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Computations of Enhanced Soot Production in Flickering Diffusion Flames

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ABSTRACT

Recent experimental measurements of soot volume fraction in a flickering CH_4/air diffusion flame show that for conditions in which the tip of the flame is clipped, soot production is ~5 times greater than that measured for a steady flame burning with the same mean fuel flow velocity. Numerical simulations of both steady and time-varying flickering CH_4/air diffusion flames are used to examine the differences in combustion conditions which lead to this observed enhancement in soot production in the flickering flames. These simulations successfully predict that the maximum soot concentration increases by over four times compared to the steady flame and show that flickering flames exhibit much longer residence times during which the local temperatures and stoichiometries are favorable for soot production.

I. INTRODUCTION

Time-varying diffusion flames exhibit a much broader range of combustion conditions than those observed in steady flames. Investigation of different combinations of residence time, temperature history, local stoichiometry, and strain and scalar dissipation rates can provide new insights into the chemistry-flowfield interactions relevant to practical turbulent combustion conditions. Recent quantitative experimental measurements of the local soot volume fraction in a flickering CH_4/air flame show that for a forcing condition in which the tip of the flame is clipped, the peak local soot volume fraction is 5-6 times greater than that measured for a steady flame burning with the same mean fuel flow velocity [1]. Direct numerical simulations of steady and flickering CH_4/air diffusion flames have been conducted to (a) quantitatively compare experimental soot volume fraction and temperature results for a steady CH_4/air flame with predictions using the integrated soot model of Syed, Stewart and Moss [2], (b) compare experimental measurements and computations of the soot volume fraction in the flickering flames, and (c) elucidate the changes in residence time, temperature, and mixture fraction which lead to the enhanced soot production observed in the flickering flames.

II. NUMERICAL METHOD

The numerical model solves the two-dimensional, time-dependent, reactive-flow Navier-Stokes equations coupled with sub-models for soot formation and radiation transport. The fluid convection [3] and diffusive transport sub-models are the same as those published previously [4], however, this model uses different chemical reaction and soot formation sub-models. The fuel consumption rate is expressed in terms of Bilger's [5] formulation

$$\omega_{CH_4} = - \rho D (\nabla\xi)^2 (d^2Y_{CH_4}/d\xi^2) ,$$

where ρ is the fluid density, and $D = 1.786\text{x}10^{-5}T^{1.662}$ [6]. Mixture fraction is expressed in the form, $\xi = (\beta - \beta_2)/(\beta_1 - \beta_2)$, where β is a weighted summation of atomic fractions [7]. The resulting production and consumption rates of CO_2, H_2O, and O_2 are then evaluated from their respective stoichiometric coefficients, while the amount of heat released is based on the amount of CH_4 depleted times ΔH_{comb}.

The soot volume fraction and number density are computed as a function of the local gas properties, based upon the simplified rate expressions of Syed et al. [2] developed from measurements in steady CH_4/air flames:

$$\frac{dn_d}{dt} = C_\alpha N_o \rho^2 T^{1/2} \chi_{fuel} e^{-T_a/T} - \frac{C_\beta}{N_o} T^{1/2} n_d^2 - \frac{(36\pi)^{1/3} W_{NSC} n_d^{4/3}}{\rho_{soot} f_v^{1/3}}$$

$$\frac{df_v}{dt} = \frac{C_\gamma}{\rho_{soot}^{1/3}} \rho T^{1/2} \chi_{fuel} e^{-T_\gamma/T} f_v^{2/3} n_d^{1/3} + \frac{C_\delta}{\rho_{soot}} C_\alpha \rho^2 T^{1/2} \chi_{fuel} e^{-T_a/T} - \frac{(36\pi)^{1/3} W_{NSC} n_d^{1/3} f_v^{2/3}}{\rho_{soot}}$$

The third term on the right-hand side of each equation represents an oxidation term, based on the Nagle and Strickland-Constable [8] rate of oxidation. Radiation transport is based on an optically-thin assumption, and absorption coefficients are calculated as a function of soot volume fraction, temperature, and mole fractions of CO_2 and H_2O.

III. RESULTS AND DISCUSSION

Steady Methane/Air Flame

The experiments and computations are based on an axisymmetric CH_4/air diffusion flame with a fuel tube diameter of 1.11 cm, an air annulus diameter of 10.2 cm, and with CH_4 and air velocities of 7.9 cm/s. Local soot volume fractions have been measured using tomographic reconstruction of extinction data obtained at 632.8 nm as well as laser-induced incandescence images (LII), with the LII method providing superior results [1]. Temperatures have been obtained from radiation-corrected thermocouple data [9]. Figure 1 shows the experimental configuration for two-dimensional imaging measurements, and Fig. 2 presents images of OH laser-induced fluorescence (marking the high-temperature reaction zone) as well as scattering from soot particles.

Comparisons between experimental and computed profiles of temperature in the steady flame show good agreement at mid-flame heights, with significant differences occurring at low and high

axial locations. Soot volume fraction comparisons between the computations and experiments show good agreement for the radial location and shape of the soot profiles, and excellent quantitative agreement for the peak concentration (within 10%) at heights of 50 to 70 mm.

Flickering Methane/Air Flame

Experimentally the methane fuel velocity was modulated by applying a variable amplitude sine wave at 10 Hz to the loudspeaker attached to the fuel plenum (Fig. 1); the mean air and fuel flow velocity were the same as the steady flame conditions (7.9 cm/s). Computational simulation of this acoustic forcing is achieved by subjecting the inflow velocity to a 10 Hz sinusoidal function. Amplitudes corresponding to 25%, 50% and 75% of the mean flow velocity have been examined, with the 50% and 75% conditions giving good qualitative agreement with the experimental flame dynamics. Figure 3 shows computed images of soot volume fraction for the 50% amplitude case. The shapes of the simulated and experimental flames are similar, and both exhibit tip clipping. The simulations correctly predict increased soot volume fractions in the clipped portions of the flickering flames, ~ 4 times greater than that for the steady flame burning with the same mean fuel flow velocity.

Pathline comparisons (Fig. 4) have been made for the soot production rates, temperatures, and local equivalence ratios as a function of residence time in the steady versus flickering flames. Pathlines were obtained by following the history of a fluid parcel which travels through the maximum sooting region in each flickering flame. These results reveal that soot inception and growth occur later in the flickering flames and extend over significantly longer residence times during which favorable temperatures and stoichiometries exist for growth. The pathlines also suggest that soot inception occurs later and at slightly higher temperatures and under leaner conditions in the flickering flames.

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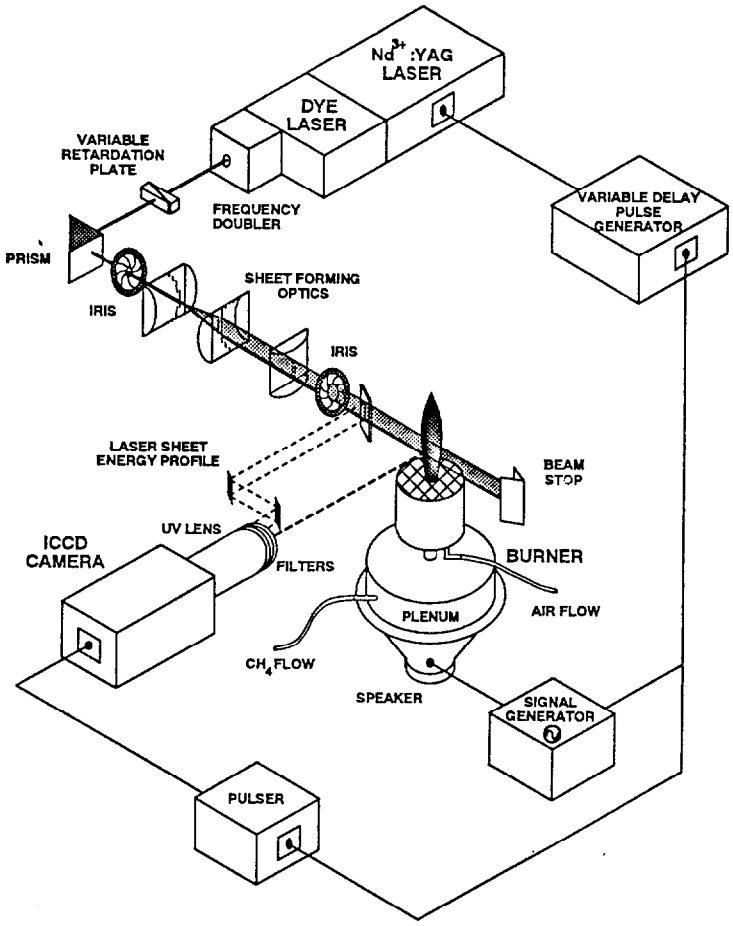

Figure 1. Experimental set-up for 2-D imaging of axisymmetric diffusion flames which are acoustically excited and phase-locked to the pulsed dye laser system operating at 10 Hz. Images are recorded using an intensified charge-coupled device (ICCD) camera.

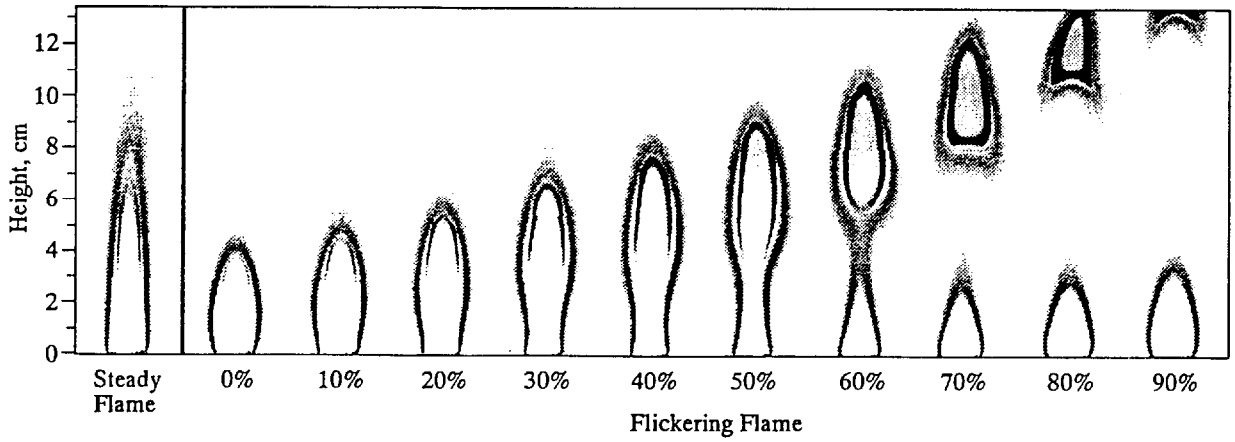

Figure 2. Laser energy-corrected OH· laser-induced fluorescence and soot scattering images in a steady and time-varying laminar CH_4/air diffusion flame using horizontally polarized light at 283.55 nm. The OH· fluorescence signals surround the intense scattering from the soot particles and serve as a convenient marker of the high-temperature reaction zone. The visible height of the steady flame is 79 mm above the fuel tube exit. Ten phase increments separated by 10 ms are shown with an arbitrary zero phase.

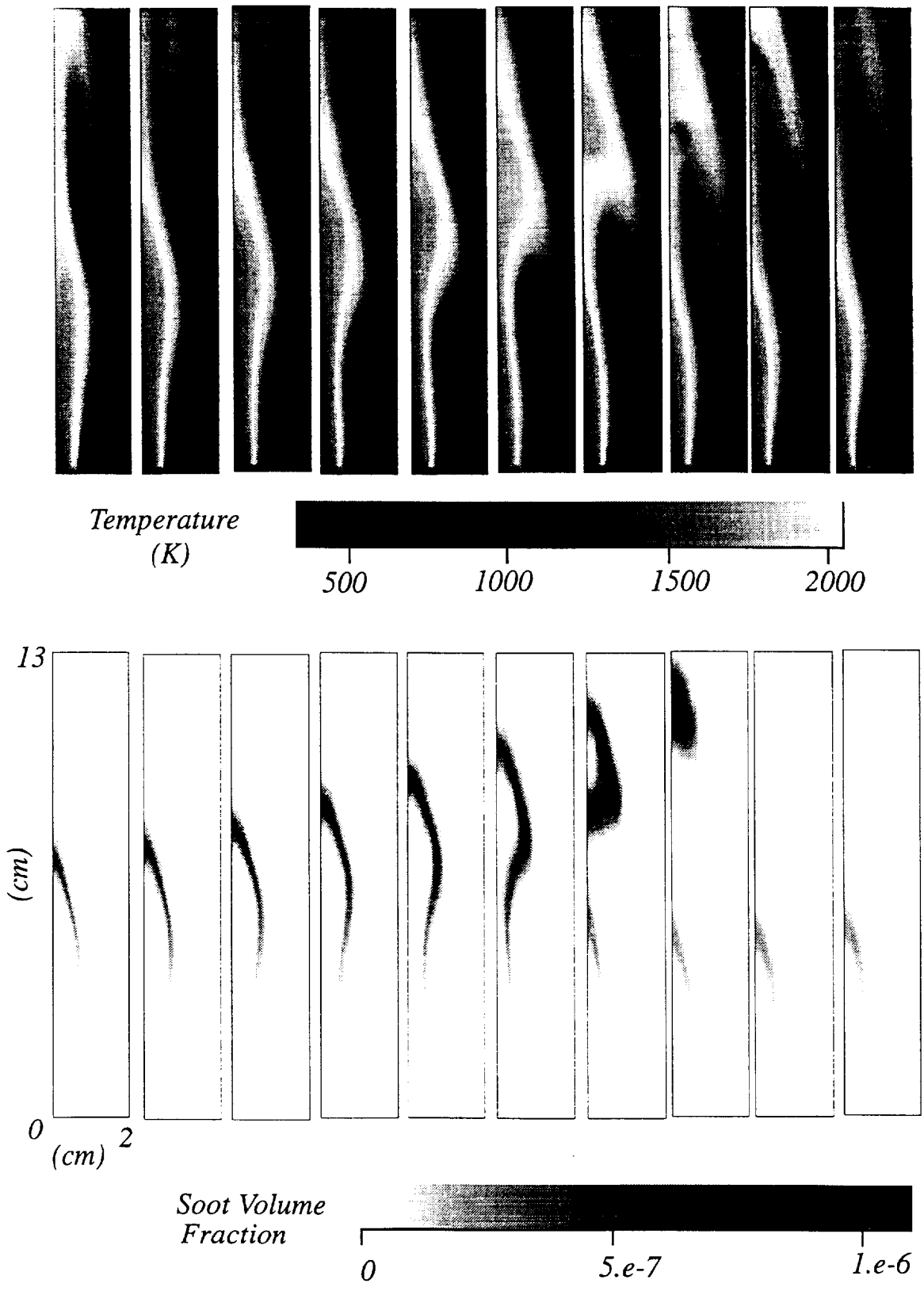

Fig. 3. Temperature and soot volume fraction computations for the flickering CH_4/air diffusion flame (50% amplitude). The time interval between frames is 10 ms.

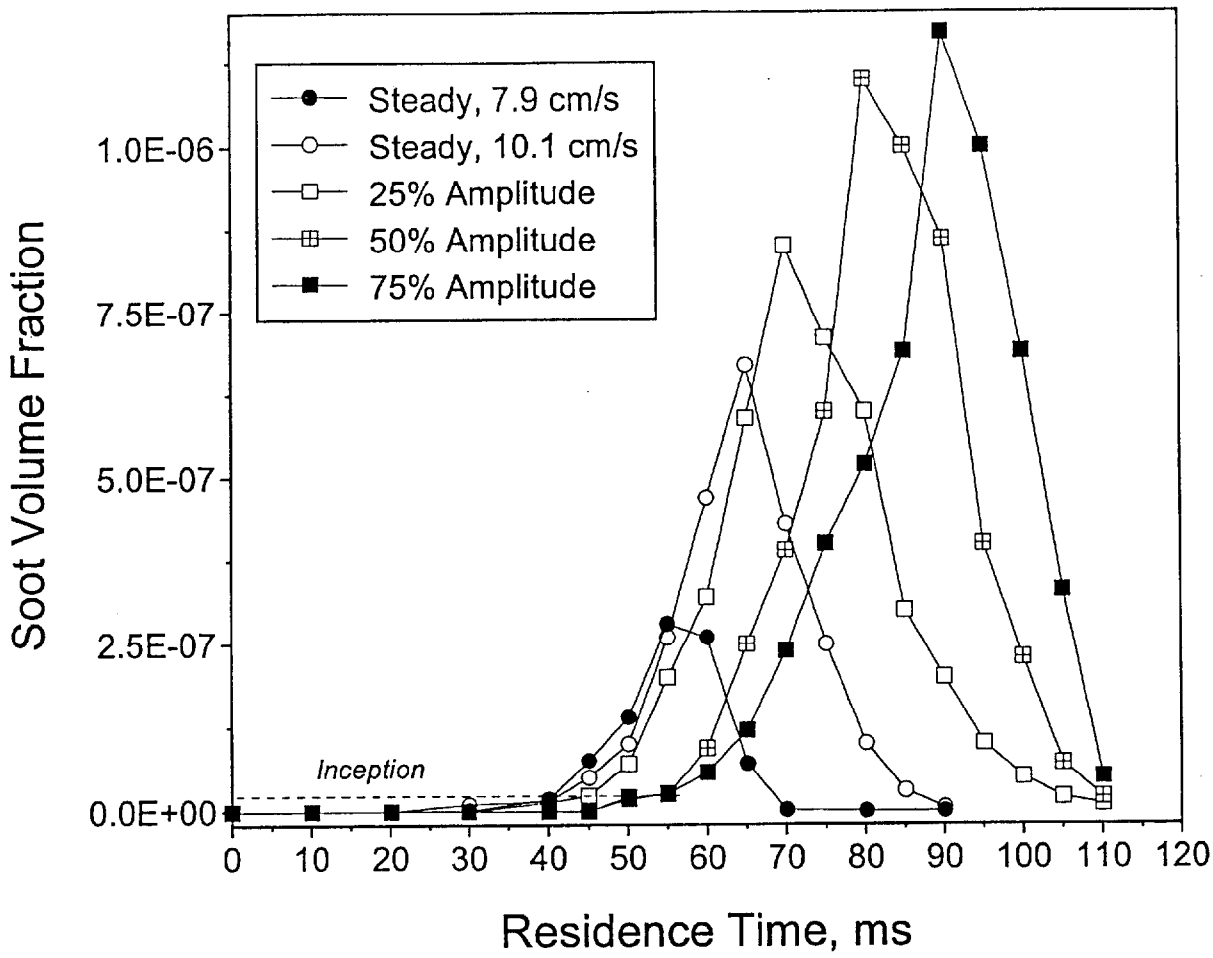

Fig. 4. Pathlines of computed soot volume fraction for two steady flame conditions and three flickering flames where the forcing amplitude of the fuel flow has been varied.

Discussion

Henri Mitler: I'm a little confused about the oxidation reaction. You said that in the model, O_2 is the principle oxidizer. I had the impression that it's the hydroxyl radical that does the damage.

Kermit Smyth: This is a very good point, in fact, I've done work that suggests that OH is the predominant oxidizer in this simple laminar diffusion flame. What we think is happening is that the Negel Strickland Constable rate overestimates soot oxidation at temperatures above 1800 K, and we have compensating errors here.

Patrick Pagni: I am very excited about your laser measurements. How do you know that the laser does not influence the size of the particles?

Kermit Smyth: In fact, the laser induced incandescence method is very likely to perturb the particle field, so repeat measurements on the same soot particles cannot be carried out with confidence. But if you're not doing that, which is certainly true here, one can make proper calibrations and get very good measurements.