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An experimental and theoretical comparison of C_3–C_5 linear ketones

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Abstract

Ketones have been recently identified as products from lignocellulosic biomass conversion. This motivates the consideration of these compounds as biofuel candidates. In order to further investigate the possibility of using these compounds as biofuels, further examinations of their fundamental combustion chemistry is required. As part of this, autoignition delay times behind reflected shock waves for stoichiometric fuel in air mixtures using acetone, 2-pentanone and 3-pentanone at 20 and 40 bar have been measured. Available comparable literature ignition delay times, including data for butanone, are also compared and used in the following analysis. Using the experimental data, correlations of the ignition delay times are derived. In addition, using knowledge of bond dissociation energies in the molecules and possible decomposition products, an explanation for the observed trends in reactivity is given. The trend in reactivity is found to be the same for both 20 and 40 bar ignition delay times, and follows the trend: 3-pentanone > butanone > 2-pentanone > acetone. Furthermore, available chemical kinetic models are compared to the measured data in order to evaluate the current understanding of ketone oxidation. Prediction performances of the different models vary widely indicating the need for further work on kinetic model development.

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1. Introduction

Declining fossil fuel resources and the general desire for a reduction of CO_2 emissions have led to a rising interest in fuel production from biomass. As part of the systematic search for suitable biofuels within the Cluster of Excellence "Tailor-Made Fuels from Biomass" (TMFB), 2-butanone was found by Hoppe et al. [4] to be a possible biofuel candidate due to a better primary breakup, higher energy density and improved knock resistance when compared to ethanol. In addition, it shows increased combustion stability at low engine load and cold boundary conditions compared to ethanol [4]. Ketones in general, also reduce soot formation when used as additives in the combustion of common fuels [5,6].

Furthermore, ketones play an important role as representative compounds for volatile organics in industrial thermal oxidizer processes [5]. Due to the light emitting abilities in laser induced fluorescence

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processes ketones like acetone or 3-pentanone are often used as fuel tracers [7–11].

Ketones can also be found as intermediate products in the combustion of larger oxygenated species like alcohols, ethers and hydrocarbons like *n*-alkanes [12]. Therefore understanding the combustion behavior of ketones and the development of detailed chemical kinetic models is an area of increasing interest. In order to adequately understand the combustion of ketones under engine relevant conditions more data at elevated pressures, above 10 bar and using fuel in air mixtures is necessary.

There exists a number of previously published fundamental studies of ketones summarized here. Experiments measuring ignition delay times for acetone can be found for temperatures of 1050–1930 K using high argon dilution between 86.88% and 99.68%, at pressures from 1.0 to 3.2 bar and equivalence ratios of 0.5–2.0 [7,13–16]. Only two previous publications contain data at elevated pressures, at approximately 12 and 13 bar [15] and 20 bar [14], but still with high dilution levels. Butanone ignition delay times were measured at 1100–1850 K, at pressures between 1 and 6.6 bar using argon dilutions of 88.00–96.75% and $\phi =$ 0.5–2.0 [17,18]. Burke et al. [1] recently published stoichiometric ignition delay times for butanone at 852–1281 K, 20 and 40 bar in air. Experimental results for 3-pentanone exist at temperatures of 1150–1850 K, pressures of 1.0–1.9 bar, $\phi = 0.5$–2.0 in argon dilutions of 86.88–99.68% [2,14,16,19]. In addition, Fikri et al. [2] measured ignition delay times for 3-pentanone in air at 10, 20 and 40 bar, $\phi = 0.5$ and 1.0. Ignition delay measurements for 2-pentanone are only considered by Lam et al. [16]. This study covered temperatures at 1350–1515 K, ≈ 2.5 bar, $\phi = 1.5$ in 99.40% argon. The results of these studies were also used for chemical kinetic modeling in these studies.

In addition, detailed chemical kinetic models were developed for the different ketones based on flame speed measurements in spherical bombs [1,7,19] on initial conditions of 298 K, ≈ 1 bar, $\phi =$ 0.8–1.6 in air. Detailed chemical kinetic models have also been developed based on data obtained from stabilized flames [5,20–22] at 298–358 K initial temperatures, 11.25 mbar to 1 bar, $\phi =$ 0.8–1.72 in air or argon [6]. In addition, model development based on continuous flow reactors [23,24] at 530–1500 K, 1–10 bar, $\phi =$ 0.14–4.0 using different mixture compositions were previously published. Additional kinetic models were developed based on species-time histories measured in shock tubes [13,16,18,25] at 900–1678 K, 1–3.2 bar, $\phi =$ 0.5–2.0, highly diluted in argon (94.00–99.75%). Decomposition reaction rate constants and hydrogen abstraction rate constants by $\dot{O}H$ radicals were measured using the shock tube pyrolysis data from Lam et al. [26,27] for acetone, butanone, 2- and 3-pentanone and Badra et al. [18] for butanone. Since the majority of data available in literature are reported at low pressures and high dilution levels, the current study targets to investigate the autoignition behavior of C_3–C_5 ketones for fuel in air mixtures up to 40 bar and to compare their measured ignition delay times.

This work presents ignition delay times measured behind reflected shock waves for acetone, 2- and 3-pentanone at 20 and 40 bar for fuel in air mixtures. Different kinetic models found in the literature are benchmarked against this data. In addition, recently published ignition delay times for butanone performed at the same conditions from Burke et al. [1] are also used for comparison.

2. Experiments

Ignition delay time measurements behind reflected shock waves are measured in the PCFC rapid screening shock tube (PCFC-RSST). The shock tube has a 3 m long curved driver section and a 4.1 m long driven section with an inner diameter of 63.5 mm. It is designed for high pressures up to 500 bar. The driven section is designed for temperatures up to 150 °C. Driver and driven sections are separated through a double diaphragm chamber housing two pre-scored aluminum diaphragms. In order to tailor the conditions behind the reflected shock, the driver section can be filled with a mixture of synthetic air and helium. The incident shock velocities were measured over the last 1.0 m of the driven section using five PCB model 113B22 pressure transducers. In order to determine the gas conditions behind the reflected shock an inhouse code was used based on the "Shock and Detonation Toolbox" [28] developed for Cantera [29]. Thermochemical data for the fuels have been taken from the literature [19]. Since no data was available for 2-pentanone at the high temperatures considered here, it was calculated using the group additivity method [30]. The results were found to be within an uncertainty of 1.6% compared to the data provided on NIST chemical webbook [31] for low temperatures.

Ignition delay times were defined between the pressure rise caused by the reflected shock and the steep pressure rise resulting from ignition, Fig. 1. This was recorded using the pressure trace obtained from the transducer closest to the endwall (9 mm).

Mixtures were prepared in a heated Teflon coated stainless steel mixing vessel. Mixture compositions were controlled by monitoring partial pressures. Static pressures were measured with a STS ATM.1st pressure sensor with a measuring range of 5 bar. In this study experiments with stoichiometric fuel in air mixtures are targeted at a constant O_2/N_2 ratio of 21/79. Oxygen and nitrogen are added after vaporizing the fuels in the mixing vessel. Both the oxygen and the nitrogen are of $\geq$ 99.999% purity and were obtained from West-

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