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A study of liquid fuel injection and combustion in a constant volume vessel at diesel engine conditions

Z. Hu [a], L.M.T. Somers [a,*], T. Davies [b], A. McDougall [b], R.F. Cracknell [b]

[a] Eindhoven University of Technology, Den Dolech 2, P.O. Box 513, 5600MB, Eindhoven, The Netherlands
[b] Shell Global Solutions (UK) Shell Research Ltd., Shell Technology Centre Thornton, P.O. Box 1, Chester CH1 3SH, United Kingdom

HIGHLIGHTS

- *N*-heptane and *i*-octane are studied at diesel engine conditions in a constant volume cell.
- Ignition delay is studied as function of pressure and temperature.
- The experiments include classical diesel combustion regimes and PCCI-like conditions.
- The Flamelet Generated Manifold (FGM) method is applied in a CFD code to model experiments.
- The model recovered the ignition delays for *n*-heptane for varying conditions.

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ABSTRACT

Experiments were performed in a constant volume vessel, with fuel sprays injected into the vessel at selected pressure and temperature conditions that are typical of a diesel engine at cold start. *N*-heptane and *i*-octane were used as surrogate fuels for diesel and gasoline, following the establishment of a semi-detailed mechanism containing skeletal mechanisms for *n*-heptane and *i*-octane, that has proved to predict autoignition delay times that agree well with experiments. Computational Fluid Dynamics (CFD) modeling of combustion for these two fuels at the selected experimental conditions were thus conducted adopting this mechanism, with the objective of studying fuel composition, temperature and pressure effects on mixing and combustion numerically. A tabulated chemistry approach called Flamelet Generated Manifolds (FGMs) has been applied for combustion modeling in the CFD solver STAR-CD. Since diesel combustion features mainly diffusion combustion, the manifold is created with 1D diffusion flame solutions from ignition and extended to steady state flamelets from low-to-high stretch rates. Effects from different fuels are examined experimentally, while effects from different conditions for *n*-heptane injection are examined from both experimental and simulation results.

1. Introduction

Due to the ever increased demand for low smoke and low NOx emissions, considerable research effort has been directed towards cleaner diesel engines, that retain the advantage of high efficiency [1–3]. Smoke can be reduced by promoting the mixing of fuel and air before combustion [1]. The NOx level can be reduced by lowering the combustion temperature. Many strategies such as low compression ratio, EGR cooling and high injection pressure have been adopted to achieve low-temperature premixed combustion [4]. HCCI (Homogeneous Charge Compression Ignition) combustion is another approach to achieve low-NOx and low-smoke in a compression ignition engine, which features autoignitive lean combustion [5,6]. However, engine control is difficult in this case and the lean mixture combustion limits the achievable load [7]. Recently, PCCI (Premixed Charge Compression Ignition) combustion has received more attention since it offers the efficiency of a conventional diesel engine, but with low smoke and NOx emissions. Through high exhaust gas recirculation (EGR) rates and strategic injection timings, PCCI combustion features non-homogeneous fuel–air mixtures, so that combustion is also mixing controlled as in conventional diesel engine, but with a longer ignition delay so to allow enough time for premixing fuel and air followed by a low temperature combustion event, therefore it achieves low smoke and low NOx target [8].

In short, PCCI combustion is when fuel and air are premixed but not fully premixed. The present work examines PCCI condition in a constant volume vessel, by varying ignition delay through varying fuels, temperature, pressure, etc. Levels of mixing are thus different

* Corresponding author. Tel.: +31 40 2472107; fax: +31 40 2433445.
E-mail address: l.m.t.somers@tue.nl (L.M.T. Somers).

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at the time of ignition, affecting overall combustion. This paper describes both experimental results and Computational Fluid Dynamics (CFD) modeling, where the latter technique is used in this study to examine local mixing.

Among many factors that affect autoignition delay, fuel ignition quality is of primary interest. Conventionally gasoline autoignition quality is defined by RON (Research Octane Number) and MON (Motor Octane Number). Typical gasoline used in Europe has a RON of 95 and MON of 85. The RON and MON are measured under the specific condition of the RON and MON tests. Furthermore, there is the Octane Index, OI, which is measured for any specified temperature and pressure in a given engine, that describes autoignition quality of fuel at various engine condition. OI = $(1-K)$ RON + $K*$ MON, and K is a constant depending only on the pressure and temperature variation in the engine [9]. The octane scale is based on primary reference fuels (PRFs), mixtures of the two paraffins *i*-octane and *n*-heptane, which correspond to octane number of 100 and 0 respectively. Diesel fuel's autoignition quality is described by Cetane Number, CN. Typical diesel used in Europe has a minimum CN of 52.

Despite the importance of the RON and MON as international standards in the automotive and oil industries, they are incomplete guides to autoignition since the PRFs and the associated RON and MON tests were initially chosen to reveal the extremes of gasoline knock behaviour [10]. It should be recognized that fuel autoignition behavior changes at various operational T and p values, so practical fuel will autoignite differently from PRF with same RON and MON, when the condition is different from those of RON and MON test. Chemical kinetics have been developed for PRFs, that can reveal autoignition behavior of PRFs at different condition; however, the autoignition chemistry for non-PRF fuels is not fully understood at the moment. Different combination of PRFs are then used to mimic real fuels for their similar autoignition behavior, *n*-heptane for diesel, *i*-octane for gasoline, etc. In this study, PRFs will be used for computational purposes, that a semi-detailed chemical kinetic mechanism by Andrae (137 species and 633 reactions [11]) will be used. It has been proved to be capable of predicting correct autoignition behavior for mixtures of *n*-heptane, *i*-octane and toluene at various pressure and temperature conditions.

2. Experiment

Two model fuels *n*-heptane and *i*-octane were used and their properties are listed in Table 1. A constant volume vessel that mimics diesel engine condition was adopted for experimental work, whose details are introduced as follows.

2.1. Combustion Research Unit

The Combustion Research Unit (CRU) in Shell Global Solutions (Retail and Automotive Fuels Technology Group, Thornton) is a constant volume vessel, manufactured by Fueltech, that can mimic combustion condition in modern diesel engines. A schematic diagram of the CRU is shown in Fig. 1.

It comes with a common rail injection system of type Bosch CRIP2 (Part No: 0445110157). It features a nozzle with seven holes, distributed evenly around the circle. A spray from each hole is injected at an angle of 79° away from the injector centerline, and the include angle for each hole is 10°, which will be used in the modeling study. Fuel is injected into the pressurized heated chamber via a common rail injector, where it mixes with hot air and ignites. The combustion process is monitored with a pressure sensor inside the chamber whilst a needle lift sensor inside the injector monitors the injection event. The chamber pressure, chamber temperature, fuel pressure, chamber gas composition and pulse width that determine injection period can all be varied by the operator. Some technical parameters of the CRU are listed in Table 2.

The needle lift sensor and the two dynamic pressure sensors in the combustion chamber and fuel line all sample at a rate of 50 kHz (intervals of 0.02 ms), giving outputs including needle lift, chamber pressure and fuel pressure. The needle lift enables the measurement of the start of injection (SOI) and the end of injection (EOI). The chamber pressure is used to determine ignition delay (the time from start of injection to autoignition, ID^0), burn period (time taken for the fuel to burn once it has autoignited) and the energy released per injection, considering the maximum pressure rise (Max dP).

Table 1
Some properties of fuels used in this study.

Fuel	RON	MON	Density (g/cc)	C	H	LHV (MJ/kg)
N-heptane	0	0	0.632	7	16	44.6
I-octane	100	100	0.688	8	18	44.4

2.2. Experimental conditions

The fuel was injected into the chamber at nine different conditions as listed in Tables 3 and 4. Conditions differed by varying the chamber temperature (T) and pressure (p). The fuel injection pressure was 900 bar, pulse width was 0.9 ms, which gave a corrected injection period of about 1.3 ms (SOI = 0 ms, EOI ≈ 1.3 ms). The determination of injection profile was very important, since it directly determined mixing and combustion. The injection rate was determined through a set of non-combusting experiments. With the injector still controlled by the CRU, a large number of injections (>100) were carried out at one set of injection parameters. The chamber was at room temperature and atmospheric pressure, so combustion did not occur. After the injections had finished, the chamber was weighed again, to allow the mass of fuel injected to be calculated. This result would then be used as a calibration to determine the injected mass for the combusting case as in this study, considering the variation of injector pressure, chamber pressure and fuel density. The injection profile for all cases could be summarised as almost the same: the injection duration was 1.3 ms, injection rate for *n*-heptane was 30 g/s, while for *i*-octane it was about 32.658 g/s, due to the density difference between the two fuels. These values can also be suitably validated by the measured maximum pressure rise in complete combustion case, as in 4th column in Table 3 (in the experimental results section).

3. Modeling

Among numerous combustion models proposed for such reacting conditions, Flamelet Generated Manifolds (FGMs) have obtained great attention [12,13]. The common practice of FGM is to solve a set of one-dimensional premixed laminar flames; an example of a flamelet is shown in Fig. 2, for a lean burn methane/air flame, solved by detailed chemistry. FGM features tabulation of reaction rates and species mass fractions as functions of primary variables (mixture fraction, reaction progress variable, enthalpy, strain rates, etc.), as will be described later.

The methodology was initially applied to Reynolds-Averaged Navier–Stokes (RANS) computations of premixed turbulent flames [15], known as laminar flamelet library. It is extended to non-premixed diesel combustion in large eddy simulation (LES) [16], whose capability for capturing local flow fluctuations is explored [17]. Recently partially premixed flames (PPFs) have been studied [18–21], the results illustrating the great potential of the FGM method in treating scenarios with varying equivalence ratio. To study diesel combustion the FGM method is extended to incorpo-