Combustion and Flame 161 (2014) 154–161

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Laminar flame propagation of atmospheric *iso*-cetane/air and decalin/air mixtures

Bo Li [a,b], Hai Zhang [a], Fokion N. Egolfopoulos [b,*]

[a] *Department of Thermal Engineering, Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Tsinghua University, Beijing 100084, China*
[b] *Department of Aerospace and Mechanical Engineering, University of Southern California, Los Angeles, CA 90089-1453, USA*

ARTICLE INFO

Article history:
Received 12 June 2013
Received in revised form 16 July 2013
Accepted 16 July 2013
Available online 12 August 2013

Keywords:
Flame propagation
Laminar flames
Kinetic modeling
iso-Cetane
Decalin

ABSTRACT

Laminar flame speeds of *iso*-cetane/air and decalin/air mixtures were measured in the counterflow configuration at atmospheric pressure and an elevated unburned mixture temperature of 443 K. Axial flow velocities were measured along the stagnation streamline using the digital particle image velocimetry. The laminar flame speeds were determined by determining the variation of a reference flame speed as a function of strain rate and computationally assisted non-linear extrapolations. The data are the first to be reported in the literature, and they were modeled using a recently developed kinetic model that includes 187 species and 6086 elementary reactions. In general, the computed results were found to be in close agreement with the data. In order to get insight into kinetic effects on flame propagation, detailed sensitivity and reaction path analyses were performed using the computed flame structures. The results revealed that at the same equivalence ratio, laminar flame speeds of *iso*-cetane/air mixtures are lower than those of *n*-hexadecane/air mixtures. Additionally, it was found that the laminar flame speeds of *iso*-cetane/air and decalin/air mixtures are sensitive largely to C_0–C_4 kinetic subset, and that the lower reactivity of *iso*-cetane compared to *n*-hexadecane could be attributed to the higher production of relatively stable intermediates.

© 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.

1. Introduction

Practical transportation fuels are derived largely from conventional petroleum sources and consist of hundreds to thousands of chemical compounds. Due to their chemical complexity, characterizing fully their combustion properties is not a viable proposition. On the other hand, surrogate fuels that contain a limited number of neat components, could be used to represent the important physical and chemical characteristics of practical fuels.

iso-Cetane (2,2,4,4,6,8,8-heptamethylnonane) and decalin (decahydronaphthalene or bicyclo[4.4.0]decane) are among the surrogate component candidates for jet and diesel fuels (e.g., [1–5]) but their combustion characteristics have not been studied to notable extent. *iso*-Cetane has been recommended as a representative branched alkane in diesel surrogate mixtures [1–4]. In addition, *iso*-cetane is a key component of primary reference diesel fuels (e.g., [5]) used to define the “cetane number” that is as a measure of the ignition propensity of the fuel in air.

In general, investigations of combustion characteristics of branched alkanes are much fewer than those of *n*-alkanes. Ranzi et al. [6] have reviewed the experimental laminar flame speeds, S_u^o, of hydrocarbon fuels that have been reported in recent years. Regarding the *iso*-octane, a key component of primary reference gasoline fuels used to define “octane number,” which has been studied in various reacting configurations (e.g., [7–14]). Dryer and Brezinsky [7] conducted oxidation experiments of *iso*-octane in a flow reactor, and found that *iso*-octane produces primarily *iso*-butylene and propylene as intermediate hydrocarbons. Liu et al. [10] studied the ignition of non-premixed counterflow flames of C_8 and C_{10} alkane isomers, and revealed that increasing the degree of branching lowers the ignition propensity. Ji et al. [14] found experimentally that S_u^o’s of *n*-octane/air mixtures are higher than *iso*-octane/air at the same equivalence ratio, ϕ. Analysis of computed flame structures [14] indicated that the low reactivity of branched isomers could be attributed to the production of unreactive, H-scavenging, resonantly stabilized intermediates.

Due to its large molecular weight and low vaporization pressure, studies of *iso*-cetane are fewer compared to *iso*-octane especially in flames. Dagaut and Hadj-Ali [15] studied the oxidation of *iso*-cetane in a jet-stirred (JSR) reactor at 10 atm, in the 770–1070 K temperature range. Concentration profiles of reactants, stable intermediates, and final products were measured and two kinetic models were used to simulate the experimental results. Oehlschlaeger et al. [3] studied the autoignition of *iso*-cetane in a shock tube and a kinetic model was proposed that resulted in good

---

* Corresponding author. Fax: +1 213 740 8071.
E-mail address: egolfopo@usc.edu (F.N. Egolfopoulos).

0010-2180/$ - see front matter © 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.combustflame.2013.07.014

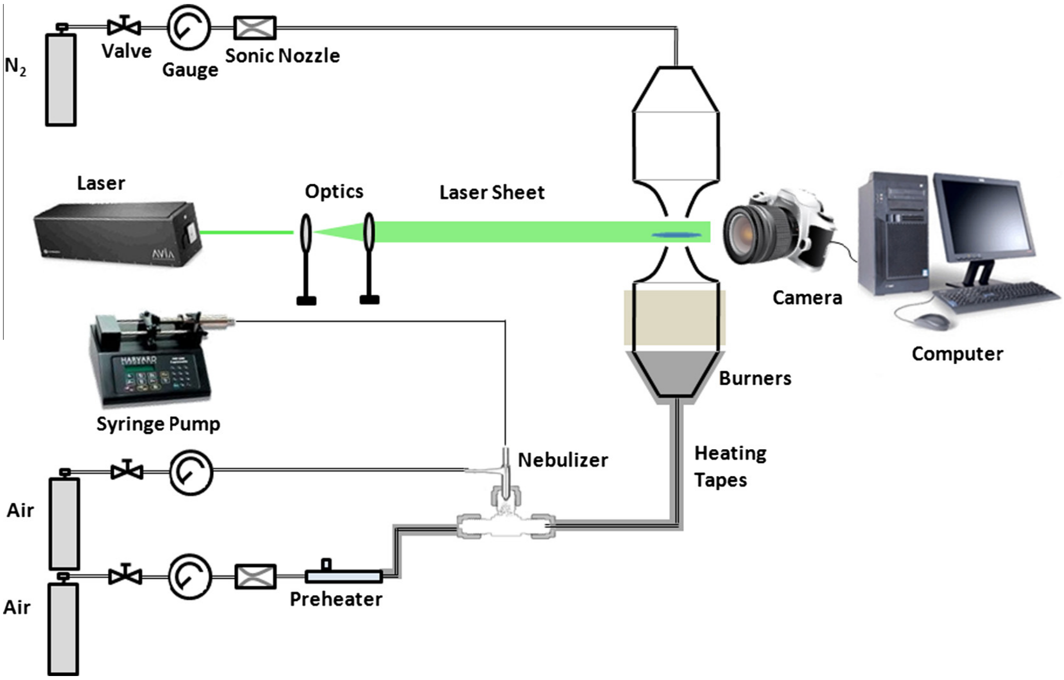

Fig. 1. Schematic of the experimental configuration.

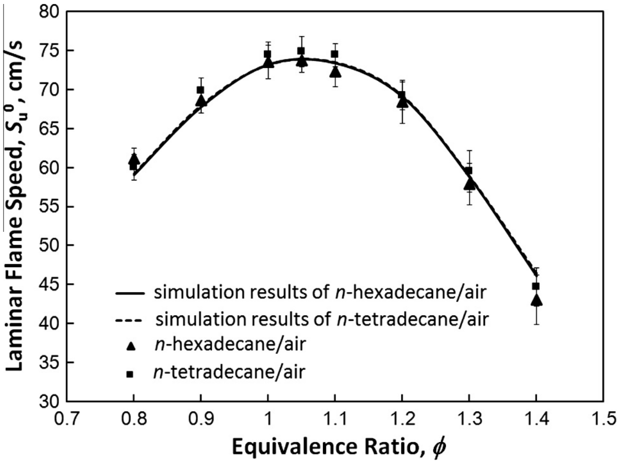

Fig. 2. Experimental and computed laminar flame speeds of *n*-tetradecane/air [24] and *n*-hexadecane/air [24] mixtures at $T_u = 443$ K and $p = 1$ atm.

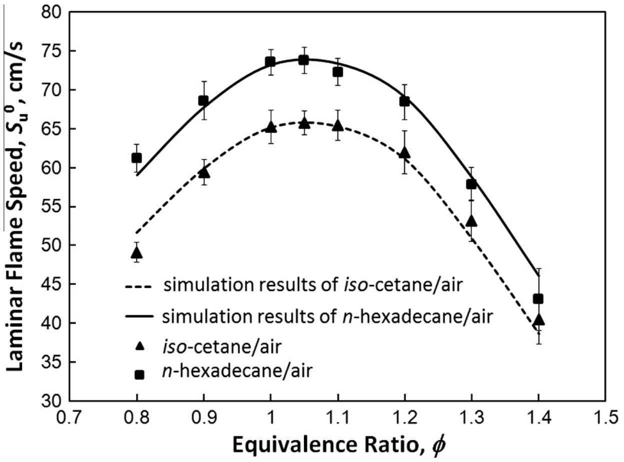

Fig. 3. Experimental and computed laminar flame speeds of *n*-hexadecane/air and *iso*-cetane/air mixtures at $T_u = 443$ K and $p = 1$ atm.

agreements between measured and computed ignition delay times. It was found also that the ignition delay times for *iso*-octane are greater than those of *iso*-cetane. Westbrook et al. [2] developed a detailed kinetic model for PRF mixtures of *n*-hexadecane and *iso*-cetane for diesel cetane ratings, and then validated it by comparisons between computed results and experimental data from shock tube ignition and JSR experiments. It was determined that *iso*-cetane exhibits lower ignition delay times than *iso*-octane and this was attributed to the different molecular structures of the fuels.

Due to its high thermal stability, decalin is among the candidates of endothermic fuel surrogates representing the multi-ring naphthenes [5,16]. Most of the existing decalin studies have focused on its pyrolysis over a wide range of pressures [17–20]. C_2–C_4 alkenes, benzene, alkyl-benzenes, and toluene have been reported as primary fuel decomposition products. Ranzi [21] developed a high-temperature detailed kinetic model for decalin. Oehlschlaeger et al. [22] measured the ignition delay times for $\phi = 0.5$ and 1.0 decalin/air mixtures in a shock tube in the 990 K-1300 K temperature range, and good agreements with model predictions were reported. Dagaut et al. [23] measured the stable species concentration profiles in a JSR with mean residence times 0.1 and 0.5 s, 750–1350 K temperatures, and 1 and 10 atm pressures. The predictions were found to be closer using a low-temperature kinetic model that was developed also in the same study. Yang and Boehman [24] investigated the oxidation of decalin in a Cooperative Fuel Research (CFR) octane-rating engine operated under motored engine conditions.

Based on the aforementioned considerations, the main goal of the present investigation was to provide archival S_u^o experimental data for *iso*-cetane and decalin flames, the first ones to be reported ever. The accurate knowledge of S_u^o is essential in kinetic model and surrogate fuel development, and in scaling turbulent flame speeds. An additional goal was to provide insight into the mechanisms that control flame propagation for these two complex fuel molecules

Download English Version:

https://daneshyari.com/en/article/168800

Download Persian Version:

https://daneshyari.com/article/168800

Daneshyari.com