

SOOT KINETICS/RADIATION INTERACTIONS IN METHANE/AIR DIFFUSION FLAMES

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Introduction

Radiation heat transfer from flames depends on the instantaneous soot volume fractions and temperatures. The major obstacle to obtaining accurate soot volume fraction predictions in flames is the strong coupling between the finite rate kinetics of soot processes and radiation [1,2]. Detailed models of soot kinetics cannot be incorporated in turbulent flame studies due to the limitations of computer resources. Therefore, many studies have concentrated on simplified global kinetics models incorporating soot nucleation, growth and oxidation mechanisms[3,4]. The local temperatures needed for the soot kinetics calculations were obtained using simplified global radiation models. However, in strongly radiating flames it has been shown that the radiation and soot kinetics calculations need to be coupled to accurately predict observed soot volume fractions[2]. The degree of this coupling in weakly radiating flames, where radiation is predominantly from gas species molecules rather than soot, has not been studied. The objective of the present work is evaluate this coupling of radiation and soot kinetics in weakly radiating flames by using the simplified soot kinetics model of Ref. [4] along with a narrow-band radiation model [5].

Theoretical Methods

The parabolic boundary layer equations for an axisymmetric laminar reacting flow [6] are:

$$\frac{\partial}{\partial x}(\rho u \Phi) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v \Phi) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu}{\sigma_{\Phi}} \frac{\partial \Phi}{\partial r} \right) + S_{\Phi} \quad (1)$$

where Φ represents velocity, mixture fraction, enthalpy, soot mass fraction and soot particle number density respectively. ρ is the density, μ is the viscosity, σ_{Φ} are the Prandtl/Schmidt numbers, and S_{Φ} are the source terms [2]. x and r are the streamwise and radial co-ordinates and u and v are the streamwise and radial velocities. The source term for the soot mass fraction equation includes soot oxidation due to O_2 [4] and OH [3]. The concentrations of major gas species are obtained from generalized state relationships and that of OH and C_2H_2 from Ref. [7]. The radiation source term was solved using a multi-ray method [2] in conjunction with the RADCAL program of Ref. [5].

Results and Discussion

The efficacy of the calculation procedure has been evaluated previously by application to strongly radiating acetylene/air diffusion flames[2]. The details of the coupling between radiation and finite rate soot kinetics in weakly radiation flames are highlighted in the present work. Figure 1 shows radial profiles at three representative axial locations in a methane/air laminar diffusion flame. The calculated stoichiometric flame height was 170 mm. Close to the burner exit, at a height of 50 mm, soot formation from acetylene molecules takes place due to the rich stoichiometry. This is close to the region of peak soot volume fractions and the local radiative fraction is around 8% at the center-line. Higher up, the soot oxidizes primarily due to reaction with the OH radicals and at a height of 100 mm, the soot levels are a factor of 10 lower. Radiative heat loss fraction, primarily due to contributions from the gas molecules has increased to around 10% and at an axial location of 160 mm, almost all the soot has oxidized with the radiative fraction reaching approximately 20% locally. Therefore, there is substantial variation in local radiative fractions and soot volume fractions over the entire flame.

Fig. 2. shows the effect of the variation in local radiative fraction on the soot volume fractions. The variation of peak soot volume fraction with axial distance is shown for four different calculations. The first calculation shown by the solid line is the fully coupled calculations including OH oxidation. The soot levels increase to about 0.07 ppm and then decrease rapidly to very low values due to OH oxidation at around two-thirds the flame height. The second calculations shown by the long dashed lines are fully coupled calculations neglecting OH oxidation. The soot levels rises to about 0.11 ppm and then decrease very slowly with soot being emitted from the tip of the flame contrary to experimental observations, highlighting the importance of OH oxidation. The last two calculations shown by the short dashed line and the dotted line assume a fixed radiation heat loss of 20% and 5% respectively. If a value of 20%, which has been observed experimentally, is used, the peak soot volume fraction reaches only about 0.03 ppm and oxidation is much slower. This is due to lower temperatures restricting both soot growth and oxidation. To match the peak observed in the fully coupled calculations an unrealistically low value of 5% radiative fraction has to be used. This causes oxidation to more rapid, and the lack of coupling makes the growth slower as seen in Fig. 2.

Fig 3 shows the development of mixture fraction and peak radial radiative fraction as a function of axial distance. Close to the burner, the radiative fraction is zero and increase to around 18% at the flame height. Thereafter, it remains roughly constant at around 19% which is the expected values for laminar methane/air diffusion flames. If oxidation of soot from OH is excluded, there is very little effect on this radiative fraction indicating that radiation is predominantly from gas molecules since the soot levels are vastly different for the two cases.

Conclusion

The coupling of gas band radiation with soot production and oxidation terms is important for correctly predicting soot levels in weakly radiating flames. OH oxidation is primarily responsible for the destruction of soot these flames.

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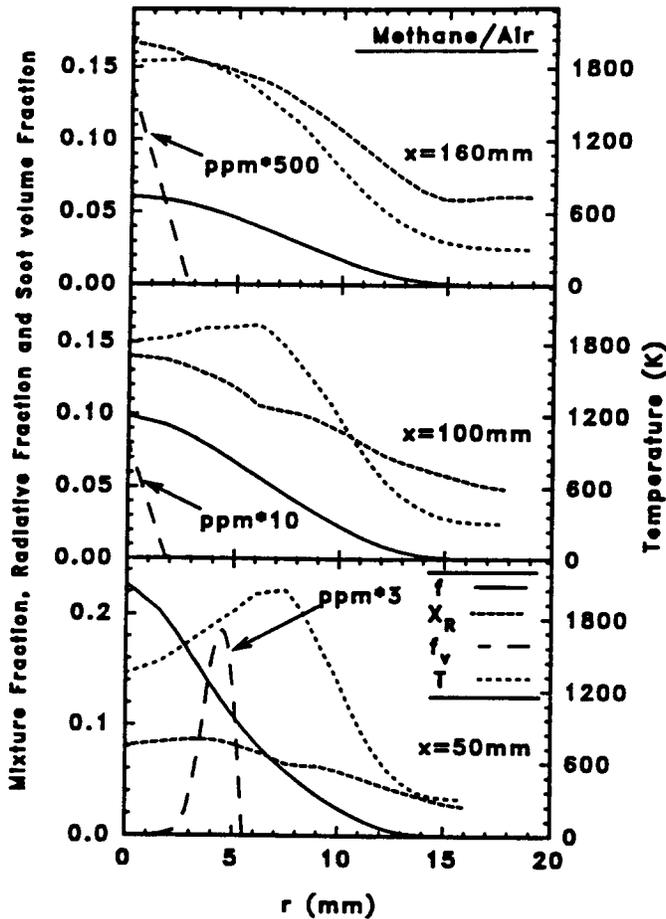


Fig. 1. Radial profiles of soot, mixture fraction, temperature and radiative fraction in a laminar methane/air diffusion flames

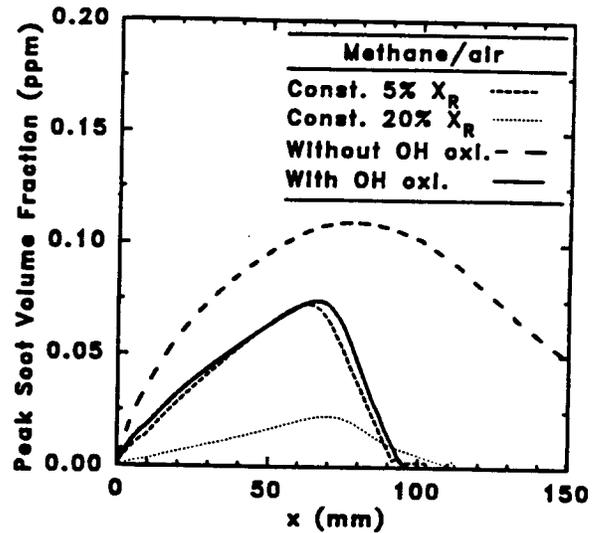


Fig. 2. Axial variation of peak soot volume fractions in a laminar methane/air diffusion flame.

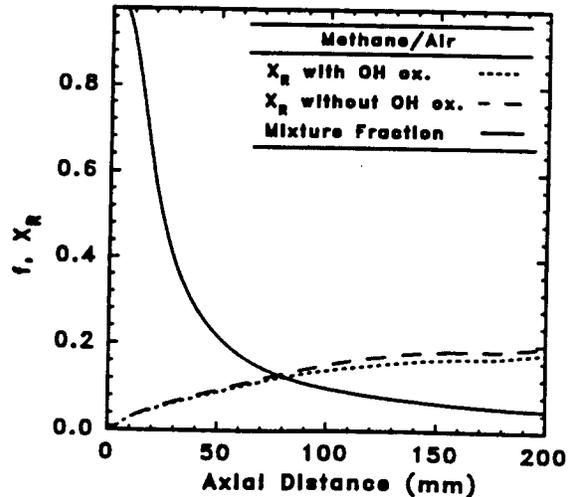


Fig. 3. Axial variation of mixture fraction and radiative fraction in a methane/air diffusion flame.