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Computation of Swirling Turbulent Diffusion Flames with a Finite-Element Method

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ABSTRACT

This paper presents a numerical algorithm for simulating turbulent combusting flows with strong swirling. The numerical scheme is in Finite-Element formulation. A hybrid approach of the TEACH type algorithm and the Artificial-Compressibility method is used to solve the Navier-Stokes equation and the continuity equation. The continuity equation is derived through a second-order Taylor series expansion. The fluid is assumed to be ideal gas. The turbulence effect is approximated by a RNG based $k-\epsilon$ two-equation model. All the governing equations are solved sequentially in a segregated manner. The numerical method is used to predict a swirling turbulent diffusion flame inside an axi-symmetric burner. The calculated results are compared with experiment data.

INTRODUCTION

Turbulent diffusion flames are nonpremixed combustion processes that are extremely complex, and often, are not well understood. Demands for increased combustion efficiency and decreased pollutant emissions have led to the need for improved methods of prediction for turbulent flows with combustion. Computational fluid dynamics (CFD) has been widely applied to the prediction of isothermal swirling turbulent flows. Though many issues still remain to be addressed, especially with regards to the modelling of turbulence in these complex flows, many researchers have adopted and modified CFD techniques to calculate turbulent flows with combustion. In this paper, we will present our research effort in modelling turbulent diffusion flames. The objective is to predict turbulent combusting flows with strong swirling. The numerical scheme is formulated in Galerkin Finite-Element approach. The combustion is assumed to be mixing-controlled. A conventional Eddy-Dissipation combustion model is used to simulate the combustion process. This method has been developed as a module for the finite-element package *Fastflo*.

GOVERNING EQUATIONS

The governing equations of the turbulent non-premixed combusting gaseous flows consist of the Favre-averaged equations of conservation, the equations derived from the turbulence model and equations from the combustion model. For generality, we present the governing equations in Cartesian tensor notation.

MEAN FLOW CONSERVATION EQUATIONS

To have a robust algorithm for predicting the complex swirling turbulent diffusion flames, we will rearrange the momentum and continuity equations slightly. Assuming that all variables are known at time t (corresponding to iteration n), we try to obtain solution at the next time step $t+dt$ (corresponding to the $n+1$ iteration).

From the continuity equation and the equation of state, after some rearrangement, we have the vector momentum equation in such a form:

$$\rho\frac{\partial \mathbf{V}}{\partial t} + (\rho\mathbf{V}\cdot\nabla)\mathbf{V} - M^2\nabla[RT\nabla\cdot(\rho\mathbf{V})]dt - \nabla\cdot[\mu_t(\nabla\mathbf{V}+\nabla\mathbf{V}^T)] = -\nabla P \quad (1)$$

the vector velocity $\mathbf{V}$ has its component U_i in the i coordinate direction, ρ represents the density of the gaseous mixture, and P is the pressure. The turbulent viscosity μ_t will be defined later by a $k-\epsilon$ turbulence model. M is the typical Mach number of the flow. M^2 is used as a scaling factor to eliminate the acoustic effect within the momentum equation.

Through a Taylor series expansion in time, and from the continuity equation, we can derive the equation for the pressure correction:

$$\frac{dP^{n+1}}{R \cdot T} - \frac{dt^2}{2} \triangle dP^{n+1} = -dt \cdot \nabla \cdot (\rho \mathbf{V}^{n+1}) \quad (2)$$

Once the $P_{t+dt} = P_t + dP^{n+1}$ is known, the density can be updated through the equation of state:

$$\rho = \frac{P}{R \cdot T} = P/[\overline{R}T \sum_{i=1}^{N} \frac{\overline{Y_i}}{M_i}] \quad (3)$$

$\overline{R}$ is the universal gas constant, M_i is the ith gas component's molecular weight, and $\overline{Y_i}$ is the mass fraction of ith species that satisfies the equation:

$$\rho \frac{\partial \overline{Y_i}}{\partial t} + (\rho \mathbf{V} \cdot \nabla)(\overline{Y_i}) = \nabla \cdot (\frac{\mu_t}{\sigma_y} \nabla \overline{Y_i}) - \overline{\omega_i} \quad (4)$$

In the Eddy-Dissipation combustion model, the energy equation is expressed as an equation for temperature:

$$\rho C_p(T) \frac{\partial T}{\partial t} + \rho C_p(T) \mathbf{V} \cdot \nabla T =$$
$$\nabla \cdot [(C_p(T)\mu_t + \lambda) \nabla T] + \overline{\omega_{fuel}} \cdot h_{react} + Q_{rad} \quad (5)$$

$C_p(T)$ is the sum of all species' specific heat at temperature T. h_{react} is the heat of reaction from the fuel, and $\overline{\omega_i}$ represents the ith species' average reaction rate. Q_{rad} is the heat input from radiation effect to be modelled later.

After boundary conditions have been specified, equations (1), (2), (3),(5), (4) can be solved, sequentially or in a coupled manner, to produce $\mathbf{V}$, P, ρ, T and $\overline{Y_i}$. However, first of all, we need to know the turbulence viscosity μ_t and the reaction rate ω_i.

RNG-BASED $k - \epsilon$ TURBULENCE MODEL

The turbulence model is a two-equation $k-\epsilon$ model based on the Renormalization Group (RNG) analysis (Yakhot et al 1986). The transport equations for the turbulence kinetic energy k and dissipation rate ϵ are:

$$\rho \frac{\partial k}{\partial t} + \rho \mathbf{V} \cdot \nabla k - \nabla \cdot [\alpha \mu_t \nabla k] =$$
$$\mu_t \sum_{i,j} \frac{\partial U_i}{\partial x_j} (\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}) - \rho \epsilon \quad (6)$$

$$\rho \frac{\partial \epsilon}{\partial t} + (\rho \mathbf{V}) \cdot \nabla \epsilon - \nabla \cdot [\alpha \mu_t \nabla \epsilon] =$$
$$C_1 \nu_t \frac{\epsilon}{k} \sum_{i,j} \frac{\partial U_i}{\partial x_j} (\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}) - C_2 \rho \frac{\epsilon^2}{k} - \rho S \quad (7)$$

The total viscosity μ_t is calculated from:

$$\mu_t = \rho \nu_{mol} [1 + (\frac{C_\mu}{\nu_{mol}})^{1/2} \frac{k}{\epsilon^{1/2}}]^2 \quad (8)$$

In this $k - \epsilon$ model, wall-function treatment is not needed for velocities along solid walls.

COMBUSTION MODEL

The Eddy-Dissipation model (Magnussen et al 1976) is adopted here to calculate the average reaction rate:

$$\overline{\omega_i} = A \cdot \rho \cdot S_i \cdot \min[Y_{fuel}, \frac{Y_{O^2}}{S_{O^2}}] \cdot \frac{\epsilon}{k} \quad (9)$$

where the free parameter A is set to 4.0, S_i is the stoichiometric coefficient of the ith species with regard to the fuel in the process of reaction. For one step chemical reaction, only one species' reaction rate needs to be determined, all other reaction rates can be determined through stoichiometric coefficients. Similarly, there is no need to solve all species mass conservation equations (4) except one. We choose to solve the averaged mass conservation equation of the product steam.

$$\rho \frac{\partial \overline{Y_{H_2O}}}{\partial t} + (\rho \mathbf{V} \cdot \nabla)(\overline{Y_{H_2O}}) = \nabla \cdot (\frac{\mu_t}{\sigma_y} \nabla \overline{Y_{H_2O}}) + \overline{\omega_{H_2O}} \quad (10)$$

where $\overline{\omega_{H_2O}}$ is given by (9). We also need to solve the conservation equation for the mean value F of mixture fraction f:

$$\rho \frac{\partial F}{\partial t} + (\rho \mathbf{V} \cdot \nabla) F = \nabla \cdot (\frac{\mu_t}{\sigma_F}) \nabla F \quad (11)$$

Once the mean value F and $\overline{Y_{H_2O}}$ are known, we can determine all other species' mean mass fractions through simple arithmetic.

RADIATIVE HEAT TRANSFER

For the radiation effect, we adopt the P_1 spherical harmonics approximation (Truelove 1990), and the gas is treated as a grey medium. In the P_1 spherical harmonics approximation, the equation for the zero-order radiation intensity I_0 is:

$$\nabla \cdot \frac{1}{K_e^*} \nabla I_0 = 3K_a(I_0 - I_b) \quad (12)$$

Here $I_b = \sigma T^4/\pi$ is the total black-body intensity of the gas at temperature T.

The heat input Q_{rad} from the radiation to the energy equation can be calculated as:

$$Q_{rad} = 4\pi K_a (I_0 - I_b)$$

NUMERICAL SCHEME

The governing equations for velocity, density, pressure, temperature, species mass fraction, and the transport equations for k and ϵ are discretized and solved in the Galerkin finite-element formulation. All the equations are fully coupled with each other, so solving such a large equation system simultaneously

would require extremely large computer memory. In addition, these equations are highly non-linear, which means this equation system has to be solved repeatedly before a converged solution is reached. Here, we will solve the equations sequentially, except that the vector momentum equation is solved with its components fully coupled. For axi-symmetric flow, only the axial and radial velocity components are coupled, while the tangential velocity is solved separately.

The iterative solution procedure for all the equations can be listed in the following 8 steps:

1. $\mathbf{V}^{n+1}$ is obtained by equation (1).
2. Equation (2) is solved to give dP. This leads to obtain density ρ^{n+1} by (3).
3. k^{n+1} is first obtained through (6).
4. Equation (7) then produces ϵ^{n+1}.
5 Total viscosity μ_t is now updated by (8).
6. Equation (11) is solved to give F.
7. $\overline{Y}_{H_2O}^{n+1}$ is produced by equation (10).
8. F^{n+1} and $\overline{Y}_{H_2O}^{n+1}$ are then used to calculate other species' mass fraction $\overline{Y}_i$. Reaction rate is worked out by (9).

NUMERICAL TEST

As an accuracy test of the algorithm presented in this paper, we compare the computed results from the numerical method with experimental data obtained inside an axi-symmetric burner (Sykes et al, 1979). The axi-symmetric burner is a model furnace with swirling natural gas flame inside. The furnace and burner arrangement are illustrated in Fig.1. The incoming air has a large swirl number of $S_w = 0.85$ at the annulus inlet. We choose the radius of burner as the characteristic length, the mean axial velocity $U = 13.7m/s$ at the air annulus inlet is taken as the characteristic velocity. The Reynolds number is $Re = 139081$, the Mach number is $M = 0.047$. Since the flow is axi-symmetric, only half of the axi-symmetric cross-section is considered. The domain is covered by a total of 7765 four-node linear elements.

The computed velocity streamlines are plotted in Fig.2. We can clearly see that in the region close to the fuel inlet, there is a very strong recirculation zone, this is caused by the sudden expansion due to combustion. This recirculation zone is also reported in the experiment. In addition, close to the inlet, there is another large recirculation region that is formed by the geometric expansion. The temperature isothermal contours are plotted in Fig.3. This figure shows a thin high temperature flame sheet extending from the air/fuel inlets. Due to the swirling velocity, this flame sheet is curved toward the outer wall. Along the central axis, the computed temperature is compared with experimental data, as shown in Fig.4. In the region close to the fuel inlet, the computed temperature rises in a slower rate than that of the experiment. This indicates the reaction rate is under-predicted. The free parameter A in the reaction rate equation (9) can be increased to make the computed temperature rise faster. In the present calculation, we have not tried to alter the A value to match experiment, the A is fixed at 4.0, as can be found in some published papers. While downstream from the fuel inlet, the temperature profile from the experiment is predicted satisfactorily, though the computed temperature is slightly higher. Overall, the calculated results agree quite well with the experiment.

CONCLUSION

In this paper, an algorithm for predicting turbulent diffusion flames has been presented. The fluid is assumed to be ideal gas. A RNG based $k-\epsilon$ turbulence model is adopted. The combustion model is a Eddy-Dissipation model. The numerical scheme is implemented in Galerkin finite-element formulation.

This numerical scheme has been used to predict the natural gas flame inside an axi-symmetric furnace. The flame inside the furnace has a strong swirling. The combusting flow is fully turbulent, and large complex recirculating zones exist inside the burner. Given the complex nature of flows associated with turbulence, strong swirling and combustion, the prediction from the numerical method agrees satisfactorily with experiment. The numerical method is able to calculate the velocity and large density variation. The recirculation zone is predicted quite satisfactorily. The temperature distribution is also reproduced well. The numerical test has demonstrated that the algorithm presented here is robust and accurate for swirling turbulent diffusion flames. Further research will be directed at comparing velocity and temperature distribution with detailed measurements.

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REFERENCES

Magnussen B.F. and Hjertager B.W. 1976, On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion, 16th Symposium on Combustion, pp.719-729, The Combustion Institute.

Sykes J. and Truelove J.S. 1979, A Finite Difference Computer Program for Calculating Turbulent and Combusting Fluid Flows, AERE Report No. R 9485, Harwell.

Truelove J.S. 1990, Models for Radiant Heat Transfer in Flash-Smelting Furnaces, Tech. Note $CRL/TN/41/90$, BHP Central Research Lab.

Yakhot V. and Orszag S.A. 1986, Renormalization Group Analysis of Turbulence: 1. Basic Theory, J. Sci. Comput., Vol.1, No.3.

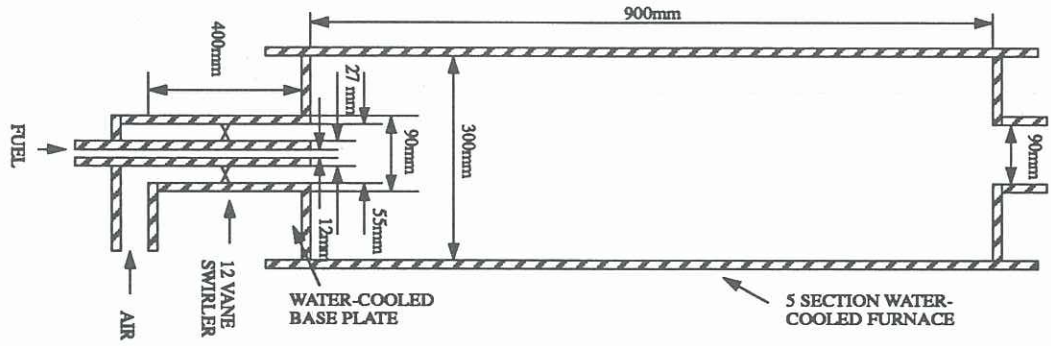

Figure 1: Furnace enclosure and coaxial burner.

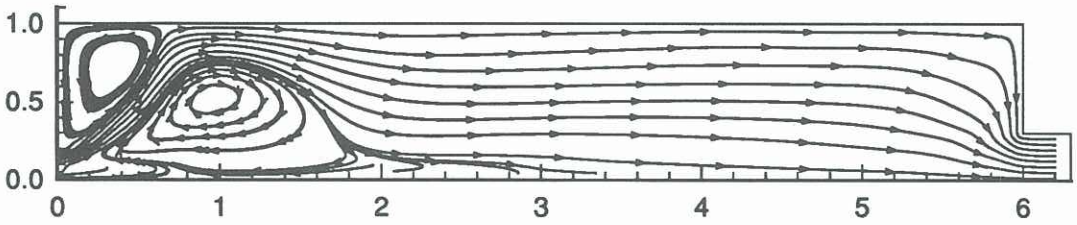

Figure 2: Velocity streamlines.

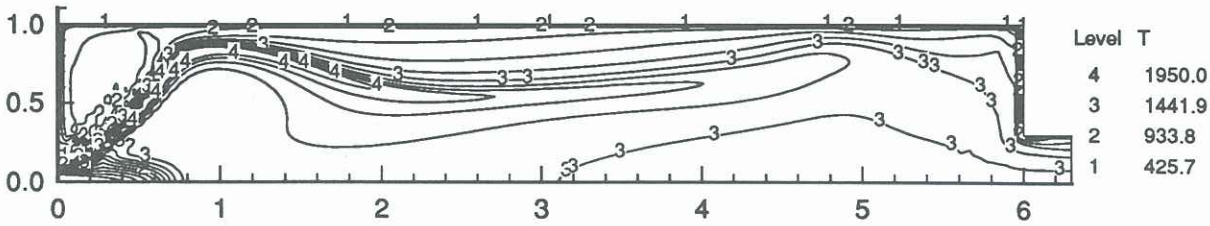

Figure 3: Temperature contour plots.

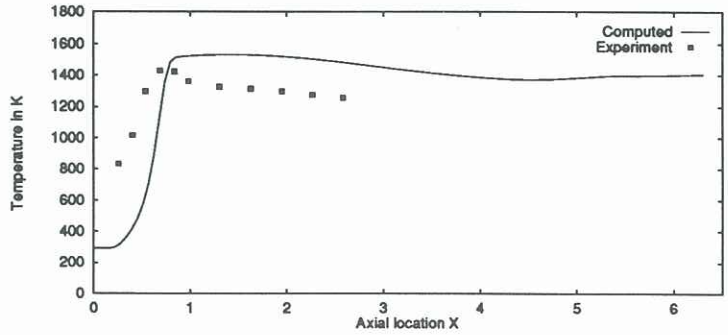

Figure 4: Temperature along the axis.