



Flame propagation of mixtures of air with high molecular weight neat hydrocarbons and practical jet and diesel fuels

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Available online 25 September 2012

Abstract

Laminar flame speeds of mixtures of air with $n\text{-C}_{14}\text{H}_{30}$, $n\text{-C}_{16}\text{H}_{34}$, a petroleum-derived JP-5 jet fuel, a camelina-derived hydrotreated renewable JP-5 jet fuel, a petroleum-derived F-76 diesel fuel, and an algae-derived hydrotreated renewable F-76 diesel fuel, were measured in the counterflow configuration at atmospheric pressure and elevated unburned mixture temperatures. Digital particle image velocimetry was used to measure the axial flow velocities along the stagnation streamline. The experiments for $n\text{-C}_{14}\text{H}_{30}/\text{air}$ and $n\text{-C}_{16}\text{H}_{34}/\text{air}$ mixtures were modeled using recently developed kinetic models, and the experimental data were predicted satisfactorily. Both experiments and simulations revealed that the laminar flame speeds of $n\text{-C}_{14}\text{H}_{30}/\text{air}$ and $n\text{-C}_{16}\text{H}_{34}/\text{air}$ mixtures are very close to each other, as expected. On the other hand, the laminar flame speeds for the four practical fuels were found to be lower than $n\text{-C}_{14}\text{H}_{30}$ and $n\text{-C}_{16}\text{H}_{34}$, due to the presence of aromatics and branched hydrocarbons. Similarly, the laminar flame speeds for the alternative fuels were found to be higher than the petroleum-derived ones, again due to the presence of aromatic compounds in the latter. Further insight into the effects of kinetics and molecular transport was obtained through sensitivity analysis.

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Keywords: n -Tetradecane; n -Hexadecane; Jet fuels; Diesel fuels; Flame propagation

1. Introduction

Jet and diesel fuels are used extensively in both the civilian and military sectors worldwide. These fuels contain hundreds of chemical components, which are largely n -alkanes, iso -alkanes, $cyclo$ -alkanes, and aromatics. Due to the chemical complexity of these compounds, the combustion characteristics of practical fuels cannot be modeled

from first principle and understood. The first step towards that goal is to perform fundamental combustion studies for both the practical fuels and the attendant surrogate compounds and their blends, so that insight is achieved into the rate-controlling processes during the conversion of chemical to thermal energy in engines.

In the past, extensive studies on global flame properties for neat liquid n -alkanes have been conducted. For example, laminar flame speeds, S_u^o , of $n\text{-C}_7\text{H}_{16}/\text{air}$ mixtures has been measured using different methodologies (e.g., [1–5]). Zhao et al. [6] studied experimentally and numerically

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S_u^0 's of n -C₁₀H₂₂/air mixtures. Kumar and Sung [7] measured S_u^0 's and extinction strain rates of n -C₁₀H₂₂ and n -C₁₂H₂₆ flames. Ji et al. [8] investigated the propagation and extinction of C₅–C₁₂ n -alkane flames, and close agreements were found between the experimental data and computed results using a recently developed kinetic model. Humer et al. [9] studied the ignition and extinction characteristics of n -C₁₀H₂₂ and n -C₁₂H₂₆ flames. Liu et al. [10] studied the ignition of non-premixed C₃–C₁₂ n -alkane flames. Although there is notable amount of work on flames of n -alkanes up to C₁₂, flame studies on heavier fuels such as, for example, in the C₁₄–C₁₆ range, are scarce or non-existing, and these heavier compounds are of direct relevance to practical fuels such as JP-5 and diesel. It should be noted, that autoignition or speciation studies of heavy fuels could be done more readily in homogeneous reactors, as ppm levels of fuels are required typically. In flames on the other hand, significant amounts of fuel need to be present to make the mixture flammable, and thus the unburned mixture temperature needs to be higher in order to achieve high enough fuel vapor pressure to exceed its partial pressure and be sustained thus in the gaseous phase.

Furthermore, compared to neat component liquid fuels, flame propagation studies of practical fuels are fewer. Various experimental methodologies have been used to investigate combustion characteristics of conventional and alternative practical fuels, such as flow reactors (e.g., [11]), shock tubes (e.g., [12]), and counterflow flames (e.g., [13]).

In terms of flame studies, Holley et al. [13] studied the ignition and extinction characteristics of non-premixed flames of various jet fuels and their surrogates. Kumar et al. [14] investigated the propagation and extinction of flames of petroleum and synthetic jet fuels. Chong and Hochgreb [15] reported S_u^0 's of flames of Jet-A, diesel, palm methyl esters, and their blends. Ji et al. [16] studied the propagation and extinction of flames of conventional and alternative jet fuels. Dooley et al. [17] developed a method for the formulation of fuel-specific jet fuel surrogates via an empirical correlation that was tested successfully against autoignition data. It is apparent that the existing flames studies of practical fuels are limited to fuels with average carbon numbers up to 12, for reasons that are similar to those discussed earlier for neat hydrocarbons. It is realized also, that there is need to extend the flame investigations to higher molecular weight fuels such as JP-5 that is used in naval aviation and diesel, which could be petroleum-derived and/or bio-derived.

In view of these considerations, the main goal of this study was two-fold. First, to extend the current experimental and computational capabilities so that fuels with carbon numbers greater than C₁₂ could be investigated in flame environ-

ments with confidence. Second, to use those capabilities and study the flame propagation for mixtures of air with n -C₁₄H₃₀, n -C₁₆H₃₄, as well as four practical naval fuels, namely a petroleum-derived JP-5 jet fuel (hereafter referred to as JP-5), a camelina-derived hydrotreated renewable JP-5 jet fuel (hereafter referred to as HRJ), a petroleum-derived F-76 diesel fuel (hereafter referred to as F-76), and an algae-derived hydro-treated renewable F-76 diesel fuel (hereafter referred to as HRD). As it will be discussed later, the carbon number of the aforementioned fuels ranges from C₁₀ to C₁₇.

2. Experimental approach

The experiments were carried out in the counterflow configuration (e.g., [3,8,10,13,16,18–20]) at atmospheric pressure. In all measurements, the burner nozzle diameters and the burner separation distance were 14 mm. The gaseous flow rates were metered using sonic nozzles, which were calibrated using a wet-test meter.

The key component of the experimental configuration is the fuel vaporization and subsequent handling throughout the heating path, as it has been reported in previous investigations by the authors for molecules up to C₁₂ (e.g., [3,8,10,13,16]). In order to study heavier compounds, the fuel vaporization and heating path had to be upgraded notably.

A high-precision syringe pump was used to control the liquid fuel flow rates. The pump has a reported accuracy of $\pm 0.5\%$, resulting in reactant concentration uncertainty of about $\pm 0.5\%$. A glass nebulizer was used to produce micron-size liquid fuel droplets, which were introduced then into a preheated air flowing in a 90° orientation with respect to the fuel spray. This cross-flow injection allows for very efficient mixing and vaporization at temperatures lower than the fuel boiling point. Additionally, it was determined through trial and error, that the cross-flow injection minimizes the unsteadiness associated with the vaporization process, which is more profound for large mass fuel loadings. Unsteady vaporization can result in notable flame unsteadiness and compromise thus the quality of the experimental data. In order to avoid fuel cracking, the temperature of the fuel/air mixture was maintained below 490 K throughout the heating path, and its control was achieved through an array of thermocouples to assure that there are no hot spots. The burners were heated with ceramic heating jackets.

A K-type thermocouple was used to monitor the temperature of the unburned mixture, T_u , at the center of the burner exit. The majority of the measurements were carried out for $T_u = 443$ K, while for n -C₁₄H₃₀/air flames one additional set

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