NUMERICAL SIMULATION OF FLOW AND TEMPERATURE FIELD INDUCED BY COFLOW LAMINAR DIFFUSION FLAMES

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Abstract For an axisymmetric, unconfined coflowing laminar diffusion methane-air flame, the coupling procedure between flow and temperature fields via Boussinesq approximation in the momentum equations is considered in this paper. The projection method is used to solve the flow field equations with the pseudo-momentum equation and energy equations solved by the Douglas-Gunn time splitting method. Instead of considering the detailed chemical reactions and thermal radiation in the flame, we consider thermal buoyancy force as the leading driving force, and use experimental data to construct the thermal source term via a least squares technique, which, in turn, will help us to understand the chemical kinetics of flames.

Key Words coflow laminar diffusion flame, Navier-Stokes equations, Boussinesq approximation, projection method, Douglas-Gunn time splitting.

1. Introduction

It is well known that combustion processes are very complex phenomena which depend upon interrelated processes of fluid mechanics, heat and mass transfer, chemical kinetics, thermodynamics, turbulence, and accompanied by change of phase in some cases. It is nearly impossible to consider the coupling process of all the factors when performing numerical simulations; thus, many calculations have been done in various areas of combustion based on simplifying assumptions. Study of (laminar and turbulent) coflow diffusion flames is an important subject associated with fuel efficiency in industrial burners, and associated resulting air pollution. Moreover, there exists a fundamental curiosity regarding the mechanisms of soot formation, the chemical and physical structures of soot, and its interaction with other physical phenomena. Since Faraday's pioneering work on the chemical history of a candle flame, which was published as early as 1861 [1], extensive (both experimental and theoretical) studies have been conducted on this subject. Yet, our knowledge is still far short of complete understanding of the phenomena.

In this paper, we employ a new method to simulate the flow and temperature field associated with an axisymmetric, unconfined coflowing laminar diffusion flame resulting from combustion of methane in air. The governing equations are the

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Navier-Stokes (N.-S.) equations in the form of the Boussinesq approximation, but with temperature-dependent transport properties. These equations are discretized by standard second-order accurate finite difference methods on a staggered grid, and solved by the projection method in the form described by Gresho [2]. This technique is formally time-accurate, but because of stability of the laminar diffusion flame, it is used as a pseudo-time marching procedure to achieve steady solutions. Pseudo-time steps are computed efficiently by employing Douglas-Gunn time splitting for the momentum and energy equations, and optimal successive overrelaxation (SOR) for the pressure Poisson equation (PPE). To the authors' knowledge, this is the first application of this method to any but model problems in Cartesian coordinates.

But the more important and novel feature of the present study is the construction, via a least squares technique and experimental data, of a heat source term in the thermal energy equation. This source term is, of course, related to the chemical kinetics of the combustion process, and once it is known, it is possible to study the fluid dynamical aspects of the flow without simulating the details of the chemistry.

2. Physical Problem and Governing Equations

2.1 Physical Problem and Coordinate System

Suppose we are going to consider the axisymmetric, unconfined coflowing laminar diffusion methane-air flame (see Figure 1). The fuel comes from the inner tube while the air comes from the outer tube. Outside the outer tube there exists an insulated solid boundary. Thus, we can select the cylindrical polar coordinate system for convenience of representing the problem.

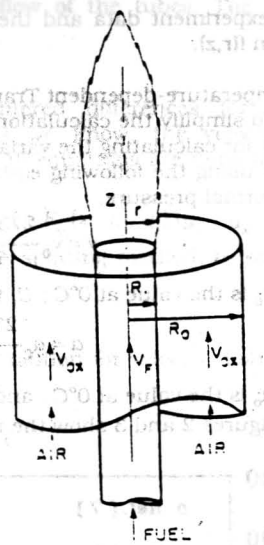


Figure 1. Physical Problem

2.2 Governing Equations

In this preliminary study, we ignore effects of chemical reactions, thermal radiation and concentration induced buoyancy force, and consider only the thermal buoyancy force as the main driving force. We take the gas of the whole region as air; then the governing equations for this problem are the continuity, momentum and energy equations, which can be expressed as follows:

$$\frac{\partial(rV_r)}{r\partial r} + \frac{\partial V_z}{\partial z} = 0 \tag{1}$$

$$\frac{\partial V_r}{\partial t} + \frac{\partial(rV_r^2)}{r\partial r} + \frac{\partial(V_rV_z)}{\partial z} = -\frac{\partial P}{\partial r} + \frac{1}{\mathrm{Re}}\{\frac{2}{r}\frac{\partial}{\partial r}[\lambda(T)r\frac{\partial V_r}{\partial r}] + \frac{\partial}{\partial z}[\lambda(T)(\frac{\partial V_r}{\partial z} + \frac{\partial V_z}{\partial r})] - \frac{2\lambda(T)V_r}{r^2}\} \tag{2}$$

$$\frac{\partial V_z}{\partial t} + \frac{\partial(rV_rV_z)}{r\partial r} + \frac{\partial(V_z^2)}{\partial z} = -\frac{\partial P}{\partial z} + \frac{1}{\mathrm{Re}}\{\frac{1}{r}\frac{\partial}{\partial r}[\lambda(T)r(\frac{\partial V_r}{\partial z} + \frac{\partial V_z}{\partial r})] + \frac{\partial}{\partial z}[2\lambda(T)\frac{\partial V_z}{\partial z}]\} + \frac{Gr}{\mathrm{Re}^2}\theta \tag{3}$$

$$\frac{\partial T}{\partial t} + \frac{\partial(rV_rT)}{r\partial r} + \frac{\partial(V_zT)}{\partial z} = \frac{1}{Pr\mathrm{Re}}[\frac{1}{r}\frac{\partial}{\partial r}(\psi(T)r\frac{\partial T}{\partial r}) + \frac{\partial}{\partial z}[\psi(T)\frac{\partial T}{\partial z}] + \frac{\dot{Q}}{\rho_\infty c_p} \tag{4}$$

where: Re is the Reynolds number, $Re = LV/\nu_0$; Gr is the Grashof number, $Gr = \frac{g\beta(T)L^3(T_0-T_\infty)}{\nu_0^2}$; Pr is the Prandtl number, $Pr = \nu_0/a_0$; θ is nondimensional temperature, $\theta = (T - T_\infty)/(T_0 - T_\infty)$.

The nondimensional kinematic viscosity $\lambda(T) = \nu(T)/\nu_0$ and thermal diffusivity $\psi(T) = a(T)/a_0$ are all temperature-dependent variables.

2.3 Thermal Source $\dot{Q}$

In Eq. (4), there exists a thermal source $\dot{Q}$ which usually depends on chemical reaction and thermal radiation, etc. As we know, the overall chemical reaction equation for the combustion of methane in air is

$$CH_4 + 2O_2 = CO_2 + 2H_2O + \Delta h ,$$

while $\dot{Q} = \Delta h A C_{CH_4} C_{O_2}^2 e^{-\frac{E_0}{RT}}$.

Here, we suppose that $\dot{Q}$ is also a function of position; that is,

$$\dot{Q} = f(r, z)\Delta h A C_{CH_4} C_{O_2}^2 e^{-\frac{E_0}{RT}} . \tag{5}$$

Using experiment data and the least squares technique we attempt to determine the function f(r,z).

2.4 Temperature-dependent Transport Properties

To simplify the calculation of momentum and energy equations, we construct the formula for calculating the variable transport properties as in Ref. [5]. Based on this we suggest using the following equations for kinematic viscosity and thermal diffusivity of air at normal pressure:

$$\nu = \nu_0 \frac{273.15 + C_1}{T + C_1} \left(\frac{T}{273.15}\right)^{2.5} , \tag{6}$$

where ν_0 is the value at 0°C ; C_1 is the constant, $C_1 = 125$; similarly

$$a = a_0 \frac{273.15 + C_2}{T + C_2} \left(\frac{T}{273.15}\right)^{2.4} , \tag{7}$$

where a_0 is the value at 0°C , and C_2 is the constant, $C_2 = 216$

Figures 2 and 3 show the results from above equations and Refs.[6,7]

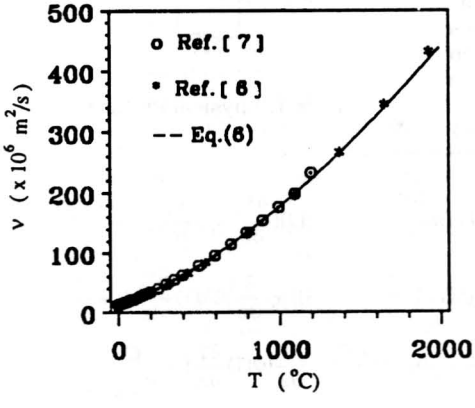


Fig. 2 Kinematic viscosity of air

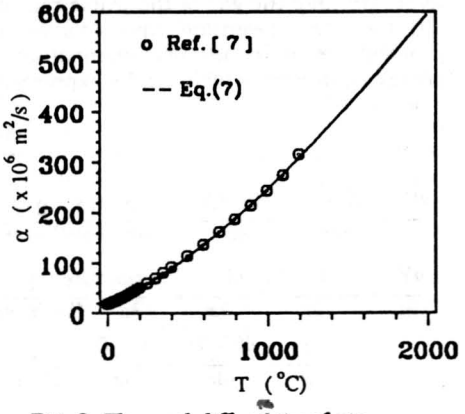


Fig. 3 Thermal diffusivity of air

3. Numerical Analysis

3.1 Computational Domain and Grids

For this axisymmetric diffusion flame problem, we may take a 2-dimensional region in cylindrical coordinates as the computational domain: $0 \le r \le RL, 0 \le z \le ZL$, with the centerline of the flame at r=0, and base of flame at z=0 for flame "type d" in K. Saito et al. [4]. RL and ZL are taken as about 10 times the radius and height of flame. 50×200 grid cells are employed in the present calculation. To avoid checkerboarding of the solution, a staggered grid (cf. [9]) as shown in Fig. 4 has been used.

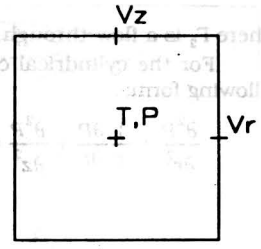


Fig. 4 Staggered Grid

3.2 Boundary Conditions

For r=0, symmetry conditions are used, i.e., $V_r = \partial V_z / \partial r = 0$. The outflow boundary conditions with the form of $\frac{\partial V_\tau}{\partial n} = 0$, $-P + \frac{1}{Re}\frac{\partial V_n}{\partial n} = 0$ are used at r=RL or z=ZL, and at z=0, the velocity distribution is specified for the outflow of the tubes. The no-slip condition is applied at the solid horizontal boundary.

3.3 Quasilinearization and Discretization

The Crank-Nicolson time integration and centered differences for spatial derivatives are used to discretize the equations. As we know, the velocity and temperature are strongly coupled in this problem, and all equations are nonlinear. We linearize them by simply using Taylor expansion, i.e.

$$F(x, y, y_x) = F(x, y, y_x)^* + F_y(x, y, y_x)^*(y - y^*) + F_{y_x}(x, y, y_x)^*(y_x - y_x^*) \qquad (8)$$

so as to use the linear solver, say, Douglas-Gunn time splitting method, to solve the equations.

3.4 Initial Conditions

To make the problem be well-posed, the initial condition for velocity distribution $\mathbf{u}(x, 0) = \mathbf{u}_0(x)$ must satisfy the following conditions:

$$\mathbf{n}\cdot\mathbf{u}_0 = \mathbf{n}\cdot\mathbf{w}(\mathbf{x}, 0) \qquad on \quad \Gamma_1$$

where Γ_1 is a solid boundary moving with velocity $\mathbf{w}$,
and

$$\nabla\cdot\mathbf{u}_0 = 0 \qquad in \quad \overline{\Omega}$$

with $\overline{\Omega}$ being the problem domain plus boundary.

To make solutions of the velocity and pressure be sufficiently smooth the initial pressure distribution should be given by (see [3])

$$\nabla^2 P = \nabla\cdot(\mathbf{f} - \mathbf{u}\cdot\nabla\mathbf{u}) \qquad in \quad \Omega \qquad (9)$$

with concomitant BCs:

$$\frac{\partial P}{\partial n} = \mathbf{n}\cdot(\nu\nabla^2\mathbf{u} + \mathbf{f} - \frac{\partial \mathbf{u}}{\partial t} - \mathbf{u}\cdot\nabla\mathbf{u}) \qquad on \quad \Gamma_1$$

and

$$P = \nu \frac{\partial u_n}{\partial n} - F_n \quad on \quad \Gamma_2,$$

where Γ_2 is a flow-through boundary.

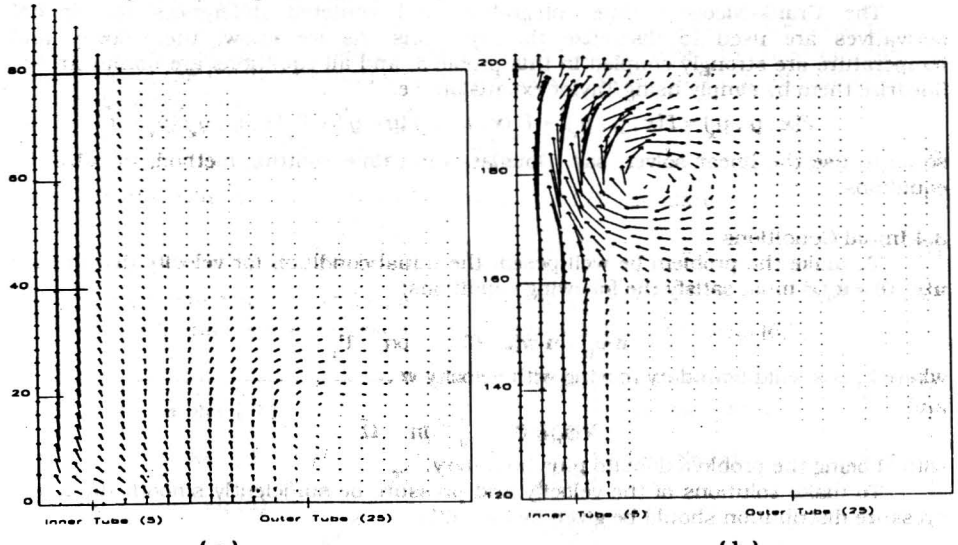
For the cylindrical coordinate system, the pressure poisson equation (8) has the following form:

$$\frac{\partial^2 P}{\partial r^2} + \frac{1}{r}\frac{\partial P}{\partial r} + \frac{\partial^2 P}{\partial z^2} = -\frac{\partial V_r}{\partial r}\cdot\frac{\partial V_r}{\partial r} - \frac{\partial V_z}{\partial z}\cdot\frac{\partial V_z}{\partial z} - 2\frac{\partial V_r}{\partial z}\cdot\frac{\partial V_z}{\partial r} - \frac{V_r^2}{r^2}. \tag{10}$$

4. Results

For the thermal energy equation, we try to use room temperature as the initial distribution and set homogeneous Neumann conditions at boundaries. From Eq. (5) we know that $\dot{Q}$ is very very small at room temperature (this is physically somewhat like a flow without ignition). Thus, we set the temperature at the centerline and base of the flame using experimental data in order to provide thermal energy.

'Projection 2 with OBC' [2] is used to solve the total flow field, leading to automatic satisfaction of the the continuity equation. The poisson equation for the potential is solved via optimal successive overrelaxation, and pseudo-momentum equations, as well as energy equation, are solved by the two-level Douglas-Gunn time splitting method. The resulting linear tridiagonal algebraic systems in each directions are solved by LU-decomposition.



(a) (b)

Fig. 5 Velocity Vector Distribution

From the calculation, we find that there exists a vortex near the flame tip at the beginning of iteration, due to the large temperature gradient there, and it moves upward during iteration. Near the centerline between the vortex and flame tip, the radial velocity is nearly zero. So we can expect that when the vortex moves out of the top outflow boundary (z=ZL), the solution will become steady. But there is a difficulty when the vortex reaches the boundary. Outflow conditions recommended in [2] appear unable to transmit the vortex through the boundary, leading the numerical instability. Nevertheless, the flow field and temperature distribution are physically realistic prior to

this time. Sample results are provided in Figs. 5 and 6. Figures 5(a) and 5(b) show the velocity vector distributions at top and bottom region of the domain near the centerline; the vertical coordinate is grid point index. Figure 6 provides the temperature distribution contour. Of particular interest is the oscillatory temperature distribution in the neighborhood of the vortex.

To implement the least squares technique, we let f in Eq. (5) also be a function of a set of parameters, say $f = f(C_1, C_2, \cdots, C_n, r, z)$. We first choose some guessed values for all the parameters, make a calculation via above procedure, and then adjust them to make

$$S = \sum_{i=1}^{N} (T_{i,cal} - T_{i,exp})^2$$

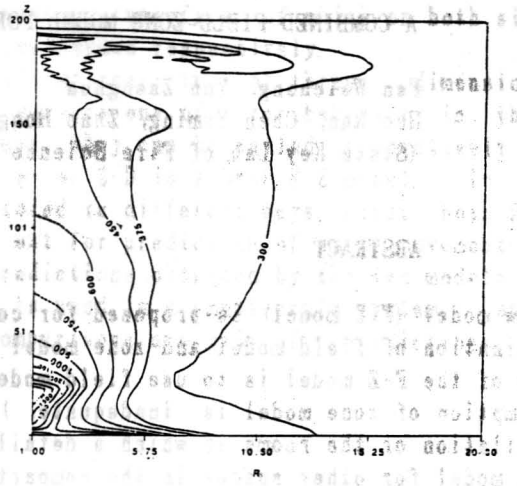


Fig. 6 Temperature Distribution Contour

a minimum. This will provide an effective chemical heat source distribution from which we expect to derive information on the nature of the chemical kinetics of the system.

5. Acknowledgements

This work was supported in part by USEPA under the grant # 1D1155NAEX and by NIST under grant # 60NANB1D1142.

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