



Full Length Article

A comparison study of cyclopentane and cyclohexane laminar flame speeds at elevated pressures and temperatures

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ABSTRACT

Laminar flame speeds of cyclopentane/air and cyclohexane/air mixtures were determined at equivalence ratios of 0.7–1.6, initial pressures of 1–5 atm, and initial temperatures of 353–453 K using the spherically propagating flame method. Four recently published models of cyclopentane and cyclohexane were validated by current experimental data and showed a reasonable agreement, especially for JetSurF2.0 model and Tian model. A comparison of cyclopentane/air and cyclohexane/air laminar flame speeds was conducted over wide conditions. A comprehensive analysis was conducted through thermal, transport and chemical kinetic effects, and the reaction path analysis and sensitive analysis were employed to further investigate the chemical kinetic effects. The results showed that the laminar flame speed of cyclohexane/air mixture is larger than that of cyclopentane/air and the discrepancy increases with the initial pressure. The discrepancy mainly results from the chemical kinetic effects. Specifically, cyclopentane generates more methyl and allyl intermediates which can consume large amounts of H radicals and induce chain terminating reactions. While, cyclohexane generates a larger amount of ethyl and 1,3-butadiene intermediates which can further yield more vinyl, and the later can induce chain branching reactions and increase the overall burning rate. Thus, it is the different distribution of the cracked products in cyclopentane/air and cyclohexane/air flames that leads to the discrepancy of laminar flame speeds.

1. Introduction

Cyclic alkanes are important components of practical fuels, which can be up to one third or more by weight in diesel [1,2]. It may contribute to the production of aromatics through de-hydrogenation reactions and further increase soot formation at high temperatures [3]. With the emergence of oil-sand derived fuels, which contains more cyclic alkanes than conventional fuels [4], cyclic alkanes will become more important in practical fuel chemistry.

Cyclohexane (CHX) is a simple representative of cyclic alkanes with a six-membered ring and until now several kinetic models have been proposed for it [4–12]. Voisin et al. [5] proposed a low and high temperature oxidation model for CHX and validated it by the species profiles in a jet stirred reactor (JSR) in the temperature range of 750–1100 K and 10 atm. Then Bakali et al. [6] revised this model and validated it through species mole fraction profiles in a JSR at 1, 2 and 10 atm. Ranzi et al. [7] compiled a detailed model for pyrolysis and oxidation of CHX, which was also validated by JSR [6] and ignition delay times in rapid compression machine (RCM) [13]. Silke et al. [4] proposed an oxidation model of CHX including low and high temperature oxidation kinetics, and a reasonable agreement had been

achieved compared to related low temperature oxidation experiments, such as JSR [5,6] and RCM [13,14]. Later, a detailed kinetic model JetSurF2.0 was developed, which can not only be used for n-alkanes, but also for CHX and mono-alkylated CHXs [9]. Based on the previous research [8], Serinyel et al. conducted a JSR experiment at temperatures ranging from 500 to 1100 K and proposed an optimized comprehensive oxidation model for CHX including low to high temperature [10]. Besides the JSR and RCM experiments, which mainly reflect low temperature oxidation of CHX, many evaluated experiments had also been conducted aimed at high temperature oxidation kinetics. Several ignition delay times have been measured in shock tubes over a wide range [15–17] and the initial pressure can be up to 61 atm [18]. As for laminar flame speeds, Davis and Law et al. [19] measured the laminar flame speeds of CHX at atmospheric pressure and temperature. Ji et al. [20] and Serinyel et al. [10] conducted relative study of CHX flame propagation at atmospheric pressure and temperature from 298 to 398 K. Wu et al. [21] measured the laminar flame speeds of CHX at 353 K and elevated pressures up to 20 atm with oxygen/helium as oxidizer. Although laminar flame speeds of CHX have been measured at elevated temperatures, the initial temperature is not high enough and there still exists some discrepancy among available experimental

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results, which is mainly due to the difference of the experimental and data processing approaches. Thus, it is necessary to provide more archival experimental data over broad conditions and investigate the laminar flame speeds of CHX at elevated temperatures and pressures.

Adjacent to CHX, cyclopentane (CPT) is another representative of cyclic alkanes with five-membered ring, which appears high-octane and knock-resistant characteristics. Due to its individual characteristics, CPT has significant influence on the ignition and combustion of gasoline surrogates, as demonstrated by Sarathy et al. [22]. However, researches relevant to CPT were much less than CHX. Sirjean et al. [15] generated a high temperature oxidation model for CPT using the EXGAS software and investigated the ignition delay time at pressure from 7.3 to 9.5 atm in a shock tube. Later, Daley et al. [18] measured the ignition delay time of CPT at elevated pressures up to 55 atm. Tian et al. [23] conducted a shock tube study at pressures of 1.1–10 atm and in the temperature range from 1150 to 1850 K, and a sub-mechanism was added to the JetSurF2.0 mechanism for the kinetic interpretation of CPT oxidation chemistry. Randazzo et al. [24] investigated the pyrolysis of CPT in a diaphragmless shock tube with laser Schlieren densitometry at nominal post-shock pressures of 35, 70, 150 and 300 Torr and temperatures of 1472–2074 K. Recently, Rashidi et al. [25] proposed a conventional oxidation kinetic model for CPT ranging from low to high temperature. To validate this model, Rashidi et al. [26,27] conducted a JSR study for low temperature oxidation of CPT and measured the ignition delay times at pressures of 20 and 40 atm over the temperature range of 650–1350 K using a shock tube and RCM. Also, the model was validated by the laminar flame speeds of Davis and Law et al. [19] at atmospheric pressure and temperature. However, until now, there are only the laminar flame speeds of CPT at atmospheric pressure and temperature [19]. As we all know, substantial experimental data over broad conditions is necessary to deepen the understanding of thermal decomposition and oxidation of CPT. Thus, the relevant study about the laminar flame speeds of CPT is limited and it is necessary to validate these models with laminar flame speeds at elevated pressures and temperatures.

Meanwhile, in order to generalize and simplify the oxidation and flame propagation process of large molecular fuels, the investigation of similarity between these large alkanes has been conducted through the comparison of laminar flame speeds. Davis and Law et al. [19] measured the laminar flame speeds for n-alkanes from C₃ to C₇ and found that it was nearly identical for the C₄–C₇ n-alkanes at atmospheric pressure and temperature. Ji et al. [28] measured the laminar flame speeds of C₅–C₁₂ n-alkanes flames at elevated temperatures and the similar results was determined respectively from C₅ to C₈ and C₉ to C₁₂. Later, Kelley et al. [29] extended the experimental condition to elevated pressures of 10–20 atm and the similar laminar flame speeds still existed for C₅–C₈ n-alkanes. However, to the best of our knowledge, the comparison of C₅–C₆ cyclic alkanes laminar flame speeds has not been investigated. Cyclic alkanes have an evident difference from n-alkanes in chemical kinetic characteristics because of the existing of ring structure. Although it is similar in laminar flame speeds for C₅–C₈ n-alkanes, that of cyclic alkanes is still unknown. Therefore, it is necessary to compare the laminar flame speeds of CPT and CHX and study the effect of initial pressures and temperatures.

Thus the objective of this study is to provide the laminar flame speeds of CPT and CHX at initial pressures from 1 to 5 atm and temperatures from 353 to 453 K. Four recently published kinetic models of CPT and CHX were validated using the present laminar flame speeds over wide experimental conditions. A comparison of CPT and CHX laminar flame speeds was carried out to investigate the effect of carbon numbers of ring structure on cyclic alkanes high temperature oxidation kinetics at various initial pressure and temperature. And a comprehensive analysis was conducted through thermal, transport and chemical kinetic effects to explain the discrepancy between CPT and CHX.

2. Experimental setup and simulation approach

Laminar flame speeds were measured with outwardly spherical flame propagation method using a combustion chamber, whose details can be found elsewhere [30,31] and only a brief introduction is given here. The chamber is cylindrical with an inner diameter of 180 mm and a length of 210 mm. Two quartz windows with the diameter of 80 mm are located on both sides of the chamber for optical access. A 1.5 kW heating tape is wrapped around the chamber and the temperature is monitored by a K-type thermocouple installed in the chamber. Before each experiment, the chamber was heated to the experiment temperature and evacuated by a pump. The liquid fuels CPT (98%) and CHX (99.5%) were injected into the heated chamber using micro syringes through a valve. To make sure that the liquid fuels had been fully vaporized, the real pressure after the injection and vaporization of liquid fuels was compared to the theoretical pressure. Then the oxygen (99.999%) and nitrogen (99.999%) were introduced through intake valves to the required partial pressure, which was monitored by a Rosemount pressure transmitter with a maximum range of 1.03 MPa. At least 10 min was awaited before ignited by the centrally located electrodes to make sure that the fuels and gases had been mixed completely. A high speed digital camera (Phantom V611) was employed to capture the spherically propagation flames at the speed of 10,000 frames per second.

The unstretched burned flame speed S_b^0 was extrapolated by the nonlinear method of Frankel and Sivashinsky [32],

$$S_b = S_b^0 - 2 \cdot S_b^0 L_b / r_f \quad (1)$$

where S_b is the stretched burned flame speed, L_b is the Markstein length and r_f is the flame radius.

Finally, the laminar flame speed S_u^0 can be determined through a simplified continuity equation across the flame front,

$$S_u^0 = S_b^0 \cdot \rho_b / \rho_u \quad (2)$$

where ρ_b and ρ_u are the burned and unburned gas density, respectively.

The uncertainty of experimental data in the present study can be attributed by various factors, such as mixture composition, initial temperature, initial pressure, ignition, buoyancy, radiation, instability, confinement, nonlinear stretch behavior and extrapolation [33]. The method proposed by Moffat et al. [34] was chosen to evaluate the overall experimental uncertainty of laminar flame speed, which took both systematic uncertainty and random uncertainty into consideration. For the present study, the systematic uncertainty was mainly caused by equivalence ratio, initial temperature and pressure, and the relationship between each factor and laminar flame speed obtained by Cai et al. [35] was used here. The relative uncertainty of equivalence ratio was within the range of $\pm (2-3)\%$ mainly induced by the uncertainties in monitoring the partial pressures of fuel, O₂ and N₂. The precision of initial temperature and pressure were controlled within ± 3 K and ± 3 kPa, respectively. Besides, the random error was taken into consideration and the experiments were repeated three times for each condition. Accounting for the radiation effect, the deviation due to radiation was also evaluated using the equation of Yu et al. [36]. Flame radius from 9 to 22 mm were chosen in extracting the laminar flame speeds to avoid the effects of ignition and chamber confinement [37,38]. And the effects of nonlinear stretch behavior and extrapolation were also included in the overall uncertainty. In total, the uncertainty of the laminar flame speeds was evaluated to be about 1–3 cm/s in this study.

Laminar flame speeds were calculated using the PREMIX model of Chemkin-PRO software [39]. Simulation was conducted using finite difference method with adaptive grid. Mixture-averaged transport and thermal diffusion accounting for Soret effect were used. To ensure the accuracy of the calculation, the solution gradient and curvature were both fixed at 0.03 and the total number of points was more than 800. Four recently published kinetic models were validated by the present

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