Measurements of Laminar Burning Velocity in a Shock Tube

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1 Introduction

The speed at which a laminar flame consumes an unburned, flammable mixture represents one of the most important quantities in combustion science. Premixed flames appear in many of the combustion systems upon which society relies. One ubiquitous occurrence of these flames is in spark ignition (SI) engines, where an understanding of flame propagation at elevated temperatures is critical not only for maximizing performance, but also for preventing inadvertent, abnormal effects such as engine knock. Due to difficulties in preparing flammable mixtures at elevated-temperature conditions in traditional, static-bomb flame speed experiments, very little flame speed data exists at engine-relevant temperatures. Here, we present the first measurements of laminar burning velocities (S_u^0) of *n*-heptane and *iso*-octane at engine-relevant, negative temperature coefficient (NTC) regime temperatures using high-speed imaging in a shock tube.

2 Experimental Setup and Data Interpretation

Flame speed measurements were performed in an extended-test-time, 11.5-cm internal diameter, stainless steel, high-purity kinetics shock tube with a 9.7-m driven section and a variable-length driver to achieve extended, constant-pressure test times [1]. Flames were initiated after the reflected shock waves using laser ignition via a Q-switched, Nd:YAG laser, frequency doubled to 532 nm. A comprehensive description and validation of the method applied in this work is detailed by Ferris et al. [2]. The laser pulse was triggered within 1 ms of the reflected shock wave – a time an order of magnitude shorter than the minimum ignition delay time for either fuel over the measurement conditions. As such, appreciable spontaneous ignition chemistry is not expected to take place in the unburned gas ahead of the flame for either fuel studied.

The growth of outwardly propagating flames was imaged through a quartz end-wall by a Phantom v710 camera coupled to a LaVision ultraviolet-sensitive high-speed intensifier. A 313-nm bandpass filter with a 10-nm FWHM isolates emission primarily attributed to electronically excited OH* radicals to visualize the flame front. Additional details regarding the development and application of shock-tube end-wall imaging are provided by Troutman et al. [3] and Tulgestke et al. [4].

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In order to extract S_u^0 from image sequences, several processing steps are required. The procedure outlined here highlights the major steps in data reduction; for a detailed discussion of the analysis, the reader is referred to the description provided by Ferris et al. [2].

Identification of the flame front is the first step in obtaining a burning velocity measurement from video records (Fig. 1). Binarization based on a statistically derived Otsu threshold [5] is used to identify the region comprising the flame in each image. The local, burned flame speed (S_b) is the rate of translation of the flame in a direction normal to its surface and relative to the burned gas. For spherical flames, a time derivative of the flame radius describes the flame speed. As laser-initiated flames tend to be, by nature of the shape of laser-induced sparks, slightly aspherical, a first-order correction is applied using the angle α between the radial-position and normal vectors corresponding to each tracked location on the flame edge ($S_b = [dr/dt]\cos\alpha$) [2].

The local stretch rate κ is also required in order to extrapolate the burned flame speed to zero-stretch (S_b^0). Most previous works employing outwardly propagating flames use a special case of stretch rate definition based on the flame radius ($\kappa = [2/r][dr/dt]$). Again accounting for the aspherical nature of the flames studied in this work, the more general definition of stretch based on the normalized rate of area change is adopted here ($\kappa = [1/A][dA/dt]$) [2]. The unstretched, burned flame speed, S_b^0, and Markstein length, L_b, were extrapolated from the S_b vs. κ data using the non-linear relation provided by Kelley et al. [6].

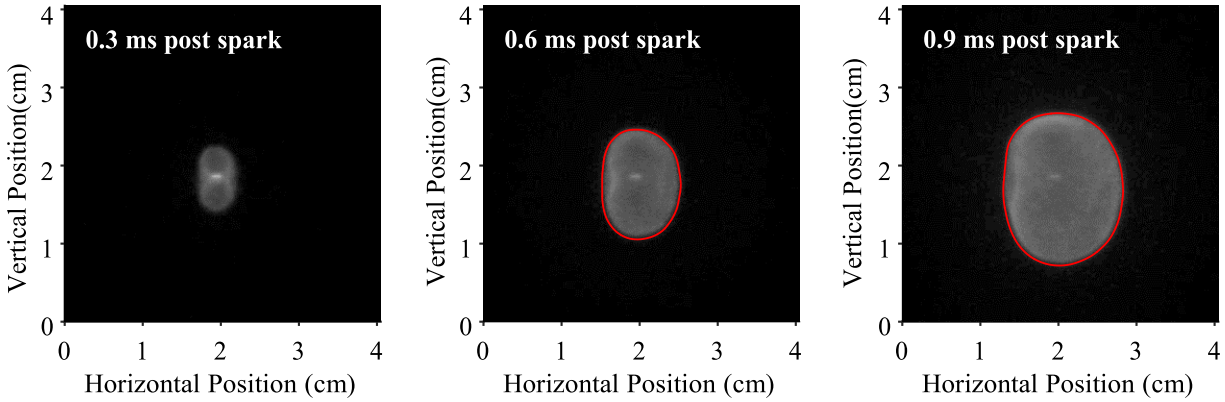

Fig. 1 Samples from an image sequence of an *n*-heptane flame in the O_2/N_2/He oxidizer mixture at 825 K and 0.95 atm. Red lines show extracted flame edge location

3 Results and Discussion

Fuel in Air (O_2/N_2)

Laminar burning velocity measurements are presented in Fig. 2 (left) for both *n*-heptane and *iso*-octane with unburned gas temperatures from 400 K to 600 K, an equivalence ratio of 0.9 in engineered air (21% O_2/79% N_2), and a nominal pressure of 1 atm (±10%). Between 425 K and 525 K, measured S_u^0 values are lower than, but follow the same temperature trend as, modeled results calculated using the PREMIX laminar flame speed code in Chemkin Pro with the specified mixture composition, 1 atm pressure, mixture-averaged transport, and a 2-cm simulation domain. The 2011 gasoline surrogate mechanism of Mehl et al. provides the kinetic, transport and thermodynamic parameters [7]. Above 550 K, an apparent change in the temperature dependence of the burning velocity is observed through an increase in the slope. Difficulties in the analysis of unstable flames begin in the vicinity of 600 K, precluding higher temperature measurements.

Markstein lengths were calculated to be positive for all flames measured, consistent with the expectation of Le greater than unity for the selected lean mixtures.

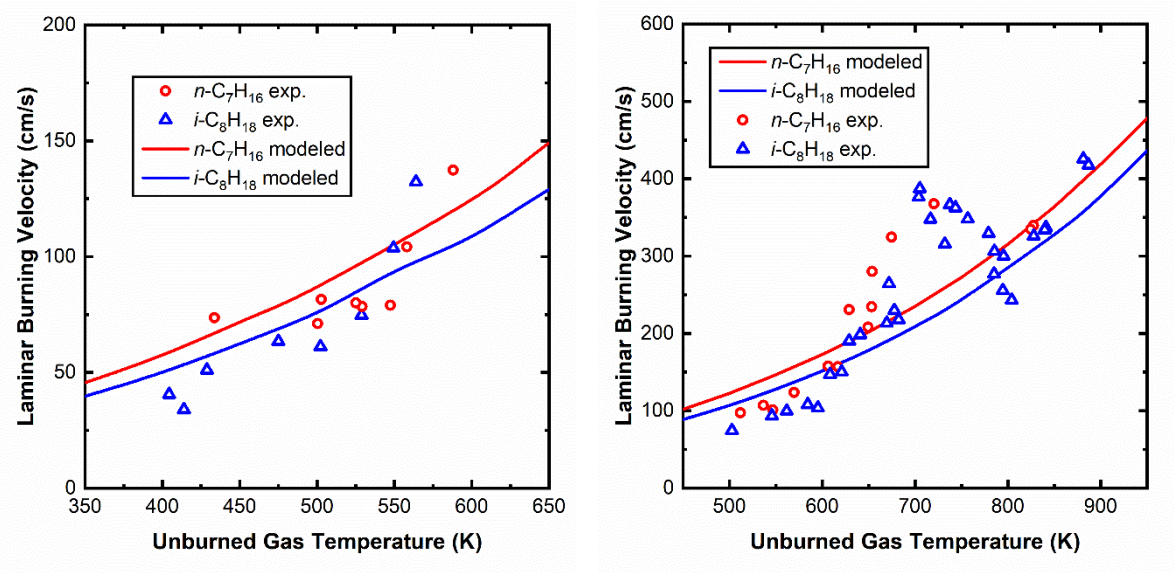

Fig. 2 Laminar burning velocity (S_u^0) measurements for φ = 0.9 experiments at 1 atm (± 10%) along with modeled results using the mechanism of Mehl et al. [7] and the PREMIX flame speed code in Chemkin Pro. Left: results for experiments conducted in engineered air (21% O_2/79% N_2). Right: results for experiments conducted in a mixture of 18% O_2, 41% N_2, and 41% He.

Fuel in O_2/N_2/He

Exchanging engineered air for a reduced oxygen, helium-containing oxidizer mixture of 18% O_2, 41% N_2, and 41% He sufficiently stabilized flames to permit measurements up to 850 K for *n*-heptane and nearly 900 K for *iso*-octane, each with an equivalence ratio of 0.9 (Fig. 2, right). To the authors' knowledge, these results represent the first constant-pressure, laminar burning velocity measurements for any large alkane fuel across the entire NTC temperature regime. Below 600 K, the measured temperature dependence of S_u^0 for both fuels agrees very well with their respective model results; the measured magnitudes of S_u^0 are about 25% lower than modeled. Beginning at 600 K, a much stronger temperature dependence than predicted by the model is observed, continuing until a peak burning velocity is reached near 700 K. Between 700 K and 800 K, the laminar burning velocity declines with increasing temperature, thus presenting the first experimental observation of a direct manifestation of NTC behavior in laminar burning velocity measurements known to the authors. Above 800 K, the burning velocity again increases with increasing temperature, albeit at a faster rate than simulated.

Discussion

These results present, to the authors' knowledge, the first experimental observation of an NTC regime in flame speed measurements, the existence of which has been predicted previously by computational studies conducted using direct numerical simulations (DNS). In particular, the low-temperature chemistry (LTC) associated with 1st-stage ignition has been predicted to lead to either the manifestation of distinct cool flames [e.g. 8] or modified chemical composition of the unburned gas that subsequently affects the propagation speed of the hot flame [9]. While a determination of which phenomenon is responsible for producing the

NTC behavior seen here is not yet possible, the ability to reproduce the relevant conditions experimentally is a significant step towards elucidating the dynamics of high-temperature flames.

The lack of NTC behavior in the modeled results presented here is believed to be an artifact of using the PREMIX flame speed code; the use of a 1-dimensional, steady-state solver and limited simulation domain may not, reasonably, be expected to accurately capture transient and complex dynamics relevant in the NTC regime. As such, the fact that the modeled results do not predict NTC flame speed behavior is not inherently an indication that the Mehl et al. mechanism is incomplete or flawed, as it contains low-temperature chemistry and is known to predict NTC ignition delay time behavior reasonably well [7]. Rather, further work is necessary to better characterize the structure and dynamics of flames in this newly accessible high-temperature regime before these new measurements can be directly employed in the optimization and validation of kinetic mechanisms.

Due to the dynamic nature of the shock-tube environment, the minimum achievable flame speed uncertainty obtainable in a shock tube is somewhat higher than that associated with static-bomb methods – a necessary tradeoff in permitting measurements to be made at significantly higher unburned-gas temperatures [2]. While a detailed treatment of uncertainty will be reserved for forthcoming archival publications [e.g. 10], a total uncertainty of about 10% is expected to provide a reasonable estimate based upon the combined contributions from the S_b vs. κ fit, thermodynamic conditions, and fuel concentration. As is apparent in Fig. 2, this level of uncertainty accounts for the scatter in measurements at similar conditions while being far too small to discount the observed NTC behavior.

An additional point of interest in the flames under study is the appearance of what might be interpreted as internal flame structure in certain temperature regimes, along with a more general destabilization of flames at higher temperatures. The destabilization, which contributed to the scarcity of data in *n*-heptane above 700 K and complicated the interpretation of the *iso*-octane measurements, may be in part due to boundary-layer effects exacerbated by the use of N_2 as a diluent; future work will explore this through the use of Ar as a diluent, which, by its monoatomic structure, is known to reduce the thickness of boundary-layers in shock tubes. A definitive interpretation of the temperature-dependent change in structure is, at present, unclear, though subsequent work by Susa et al. has provided evidence that multi-stage flame structures may be involved [11]. Further investigation of flame structure at high-temperatures presents an important direction for future studies using the shock-tube method.

4 Conclusion

This work presents the first experimental measurement of laminar burning velocities for the primary reference fuels *n*-heptane and *iso*-octane across the NTC temperature regime under constant-pressure conditions. The findings provide direct experimental evidence to support the presence of an NTC regime in the laminar burning velocities of fuels known to exhibit NTC ignition behavior, as has been predicted through DNS studies. These findings highlight the value of continued study of high-temperature flame phenomena, both through the application of novel experimental methods and the DNS methods established in the literature. Furthermore, the shock-tube flame speed method promises to provide important new datasets against which future detailed reaction mechanisms might be validated, leading to improved performance under engine-relevant conditions.

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