**Flame Structure of Counterflow n-Heptane/Air Partially Premixed Flames**

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**INTRODUCTION**

Liquid fuels represent perhaps the most important energy source, since they are used in numerous propulsion and energy conversion applications. The characteristics of liquid fuel combustion are extremely complex because the fuel is introduced into the combustion chamber in the form of a spray that consists of droplets with a wide size and velocity distribution, resulting in disparate vaporization rates. This non-uniform evaporation process in practical spray combustion systems is very difficult to model so that a fundamental investigation that begins from simpler configurations is very useful. Such an investigation can also facilitate the validation of theoretical/computational models through experimental measurements of flames established in such simpler configurations. However, there is a paucity of such measurements in the literature [1,2]. Although most practical liquid fuels are blends of several components, we have selected n-heptane as a surrogate fuel in this investigation for sake of simplicity. Due to their diverse applications and fundamental relevance, partially premixed flames have been investigated extensively in recent years. Most of these studies, however, have focused on methane-air flames [1,3–9], motivated perhaps by the fact that extensive experimental data have been reported for these flames and detailed reaction mechanisms are available to model the methane-air chemistry. Except for some recent studies [1,9–13], partially premixed flames burning higher hydrocarbon fuels, especially liquid fuels, have not been investigated.

In this investigation, we report on an experimental-computational investigation of n-heptane partially premixed flames established in a counterflow burner. The objective of this study is to report detailed experimental data that can be subsequently used for the validation of computational models and reaction mechanisms involving simulations of liquid fuels in general, and n-heptane in particular.

**EXPERIMENTAL APPARATUS**

Experimental results have been obtained for flames established in a counterflow burner. The separation distance between the counterflow nozzles of the burner is 15 mm and the jet diameter is 27.38 mm. The fuel emerges from the bottom nozzle. A nitrogen curtain is established through an annular duct surrounding the fuel jet in order to isolate the flame from ambient disturbances. The nitrogen and burned gases are exhausted and cooled through another annular duct around the oxidizer nozzle. A detailed schematic of the experimental setup is presented in Fig. 1.

The velocities of the two streams are chosen to conform to the global strain rate [3],

\[ a_g = \frac{2|V_O|}{L} \left( 1 + \frac{|V_F|}{|V_O|} \frac{\rho_F}{\rho_O} \right) \]
Fig. 1  Schematic of the experimental apparatus.

and to satisfy the momentum balance,

$$\rho_O V_O^2 = \rho_F V_F^2$$

The oxidizer is air at room temperature while the fuel stream consists of mixtures of nitrogen and prevaporized n-heptane. The fuel nozzle is heated and the temperature is controlled to maintain the fuel-containing stream at a 400 K temperature at the burner exit. Nitrogen and n-heptane are mixed in a prevaporizer, which consists of a stainless steel chamber that is electrically heated. The desired mass flowrate of n-heptane into the prevaporizer is maintained by a liquid pump. Half of the chamber is filled with glass beads to impede the flow, thereby increasing its residence time in the chamber and, hence, enhancing the heat transfer to the liquid fuel. The temperature of the fuel vapor exiting the chamber is monitored by a thermocouple.

Temperature profiles of various flames have been obtained using a thin Pt-Rh thermocouple with a bead diameter of 0.508 mm and wire diameter of 0.127 mm.

**REACTION MECHANISM**

The kinetic mechanism (SOX) used to model the flames has been developed by extending a detailed oxidation scheme which can be used for several fuels. Due to the hierarchical modularity of the mechanistic scheme, this model is based on a detailed sub-mechanism of C_1-C_4 species. Assuming analogy rules for similar reactions, only a few fundamental kinetic parameters are required for the progressive extension of the scheme towards heavier species. The resulting kinetic model of hydrocarbon oxidation from methane up to n-tetradecane consists of about 250 species and 5,000 reactions. Almost all the reactions considered in this work have been already published and the complete scheme is available upon request [14].

The subset of n-heptane oxidation reactions in the mechanism have been extensively tuned by validating experimental measurements for pure pyrolysis conditions, oxidation in a jet stirred and plug flow reactors, and on a large set of shock tube experiments [15]. The polycyclic aromatic hydrocarbons (PAHs), well known for being soot precursors, are described with large detail inside the scheme. The formation of the first aromatic rings by the C_2 and C_4 chemistry and by the resonantly stabilized radicals like propargyl and cyclopentadienyl (C_5H_5 and C_5H_5) has been carefully investigated in previous investigations [16,17]. Further growth of PAH species up to coronene (C_{24}H_{12}) is also modelled through the well known HACA mechanism (Hydrogen Abstraction Carbon Addition) [18]. The main consumption reactions of aromatics and PAHs are H abstraction reactions by H and OH radicals. This high temperature reaction
mechanism has been validated by a large amount of experimental data [16,17].

**Fig. 2a** Experimental (symbols) and simulated (lines) temperature profiles at a strain rate of 50 s$^{-1}$.

Numerical simulations have been done with OPPDIF, a program from CHEMKIN package [19] that is capable of modeling combustion between two opposed jets. The code has been modified to handle the complex reaction mechanism that was previously described, and to account for thermal radiation through the optically thin model. Thermodynamic properties were mainly obtained from Burcat [20]. Unavailable properties have been estimated by using group additivity and difference methods [21]. Transport properties have been obtained from the CHEMKIN database [22] wherever available, while unavailable data has been deduced by analogy with known species.

**RESULTS AND DISCUSSION**

Experiments were performed by varying the global strain rate and the equivalence ratio. Partially premixed n-heptane flames exhibit a characteristic double flame structure. There is an azure flame on the fuel side due to the partial oxidation of heptane by the air present in the fuel-rich stream. Unburned fuel and intermediate combustion species such as CO and H$_2$ are then carried to the blue non-premixed flame where they are oxidized by air.

**Fig. 2** Experimental (symbols) and simulated (lines) temperature profiles at a strain rate of 75 s$^{-1}$ (b) and 100 s$^{-1}$ (c).

We will report three sets of results for three different strain rates. For each strain rate, we will compare temperature profiles for flames established with several values of equivalence ratios $\phi$ of partial premixing. Figure 2a presents values of temperature for flames established at a global strain rate of 50 s$^{-1}$ and at equivalence ratios decreasing from 10 to 3. The experimental values are compared with numerical simulations and the temperature measurements have been
corrected for radiation heat loss. The double flame structure is evident from the broad temperature profiles. Decreasing the equivalence ratio of premixing, i.e. making the fuel stream composition closer and closer to a stoichiometric mixture, the premixed flame shifts towards the fuel nozzle, and the peak temperature increases. For the case $\phi=3.0$ the oxidizer concentration is such that the premixed flame is almost attached to the fuel nozzle. The oxidizer side of temperature profile is slightly affected by the variation of equivalence ratio of premixing. The location of the non-premixed flame is unchanged, while the peak temperature slightly increases. The same trend can be observed in Figs. 2b and 2c in which similar experimental results are presented for strain rates of 75 s$^{-1}$ and 100 s$^{-1}$ respectively. The profiles in general become sharper at higher strain rates because flow velocities increase. The same holds for the cases $a_g=50s^{-1}$ and $\phi=3$, and $a_g=100s^{-1}$, $\phi=3.5$. The simulated profiles reflect this behavior and the peak temperature values are in good agreement with the experimental results.

REFERENCES