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COMPUTATIONAL AND EXPERIMENTAL STUDY OF LAMINAR FLAMES

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During the past year we have made substantial progress in both the computational and experimental portions of our research. In particular, we have continued our study of non-premixed axisymmetric methane-air flames. Computations were performed at the CNSF at Cornell University and locally at Yale on a Stardent GS-2500 which was purchased recently in part with DOE funds. The calculations completed during the current progress year and scheduled for presentation at the 4th International Conference on Numerical Combustion represent the first time that multidimensional elliptic flames with two carbon atom chemistry have been computed using a shared memory parallel computer. The results of this investigation have enabled us to probe the fluid dynamic-thermochemistry interaction and its effect on the structure of coflowing methane-air diffusion flames. We discovered that the height of a flame is extremely sensitive to the boundary condition employed at the surface of the burner. The use of a zero vorticity boundary condition typically produced flames whose height differed by as much as 15-20% over the experimental results. When the vorticity at the base of the flame was related to the axial gradient of the radial velocity, computed flame heights were in close agreement with those determined experimentally. Our study also continued to focus on the applicability of different chemistry in the modeling of nonpremixed combustion. Both detailed and reduced chemical mechanisms were used in the studies. We discovered that a reduced four-step methane-air mechanism employing steady-state and partial equilibrium assumptions but developed for one-dimensional systems could be used to predict accurate structure of a two-dimensional system. We also continued our investigation of mole fraction versus mixture fraction correlations for flamelet models of nonpremixed turbulent combustion. It has been suggested that reliable and accurate prediction of the instantaneous local extinction of a turbulent diffusion flame may require application of laminar flamelet models to more complex systems. If multidimensional effects are important, then computations of axisymmetric coflow flames are the natural candidates for the flamelet libraries. To this end we continued a series of calculations designed to compare temperature and species profiles as a function of the mixture fraction for various values of the scalar dissipation. In a flamelet model of nonpremixed turbulent combustion the flamelets are stored in a library as a function of the scalar dissipation. Using the same value of the scalar dissipation at the point of local stoichiometric mixture, we continued investigating the differences between the structure of stretched counterflow flames and corresponding one-dimensional "slices" of our two-dimensional coflow model along the gradient of the mixture fraction coordinate. Preliminary results indicate that substantial differences occur between the two configurations as the value of the scalar dissipation increases.

Experimentally, we have continued our investigation of axisymmetric laminar flames using laser imaging techniques. Advances have been made in several areas. In order to compare the concentration of minor species with those predicted by the computations, a series of fluorescence measurements was initiated. In our initial experiments, the OH concentration was measured by laser-induced fluorescence (LIF). For these measurements, the second harmonic from a Nd:YAG laser (10 Hz, 180 mJ/pulse) pumped a dye laser with dye Rhodamine 590 and then was frequency doubled by a KDP crystal, providing 1.5 mJ/pulse in the ultraviolet (UV). The UV beam was tuned to the $P_1(2)$ absorption transition (282.58 nm) of the OH $A^2\sum^+(\nu' = 1) \leftarrow X^2\prod(\nu'' = 0)$ system and was focused to a line intersecting the flame using a 250 mm focal length quartz lens. The LIF signal was collected normal to the UV beam with a pair of quartz lenses (fl = 100 mm and fl = 80 mm) and focused onto an intensified cryogenically cooled CCD detector. A narrow band UV interference filter (center wavelength = 310.0 nm, FWHM = 8.9 nm) was placed in front of the detector and the OH fluorescence in the $A^2\sum^+(\nu' = 0) \leftarrow X^2\prod(\nu'' = 0)$ band at 309 nm was observed. The intensifier was gated coincident with the laser pulse and the signal was integrated over 50 laser shots at each downstream location. The burner was then moved to a different downstream location and another line image recorded. The series of line images was then combined to produce the relative OH concentration image (without temperature and quenching corrections). To obtain absolute concentration values, a premixed flat-flame calibration burner was used. Quenching corrections will be possible by making use of the species and temperature measurements provided by the Raman measurements. We are currently in the process of extending our fluorescence measurements to include CH.

Journal Publications

1. M. D. Smooke and M. B. Long, "Computational and Experimental Study of a Laminar Axisymmetric Methane-Air Diffusion Flame," *Twenty-Third Symposium International on Combustion*, (1991).

2. M. D. Smooke and V. Giovangigli, "Extinction of Tubular Premixed Laminar Flames with Complex Chemistry," *Twenty-Third Symposium International on Combustion*, (1991).

3. M. D. Smooke, J. Crump, K. Seshadri and V. Giovangigli, "Comparison Between Numerical Calculations and Experimental Measurements of the Structure of Diluted Methane Air Premixed Flames," *Twenty-Third Symposium International on Combustion*, (1991).

Other Publications

1. M. D. Smooke and V. Giovangigli, "Numerical Modeling of Axisymmetric Laminar Diffusion Flames," to be published *Impact of Computing in Sci. and Eng.*, (1991).

2. Y. Xu and M. D. Smooke, "Application of a Primitive Variable Newton's Method for the Calculation of Axisymmetric Laminar Diffusion Flames," submitted to *J. Comp. Phys.*, (1991).

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