



Cyclopentane combustion. Part II. Ignition delay measurements and mechanism validation



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ABSTRACT

This study reports cyclopentane ignition delay measurements over a wide range of conditions. The measurements were obtained using two shock tubes and a rapid compression machine, and were used to test a detailed low- and high-temperature mechanism of cyclopentane oxidation that was presented in part I of this study (Al Rashidi et al., 2017). The ignition delay times of cyclopentane/air mixtures were measured over the temperature range of 650–1350 K at pressures of 20 and 40 atm and equivalence ratios of 0.5, 1.0 and 2.0. The ignition delay times simulated using the detailed chemical kinetic model of cyclopentane oxidation show very good agreement with the experimental measurements, as well as with the cyclopentane ignition and flame speed data available in the literature. The agreement is significantly improved compared to previous models developed and investigated at higher temperatures. Reaction path and sensitivity analyses were performed to provide insights into the ignition-controlling chemistry at low, intermediate and high temperatures. The results obtained in this study confirm that cycloalkanes are less reactive than their non-cyclic counterparts. Moreover, cyclopentane, a high octane number and high octane sensitivity fuel, exhibits minimal low-temperature chemistry and is considerably less reactive than cyclohexane. This study presents the first experimental low-temperature ignition delay data of cyclopentane, a potential fuel-blending component of particular interest due to its desirable antiknock characteristics.

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1. Introduction

Recent developments in climate change policies [1] and fuel economy projections [2] portend major shifts in energy production and consumption trends. In an unprecedented occurrence, 195 countries signed the Paris Agreement whereby they pledged to reduce greenhouse gas (GHG) emissions and limit the increase in global average temperature to well below 2 °C above pre-industrial levels by the year 2020 [1]. At the same time, the global demand for energy is expected to increase as the world's population and Gross Domestic Product (GDP) increase, particularly in China and India [2]. In order for the projected increase in energy demand

to be met within the constraints of legally binding climate change agreements, the fuel industry has to evolve. The latest Energy Outlook report published by British Petroleum (BP) shows that, even though conventional fossil fuels are projected to meet two-thirds of the increase in energy demand out to 2035, renewables and unconventional fossil fuels will grow faster [2]. Shale-derived fuels are among the emerging new sources of energy that are expected to grow quickly in the near future due to technological advancements [2]. These, among others, are the fuels of the future, and they are primarily composed of alkanes and cycloalkanes, followed by aromatics and bicyclic hydrocarbons [3]. The combustion chemistry of alkane fuel components is relatively well researched; however, that of cycloalkanes is not, despite the proven importance of cycloalkane functionality in the oxidation of real fuels [4]. In general, investigating fuel chemistry ultimately allows for the control of fuel efficiency and emission via targeted fuel and engine design.

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The most prominent cyclic backbone in practical fuels is cyclohexane [3]. Accordingly, studies on cycloalkane combustion are mostly concerned with cyclohexane and methylcyclohexane, which are regarded as representatives of the naphthenic fraction in conventional fuels [5–10]. These studies show that cyclohexane and its derivatives are less reactive than their non-cyclic counterparts due to the conformational inhibition of ROO/QOOH isomerization pathways, which promotes the formation of non-reactive olefins [11,12]. They also emphasize the importance of these species in soot formation mechanisms [13]. Since cycloalkane chemistry and kinetics are strongly influenced by the ring size [12], and because other cycles are also prominent in practical fuels, it is important to investigate components other than cyclohexane.

In this study, we investigate the low- and high-temperature reactivity and ignition properties of cyclopentane, a high-octane, knock-resistant cycloalkane, commonly found in gasoline and a suitable blending component [14]. Previous experimental studies of cyclopentane ignition delay are generally limited to high-temperature conditions. Daley et al. [15] measured the ignition delay of cyclopentane in a shock tube (ST) under engine-relevant conditions for lean and stoichiometric fuel/air mixtures, at pressures of 13 and 45 atm, and at temperatures between 847 and 1379 K [15]. Tian et al. [16] and Sirjean et al. [17] also provided ST ignition delay measurements of cyclopentane within the temperature range of 1100–1800 K and at pressures of up to 8.4 bar, for fuel-lean, stoichiometric and fuel-rich conditions [16,17]. The fuel/oxidant mixtures were diluted in argon at fuel concentrations of 0.5 and 1.0% [16,17]. The measured data were used to validate high-temperature cyclopentane oxidation mechanisms developed based on the JetSurF2.0 mechanism [16] or using the EXGAS software [17]. Davis and Law [18] measured premixed laminar flame speeds for cyclopentane/air mixtures at a range of equivalence ratios. They found that cyclopentane/air mixtures exhibited similar laminar flame speeds as *n*-pentane, *n*-hexane, and cyclohexane.

Herein, we present ignition delay experiments that span a wider range of conditions than in previous studies and are also relevant to internal combustion engines. High-temperature experiments were conducted at the high-pressure shock tube (HPST) facilities at King Abdullah University of Science and Technology (KAUST) and the National University of Ireland, Galway (NUIG), whereas the rapid compression machine (RCM) at NUIG was used to carry out measurements at low to intermediate temperatures. The new data span temperatures between 650 and 1350 K, pressures of 20 and 40 atm, and use fuel/air mixtures at equivalence ratios of 0.5, 1.0 and 2.0. A detailed kinetic oxidation model comprising low- and high-temperature reaction classes is tested against the ignition and flame speed data available in the literature, as well as the new data. Details of the kinetic model development may be found in Part 1 of this study, entitled “Mechanism development and computational kinetics”. The model was also tested against speciation data measured in a jet-stirred reactor, as detailed in [19].

2. Experimental methods

2.1. KAUST high-pressure shock tube (HPST)

High temperature ignition delay measurements (1000–1300 K) were performed using the HPST facility at KAUST at pressures of 20 and 40 atm. The HPST has been reported previously in literature [20]; hence, only brief overview will be given here. The driven section of the shock tube is 6.6 m long while the driver section length can be varied to a maximum length of 6.6 m. The shock tube has an inner diameter of 10 cm and the inner surface is electro-polished to reduce boundary layer effects. The driver and driven sections are separated by pre-scored aluminum diaphragms in a

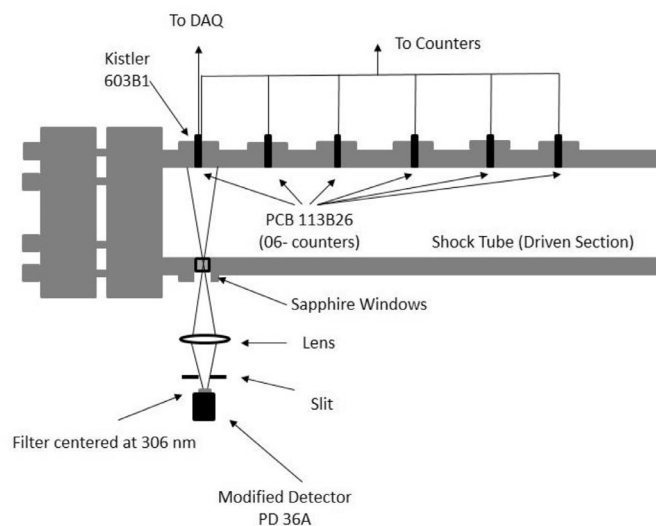


Fig. 1. Schematic of the KAUST high-pressure shock tube (HPST) used for ignition delay time measurements.

double-diaphragm mid-section. The double diaphragm mid-section allows better control of diaphragm burst pressures p_4 and hence an excellent control of reflected shock temperatures T_5 and pressures p_5 . The driven section is connected to a turbopump that can be used to achieve a vacuum pressure as low as 10^{-5} Torr. The test mixture consisting of cyclopentane (purchased from Sigma Aldrich with a purity of 99%), oxygen, nitrogen and/or helium (purchased from AH gases at 99.999% purity) was prepared manometrically by using a magnetically-stirred mixing vessel. For each set of measurements, the mixtures were allowed to mix for at least one hour before starting the experiments.

In order to measure the shock velocity, six piezoelectric pressure transducers are located axially along the last 3.2 m of the driven section of the shock tube. Post reflected shock conditions (T_5 and p_5) were calculated by using shock jump relations and known thermodynamic properties of test mixtures. A Kistler 603B1 pressure transducer located at 1 cm from the endwall was used to measure the sidewall pressure. Sidewall OH* emission was measured through a sapphire window at 1 cm from the endwall by using a photodetector and a narrow band-pass optical filter. A schematic of the experimental setup is shown in Fig. 1. Ignition delay time (IDT) is defined as the time between the arrival of the reflected shock wave at the sidewall optical location and the onset of ignition. Both sidewall pressure and OH* emission determinations are shown in Fig. 2 and agree within 5% of each other. The post-reflected pressure gradient (dp_5/dt) is nearly 3%/ms for the test conditions presented in this work, and this is accounted for in the simulations using a volume time history [21]. The uncertainty on the HPST experimental measurements is approximately $\pm 20\%$. Uncertainties in the reflected shock temperature and pressure are $< 1\%$ and are mainly due to errors in measuring incident shock velocity and thermodynamic parameters. Uncertainty in the mixture (fuel/air) composition is estimated to be less than 5% and results from the error in the measured partial pressures during mixture preparation. The pressures were measured using MKS Baratron Capacitance Manometers which have a manufacture specified uncertainty of 0.12% of the reading.

2.2. NUIG high-pressure shock tube (HPST)

High-temperature ignition delay times (1000–1300 K) were measured for stoichiometric mixtures of cyclopentane in a 21% O₂: 79% N₂ bath gas were measured behind reflected shocks within

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