prior reaction with ozone

Alessandro Schönborn [a,*], Paul Hellier [b], Nicos Ladommatos [b], Christian P. Hulteberg [c], Göran Carlström [d], Parisa Sayad [e], Jens Klingmann [e], Alexander A. Konnov [f]

[a] SINTEF Energy Research, Kolbjørn Hejes vei 1 A, 7034 Trondheim, Norway
[b] Department of Mechanical Engineering, University College London, Roberts Building, Torrington Place, WC1E 7JE London, UK
[c] Department of Chemical Engineering, Lund University, P.O. Box 124, SE-221 00 Lund, Sweden
[d] Centre for Analysis and Synthesis, Department of Chemistry, Lund University, P.O. Box 124, SE-221 00 Lund, Sweden
[e] Lund University, Division of Thermal Power Engineering, P.O. Box 118, SE-221 00, Lund, Sweden
[f] Lund University, Division of Combustion Physics, P.O. Box 118, SE-221 00 Lund, Sweden

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ABSTRACT

The autoignition timing of 1-hexene was controlled in a Homogeneous Charge Compression Ignition (HCCI) engine by reacting the fuel with ozone-containing air prior to its combustion. The experiments were conducted in a single cylinder research engine instrumented with a cylinder pressure sensor. The fuel was chemically characterised using Nuclear Magnetic Resonance (NMR) spectroscopy before and after its reaction with ozone. The NMR analyses showed that this preliminary reaction produced several oxygenated products within the fuel, and was likely to have resulted in the formation of ozonide molecules having a peroxidic structure with several oxygen molecules in series. To understand how this would affect the ignition reactions, the ignition process was modelled numerically using a single-zone chemical kinetic reactor model. The modelling suggested that peroxide molecules decomposed during the compression of the reactants in the engine and advanced ignition timing by promoting early decomposition of the fuel through the formation of radicals.

## 1. Introduction

Partially premixed combustion concepts for internal combustion engines, such as Homogeneous Charge Compression Ignition (HCCI) and Reactivity Controlled Compression Ignition (RCCI), are promising technologies for combining high fuel conversion efficiency with lower emissions of soot and nitrogen oxides (NOx) [1]. The indicated thermal efficiency of RCCI in particular, has been reported to reach 55–60% even in light-duty engines [2]. In HCCI and RCCI, the autoignition and combustion processes are entirely controlled by the chemical kinetics of the reactants. This results in a fast combustion process around the point of maximum geometrical compression of the charge i.e. at piston top-dead-centre (TDC) when the engine is operating optimally. Yet, changes in engine air charge temperature and pressure, or variations in engine load and speed, require the chemical kinetics to be controllable, in order to achieve ignition around TDC under all conditions [3]. One way to ensure that ignition takes place around TDC at varying engine operating conditions is to control the ignition quality of the fuel. This can be achieved by blending two fuels of varying ignition qualities [4], such as petrol and diesel fuel. The disadvantage of this approach is that an engine would require two fuels to operate, which would have to be kept in separate fuel tanks.

The development of a single 'smart' fuel, the ignition quality of which can be varied, could provide a more rational approach to this concept [5,12]. This work aims to highlight the potential of developing 'smart' fuels of variable ignition quality as a practical way of achieving high-efficiency RCCI combustion.

A simplified schematic of an RCCI engine using this approach is shown in Fig. 1. Fig. 1 illustrates how a single fuel may be used to provide two fuel streams of varying ignition qualities to an engine, by reacting one of the fuel flows in a reactor prior to its combustion. Two separate injection systems may be used to stratify the reactivity of the fuel and air mixture within the cylinder. By blending unreacted fuel with reacted fuel in varying proportions during the experiments, the point of ignition of the fuel and air charge can be adjusted within the engine cycle. A buffer tank may be used to store reacted fuel, in order to de-couple the speed of reaction of the fuel with ozone, from the rapid changes in fuel quality required by the engine.

A reliable low-temperature reaction of the fuel prior to combustion can be achieved using ozone ($O_3$). Ozone can be produced in compact devices at efficiencies of 340 g/kWh [6], and the reaction with fuel can produce peroxide species known to advance the time of ignition [5]. The ozone required to convert 1000 ppm of fuel into a peroxide, could theoretically be achieved with less than 1% of the fuel energy. Ozone may also be used to advance ignition directly, as has been demonstrated

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* Corresponding author at: SINTEF Energy Research, Kolbjørn Hejes vei 1 A, 7034 Trondheim, Norway.
*E-mail address:* alessandro.schonborn@sintef.no (A. Schönborn).

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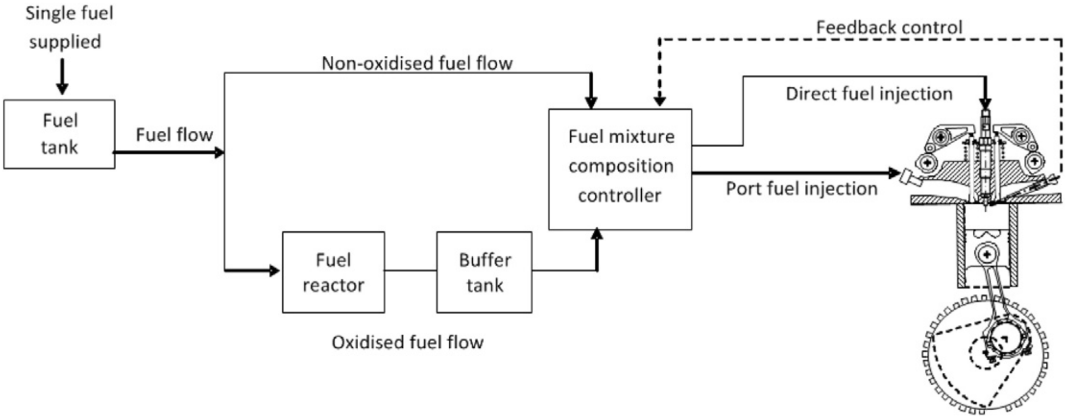


**Fig. 1.** Engine system using single fuel with variable ignition quality.

by Flynn et al. [7], Foucher et al. [8], and Masurier et al. [9,10]. Using an ozonised liquid fuel instead of gaseous ozone directly, may have the advantage of better cycle-to-cycle control, ease of stratification as well as limiting ozone destruction and energy losses occurring due to gaseous compression and injection of ozone.

In the present work, the ability of 1-hexene to control its ignition timing by altering its molecular structure in a reaction with ozone was investigated. Alkenes are known to be prone to reactions with ozone via cleavage of their double-bonds [11]. It was thus chosen to use 1-hexebe as an alkene of suitable size and volatility as model fuel for this work. A series of engine experiments were conducted in a single-cylinder direct injection diesel engine using a nearly homogeneous charge of fuel and air. Such HCCI combustion conditions allowed investigating the potential use of this ‘smart’ fuel approach in controlling combustion phasing, and allowed simple chemical kinetic modelling. It is hoped that once the fuel-and ozone reactions and the combustion chemistry of its products are better understood, this ‘smart’ fuel approach may be extended to stratified reactant mixtures, as applicable to RCCI combustion conditions.

## 2. Experimental methods

### 2.1. Engine characteristics

The engine was an automotive production engine (Ford Duratorq TDCi) customised to a single cylinder design using a single cylinder engine block (Ricardo Hydra). The compression ratio of the engine was 15:1, and the engine intake air was naturally aspirated at a constant temperature and absolute pressure of 300 K and 102 kPa. The head, cylinder bore, stroke, piston and injectors were identical to the original automotive engine. Fuel was injected into the air intake duct approximately 1 m upstream of the inlet valves. The engine speed was controlled to a constant speed of 1200 rpm using a direct-current dynamometer. Detailed engine specifications are given in Table 1.

**Table 1**
Engine specification.

| Engine model | Ford Duratorq 2003 |
|---|---|
| Number of cylinders | 1 |
| Cylinder bore | 86 mm |
| Crankshaft stroke | 86 mm |
| Swept volume | 499.56 $cm^3$ |
| Compression ratio | 15: 1 |
| Maximum cylinder pressure | 15 MPa |
| Piston design | Central ω-bowl in piston |
| Oil type | 10 W40 |
| Water temperature | 85 °C |

### 2.2. Fuel injection system

The fuel and air mixture were premixed in the intake duct of the engine over 10 diameters upstream of the intake valves. The fuel was injected using a solenoid-actuated multihole injector (Ford), and was supplied using a sealed tank pressurised to a constant gauge pressure of 300 kPa using air. A schematic of this system has been described earlier [5].

### 2.3. Instrumentation

The cylinder of the engine was instrumented using a piezoelectric pressure transducer (Kistler 6056 AU38) coupled to a charge amplifier (Kistler Type 5011) to provide measurements of the cylinder pressure at 1/5° crank angle intervals. The sampling was timed using an optical shaft encoder (Encoder Technology EC85), and pegged to an absolute reference pressure at bottom-dead-centre (BDC) of every engine cycle. The reference pressure was measured using a piezo-resistive pressure transducer (Druck PTX 7517-3257) located 160 mm upstream of the inlet valves. The cylinder pressure was measured for at least 100 engine cycles for each experiment, and averaged. The composition of the exhaust gases was determined using an automotive gas analysing system (Horiba MEXA9100 HEGR), consisting of a chemiluminescence analyser for $NO_x$, non-dispersive infrared (NDIR) analysers for CO and $CO_2$, a flame ionisation detector for unburned hydrocarbons and a magneto-pneumatic gas analyser for $O_2$. The number and size of particulates in the exhaust gases was determined using a differential mobility particle spectrometer (Cambustion DMS500) [13]. The particulate sampling probe was heated to 65 °C and a two-stage dilution process was used having a primary dilution ratio of 1:4, and a secondary dilution ratio of 1:35.

### 2.4. Fuel properties and reaction with ozone

The fuel used in the engine experiments consisted of 1-hexene, 1-hexene reacted with ozone-containing air, and a 50% volumetric mixture of these two. 1-hexene was obtained from a specialist chemical supplier (Sigma-Aldrich) and had an assay of at least 97%. The ozone in the ozone-containing air was generated using a corona-discharge, and had a mole fraction of approximately 4%. The ozone-containing air was passed through a quantity of 250 g 1-hexene using a stainless-steel tube of 250 mm length, 4 mm internal diameter and 6 mm external diameter. This process was applied to the fuel for 4 h, and was carried out at a temperature of 293 K, and an absolute pressure of 102 kPa. The reaction time of fuel with ozone used in these experiments was long compared to the rapid cycle-to-cycle changes in fuel quality required by the engine. This long time was chosen to ensure ample

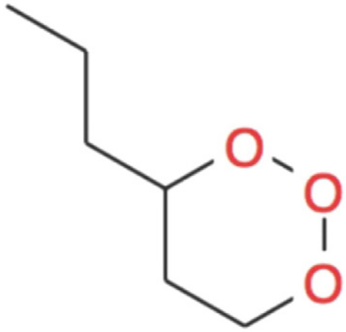


**Fig. 2.** Possible structure of ozonide produced in the fuel during its reaction with ozone-containing air.

conversion of the fuel with ozone for these initial experiments. Conceptually, a buffer tank for reacted fuel (Fig. 1) would provide a simple solution for using a comparatively slow reaction of the fuel with ozone, in conjunction with the requirements for fast changes in fuel quality demanded by the engine. Yet, during the reaction process, the formation of a white mist was observed in the ozone-containing air bubbles passed through the 1-hexene within seconds. This may indicate that some reactions were significantly faster than 4 h. Further work will be necessary to examine the reaction times of the fuel with ozone, and establish time-dependent product concentrations.

### *2.5. Fuel NMR analyses*

The products of the reaction of the 1-hexene with ozone-containing air at the described conditions could not be predicted using existing schemes, and thus had to be determined analytically. NMR experiments were acquired at 25 °C on a Bruker Avance III HD 500 MHz NMR spectrometer, equipped with a 5 mm SmartProbe BBFO probehead. Two samples were analysed. One containing approximately 500 μl of 1-hexene, which had reacted with ozone-containing air, and one containing approximately 500 μl of untreated 1-hexene. 50 μl of toluene-d8 ($C_6D_5CD_3$, Dr. Glaser AG Basel, 99.5% D) were added to both samples for the field frequency lock. NMR chemical shifts are referenced internally to the residual, most down-field $^1$H resonance of the aromatic resonances of toluene at 7.09 ppm for $^1$H, and 128.0 ppm for the attached $^{13}$C.

A comparison of the $^1$H NMR spectra of the two samples identified several peaks of low intensity, only present in the sample of ozone-treated 1-hexene. Several of these occurred at a chemical shift indicating oxidation products. The $^1$H NMR spectrum was completely dominated by the intense resonances from protonated 1-hexene, but additional two-dimensional (2D) $^1$H–$^1$H–TOCSY, $^{13}$C–HSQC, and $^{13}$C–HMBC experiments could still allow for spin system characterisation and tentative identification of three of the four main reaction products, as formic acid, 1-pentanal, and 1,2-epoxypentane. For a fourth main reaction product, the NMR data did not provide conclusive evidence for identification. The data indicated the existence of six protonated carbon atoms, with two of the carbons having resonances at the unusually high chemical shifts values of 68.6 and 79.7 ppm. This is likely due to that both carbons were attached to oxygen atoms, probably at either end of a peroxide or ozonide group. An example of a plausible structure is given in Fig. 2.

The concentrations of the various reaction products were estimated by comparison of their peak intensity to the intensity of the $^{13}$C satellites of the resonances from 1-hexene, also observed in the spectrum. The natural abundance of $^{13}$C was 1.07%. The mole fraction of pentanal was 0.2%, and the ratio of 1-pentanal:formic acid:epoxide:peroxide was 3:1.5:1:1.

For resonances observed in the 1D $^1$H NMR spectrum, the peak multiplicity (s, singlet; m, multiplet; dd, double doublet) and number of $^1$H atoms are indicated in the NMR chemical shift listings, below, together with the $^{13}$C NMR chemical shifts if they could be determined.

Formic acid: $^1$H-NMR/$^{13}$C-NMR (500 MHz/125 MHz, 1-hexene) ppm 7.66(s, 1 H)/162.9.

1-pentanal: $^1$H-NMR/$^{13}$C-NMR (500 MHz/125 MHz, 1-hexene) ppm 9.53(t, 1 H)/199.0, 2.12/43.6, 1.45, 1.23, 0.84.

1,2-epoxypentane: $^1$H-NMR/$^{13}$C-NMR (500 MHz/125 MHz, 1-hexene) ppm 2.65(m, 1 H)/51.5, 2.46(dd, 1 H)/45.6, 2.18(1 H)/45.6, 1.35, 0.87.

Unidentified product: $^1$H-NMR/$^{13}$C-NMR (500 MHz/125 MHz, 1-hexene) ppm 3.97(m, 1 H)/79.7, 3.80(m, 2 H)/68.6, 2.38(m), 1.91, 1.53, 1.29, 0.86.

## 3. Combustion experiments

In a series of combustion experiments control of the autoignition timing of 1-hexene in an engine was achieved by reacting a variable portion of the 1-hexene with ozone-containing air prior to its introduction into the engine. The engine was operated at a constant speed of 1200 rpm, and constant indicated mean effective pressure (IMEP) of 0.45 MPa. The fuelling was adjusted to produce constant power during all experiments. First, 1-hexene was injected into the engine, followed by 1-hexene reacted with ozone-containing air, and finally a 1:1 volumetric mixture of the two was injected. The cylinder pressure and apparent heat release of combustion of these experiments are shown in Fig. 3.

Fig. 3 a) shows that the peak cylinder pressure progressively increased as the fraction of 1-hexene oxidised with ozone was increased within the fuel. Fig. 3 b) shows that the increased peak cylinder pressure was accompanied by an advance in the heat release of the fuel towards

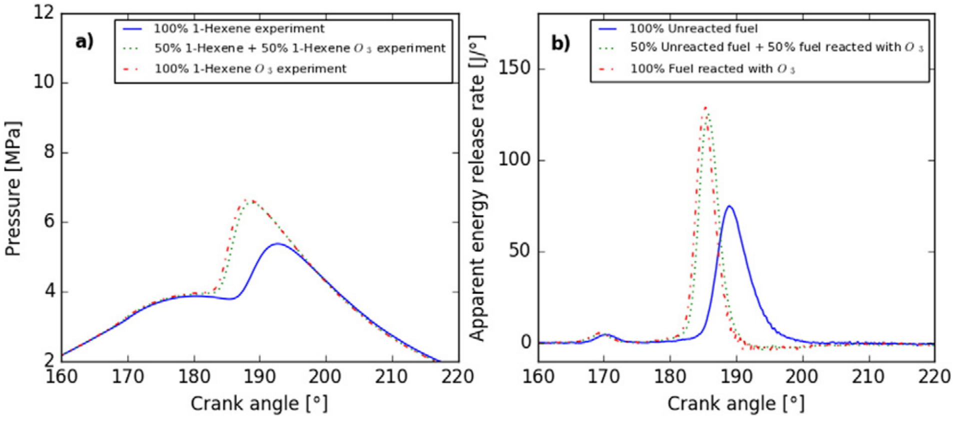


**Fig. 3.** Engine experiments conducted in HCCI combustion mode showing a) cylinder pressure and b) apparent heat release rate of combustion.

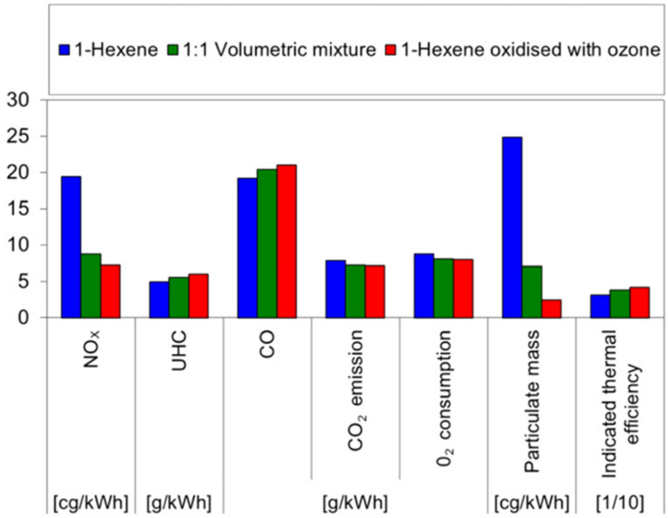


**Fig. 4.** Experimentally-measured indicated efficiency and exhaust gas emissions of the engine.

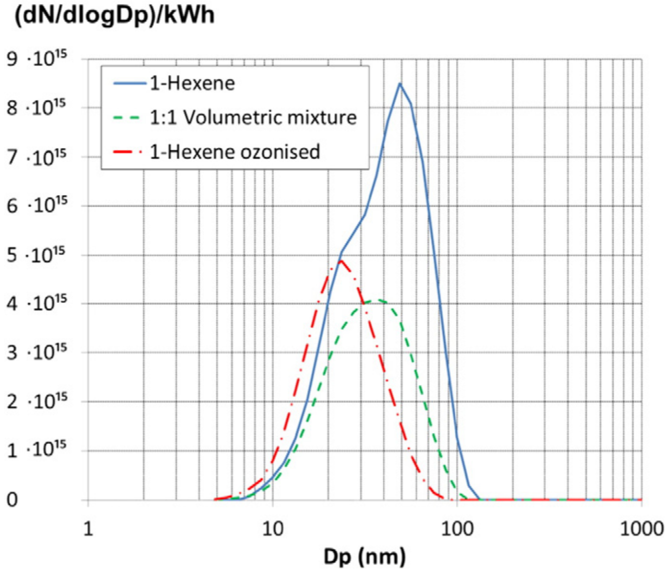


**Fig. 5.** Experimentally measured power-specific particulate size spectral density.

TDC (180° crank-angle (CA)). The heat release rate in Fig. 3 b) shows that a significant proportion of low-temperature heat release occurred around 170° CA for all fuels. This low temperature heat release had a slightly higher peak value and occurred slightly earlier for 1-hexene oxidised with ozone, than for unreacted 1-hexene. This suggests that the low-temperature ignition reactions were affected by the oxidation of the fuel with ozone. The high-temperature heat release which occurred just after 180° CA, was advanced and had a higher intensity when the 1-hexene was oxidised with ozone.

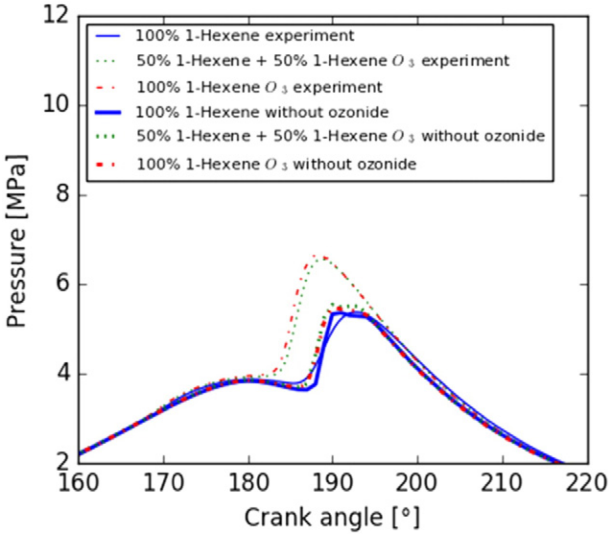


**Fig. 6.** Cylinder pressure calculated in chemical kinetic simulation of the HCCI cycle when excluding the ozonide molecule, and comparison with experiments.

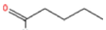
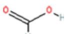
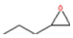
Fig. 4 shows the indicated thermal efficiency and exhaust gas emissions of the engine. The engine efficiency increased as the ignition timing of the engine was advanced by reacting the fuel with ozone prior to its introduction to the combustion chamber. This may be expected since the earlier ignition timing just after TDC tends to be more favourable for high cycle efficiency from a cycle perspective [4]. The higher peak cylinder pressures shown in Fig. 3 a) suggest that the combustion of 1-hexene reacted with ozone took place at higher reaction temperatures than the original 1-hexene. Such higher pressure and temperature conditions are likely to have improved the combustion efficiency of the fuel and air mixture. Fig. 5 shows the size-spectral density of the particulates recorded using the differential mobility spectrometer. The emission of total particulate mass was higher for unreacted 1-hexene than when 1-hexene was reacted with ozone prior to combustion. This may again be correlated with the higher reaction pressures and temperatures associated with the 1-hexene, resulting in improved burnout of soot particles.

The size spectral density of larger particulates around 100 nm in diameter decreased for fuel reacted with ozone prior to combustion, which may be a sign of improved burnout of soot-particles for the advanced ignition timing.

## 4. Chemical kinetic modelling

In order to investigate the reasons for the change in ignition timing when the fuel was reacted with ozone prior to injection into the engine, the engine experiments were simulated using a single-zone homogeneous reactor model and the chemical kinetic mechanism developed by Zhang et al. [14]. The modelling was implemented in the Cantera 2.2.0 software tools. As discussed by Hammond et al. [15] homogeneous chemical kinetic reactor models are unable to capture the physical details of the engine such as temperature and reactant stratification, and

**Table 2**
Fuel composition in chemical kinetic simulations.

| Name | Sum formula | Structure | Mole fraction in unreacted 1-hexene | Mole fraction in 50/50 mixture | Mole fraction in ozonised 1-hexene |
|---|---|---|---|---|---|
| 1-hexene | C6H12–1 |  | 1 | 0.997833 | 0.995667 |
| Pentanal | C5H10O1–5 |  | 0 | 0.001 | 0.002 |
| Formic acid | CH$_2$O$_2$ |  | 0 | 0.0005 | 0.001 |
| Epoxide | C$_5$H$_{10}$O |  | 0 | 0.000333 | 0.000667 |
| 1-hydroperoxyhexane | C$_6$H$_{14}$O$_2$ |  | 0 | 0.000333 | 0.000667 |

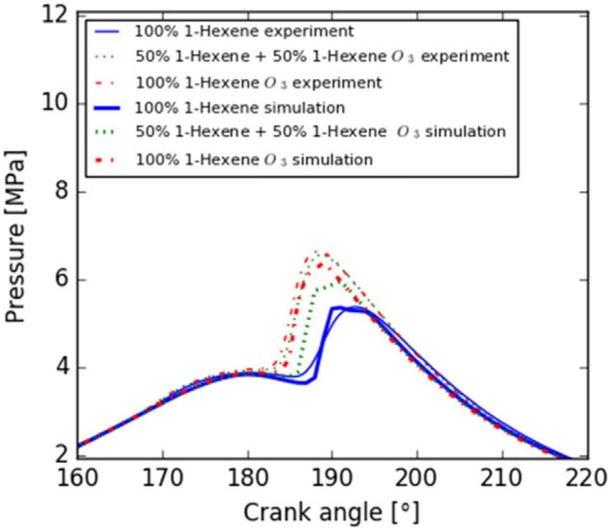


**Fig. 7.** Cylinder pressure calculated in chemical kinetic simulation of the HCCI cycle by modelling the ozonide as 1-hydroperoxyhexane, and comparison with experiments.

will not predict heat release rates and emissions correctly, but they are reliable for predicting the ignition timing trends in the engine.

The reaction conditions and cylinder pressure of the engine was calculated using a slider-crank model computed in the Python 3.4 programming language. The initial temperature of the reactants was not measured in the engine experiments, but would be expected to be significantly higher than the inlet air temperature of 300 K, due to the heat transfer from the intake valves and walls. This temperature was tuned in the chemical kinetic model, so as to match the ignition of pure 1-hexene in the model with that in the experiments. This yielded an initial reactant temperature of 407 K, which is reasonable for a continuously firing warmed-up engine. The fuel composition of the experiments in which 1-hexene reacted with ozone was simulated were based on the NMR analyses, but had to be adapted with some assumptions and simplifications, in order to be able to model the experiments using the existing chemical kinetic mechanism. The 1-hexene reacted with ozone-containing air was modelled as 1-hexene containing the four most important reaction products, or surrogates. The four main reaction products were 1-pentanal, formic acid, 1,2-epoxypentane, and the ozonide or peroxide which could not be fully identified, but whose likely molecular structure is shown in Fig. 2. The fuel composition for the fuels is given in Table 2.

If only the identified compounds consisting of 1-pentanal, formic acid, 1,2-epoxypentane were included in the chemical kinetic model, no clear advance of the ignition timing was observed in the chemical kinetic computations. This is shown in Fig. 6, which shows the cylinder pressure traces of the HCCI engine experiments together with the cylinder pressure traces computed by the chemical kinetic model, when the ozonide molecule is replaced by simple 1-hexene.

Fig. 6 suggests that the advance in ignition timing cannot be explained by the formation of the identified reaction products in the fuel alone.

An effort was made to model the effect which the ozonide may have on ignition timing. Since the molecule shown in Fig. 2, could not be modelled using existing chemical kinetic mechanisms, it was decided to model its peroxidic property using a molecule of similar molecular structure. The molecule 1-hydroperoxyhexane was chosen as a simplified surrogate molecule for the ozonide shown in Fig. 2, because of its structural similarity in containing six carbon atoms and at least one oxygen to oxygen bond. Fig. 7 shows a comparison of the calculated cylinder pressure from the homogeneous combustion model, with the engine experiments if the reaction products were modelled as 1-pentanal, formic acid, 1,2-epoxypentane and by 1-hydroperoxyhexane.

The calculations showed that a clear advance in ignition timing was observed when 1-hydroperoxyhexane was included in the fuel composition. Fig. 7 shows that this trend is in agreement with the experimental data recorded in the engine, although small differences in cylinder pressure are visible. The main difference is that the experiments showed a slightly stronger advance in ignition timing, and a more pronounced increase in peak cylinder pressure for 1-hexene reacted with ozone containing air. The chemical kinetic simulations allowed exploring the mechanism behind the advancement of ignition timing in further detail. Fig. 8 shows a reaction path diagram of the reactor model at 90° CA

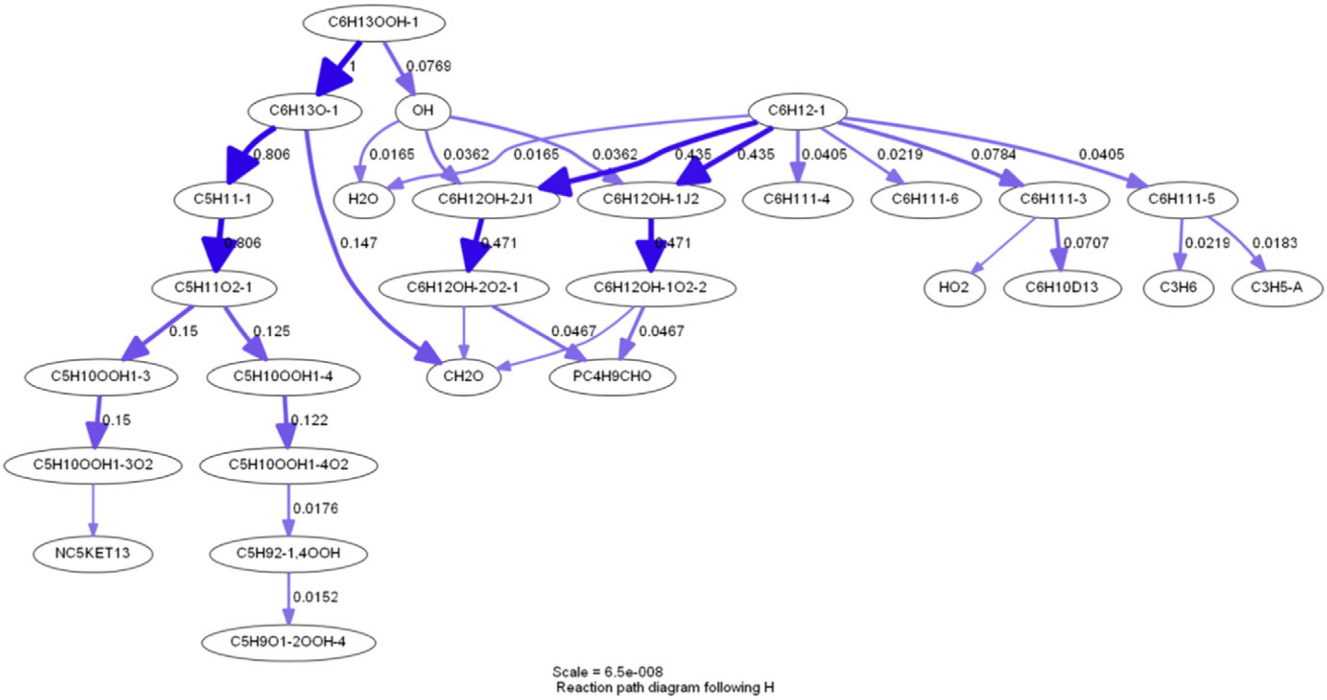


**Fig. 8.** Reaction paths of 1-hexene reacted with ozone at 90° CA before TDC.

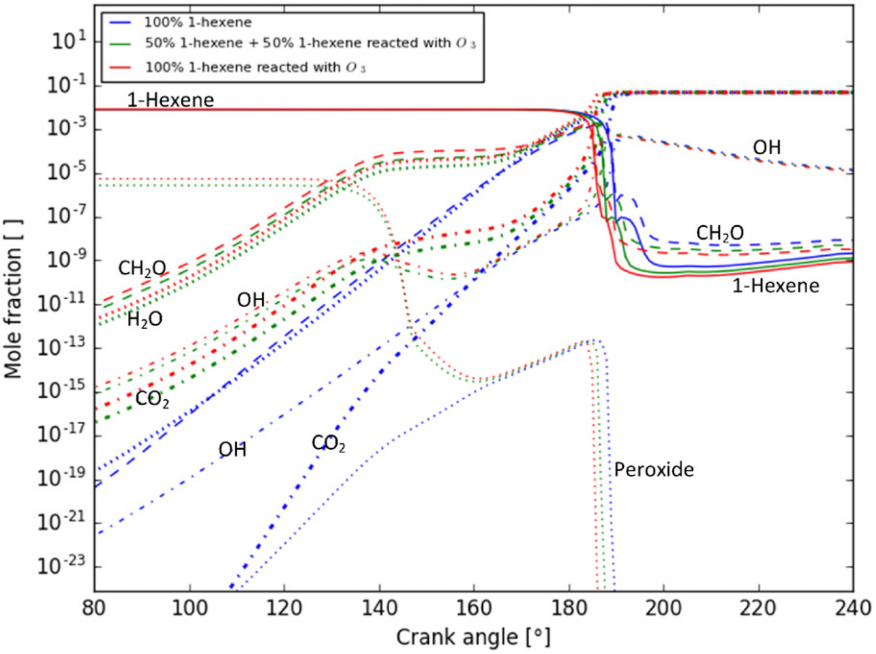


**Fig. 9.** Species concentration during ignition for 1-hexene oxidised with ozone.

before TDC, illustrating how the presence of 1-hydroperoxyhexane (C6H13OOH-1) influenced the decomposition of 1-hexene by supplying hydroxyl (OH) radicals during the induction period. Fig. 9 shows that decomposition of 1-hydroperoxyhexane accelerated progressively from 80 to 140° CA with the peak decomposition taking place around 142° CA.

During the induction period, the decomposition of 1-hydroperoxyhexane led to the formation of OH radicals, which supported the conversion of 1-hexene. The OH radicals were shown to attack the 1-hexene (C6H12–1) molecules early during the ignition process (90° before engine TDC), and assist their decomposition into (C6H12OH–2J1), (C6H12OH–1J2), and $H_2O$, as well as formaldehyde (CH2O). Fig. 9 illustrates in detail how the mole fractions of these species evolved over time, for the specific case of the 1-hexene oxidised with ozone.

The conversion of the fuel into its final products $CO_2$ and $H_2O$ was marked by a peak concentration of $CH_2O$ during the early high-temperature ignition phase around 180° CA, followed by OH during the final stages of combustion around 188° CA. The $CH_2O$ was almost entirely decomposed during the combustion process, leaving a fraction of <1 ppm of $CH_2O$ in the exhaust gases for 1-hexene reacted with ozone as well as for neat 1-hexene. Formaldehyde emissions from the ozonides would thus not be anticipated to pose a significant problem.

## 5. Conclusions

A series of engine experiments were conducted to investigate the possibility of altering the molecular structure and composition of a fuel, in order to control its ignition timing.

The main conclusions of this study may be summarised as follows:

1. Ignition timing of a 1-hexene and air reactant mixture can be advanced using prior reaction of the fuel with ozone-containing air.
2. Chemical analyses of the fuel after reaction with ozone-containing air suggest that ozonides formed within the fuel.
3. Ignition advance was likely to be promoted by early decomposition of peroxidic structures amongst the molecules, which can advance the main ignition timing through formation of reactive intermediates such as OH radicals.

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