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Numerical Simulation of a Coflow, Laminar Diffusion C_2H_4 /Air Flame

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Introduction

The growing demands for high fuel efficiency and low pollutant emissions impact the design of combustion devices, and have further motivated a great deal of research interest in modeling multidimensional laminar and turbulent flames. The solution of multidimensional flames requires the calculation of a large system of elliptic governing equations. The governing equations of chemical species in combustion process are strongly coupled with the equations of fluid motion and energy transport. Moreover, these equations are highly nonlinear due to the exponential dependence of the chemical source terms on the temperature. Therefore numerical simulation of multidimensional flames is an extremely challenging problem.

The advances in the development of high speed workstations with massive amounts of memory has enabled combustion scientists to successfully numerically investigate some simple flame configurations with detailed chemistry and complex transport properties, such as the simulation of counterflow and one dimensional flames. The interaction of heat and mass transfer and chemical reaction in practical combustion systems requires the study of multidimensional flames. The two-dimensional axisymmetric laminar diffusion flame is a relatively simple, but very typical, multidimensional flame configuration, for which many experiments have been conducted. In this paper, such a diffusion flame is numerically investigated in consideration of the complex transport and thermal properties. As a first attempt at a multifaceted problem, and for providing better initial conditions for the simulation by a detailed chemistry model, a simplified two-step reaction scheme is used. The fully elliptic problem is treated.

Governing Equations and Numerical Method

The investigated flame is a coflow laminar diffusion flame in which a cylindrical fuel stream is surrounded by a coflowing air jet. In cylindrical coordinates (r, z) , the governing equations are [1]

$$\frac{\partial}{\partial r}(r\rho v) + \frac{\partial}{\partial z}(r\rho u) = 0 \quad (1)$$

$$\begin{aligned} \rho v \frac{\partial u}{\partial r} + \rho u \frac{\partial u}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial u}{\partial r} \right) + 2 \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) \\ - \frac{2}{3} \frac{\partial}{\partial z} \left(\frac{\mu}{r} \frac{\partial}{\partial r} (rv) \right) - \frac{2}{3} \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial v}{\partial z} \right) + \rho g_z \end{aligned} \quad (2)$$

$$\begin{aligned} \rho v \frac{\partial v}{\partial r} + \rho u \frac{\partial v}{\partial z} = -\frac{\partial p}{\partial r} + \frac{\partial}{\partial z} \left(\mu \frac{\partial v}{\partial z} \right) + \frac{2}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial v}{\partial r} \right) \\ - \frac{2}{3} \frac{1}{r} \frac{\partial}{\partial r} \left(\mu \frac{\partial}{\partial r} (rv) \right) - \frac{2}{3} \frac{1}{r} \frac{\partial}{\partial r} \left(r \mu \frac{\partial u}{\partial z} \right) + \frac{\partial}{\partial z} \left(\mu \frac{\partial u}{\partial r} \right) \end{aligned} \quad (3)$$

$$\begin{aligned} c_p \left(\rho v \frac{\partial T}{\partial r} + \rho u \frac{\partial T}{\partial z} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) \\ - \sum_{k=1}^{KK} \left[\rho c_{pk} Y_k \left(V_{kr} \frac{\partial T}{\partial r} + V_{kz} \frac{\partial T}{\partial z} \right) \right] - \sum_{k=1}^{KK} h_k W_k \omega_k + q_r \end{aligned} \quad (4)$$

$$\begin{aligned} \rho v \frac{\partial Y_k}{\partial r} + \rho u \frac{\partial Y_k}{\partial z} = -\frac{1}{r} \frac{\partial}{\partial r} (r \rho Y_k V_{kr}) - \frac{\partial}{\partial z} (\rho Y_k V_{kz}) + W_k \omega_k, \\ k=1,2,\dots, KK \end{aligned} \quad (5)$$

where ρ is the mixture density; W_k the molecular weight of the k^{th} species; λ the mixture thermal conductivity; c_p the specific heat of the mixture under constant pressure; c_{pk} the specific heat of the k^{th} species under constant pressure; ω_k the mole production rate of the k^{th} species per unit volume; h_k the specific enthalpy of the k^{th} species; g_z the gravitational acceleration in the z direction; μ the viscosity of the mixture; Y_k the mass fraction of the k^{th} species; V_{kr} and V_{kz} the diffusion velocities of the k^{th} species in r and z directions; and KK the total species number. The last term on the right side of eq. (4) is the radiation heat loss, which is obtained by an optically thin model [2]

$$q_r = -4k_p \sigma (T^4 - T_0^4) \quad (6)$$

where σ is Stefan-Boltzman constant; k_p is the Planck mean absorption coefficient; T_0 is the ambient temperature. It is assumed that the significant radiating species are CO_2 , CO and H_2O .

The diffusion velocities are written as:

$$V_{kr} = -\frac{1}{Y_k} D_k \frac{\partial Y_k}{\partial r}, \quad k=1,2,\dots, KK \quad (7)$$

$$V_{kz} = -\frac{1}{Y_k} D_k \frac{\partial Y_k}{\partial z}, \quad k=1,2,\dots, KK \quad (8)$$

D_k is related to the binary diffusion coefficients through the relation

$$D_k = \frac{1 - X_k}{\sum_{j \neq k}^{KK} X_j / D_{jk}}, \quad k=1,2,\dots, KK \quad (9)$$

where X_k is the mole fraction of the k^{th} species, and D_{jk} is the binary diffusion coefficient.

In order to ensure the net species diffusion flux to be zero, a correction diffusion velocity is used [3]. The system is closed with the equation of state and appropriate boundary conditions on each side of the computational domain. The SIMPLE numerical scheme [4] is used to solve the governing equations. The diffusion terms in the conservation equations are discretized by the central difference method and the convective terms are discretized by the upwind difference method.

The fuel studied for this coflow diffusion flame is ethylene. A simplified two-step reaction model [5] with six species (C_2H_4 , CO_2 , H_2O , O_2 , N_2 , CO) is used in the simulation.



$$k_{R1} = 2.4 \cdot 10^{12} \cdot \exp(-30/RT) \cdot [\text{C}_2\text{H}_4]^{0.1} \cdot [\text{O}_2]^{1.65} \quad (10)$$

$$k_{R2} = 10^{14.6} \exp(-40/RT) \cdot [\text{CO}] \cdot [\text{H}_2\text{O}]^{0.5} \cdot [\text{O}_2]^{0.25} \quad (11)$$

$$k_{-R2} = 5 \cdot 10^8 \cdot \exp(-40/RT) \cdot [\text{CO}_2] \quad (12)$$

where k_{R1} is the reaction rate of R1, and k_{R2} and k_{-R2} are the forward and backward reaction rates of R2 respectively.

All the thermal and transport properties for these species are obtained from CHEMKIN and TPLIB databases [3,6].

Result and Discussions

Figure 1 shows the simulated flame temperature distribution. Compared to the experimental result obtained by a NRC research group [7], given in Fig. 2, the flame height from the numerical results is similar to that from the experiment and the temperature distribution throughout the flame envelope is reasonable. For both the experiment and the simulation, results show that the maximum temperature contours do not converge on the axis. This is due to the radiation heat loss, as numerical results without radiation heat loss do not present this feature.

It is noted that the calculated temperatures in the upper half of the flame are higher than the experimental results. This difference is likely due to the simplified two-step reaction model. First, the simplified two-step reaction model neglects the existence of some important species and free radicals in the flame, such as H_2 , OH , O and H and others. These species and radicals are normally found to lower the flame temperature. Secondly, although CO is included in the reaction model, the reaction rate of CO to CO_2 may not be appropriate, which results in a lower CO concentration. Fig. 3 presents the calculated CO mass fraction distribution in the laminar diffusion flame. The peak calculated CO concentration of 0.3% is substantially lower than the typical value numerically obtained for a counterflow diffusion flame configuration [8]. This lower CO concentration contributes to a higher flame temperature, as the specific heat for CO is substantially less than for CO_2 and certain amount of heat is released from the combustion of CO .

Figure 4 shows the fuel C_2H_4 mass fraction distribution, and Figures 5 and 6 show CO_2 and H_2O mass fraction distributions, respectively. We note that most of the ethylene is consumed within 1.0 cm of the fuel jet. Large quantity of H_2O is produced soon after the ethylene has been consumed. Carbon dioxide is produced a little further downstream of the water production region

due to the two-step reaction model. Therefore the concentration distributions of these main species are qualitatively reasonable.

Conclusions

The simulation of a coflow laminar diffusion flame by a two-step simplified reaction model and detailed thermal and transport properties can give qualitatively reasonable result for flame height, flame temperature and main species concentration distributions. However, the CO concentration from the simulation is much lower than expected, and the temperature in the upper flame region is higher than the experimental result, which is attributed to the simplified reaction model.

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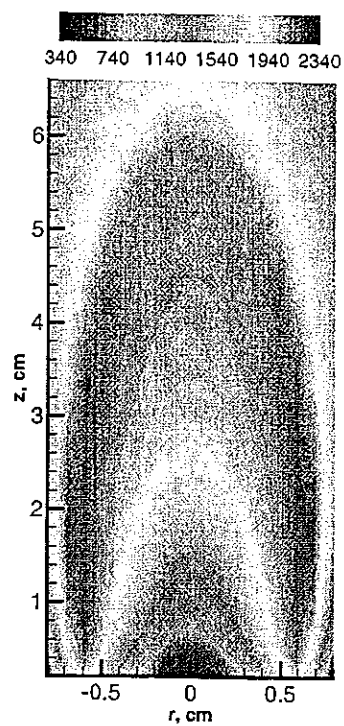


Fig.1 Flame temperature, K
(Simulation)

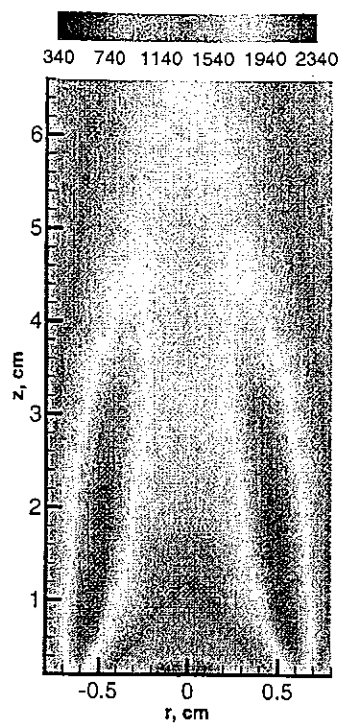


Fig.2 Flame temperature, K
(Experiment)

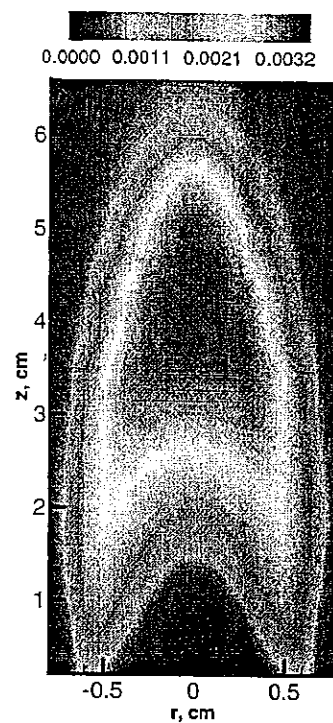


Fig.3 CO mass fraction
(Simulation)

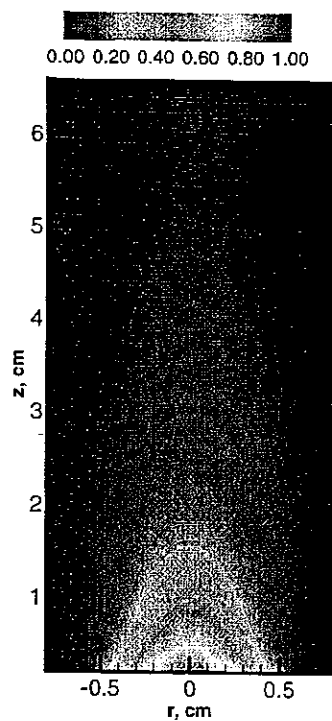


Fig.4 C_2H_4 mass fraction
(Simulation)

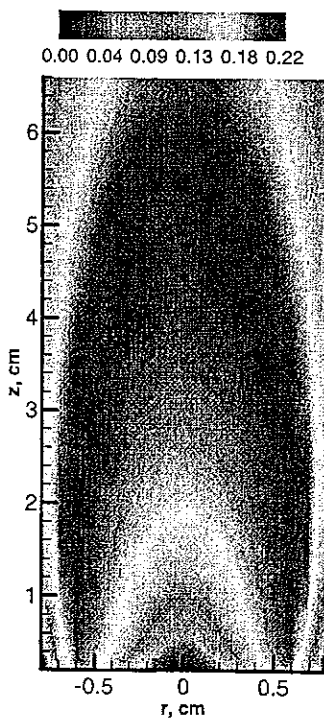


Fig.5 CO_2 mass fraction
(Simulation)

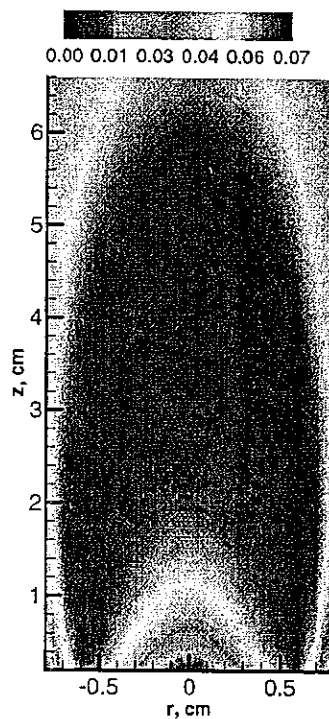
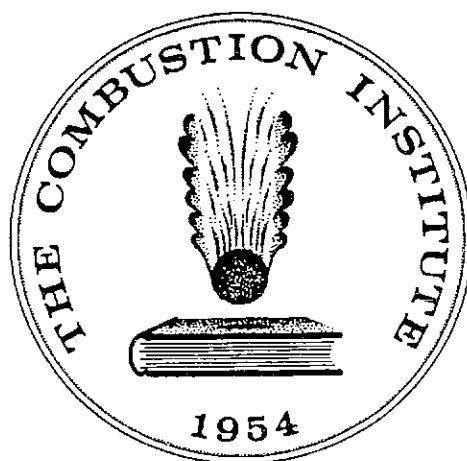


Fig.6 H_2O mass fraction
(Simulation)

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