



Full Length Article

Shock tube study of *n*-nonane/air ignition over a wide range of temperaturesKangle Yong^a, Jiuning He^a, Weifeng Zhang^a, Leyong Xian^a, Changhua Zhang^a, Ping Li^{a,*}, Xiangyuan Li^b^a Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China^b College of Chemical Engineering, Sichuan University, Chengdu 610065, China

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ABSTRACT

Ignition delay experiments for gas phase *n*-nonane/air mixtures have been performed behind reflected shock waves over a wide temperature range of 684–1448 K, pressures of 2.0–15.0 atm, and equivalence ratios of 0.5, 1.0, and 2.0. Ignition delay times were determined using electronically excited CH emission and reflected shock pressure signals monitored at the sidewall of the shock tube. A negative-temperature-coefficient (NTC) behavior of *n*-nonane/air ignition was observed at temperatures of 800–950 K. Dependence of ignition delay time upon temperature, pressure, and equivalence ratio was investigated systematically. High temperature ($T > 1000$ K) results show that the effect of equivalence ratio on ignition delay times is different at low and high pressures. In the NTC region, ignition delay times are highly sensitive to equivalence ratio and pressure. The present ignition data are in satisfactory agreement with predictions of two widely used chemical kinetic mechanisms. Sensitivity and reaction pathway analyses reveal that the dominating reactions affecting ignition delay times and reaction pathways during ignition process for *n*-nonane/air are quite different at high and low temperatures. Comparison of *n*-nonane/air ignition delay times with those of other larger *n*-alkanes (*n*-heptane, *n*-octane, *n*-decane, *n*-dodecane, and *n*-tetradecane) indicates that the length of *n*-alkanes chain influences little on ignition delay times of *n*-alkanes. The present results are useful for understanding ignition characteristics of *n*-nonane and providing experimental data to validate chemical kinetic mechanisms for *n*-nonane.

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1. Introduction

Practical fuels, such as diesel and jet fuels, are complex mixtures consisting of hundreds of hydrocarbon species. The species can be classified into alkanes, alkenes, cycloalkanes, and aromatics according to their molecular structures and functional groups [1]. Normal alkanes occupy a large volumetric percentage in diesel and jet fuels [2–4], study on the combustion properties of *n*-alkanes is necessary for understanding combustion properties of practical fuels. Ignition delay time is an important parameter for describing combustion properties of the fuels. Till now, experimental investigations on ignition delay times of *n*-alkanes from methane to *n*-octane are abundant [5–17], and ignition delay times measurements on *n*-decane, *n*-dodecane and other heavy hydrocarbons are also available [18–20]. Ciezki and Adomeit [14] measured *n*-heptane/air ignition delay times in a shock tube at the temperature range of 750–1250 K and pressures of 3–42 atm. Sar-

athy et al. [17] reported ignition delay times of *n*-octane/air at temperatures from 644 to 1327 K and pressures of 20 atm in a heated shock tube. Pfahl et al. [18] measured *n*-decane/air ignition delay times in a heated shock tube at elevated pressures of 13–50 atm in the temperature range of 650–1300 K. Shock tube ignition delay times of *n*-dodecane/air at temperatures of 727–1422 K and pressures of 15–34 atm have been reported by Vasu et al. [19]. Shen et al. [20] reported ignition delay times of *n*-heptane, *n*-decane, *n*-dodecane and *n*-tetradecane in air over temperatures of 786–1396 K and at pressures of 9–58 atm. However, experimental study on ignition delay times of *n*-nonane is scarce. Ignition delay times of *n*-nonane/Ar mixtures have been experimentally studied at limited conditions [16,21]. Davidson et al. [16] reported shock tube ignition delay times of *n*-nonane/Ar mixtures with 4% oxygen concentration at pressures of 1.0–4.0 atm and equivalence ratios of 0.5 and 1.0. Rotavera and Petersen [21] measured ignition delay times of *n*-nonane diluted in argon in a shock tube at pressures near 1.5 and 10.4 atm with equivalence ratios of 0.5 and 1.0. All of these measurements are carried out only at high temperatures ($T > 1230$ K). To our knowledge, no research has been reported on ignition delay times for mixtures of *n*-nonane in air. Moreover, *n*-

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nonane is present in petroleum-based fuels [22,23], especially in Chinese RP-3 jet aviation fuel at a level of more than 5% in weight percent. Thus, measurements on ignition delay times of *n*-nonane/air mixtures at a wide range of conditions are worthwhile.

For kinetic mechanisms about *n*-nonane ignition, Westbrook et al. [24] proposed a detailed mechanism (LLNL mechanism) to describe the pyrolysis and oxidation of *n*-alkane hydrocarbons from *n*-octane to *n*-hexadecane over a wide range of temperatures. JetSurf v2.0 mechanism [25], which consists of 348 species and 2163 reactions, is another one can be used to predict ignition delay times for *n*-nonane at high temperatures.

In current work, ignition delay times of *n*-nonane/air were measured at wide experimental conditions. Effects of temperature, pressure, and equivalence ratio on ignition delay times were discussed. The new data were compared with predictions of kinetic mechanisms. In addition, the measured ignition delay data were compared to those of other five large *n*-alkanes. Finally, sensitivity and reaction pathway analyses were carried out to identify key reactions and fuel consumption pathways during the ignition process of *n*-nonane.

2. Experimental methods

Experiments were carried out in a heated shock tube with an internal diameter of 10.0 cm. A double-diaphragm section divides the shock tube into a 6.0 m driver and a 5.0 m driven sections. Polycarbonate diaphragms with different thickness were employed to generate different shock pressures. The shock tube and mixing tank were evacuated to pressures below 1 Pa with a rotary vane vacuum pump prior to experiments. Fuel mixtures were prepared in a 40 L stainless steel tank and mixed at least 2 h prior to experiments by molecular diffusion. The mixing tank and associated manifold were heated to 100 °C to avoid condensation of the fuel. The saturated vapor pressure of *n*-nonane is approximately 0.21 atm at 100 °C, and the partial pressures of gas-phase *n*-nonane were kept less than 0.07 atm in present experiments. The initial pressure of gas-phase fuel was monitored using a thin-capacitance manometer. Partial pressures of oxygen and nitrogen were measured by a pressure gauge. Estimated uncertainty in reactant mixture composition is within 1%. Pure helium was used as the driver gas for measurements requiring test times shorter than 2.0 ms, tailored helium/argon driver gas mixtures were used to extend test times up to 20 ms for all other experiments.

The driven section was wrapped with heating coils and uniformly heated to 80 °C to prevent condensation of *n*-nonane/air mixtures. Six independent current circuits were used to provide a uniform temperature distribution within the uncertainty of ± 3 °C along the driven section. Four fast-response piezoelectric pressure transducers (PCB 113B) located along the driven section with the same length interval of 18.9 cm were used to determine the incident shock velocity. Three time intervals were recorded by a digital phosphor oscilloscope (Tektronix DPO5054). Three incident shock velocities were determined respectively and linearly extrapolated to obtain the incident shock velocity at the endwall. The uncertainty in the incident shock velocity is estimated at $\pm 0.6\%$. The temperature and pressure behind reflected shock wave were calculated by the one-dimensional normal shock relations using the measured initial temperature and pressure in the driven section, the incident shock velocity at the endwall, the mixture composition, and the thermodynamic properties of the reactant mixtures. The uncertainty in the temperature and pressure behind reflected shock wave is estimated to be $\pm 1\%$ and $\pm 2.5\%$, respectively.

Measurements of ignition delay time were made by detecting the arrival of reflected shock wave and the occurrence of CH* emis-

sion at the sidewall observation location (15 mm from the endwall). Light emission during ignition process was exported using a quartz optical fiber connected to a grating monochromator coupled with a photomultiplier tube. The grating monochromator was set at 431 nm to capture the CH* emission. The ignition delay time (τ_{ign}) is defined as the interval between the arrival of the reflected shock wave determined by the jump of pressure signal and the onset of ignition indicated by the steepest rise of the CH* emission at the observation location. An example of *n*-nonane/air ignition delay time is shown in Fig. 1. In present experiments, the variation in pressure with the reflected shock conditions was found to be in the range of $(dP/dt)(1/P_0) = 1\text{--}5\%$ m s^{-1} , and the typical variation in pressure is 3% m s^{-1} . The date of pressure histories for experiments at representative low-temperature conditions are given in Supplementary Material A. This pressure gradient should be considered in model predictions for these experiments, especially for longer ignition delay times than 1.5 ms.

Considering the uncertainties in reflected shock wave temperature and pressure, the uncertainty in reactant mixture composition, and the uncertainty in determination of ignition delay time from measured signals, the overall uncertainty of ignition delay times is estimated within $\pm 20\%$.

3. Results and discussion

Ignition delay times of *n*-nonane/air mixtures at temperatures of 684–1448 K, pressures of 2.0–15.0 atm, and equivalence ratios of 0.5, 1.0, and 2.0 have been obtained, and the NTC behavior of the ignition delay time was observed at temperatures of 800–950 K. The results are presented in Figs. 2–7, and the raw ignition delay data are tabulated in Supplementary Material B.

3.1. High-temperature ignition delay times

The measured high temperature ignition delay times are shown in Figs. 2 and 3, ignition data have been scaled to nominal pressures of 2.0, 5.0, 9.0, and 15.0 atm using the common relationship $\tau_{\text{ign}} \propto P^{-1}$ in advance. The results show that the increasing temperature or pressure leads to decreasing ignition delay time, but the effect of equivalence ratio on ignition delay times is complex.

In order to know the sensitivity of the fuel's reactivity to temperature, current high-temperature data are correlated using an Arrhenius-type expression of $\tau_{\text{ign}} = A \times \text{Exp}(Ea/RT)$, where the ignition delay time τ_{ign} is in microsecond, A is a constant, T is the ignition temperature in Kelvin, R is the universal gas constant with the

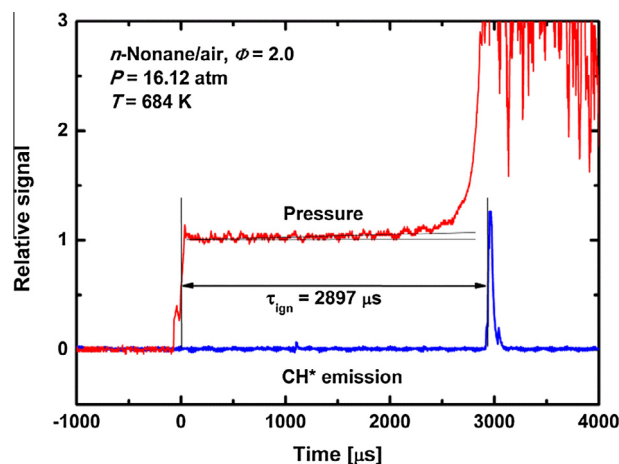


Fig. 1. Example of *n*-nonane/air ignition delay time determination.

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