



Laminar flame speeds of transportation-relevant hydrocarbons and jet fuels at elevated temperatures and pressures

Xin Hui^{a,b}, Chih-Jen Sung^{b,*}

^a Department of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland, OH 44106, USA

^b Department of Mechanical Engineering, University of Connecticut, Storrs, CT 06269, USA

HIGHLIGHTS

- ▶ Measured laminar flame speeds of *n*-decane, *n*-dodecane, *iso*-octane, toluene, *n*-PB, TMBs, Jet-A, S-8, and a Jet-A surrogate.
- ▶ Covered equivalence ratios of $\phi = 0.7$ –1.3, preheat temperatures of $T_u = 350$ –470 K, and pressures of $P = 1$ –3 atm.
- ▶ Compared experimental results with computed values obtained by using various published kinetic models for different fuels.
- ▶ Evaluated the effect of preheat temperature on laminar flame speed.
- ▶ Determined the effect of pressure on mass burning flux by extracting the overall reaction orders of various fuels.

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ABSTRACT

Laminar flame speeds of several fuel/air mixtures were experimentally determined over equivalence ratios of $\phi = 0.7$ –1.3, preheat temperatures of $T_u = 350$ –470 K, and pressures of $P = 1$ –3 atm in a high-pressure counterflow setup. Fuels investigated in this work included neat components relevant to liquid transportation fuels, such as *n*-decane, *n*-dodecane, *iso*-octane, toluene, *n*-propylbenzene, 1,2,4-trimethylbenzene, and 1,3,5-trimethylbenzene, a conventional Jet-A labeled as POSF 4658, an alternative jet fuel, S-8, labeled as POSF 4734, and a four-component Jet-A surrogate composed of *n*-dodecane, *iso*-octane, *n*-propylbenzene, and 1,3,5-trimethylbenzene. The experimental results were also compared with computed values obtained by using various published kinetic models for different fuels. In general, the simulated results are in fair agreement with the experimental data, considering the uncertainties in both experiments and kinetic models. Further analysis on experimental data was conducted to assess the effects of preheat temperature on laminar flame speed and pressure on mass burning flux. From the variation of mass burning flux with pressure, the overall reaction orders of various fuels were extracted. The present flame propagation data at elevated pressures for large hydrocarbons can be used in surrogate formulation and mechanism validation for liquid transportation fuels.

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1. Introduction

Hydrocarbons are the primary energy source for the modern civilization. It is estimated that as much as 58% of the world's energy consumption comes from the crude oil and natural gas [1]. It is also expected that liquid hydrocarbons will continue to dominate the transportation sector due to their high energy density and liquid form which makes them easy to transport. Further, the aviation sector burns about 5.8% of total oil consumed in the world [2]. Improving the fuel efficiency and reducing the pollutant

emissions of jet engines has been a major area of focus for the aircraft manufacturer. Since the combustion behavior of liquid hydrocarbons can have a great impact on the engine performance, a better understanding of liquid hydrocarbon combustion is of fundamental and practical importance in developing high-efficiency and clean-burning aeropropulsion engines of next generation.

As gasoline and diesel fuels, jet fuel is a mixture of a large number of different hydrocarbons from different molecular classes including straight chain paraffins, branched chain paraffins, cycloparaffins, and aromatics [3,4]. The complexity of jet fuel makes it impossible to directly simulate its combustion behaviors. A promising approach to overcome this difficulty is to first develop a surrogate fuel that can emulate the combustion characteristics of the target jet fuel. In general, a surrogate fuel is defined as a mixture of a limited number of hydrocarbons whose

* Corresponding author. Address: Department of Mechanical Engineering, University of Connecticut, 191 Auditorium Road, Storrs, CT 06269-3139, USA. Tel.: +1 860 486 3679; fax: +1 860 486 5088.

E-mail address: cjsung@engr.uconn.edu (C.-J. Sung).

composition can be formulated in order to best match real fuel properties, such as physical properties, chemical properties, or even both [5]. With their relatively small number of components, detailed chemical kinetics and transport properties of surrogate fuels can be developed to predict combustion performance of the target real fuels, such as ignition, flame stability, extinction, and emission characteristics, as long as the detailed kinetic models are validated against reliable fundamental combustion data. It is noted that the formulation of surrogate fuels and the validation of the associated detailed kinetic models both require a comprehensive understanding of combustion behaviors for real fuels and their reference components. Therefore, there is a growing interest in developing a fundamental combustion database of liquid hydrocarbons that are relevant to the practical transportation fuels.

For real jet fuels in particular, such as JP-8 and Jet-A, extensive surrogate fuels have been proposed over the last decade [6–23]. JP-8, a kerosene-type fuel, is widely used by US military to power aircraft and other high performance vehicles, while Jet-A is the commercial equivalent of military JP-8 and differs only by trace amounts of additives [24]. In an early study, Schulz [6] first proposed a 12-component surrogate fuel for JP-8, and compared the oxidative stability of the surrogate with real fuel. To develop a surrogate that emulates the high-temperature oxidation process of real kerosene fuel, Gueret et al. [7] compared a kerosene fuel with a three-component surrogate fuel, composed of 79% *n*-undecane, 10% *n*-propylcyclohexane, and 11% 1,2,4-trimethylbenzene by mole, in a jet stirred reactor, and developed a quasi-global chemical kinetic mechanism. Using *n*-decane as single component surrogate, Dagaut et al. [9] was able to reproduce experimental data of Jet-A1 in a jet stirred reactor, and their results showed a strong analogy between *n*-decane and kerosene oxidation kinetics. Humer et al. [19] defined three surrogate fuels (made up of *n*-decane, *n*-dodecane, methylcyclohexane, toluene, and *o*-xylene) and compared their extinction and autoignition with JP-8, Jet-A, and other two surrogates proposed by Violi et al. [11] and Agosta [12], respectively. Recently, Honnet et al. [21] proposed the Aachen surrogate (20% 1,2,4-trimethylbenzene and 80% *n*-decane by weight) for Jet-A and the associated semi-detailed mechanism. Later, Dooley et al. [22] first proposed a three-component Jet-A surrogate, composed of *n*-decane, *iso*-octane, and toluene, and compared the surrogate with Jet-A for a variety of experimental data, showing a good agreement in terms of experimental comparison between the surrogate and the target real fuel. Since further analysis suggested that large molecular weight hydrocarbons are required to match the typical threshold sooting index and molecular weight of Jet-A, Dooley et al. [23] subsequently formulated a four-component surrogate, composed of *n*-dodecane, *iso*-octane, 1,3,5-trimethylbenzene, and *n*-propylbenzene. The appropriateness of this four-component surrogate formulation was demonstrated through the experimental measurements of various gas phase combustion kinetic phenomena of the surrogate mixture and of the target Jet-A fuel [23].

Based on the literature jet fuel surrogates discussed above, the neat components often include a long straight chain paraffin, *n*-decane [6,7,9,10,13,17,19,21,22] or/and *n*-dodecane [6,11–14,19,23], as well as aromatics such as toluene [7,10,19,22], trimethylbenzene [7,17,21,23], and *n*-propylbenzene [23]. Some surrogates also have the highly branched *iso*-octane [6,11,12,14,22,23] to represent the branched components in jet fuels. At the present time, the kinetics of these representative components is still not fully understood. Moreover, understanding the effect of pressure on the flame properties for these large hydrocarbons is imperative for the development of advanced combustion technology. Consequently, fundamental flame data of liquid hydrocarbons from different molecular classes over a wide range of experimental

conditions play an essential role in the development and validation of surrogate fuels as well as their associated kinetic models.

The laminar flame speed of a combustible mixture as a function of preheat temperature, pressure, and composition is an important fundamental flame property reflecting the net effects of diffusivity, exothermicity, and reactivity of the given mixture. Hence, laminar flame speeds have been widely used to validate kinetic models. In recent years, several studies have been performed to determine the laminar flame speeds of liquid hydrocarbons by different experimental techniques. For example, in counterflow flames, Kumar et al. [25–27] measured the laminar flame speeds of preheated *n*-heptane, *iso*-octane, *n*-decane, *n*-dodecane, Jet-A, and S-8 (a synthetic jet fuel produced by the Fischer–Tropsch process from synthesis gas derived from natural gas) at atmospheric pressure. In a follow-up study, Hui et al. [28] measured the atmospheric laminar flame speeds of aromatic species, including toluene, 1,2,4-trimethylbenzene, 1,3,5-trimethylbenzene, and *n*-propylbenzene, at a preheat temperature of 400 K. Ji et al. [29] measured the laminar flame speeds of C₅–C₁₂ *n*-alkanes at a preheat temperature of 403 K and atmospheric pressure. In spherical flames, Kelly et al. [30,31] measured the laminar flame speeds of C₅–C₈ *n*-alkanes and *iso*-octane at a preheat temperature of 353 K and pressures up to 20 atm. Johnston and Farrell [32] measured the laminar flame speeds of aromatic species, including ethylbenzene, *n*-propylbenzene, toluene, and *m*-xylene, at a preheat temperature of 450 K and a pressure of 3 atm. The readers interested in laminar flame speeds of hydrocarbons are referred to a comprehensive review recently summarized by Ranzi et al. [33].

Recognizing the growing need for extended fundamental flame datasets of transportation-relevant fuels at elevated pressures, the objective of the present study was to provide experimental laminar flame speed data at elevated temperatures and pressures for large liquid hydrocarbons including *n*-decane, *n*-dodecane, *iso*-octane, toluene, 1,2,4-trimethylbenzene (1,2,4-TMB), 1,3,5-trimethylbenzene (1,3,5-TMB), and *n*-propylbenzene (*n*-PB), along with a comparison with computed values using chemical kinetic models available in the literature. We also extended the studies of Kumar et al. [27] and Dooley et al. [23] by measuring the high-pressure laminar flame speeds of real jet fuels and the four-component surrogate, *n*-dodecane/*iso*-octane/1,3,5-TMB/*n*-PB = 40.41/29.48/7.28/22.83 by mole percentage, for comparing the burning rates of Jet-A and S-8 and for further assessing how well the Jet-A surrogate performs in emulating the premixed combustion of the target jet fuel at elevated pressures, respectively. Based on the present experimental datasets, additional analysis was also performed to assess the effects of mixture preheat temperature and pressure on burning rate.

In the following sections, we shall sequentially detail the experimental setup and the methodology for determining laminar flame speed as well as the computation specifications for simulating flame propagation, followed by the result presentation and discussion.

2. Experimental specification and methodology

2.1. Experimental setup

To measure the flame speeds at elevated temperatures and pressures, a high pressure counterflow setup was developed and used. The experimental apparatus consisted of a higher pressure chamber, a counterflow burner setup, a liquid fuel vaporization system, a flow controlling system, and a digital particle image velocimetry (DPIV) system, as shown in Fig. 1. The high pressure chamber body was made of half-inch thick stainless steel and had 10 in. in diameter and 13 in. in height. This chamber can be

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