13th Australasian Fluid Mechanics Conference
Monash University, Melbourne, Australia
13-18 December 1998

Computing Diffusion Flames With Multi-stage Combustion Models

Nick Stokes and Zili Zhu

CSIRO Mathematical & Information Sciences
Clayton, Victoria, AUSTRALIA

ABSTRACT

In this paper, we use two combustion models to simulate swirling turbulent flows with combustion in furnaces. The models are one-step and three-step eddy-dissipation models, and are used to predict a non-premixed diffusion flame in a furnace for which experimental data has been gathered.

The numerical scheme is formulated in Galerkin finite-element approach, and implemented using the FEM package *Fastflo*. Segregated solution procedure is adopted for the governing equation system. Ideal gas model is assumed for the gas mixture. Turbulence effect is modelled by a RNG based $k-\epsilon$ two equation approach.

INTRODUCTION

Numerically simulating fluid flows with combustion requires both turbulence modelling and the modelling of chemical reactive processes. Numerically this is difficult and expensive, but the processes are very important in many industrial sectors, and numerical modelling of such complex processes is a valuable contribution to improving efficiencies of combustion processes.

Combustion processes often have more than 200 reactions, and over 50 species. Reduced global chemical kinetic schemes that are capable of capturing major features of the complex combustion processes are required. Even though reduced global reaction schemes cannot offer very detailed solutions, they can provide important information on combustion processes. In this aspect, they are regarded as practical and efficient tools in many industrial applications. In this paper, we compare two such reduced global kinetic schemes used to predict swirling diffusion flames in furnaces.

Since 1972, there have been a number of modified $k-\epsilon$ turbulence models (Yakhot and Orszag, 1986). The more recent RNG-based $k-\epsilon$ model offers the advantage of having the same form for both low and high Reynolds numbers, and no wall-function is needed for velocities close to solid walls. In this paper, we will use a RNG-based $k-\epsilon$ model to account for turbulence effect. The numerical scheme presented is based on an artificial-compressibility approach, and sequential solution procedure is adopted.

GOVERNING EQUATIONS

The state variables for a turbulent flow with combustion are: the Favre-averaged velocity vector $\mathbf{V}$, pressure P, temperature T, and density ρ, in addition to the mass fraction Y_i of the ith chemical component. Other important variables are turbulent kinetic energy k, dissipation rate ϵ and the chemical reaction rates ω_i of the ith species. The unknowns are then k, ϵ and ω_i.

Mean Flow Momentum Equations

For turbulent gaseous flows, the conservation equation for momentum is the Reynolds-averaged Navier-Stokes equation:

$$\rho\frac{\partial \mathbf{V}}{\partial t}+(\rho\mathbf{V}\cdot\bigtriangledown)\mathbf{V}-\bigtriangledown\cdot[\mu_t(\bigtriangledown\mathbf{V}+\bigtriangledown\mathbf{V}^T)] +\frac{2}{3}\bigtriangledown(\mu_t\bigtriangledown\cdot\mathbf{V})=-\frac{1}{M_a^2}\bigtriangledown P-\frac{2}{3}\bigtriangledown(\rho k) \quad (1)$$

where μ_t is the turbulence total viscosity. M_a^2 is a characteristic Mach number.

The mass conservation law is expressed as a continuity equation:

$$\frac{\partial \rho}{\partial t}+\bigtriangledown\cdot\rho\mathbf{V}=0 \quad (2)$$

The constitutive relationship between density ρ and pressure P is referred to as the equation of state:

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

Here, $\overline{R}$ is the universal gas constant, M_i is the molecular weight of the ith gas component, and $\overline{Y_i}$

is the mass fraction of ith species, which satisfies the mass conservation equation:

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

where $\overline{\omega_i}$ represents the ith species' average reaction rate, and σ_y is the turbulent Schmidt number for Y_i.

Energy Conservation Equation

We also have to solve the conservation equation of energy to obtain temperature. The energy equation is expressed as a conservation equation for enthalpy H:

$$\rho\frac{\partial H}{\partial t}+\rho\mathbf{V}\cdot\nabla H=\nabla\cdot[(\frac{\mu_t}{\sigma_t}+\frac{\lambda}{C_p})\nabla H]+Q_{rad} \quad (5)$$

where λ is the heat conduction coefficient and σ_t is the turbulent Prandtl number, and Q_{rad} is the heat input from the radiation effect to be determined later.

The enthalpy H is related directly to temperature by:

$$H=\int_{T_0}^{T}C_p(T,Y_1,Y_2,\cdots,Y_N)\cdot dT+\sum_i(h_i^0\cdot Y_i) \quad (6)$$

$C_p(T)$ is the sum of all species' specific heat at temperature T. h_i^0 is the enthalpy of formation of the ith species at temperature T_0.

A RNG-based $k-\epsilon$ Turbulence Model

We use a RNG-based $k-\epsilon$ two-equation model (Yakhot and Orszag, 1986) to consider the effect of turbulence on diffusion flames. The transport equation for the turbulent kinetic energy value k is:

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

and the governing equation for the turbulence dissipation rate ϵ is:

$$\rho\frac{\partial\epsilon}{\partial t}+(\rho\mathbf{V})\cdot\nabla\epsilon-\nabla\cdot[\alpha\mu_t\nabla\epsilon]=-\rho S+2C_1\mu_t\frac{\epsilon}{k}\sum_{i,j}\frac{\partial U_i}{\partial x_j}S_{ij}-\frac{2}{3}C_1\rho\epsilon(\nabla\cdot\mathbf{V})-C_2\rho\frac{\epsilon^2}{k} \quad (8)$$

$C_1=1.42$, $C_2=1.68$ and $\alpha=1.39$. The total viscosity μ_t is calculated from:

$$\mu_t = \rho\nu_0[1+(\frac{C_\mu}{\nu_0})^{1/2}\frac{k}{\epsilon^{1/2}}]^2 \quad (9)$$

here, $C_\mu=0.0845$, ν_0 is the molecular kinetic viscosity of the fluid.

TWO COMBUSTION MODELS

Single-step Eddy-dissipation Combustion Model

The one-step global reaction scheme for methane is:

$$CH_4+2O_2-->CO_2+2H_2O$$

The chemical reaction rate can be determined by a eddy-dissipation model (Magnussen and Hjertager, 1976):

$$\overline{\omega_i}=A\cdot\rho\cdot S_i\cdot\min[Y_{CH_4},\frac{Y_{O_2}}{S_{O_2}}]\cdot\frac{\epsilon}{k} \quad (10)$$

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.

Only one reaction rate needs to be determined, and only one averaged mass conservation equation (4) for steam H_2O is solved:

$$\rho\frac{\partial\overline{Y_{H_2O}}}{\partial t}+(\rho\mathbf{V}\cdot\nabla)(\overline{Y_{H_2O}})=\nabla\cdot(\frac{\mu_t}{\sigma_y}\nabla\overline{Y_{H_2O}})+\overline{\omega_{H_2O}} \quad (11)$$

where $\overline{\omega_{H_2O}}$ is determined by (10).

An average mean value of mixture fraction F satisfies the following conservation equation:

$$\rho\frac{\partial F}{\partial t}+(\rho\mathbf{V}\cdot\nabla)F=\nabla\cdot(\frac{\mu_t}{\sigma_F})\nabla F \quad (12)$$

where σ_F is the turbulent Schmidt number for F.

Three-step Eddy-dissipation Combustion Model

The three-step reduced global reaction scheme for methane is (Ha and Zhu 1997):

1. $CH_4+\frac{1}{2}O_2-->CO+2H_2$
2. $CO+\frac{1}{2}O_2<-->CO_2$
3. $H_2+\frac{1}{2}O_2-->H_2O$

For this three-step reaction scheme, the eddy-dissipation reaction rate at each reaction step is determined by:

$$\overline{\omega_i}=A\cdot\rho\cdot\min[Y_{reactant},\frac{Y_{O_2}}{S_{O_2}}]\cdot\frac{\epsilon}{k} \quad (13)$$

For multi-step reaction schemes, the mass fraction Y_i of each species has to be solved one by one by their conservation equation (4). In this case, we need to solve a total of six mass conservation equations (4).

Radiative Heat Transfer The P_1 spherical harmonics approximation (Truelove, 1990) is used, in which the gas is treated as a grey medium, and the zero-order radiation intensity I_0 satisfies:

$$\nabla\cdot\frac{1}{K_e^*}\nabla I_0=3K_a(I_0-I_b) \quad (14)$$

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

For the energy equation (5), the right hand side heat source Q_{rad} from the radiation can thus be calculated as:

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

NUMERICAL METHOD

The Navier-Stokes momentum equation (1), the continuity equation (2) and the equation of state (3) are used to calculate $\mathbf{V}$, P and ρ. The momentum equation is solved separately from the continuity equation and the equation of state.

At the nth iteration, with time step δt, from the continuity equation (2) and the state equation (3), we can derive a separate equation (Zhu, 1994) for the pressure correction δP^{n+1}:

$$\frac{\delta P^{n+1}}{R \cdot T} - \frac{(\delta t)^2}{2} \triangle \delta P^{n+1} = -\delta t \cdot \nabla \cdot (\rho \mathbf{V}^{n+1}) \quad (15)$$

This equation will be used to obtain the pressure $P^{n+1} = P^n + \delta P^{n+1}$.

The governing equations, solved sequentially, are: (1) for velocity, (3) for density, (15) for pressure, (5) for enthalpy, (4) for species mass fraction Y_i, (7) for the turbulent kinetic energy k and (8) for ϵ.

For the three-step combustion model the numerical algorithm is:
(1). $\mathbf{V}^{n+1}$ is obtained by equation (1).
(2). Equation (15) is solved to give δP. This leads to obtain density ρ^{n+1} by (3).
(3). k^{n+1} is first obtained through (7).
(4). Equation (8) then produces ϵ^{n+1}.
(5). Total viscosity μ_t is now updated by (9).
(6). Reaction rate $\overline{\omega_i}$ is calculated by (13).
(7). $\overline{Y}_i^{n+1}$ is computed by equations (4).
(8). Heat input Q_{rad} is calculated by (14).
(9). Enthalpy H is solved by (5).
(10). Temperature is computed by (6).
A local iterative loop is performed for steps (6),(7),(8),(9) and (10) before a global iteration is started for the next time step.

COMPARISON WITH EXPERIMENT DATA

The present method is used to simulate a combustion process in a natural gas fired diffusion flame burner. Swirling air comes into the burner through an annulus while natural gas comes into the combustion chamber through a central injector. Extensive experimental data has been gathered and published by Spadaccini et al, 1976. A schematic of this burner is shown here in Figure 1 where $R_0 = 6.15cm$ and the swirl number is $S_w = 0.3$. Figure 2 gives the temperature results from one and three step combustion models,

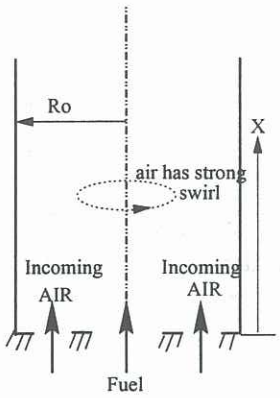
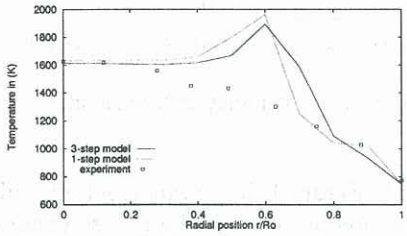
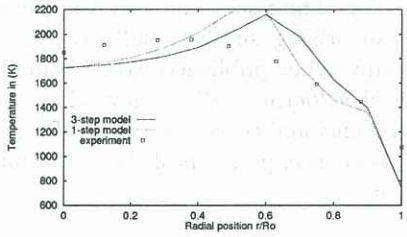


Figure 1: Schematic of the burner.



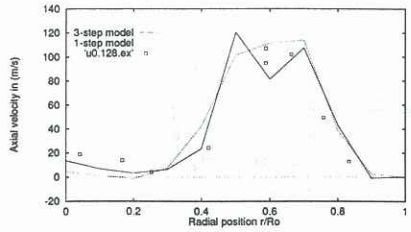
Temperature radial distribution at $X/Ro = 1.2$



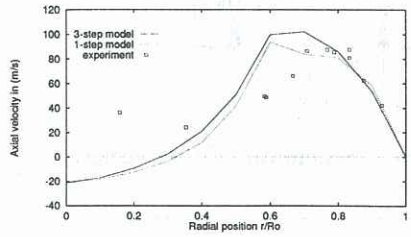
Temperature radial distribution at $X/Ro = 3.98$

Figure 2: Temperature comparison.

these results are presented as temperature radial distributions as compared against experimental data at two axial locations from the air/fuel inlets. From this figure, we can see that the three-step model gives a more accurate solution than the one-step model. However, both models over-predict the temperature around $r/R_0 = 0.6$ which is the combustion front. Figure 3 shows axial velocity distribution at two axial locations. At $X/R_0 = 0.256$, both models agree quite satisfactorily with the experimental data, the three-step model is more accurate than the one-step model for $r/R_0 < 0.3$. For $X/R_0 = 0.972$, both combustion models predict a large flow reversal, while the experimental data shows that there is no flow reversal at all. The discrepancy cannot be explained, as with such strong swirl, there should be strong flow reversal in the central core area close to the fuel inlet. However, it was observed that a very strong unsteady flame exists close to the fuel injector. The tangential velocity results

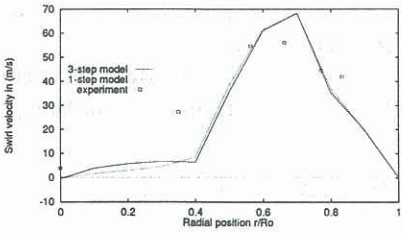


Axial velocity distribution at $X/R0 = 0.256$

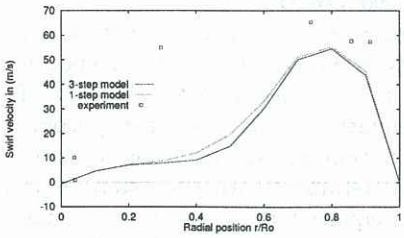


Axial velocity distribution at $X/R0 = 0.972$

Figure 3: Axial velocity comparison.



Swirl velocity distribution at $X/R0 = 0.256$



Swirl velocity distribution at $X/R0 = 0.972$

Figure 4: Tangential velocity comparison.

are presented in Figure 4. The two models give almost identical predictions, and large discrepancy with experimental data can be seen for the results at $X/R_0 = 0.972$. The results for the tangential velocity is not surprising, similar results were documented in many other published work on modelling tangential velocities. We believe that the flow's three-dimensionality is the cause of such discrepancy between experimental data and numerical solutions.

CONCLUSION

In this paper, we have presented a numerical method for predicting diffusion flame in burners. The fluid flow in the burners can have strong swirl. We have implemented the numerical to simulate a natural gas fired axisymmetric burner for which extensive experimental data was gathered. Two combustion models were used to simulate the combustion process, and a RNG-based $k - \epsilon$ model was implemented to account for the turbulence effect. The numerical results from the presented method have been compared with experimental data. The prediction on temperature and axial velocity generally agree well with experimental results, while the tangential velocity prediction has certain discrepancy in regions far away from the fuel injector.

As demonstrated in this paper, the numerical solution can predict main features of complex swirling flows with combustion. The numerical scheme is easy and less expensive to use. It can certainly be used on a daily basis as a practical and efficient tool in the study of combustion processes in industrial burners.

ACKNOWLEDGEMENT

This research work is carried out as part of the development of the general finite-element PDE package *Fastflo*, following earlier work funded by BHP Research.

REFERENCES

YAKHOT, V. and ORSZAG, S.A. "Renormalization Group Analysis of Turbulence: 1. Basic Theory", **J. Sci. Comput.**, Vol.1, No.3, 3-55, 1986.

MAGNUSSEN, B.F. and HJERTAGER, B.W. "On Mathematical Modeling of Turbulent Combustion with Special Emphasis on Soot Formation and Combustion", **16th Symposium on Combustion**, 719-729, The Combustion Institute, 1976.

HA, J. and ZHU, Z. "Simulation of Reactive Flows in Burners", **Int. Conf. on Computational Fluid Dynamics in Mineral & Metal Processing and Power Generation**, Melbourne, Australia, 1997.

Spadaccini, L.J., Owen, F.K. and Bowman, C.T. "Influence of Aerodynamic Phenomena on Pollutant Formation in Combustion", U.S. Dept. of Commerce, Technical Report FB-258 904 EPA-600/2-76-247a, 1976.

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

ZHU, Z. "Artificial-Compressibility Method with Upwinding", **Computational Techniques and Applications: CTAC93**, 502-510, Ed. Stewart, D., Gardner, H. and Singleton, D., World Scientific Publishing, 1994.