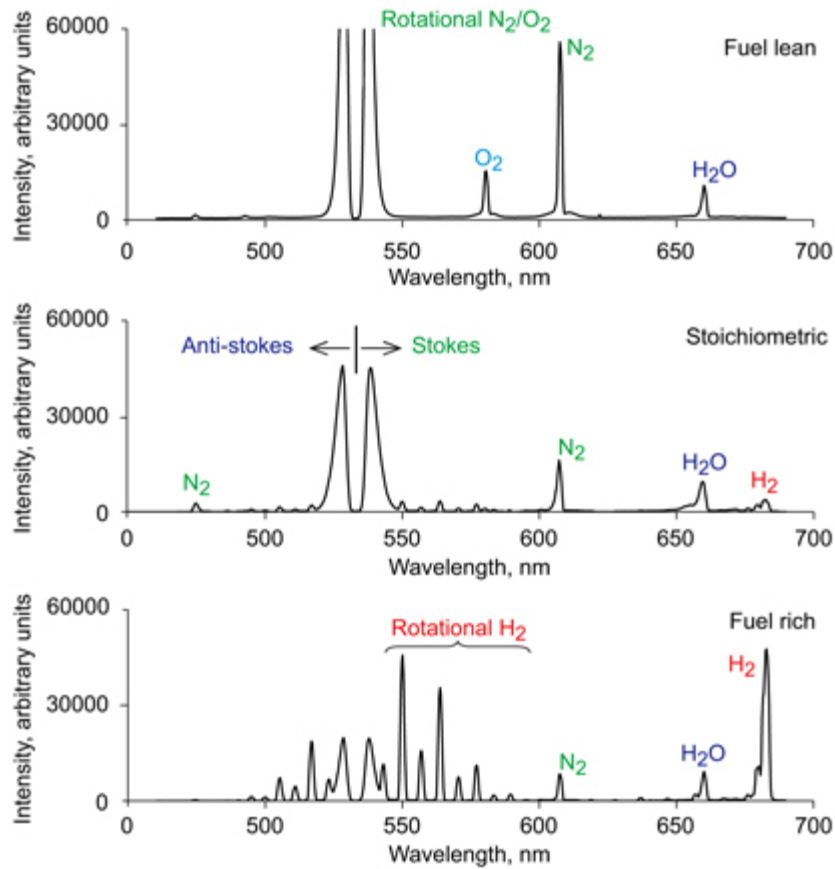


Transferable Calibration Standard Developed for Quantitative Raman Scattering Diagnostics in High-Pressure Flames

Researchers from NASA Glenn Research Center's Combustion Branch and the Ohio Aerospace Institute (OAI) have developed a transferable calibration standard for an optical technique called spontaneous Raman scattering (SRS) in high-pressure flames. SRS is perhaps the only technique that provides spatially and temporally resolved, simultaneous multiscalar measurements in turbulent flames. Such measurements are critical for the validation of numerical models of combustion. This study has been a combined experimental and theoretical effort to develop a spectral calibration database for multiscalar diagnostics using SRS in high-pressure flames. However, in the past such measurements have used a one-of-a-kind experimental setup and a setup-dependent calibration procedure to empirically account for spectral interferences, or crosstalk, among the major species of interest. Such calibration procedures, being nontransferable, are prohibitively expensive to duplicate. A goal of this effort is to provide an SRS calibration database using transferable standards that can be implemented widely by other researchers for both atmospheric-pressure and high-pressure (<30 atm) SRS studies. A secondary goal of this effort is to provide quantitative multiscalar diagnostics in high-pressure environments to validate computational combustion codes.

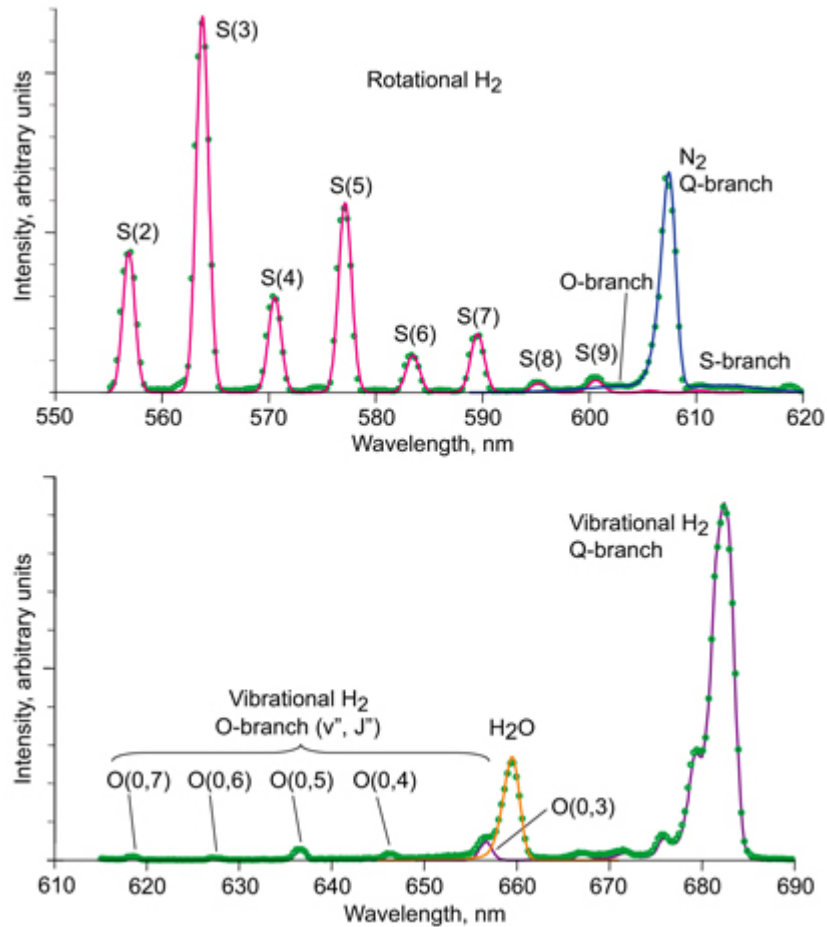


Typical Raman spectra from a 10-atm premixed H₂-air flame at three different equivalence ratios, Φ (from fuel lean, $\Phi = 0.16$, to fuel rich, $\Phi = 4.90$). Note that there is O₂ in the fuel lean data, but not in the fuel rich data, where H₂ appears in large quantities. Data were averaged over 200 laser shots.

Long description of figure 1. Fuel-lean, stoichiometric, and fuel-rich graphs of intensity versus wavelength in nanometers, showing rotational nitrogen/oxygen, anti-stokes and stokes areas, and rotational hydrogen.

To provide quantitative measurements of major species concentration and temperature in high-pressure flames using SRS, researchers must compensate for the spectral interferences, or crosstalk, between different molecular species by using a temperature-dependent calibration matrix. We implement the spectral calibration by using a high-pressure combustion facility that utilizes a specially designed fully premixed gaseous multifuel burner mounted inside a 60-atm pressure vessel that provides optical access for the SRS measurement (refs. 1 to 3). By collecting SRS spectra (400 to 700 nm, with a 0.3-nm resolution) from a variety of high-pressure (10 to 30 atm) hydrogen-fueled flames operating over a wide range of equivalence ratios (see the preceding graphs), we can correlate the pixel-integrated spectral response from the SRS process to the molecular species densities calculated from the chemical equilibrium. The chemical equilibrium calculations are based on precisely measured (0.5-percent accuracy) fuel-oxidizer flow rates at an assigned temperature and pressure. Since the temperature is measured spectroscopically with an accuracy of better than 10 K, we do not require the assumption

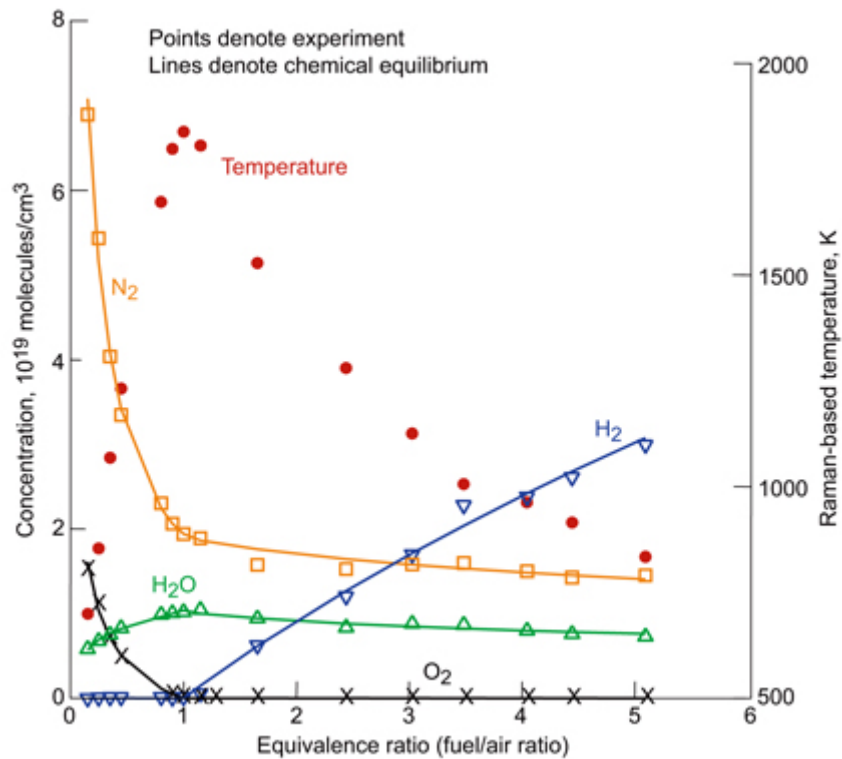
of adiabatic equilibrium. The excellent agreement between the data and chemical equilibrium calculations is shown in the following graphs. In addition to the experimental SRS calibration process, we also theoretically model the Raman scattering to quantitatively analyze the spectral interferences (ref. 4). The final graph compares the model and experimental data, showing excellent agreement. The spectral modeling aids the development of the calibration matrix functional form, and ultimately, improves the calibration accuracy.



Quantitative species concentration and temperature data from a high-pressure (10-atm) hydrogen-air calibration flame obtained using spontaneous Raman scattering. The calibration burner, a novel fully premixed design, was developed especially to provide hot products of combustion that are at chemical equilibrium. The points represent the Raman scattering measurements, and the lines represent the values predicted by chemical equilibrium at the Raman-measured temperature, and are not fits to the data points. These results represent the first use of the newly Glenn-developed transferable standard for Raman scattering in high-pressure flames. This database is unique in its ability to allow other research groups to use Raman scattering as a tool for quantitative measurements in combustion systems.

Initially, spectrally simple hydrogen-air flames were used to provide hot combustion products such as nitrogen (N₂), oxygen (O₂), water (H₂O), and hydrogen (H₂) over a wide

temperature range. We then moved progressively to more spectrally complicated carbon-containing fuels to include the SRS signals from carbon monoxide and carbon dioxide. Using a technique that we developed previously for the analysis of Raman spectra at high pressures, we determined accurate thermodynamic temperatures and Raman signal intensities for each molecular scattering species in fuel-lean and fuel-rich regions. These intensities were then used to generate the calibration matrix database for all major species and their associated spectral crosstalk effects as a function of temperature (ref. 5). Using this calibration matrix, we could then demonstrate, for the first time, quantitative multiscalar measurements of species concentration and temperature in premixed H₂-air flames at 10 atm by using spontaneous Raman scattering in conjunction with a transferable standards calibration database.



Comparison of predicted Raman spectra and measurements for a 10-atm ($\Phi = 2.04$) H₂-air flame. A temperature of 1425 K (obtained from the rotational Raman measurement of H₂) was used for the simulation. Excellent agreement is shown even though no adjustable fitting parameters were used.

Long description of figure 3. Graph of concentration in 10¹⁹ molecules per cubic centimeters versus equivalence ratio (fuel-to-air ratio) and Raman-based temperature in kelvin, showing experimental data and chemical equilibrium..

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