Characterization of Flows with Chemical Reactions in Energy Conversion Processes

T.-W. LEE
Department of Mechanical and Aerospace Engineering
Arizona State University
Tempe, Arizona
USA

Abstract: - Energy conversion processes typically involve flows with chemical reaction in complex geometries, e.g. combustors, fuel cells, heat recovery steam generators. In many instances, an understanding of these flows is needed for optimization of the efficiency, pollutant emission and thermal control. Characterization of these flows to achieve that may be a relatively simple flow visualization, routine probe measurements, advanced optical diagnostics or computational simulations validated by experimental data. In this paper, I will present some examples of the characterization methods, based on our recent work.

Key-Words: - Energy, Chemical Reactions, Diagnostics

1 Introduction

In the interest of space and time, I will only describe our work on laser-induced breakdown spectroscopy in the written version of the paper. Other material will be presented during my talk.

Laser-induced breakdown spectroscopy (LIBS) has emerged as a powerful diagnostic method in many application areas, including combustion systems [1-4]. In an earlier paper [2], we reported on a comparison of LIBS temperature measurements with thermocouple measurements [5] to show that the LIBS signal dependence on the local gas density can be exploited under constant-pressure conditions to extract the temperature data. However, in that study we were only able to look at the centerline data for two reasons: (1) validation data were available only along the centerline; and (2) moving away from the centerline increased the flame oscillations resulting from the intense laser energy deposition by LIBS probe beam. In this study, we report new results that expand upon the LIBS capabilities to measurements of the radial temperature profiles in a laminar flame achievable by circumventing the laser-induced pressure perturbations. Also, a comparison is made between the LIBS and spontaneous Raman scattering measurements of temperature. Raman scattering can be used for temperature measurements due to the energy distribution among the molecular vibrational states that change as a function of temperature. In particular, the ratio of the Stokes and anti-Stokes Raman signals is a predictable function of temperature that can also be calibrated. However, the Raman scattering method suffers from low anti-Stokes signals at temperatures below 1000 K and also from susceptiblity to interference from Rayleigh and Mie scattering. LIBS circumvents most of these difficulties due to its strong signal levels and temperature dependence that can easily be calibrated.

2 Problem Formulation

A schematic of the diagnostic setup is shown in Fig. 1. A Nd:YAG laser operating at 30 Hz with a frequency-doubled 532 nm output was used as an excitation source. The beam was focused using a 100 mm focal-length lens with an initial beam diameter of approximately 10 mm. For Raman measurements, an additional cylindrical lens was inserted in the light path in order to decrease the laser energy density. The resulting laser-induced breakdown signal (the radiation from the spark) was collected using a 100 mm-diameter, 350 mm focal-length lens, collimated and passed through filter elements (to block out the Mie scattering and spurious reflection), and focused onto the entrance slit of a spectrometer. A cooled ICCD imaging detector was mounted on the exit slit of the spectrometer to provide spectral data. For synchronization and timing, internal digital timers were used. For Raman scattering, the ICCD gate was aligned with the laser pulse, while for LIBS the gate delay needed to be optimized to discern the atomic peaks in the spectra.

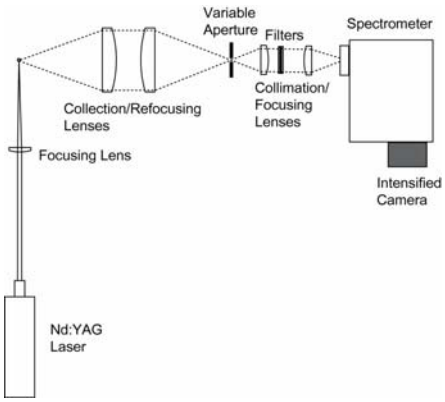

Fig. 1. A schematic of the diagnostic setup.

A Hencken burner (1 in^2 flow area with a 0.5 inch wide shroud flow) was used to produce stable laminar flames, using methane and air under partially premixed conditions. The Hencken burner geometry essentially allows for effective mixing of the fuel and air streams when operated in partially premixed conditions. Although LIBS works even in highly sooting flames [2], Raman scattering measurements cannot be done in sooting flames due to strong soot Mie scattering. Therefore, an equivalence ratio of 5 was selected for methane-air flames, where both Raman and LIBS measurements could be performed. The fact that LIBS measurements can be made in harsh flame environments even under highly sooting conditions makes LIBS a powerful diagnostic tool in combustion measurements [2]. The flow rates were monitored and set to 50 cm^3/s, for the fuel-air mixture at an equivalence ratio of 5, by a set of digital thermal mass flowmeters. The mean velocity based on this flow rate and the burner cross-sectional area was 7.75 cm/s. In addition, a shroud of nitrogen co-flow outside the flame was used at a flow rate of 8.3 cm^3/s.

3 Problem Solution

Figure 2 shows the LIBS and Raman spectra. Broadband spectra were acquired for both LIBS and Raman to resolve various peaks. In the LIBS spectra, the elemental carbon, nitrogen and oxygen peaks are prominent in the 640 to 800 nm spectral range covered. Nitrogen and oxygen appear since the fuel is partially premixed with air. As one moves away from the centerline (r = 0), the decrease in the peak heights is quite evident following the temperature increase closer to the flame. The LIBS peak heights are proportional to the number density, and therefore inversely proportional to temperature. For the Raman spectra, both the anti-Stokes and Stokes bands for the major molecular species are visible. At lower temperatures, however, the anti-Stokes peaks become too small to be useful for temperature measurements [5]. Also, spontaneous Raman signal is easily overwhelmed in any kind of sooting environment by Mie scattering. This makes LIBS a viable tool for temperature measurements in flames.

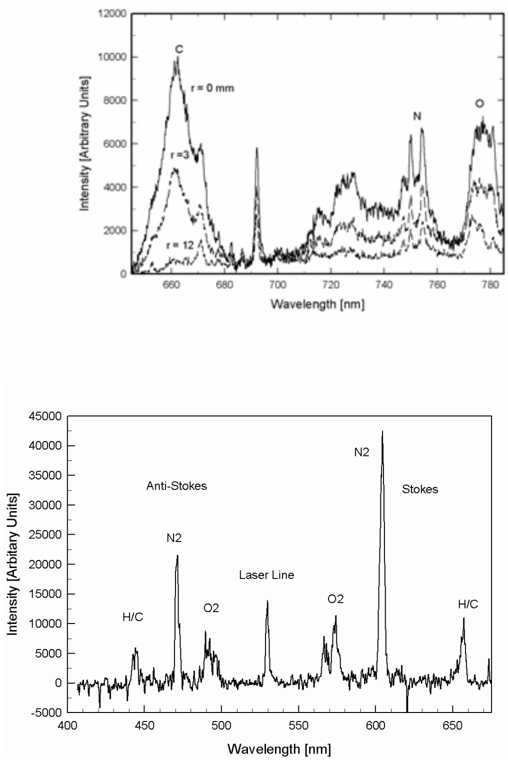

Fig. 2. LIBS (above) and SRS (below) spectra showing distinct peaks for atomic and molecular species, respectively.

Figure 3 shows a comparison of the temperature measurements by LIBS and Raman scattering. The temperature is normalized by the centerline temperature, which is the calibration temperature [6] used for both LIBS and Raman signal conversion to temperature data. The centerline temperature data were taken from Bennett et al. [6] at the same equivalence ratio of 5 and at the same axial locations normalized by the flame height. The temperature is low at the centerline and increases to the flame temperature as the radial distance increases for $Z/H_T = 0.4$. At higher positions in the flame, thermal diffusion causes the temperature profile to flatten until it starts to assume a "top-hat" profile by $Z/H_T = 0.75$. The LIBS and Raman temperature measurements are in good agreement, except at $Z/H_T = 0.4$ where the LIBS profile is inside of that from Raman. Also, the Raman measurements are only feasible for temperatures above 1000 K, and thus only those points are plotted in Fig. 3.

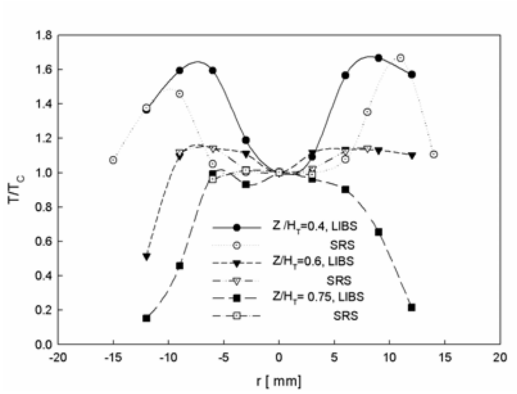

Fig. 3 Comparisons of centerline-normalized temperatures measured using LIBS (dark symbols) and SRS (open symbols).

For the current Nd:YAG laser (New Wave Research, Model Tempest) operating at 30 Hz, the spark-induced oscillations were not observed. This laser had a pulse duration of 3 to 5 ns, and a smaller initial beam diameter of 5 mm, in comparison to the 8 mm used in our previous study [2]. In addition, due to the higher available laser energy, longer focal-length lens could be used for the laser focusing. The defocusing (relative to our previous optical setup) involved in the current optical configuration all but eliminated the pressure perturbations that precluded any radial profile measurements in our previous study. However, the defocusing has an effect of reducing the spatial resolution. The fact that the LIBS can be used as a temperature probe even in highly-sooting flame environment (as demonstrated in [2]) makes it a very useful combustion diagnostic, if the focusing optics are optimized for the flame environment. For example, in laminar flames long focal-length focusing is appropriate to avoid pressure fluctuations at high energy densities, while in turbulent flames the flow recovery time scale is fast and more spatial resolution can be achieved with tight focusing of the probe beam.

4 Conclusion

Further details of the diagnostic and computational characterization methods will be provided in my PowerPoint presentation.

Ε*υχαριστω*!

References:
[1] Ferioli, F., Puzinauskas, P.V. and Buckley, S.G. (2003), *Applied Spectroscopy*, 57, 1183.
[2] Lee, T.-W. and Hegde, N. (2005), *Combustion and Flame*, 142, 314.
[3] Blevins, B.G., Shaddix, C.R., Sickafoose, S.M., and Walsh, P.M. (2003), *Applied Optics*, 42, 6107.
[4] Flower, W.L., Peng, L.W., Michael, M.P., Bergan, N.B., Johnsen, H.A., Ottesen, D.K., Westbrook, R.F., Lindsey, V. (1994), *Fuel Process Technology*, 39, 227.
[5] Hicks, Y.R., DeGroot, W.A., Locke, R.J. and Anderson, R.C. (2002), NASA-TM-2002-211588.
[6] Bennett, B.A., McEnally, C.S., Pfefferle, L.D., Smooke, M.D., 2000, *Combustion and Flame*, 123, 522.