Experimental and Numerical Study of a Laminar Nonpremixed Hydrogen Flame

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Keywords: Laminar nonpremixed flame, Raman scattering, LIPF, Flamelet model.

Introduction

Laser-based non-intrusive techniques, with adequate temporal and spatial resolution, have been applied to measure the state properties of gases in combustion environments for many years (Eckbreth, 1996). One laser-based technique, spontaneous Raman scattering, has the capability of providing simultaneous measurements of temperature and all major species concentrations in hydrogen and hydrocarbon diffusion flames. Although Raman scattering has a relatively weak signal, it has been applied to simultaneously measure temperature and all major species concentrations in turbulent hydrogen diffusion flames (Drake et al., 1986; Cheng et al., 1992; Barlow and Carter, 1994), hydrogen diluted with argon flames (Magre and Dibble, 1988; Chen and Mansour, 1996) and hydrocarbon flames (Dibble et al., 1987; Bergmann et al., 1998; Nguyen et al., 1996; Nooren et al., 2000). From the search of published literatures, most reports are on the measurements of turbulent flames. There is a need to provide laminar flame data for validation of combustion models. A goal of this paper is to provide a fine resolution and accurate database for comparisons with comprehensive flamelet model (Peters, 1984) of laminar hydrogen jet diffusion flame.

Experimental Apparatus

The schematic diagram of the UV Raman system is shown in Figure 1. A narrowband KrF excimer laser (Lambda Physik LPX-250T) produces UV light that is tunable from 247.9 to 248.9 nm with a bandwidth of 0.003 nm. The maximum pulse energy is 450 mJ with pulse duration of 20 ns. For the present experiment, the laser pulse energy is set to 150 mJ to avoid laser-induced air breakdown. The laser is tuned to 248.56 nm to minimize fluorescence interference from OH and O₂. Light scattered by the 200 mm focusing lens is measured by a PMT to provide a relative measure of the laser pulse energy. The laser is focused toward the multi-element, uncooled, flat-flame diffusion "Hencken" burner or the jet. The "Hencken" burner produces a homogenous laminar post flame zone that is used for evaluation and calibration of the Raman system. The laser beam is focused by a single 200 mm spherical lens to a 0.02×0.04 mm profile in the sample volume where the largest dimension is parallel to the direction of the jet flow. The probe length as determined by the magnification ratio of collection optics (2.34) and the opening slit of spectrometer (100 µm) is 0.04 mm in the direction of beam propagation. Stokes Raman and fluorescence signals emanating from the sample volume are collected and focused by a Cassegrainian optics (magnification ratio 2.34) through a 10 mm thick butyl acetate liquid filter and relayed to the entrance slit of a 0.275 m, f/3.8 spectrometer (Acton Research Co., SpectraPro-275) with a 1200 grooves/mm grating (3 nm/mm dispersion) and a 0.5 m, f/4 spectrometer (SPEX-500M) with a 1800 grooves/mm grating (1.1 nm/mm dispersion) for dispersion and separate measurement. An intensified CCD camera (Princeton Instruments, 576 x 384 array, 22 x 22 µm pixels) is aligned at the exit plane of the spectrometer for monitoring the Stokes Raman and fluorescence signals. The Raman and fluorescence signals are digitized with a 14-bit A/D card connected to a personal computer for data reduction. The spectral coverage of the 0.5 m spectrometer is 13.8 nm, which is insufficient to measure all the major species Raman signals. Hence, it is used for the O_2 (258.4 nm) and N_2 (263.7 nm) Raman signal measurements. The spectral coverage of the 0.275 m spectrometer is 36.3 nm, which is used to measure H_2O (273.2 nm) and H_2 (277.1 nm) Raman signals as well as OH (297 nm) fluorescence in hydrogen flames. Both the 0.5 m and 0.275 m spectrometers are aligned by placing a 200 µm wire at the center of the probe volume and centering the image onto the respective slits. This procedure ensures that both N_2 Stokes and anti-Stokes Raman signals are measured from the same sample volume. The flow facility is a 1 mm inner diameter vertical straight tube. Fuel is introduced through the jet into the still atmospheric air without coflow. The jet is mounted on a 3-D translation stage while the optical system remains fixed.

Calibration and Data Reduction

The Raman system is calibrated with the flat-flame "Hencken" burner operated at several known equivalence

ratios from lean to rich. The calibration procedure for major species and OH concentration measurements is similar to that described elsewhere (Cheng et al., 1992). The perfect gas law is used to arrive at the temperature measurement by adding the number densities of the major species. The mixture fraction, f, is a conserved scalar that describes the state of mixing between fuel and oxidizer. The mixture fraction is calculated from the Raman scattering measurements of the major species concentrations for each laser shot as the mass originating from the fuel stream divided by the total mass (Magre and Dibble, 1988). The contribution of H₂O in the room air and the flame radicals (i.e., OH, H) to the mixture fraction calculation is small (< 0.001) and is neglected. The mixture fraction is 1 in pure hydrogen, 0 in pure air, and 0.0283 at stoichiometric. The results of calibration of the single pulse Raman system over a wide range of fuel/air ratios in the Hencken burner are shown in Figs. 2-5. At each fuel/air ratio, 200 laser shots are recorded. The mean and standard deviation values for each flame condition are presented by symbols and error bars and are compared to theoretical adiabatic equilibrium curves. The variations of mixture fraction are correlated to all major species concentrations. The experimental relative standard deviation for single-shot N₂ concentration measurements is 3% at

room temperature and 7% in a stoichiometric flame at 2300 K (see Fig. 4c). The relative standard deviation for temperature and OH concentration measurements is 13% and 19% in the stoichiometric flame, respectively. The well-calibrated Raman system is then capable of analyzing flows where conditions are unknown.

Results and Discussion

A laminar hydrogen jet diffusion flame is formed by injecting fuel through a straight tube (D = 1 mm) into still atmospheric air. The jet has an exit velocity of 36 m/s, which is calculated based on the flowrate and the jet exit diameter (Reynolds number = 330). Raman and LIPF measurements are made in the radial and axial directions. At each measurement location 200 independent laser shots are taken. For each single laser shot, the thermodynamic state properties (e.g., temperature and species concentrations) are measured in the flame. Other quantities such as density and mixture fraction can be calculated. Figures 6-8 show the measured radial and axial profiles of the mean temperature, major species (O₂, N₂, H₂O, H₂), and OH concentrations with the calculated results obtained from a postprocessing of flamelet model (Seshadri et al., 1990) for the flame. The experimental data are indicated by symbols and those from the flamelet model are denoted by solid lines. The predicted data are derived from the measured mixture fraction and a flamelet library. Figure 6 details the radial profile across the potential core at x/D = 1. The temperature rapidly rises from the cool unburned core to 2008 K, where it plateaus across the reaction zone. As expected, the maximum flame temperature and the peak OH location occur at the stoichiometric contour defined by the intersection of the H₂ and O_2 concentration profile. The peak OH concentration (X_{OH} = 0.01833) is about a factor of 3 higher than the equilibrium value that corresponds to a measured mixture fraction. This superequilibrium OH concentration is caused by the slow three-body recombination reactions and hence results in a flame temperature lower than adiabatic temperature (Cheng et al., 1992). Comparisons between the predicted and measured data are in favorable agreement except that for OH concentration. The flamelet model predicts a broader distribution of OH radicals. Figure 7 shows the radial profile for the flame at x/D = 5. At this axial location, the N₂ has diffused into the central jet and the temperature and peak OH shift toward outer radial position. The maximum temperature has reached to 2224 K and is also located with the peak OH at the stoichiometric contour. The depressing of temperature is also due to superequilibrium OH effect. The maximum value of OH is 0.017. Comparisons of the predicted and measured data also indicate that the flamelet model predicts a broader OH distribution at this axial position. Figure 8 shows the axial profile along the centerline of the flame. The measured maximum temperature and OH concentration locate at x/D =60, where is close to the axial position of the stoichiometric contour. Note that the predicted major species concentrations are in good agreement with the measured values. However, the flamelet model overpredicts the temperature and OH concentrations.

Conclusions

UV Raman scattering combined with LIPF has been applied to a laminar hydrogen jet diffusion flame. The spatial resolution is improved over previous UV Raman system. Simultaneous, temporally and spatially resolved point measurements of temperature, major species concentrations (O_2 , N_2 , H_2O , H_2), and hydroxyl radical concentration (OH) are measured. In addition to obtaining an accurate and detailed mapping of temperature and species concentrations, we found that fuel has not been completely consumed up to x/D = 60. We also found that the measured maximum OH concentration coincides with the location of maximum temperature at x/D = 1 and 5. The comparisons between the measured and calculated data indicate that the flamelet approach predicts favorable results for temperature and major species concentrations but not for OH radicals. Further investigations of the reaction mechanisms are needed for the flamelet model.

Acknowledgements

This research was supported by the National Science Council of the Republic China under Grant Number NSC-90-2212-E-216-019 (TSC), NSC-90-2212-E-006-156 (YCC), and NSC-90-2212-E-006-159 (TSL).

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Fig. 1. Schematic diagram of UV Raman.



Fig. 2. Calibration result for temperature measurements.



Fig. 3. Calibration result for Q_2 and N_2 concentration measurements.



Fig. 4. Calibration result for H₂O and H₂ concentration measurements.



5. Fig. Calibration result for OH concentration measurements.



Fig. 6. Radial profiles of mean temperature, major species, and OH mole fractions at x/D = 1. The OH scale is magnified for clarity.



species, and OH mole fractions at x/D = 5.



Fig. 8. Axial profiles along the centerline of the flame.