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A shock tube study of iso-octane ignition at elevated pressures: The influence of diluent gases

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Abstract

The ignition of iso-octane/air and iso-octane/O_2/Ar ($\sim$20% O_2) mixtures was studied in a shock tube at temperatures of 868–1300 K, pressures of 7–58 atm, and equivalence ratios $\Phi = 1.0$, 0.5, and 0.25. Ignition times were determined using endwall OH^* emission and sidewall piezoelectric pressure measurements. Measured iso-octane/air ignition times agreed well with the previously published results. Mixtures with argon as the diluent exhibited ignition times 20% shorter, for most conditions, than those with nitrogen as the diluent (iso-octane/air mixtures). The difference in measured ignition times for mixtures containing argon and nitrogen as the diluent gas can be attributed to the differing heat capacities of the two diluent species and the level of induction period heat release prior to ignition. Kinetic model predictions of ignition time from three mechanisms are compared to the experimental data. The mechanisms overpredict the ignition times but accurately capture the influence of diluent gas on iso-octane ignition time, indicating that the mechanisms predict an appropriate amount of induction period heat release.

Keywords: Shock tube; Ignition; Iso-octane; Diluent; Argon; Nitrogen

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1. Introduction

Iso-octane (2,2,4-trimethylpentane), a primary reference fuel for octane rating in spark ignition engines, has drawn considerable interest as a model compound for branched alkane components found particularly in gasoline [1], but also those found in diesel [2] and jet fuels [3]. Due to its relevance to practical liquid fuels, iso-octane has been the subject of many experimental and kinetic modeling studies. Experimental investigations of iso-octane oxidation and ignition have been carried out in shock tubes [4–11], rapid compression machines (RCMs) [12–19], flames [20–22], jet stirred reactors [23–26], and flow reactors [27,28]. In these studies a variety of kinetic measurements have been made including ignition times, radical species concentrations, stable species concentrations, and flame speeds.

Ignition delay times, the subject of this work, are an important validation target for the development of kinetic mechanisms and have been measured for iso-octane in both shock tubes and RCMs. Nixon et al. [4], Vermeer et al. [5], Burcat et al. [6], Oehlschlaeger et al. [7], Fieweger et al. [8,9], Davidson et al. [10], and Vasu et al. [11] have previously investigated iso-octane ignition in shock tubes for, in

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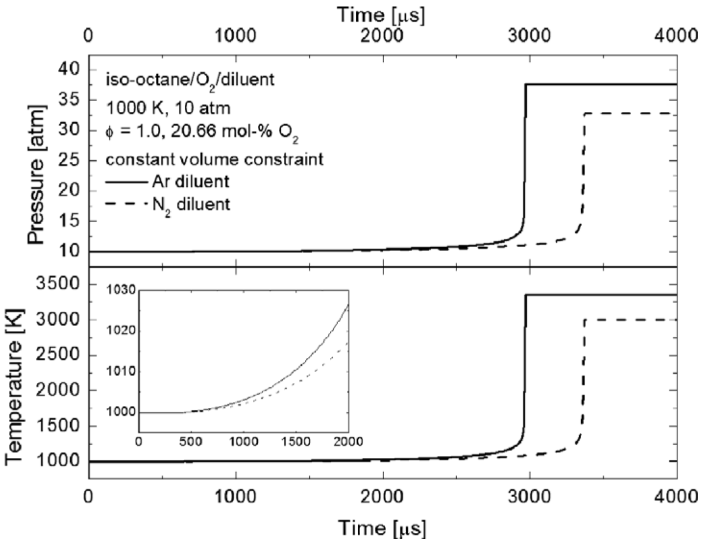

Fig. 1. Comparison of temperature and pressure time-history predictions for iso-octane ignition with Ar and N_2 as diluent gases, simulation performed using the Curran et al. [33] mechanism.

combination, a large range of conditions: pressures from 1 to 50 atm, temperatures from 700 to 2000 K, and for a large variety of lean to rich mixtures ranging in fuel concentration from very dilute (100 ppm iso-octane) in argon to stoichiometric in air (1.65% iso-octane). Halstead et al. [12], Griffiths et al. [13], Minetti et al. [14], Tanaka et al. [15], and Wooldridge and co-workers [16–19] have examined the ignition of iso-octane in RCMs for temperatures ranging from 650 to 1050 K at pressures from 8 to 40 atm. These previous studies have characterized ignition times for iso-octane mixtures over a broad range of conditions, including the low-temperature negative temperature coefficient (NTC) regime, and allowed for the assessment of iso-octane kinetic mechanisms. Kinetic modeling studies for iso-octane have been carried out by several authors including the development of detailed mechanisms [20,29–34] and skeletal/reduced mechanisms [15,35,36] for integration into computational fluid dynamics (CFD) calculations.

Shock tubes are a common choice for the investigation of ignition phenomena due to the nearly instantaneous heating ($\sim$1 ns) of the reactant mixture by the shock wave, the near adiabatic constant-volume behavior of the shock tube reflected-shock environment, the ability of shock tubes to access a range of conditions of interest to practical combustion devices, and the ease of applying optical diagnostics to shock tube experiments. When studying the ignition of a fuel compound in a shock tube, the choice of reactant mixture is important and there are several options depending on the goal of the experiment. These options include the choice of diluent gas.

Monatomic argon is often used as a diluent gas because its lack of a vibrational mode eliminates consideration of the timescale for vibrational relaxation when calculating the postshock conditions. Additionally, reflected shock pressure profiles for argon mixtures usually display less noise due to the lack of (or smaller) sidewall bifurcation relative to nitrogen. Hence, optimized reflected shock conditions are typically obtained using dilute mixtures in argon. However, dilute mixtures in argon are dissimilar in composition to those used in combustion engines, where air is typically the oxidizer and at stoichiometric conditions the fuel concentration is near 1 mol%. Therefore, experiments performed in air and at elevated pressures are desired for the validation of oxidation mechanisms used at combustion engine conditions.

The choice of diluent gas can also influence shock tube ignition measurements through the diluent heat capacity. As heat is released during the radical growth period prior to ignition the temperature rises more quickly for a monatomic diluent than for a diatomic diluent, which accelerates the ignition process. However, the influence of replacing nitrogen with argon on ignition time measurements is typically considered to be small. Würmel et al. [37] and Davidson and Hanson [38] recently demonstrated the difference in simulated iso-octane ignition times for argon and nitrogen diluent mixtures. Based on kinetic calculations, they show that argon mixtures exhibit shorter (approximately 20%) ignition times than nitrogen mixtures, a result of the lower heat capacity of argon. A similar calculation is shown in Fig. 1 for iso-octane ignition (adiabatic constant-volume constraint) with argon and