18th International Colloquium on the Dynamics of Explosions and Reactive Systems July 29-August 3, 2001, Seattle, USA

MODELLING OF TURBULENT JET FLAMES

W.T. Chan Energy and the Environment, Advantica Technologies Ltd. (A Lattice Group Company), Ashby Road, Loughborough, Leicestershire LE11 3GR, United Kingdom T. J Craft, Y. Zhang Thermodynamics and Fluid Mechanics Division, Mechanical Engineering Department, UMIST, PO Box 88, Manchester M60 1QD, United Kingdom

ABSTRACT

This paper is concerned with the computational modelling of turbulent diffusion flames. The study places particular emphasis on the testing of turbulence models, as many of these have in recent years been widely tested in non-reacting flows, and their strengths and weaknesses in such flows have become reasonably well understood. The performance of both linear and non-linear gradient transport models and second-moment closure (SMC) approaches are investigated. The study highlights the modelling of the stresses and scalar fluxes. It is demonstrated that a turbulence model which resolves the anisotropy of the turbulence could improve the prediction of the spread of the jet flames and flow properties at the outer edge of the flames.

INTRODUCTION

Most popular turbulence models can be classified as gradient transport or second-moment closure models. A gradient transport type of model represents the simplest and is the most widely adopted approach for predicting the turbulent stresses and the scalar fluxes in turbulent flows. It offers great simplicity, robust solution and often leads to reasonable results in simple flow situations. Unfortunately this type of modelling approach does not resolve the anisotropy of the turbulence and does not respond adequately to complex flow situations found in practical combusting flow situations. For this reason a more universal approach, which accounts for at least some of the transport effects of flows, such as second-moment closures (SMCs), has gradually replaced the gradient transport concept (eg. see Lindstedt & Vaos, 1999; Chan & Zhang, 1999). In recent years, various levels of complexity of SMC have been suggested and applied successfully in the computations of some complex non-reacting flows (Jones & Musonge, 1983; Shih & Lumley, 1985; Launder, 1989). On the basis of these, it would certainly appear to be advantageous to apply an advanced model for the prediction of combusting flows.

So far, much effort has been put into the development and application of "pressure-strain correlations" models. The modelling of the "pressure-scalar correlations" (a corresponding process appearing in the scalar flux transport equation), on the other hand, has received limited attention and has not yet been widely applied for predicting combusting flows. One of the reasons for this is the uncertainty of using sophisticated correlations, which may not have been so widely tested, for approximating a turbulent combusting environment. Another important issue is the computing cost. Due to these factors, a non-linear gradient transport model (Craft et al, 1996) is also investigated in the present study.

MATHEMATICAL DESCRIPTIONS

The numerical computations are generated with a finite volume elliptic solver, using a version of the UMIST code TEAM (Huang & Leschziner, 1983). All governing equations are written in density-weighted form. To obtain the discretized equations, the QUICK scheme (Leonard, 1979) is employed for the convection of mean velocities and mixture fraction and PLDS (Patankar, 1980) is used for the convection of turbulence quantities. A reasonably fine mesh is used in the present computations in order to prevent false diffusion. SIMPLE (Patankar, 1980) is used in the pressure correction algorithm.

Overall four turbulence modelling approaches are employed. They are a linear EVMs (Launder & Sharma, 1974), a linear SMC (based on the work of Rotta, 1951; Naot et al, 1970; Monin, 1965; Owen, 1973) and a non-linear SMC (Craft & Launder, 1996). An attempt has been made to extend the earlier non-reacting flow studies at UMIST to improve the ε equation by making $c_{\varepsilon 2}$ sensitive to the anisotropy invariants A_2 and A and adding an extra source term dependent on the mean strain. This modification is given in Equation 1. The full details of model descriptions can be found in the recent study of Chan (2000) and therefore are not presented here.

$$\frac{d\varepsilon}{dt} = \frac{\varepsilon^2}{k} \left[-\frac{1.80}{\left(1 + 1.54A_2^{0.5}A\right)} + 0.4 \left\{ \frac{P}{\varepsilon} + \frac{V_l}{\varepsilon} \left(\frac{\partial U_l}{\partial x_k} \right)^2 \right\}^2 + d_{\varepsilon} - \overline{u_k''} \frac{\varepsilon}{k} \frac{\partial \overline{P}}{\partial x_k}$$
(1)

To focus on the turbulence modelling aspects, and minimise the complexity of the present study, the "conserved scalar" approach is applied to describe the combustion process. A presumed β -PDF and strained laminar flamelet models using detailed chemistry for methane-air combustion have been employed. The laminar counterflow diffusion flame calculation results, with skeletal kinetic mechanisms (Smooke & Giovangigli, 1991), involving 35 elementary reactions, performed by Peeters (1995), have been used for the present natural gas jet flame calculations. The calculation was performed at a strain rate of 100s⁻¹ and a laminar flame velocity of 0.5ms⁻¹. No radiation was included and the Tsuji-geometry (Tsuji, 1982) was used.

In the present work, an attempt was made to include model for the local extinction of flames. A stretched laminar flamelet model was used and is based on the work of Liew et al (1984). Since this does not introduce any additional variables, the simplicity of the present modelling approach is retained. The time-dependent calculations of the scalar dissipation rate by Liew et al (1984) suggested that the criterion of quenching is $40s^{-1}$ for methane-air flames. However, a lower quenching limit of $15s^{-1}$ has been used.

GEOMETRY AND BOUNDARY CONDITIONS

Two sources of experimental data have been carefully selected. The experimental work by De Vries (1994) and Stroomer (1995) at Delft University of Technology (Technische Universiteit Delft) is particularly preferred as it contains both non-reacting and reacting flow measurement data with the same burner configuration. The joint experimental study of piloted jet flames of pure methane conducted at the University of Sydney and Sandia National Laboratories (Masri et al, 1988, 1990) has also been selected for the investigation. In all calculations, the numerical procedures remain unchanged. The purpose is to compute each test case with a single code so that any differences arising from different numerical procedures can be avoided, allowing the accuracy of the models to be evaluated more effectively.

A grid of 200 x 150 nodes covering a domain of 150 x 35 jet diameters, equivalent to 0.9m long and 0.2m wide, is used in the calculations of the Delft flame. Previous experience has demonstrated that a grid independent result can be achieved on a grid of around 150 x 60 nodes. The grid is compressed around the

nozzle exit in both axial and radial directions. Since the computational domain for the calculation of the Sydney-Sandia flames is quite similar to that of the Delft flame, a 150×70 grid covering the domain of 100×35 jet diameters (720mm x 252mm) was used to ensure a grid independent solution.



Figure 1: Radial profiles of mean axial velocity X/D=8.33 and rms axial velocity fluctuations at X/D=25

RESULTS AND DISCUSSION

Calculation results of \tilde{U} and *Urms* for Delft flame using the cubic SMCs, are compared with the standard linear SMC results and the measured data in Figure 1. A good description of the flame width is observed in the upstream region when the cubic SMC is employed. Moreover, excellent results are achieved by using the cubic SMC together with the "modified" ε transport equation (Equation 1). It seems that the model is able to account properly for the anisotropy of turbulence in flames.

Figure 2 shows the measured and predicted temperature profiles, comparing predictions of the standard EVM, SMC and cubic SMC models are plotted. Attention is drawn to the predictions of the cubic SMC with Equation 1. The inclusion of Equation 1 generates a more realistic level of the dissipation rate, leading to better predictions of the turbulent stresses, fluxes, and the scalar dissipation rate \mathcal{E}_z . This modelling combination thus provides excellent predictions of the spreading rate of the flame, and the measured temperature, not only in the centre part of the flame but also around its edge. The two figures suggest that the width of the flame is better predicted than with the other models. The model avoids the weakness of the EVM, which underestimates the temperature across the flame, and of the standard SMC, which gives an overestimation of the temperature.



Figure 2: Radial profiles of mean temperature at *X/D*=8.33 and 41.67

Figure 3 shows the measured and computed mean temperature profiles at two axial locations using the stretched laminar flamelet model (SFM) to account for the frequent local extinction found in the Sandia-Sydney M-Flame. The turbulence model used for the calculations is the cubic SMC for both the \sim

turbulent stresses and fluxes. The scalar dissipation rate χ is estimated as $\chi = R \frac{\varepsilon}{k} z^{n^2}$ where the mixture

fraction variance is calculated from its own transport equation and the time scale ratio, R, is taken as a constant of 2. At X/D=30, improvements in the predictions at the centre of the flame using the SFM can be seen. Unfortunately, the results are still far from reality and the computed maximum temperatures remain 400degC higher than the measured values. It is suggested that the effect of stretching in the model is not sufficient. To address the problem, one possibility might be to employ multiple-strained laminar flamelet profiles so that a family of strained laminar flamelet profiles can be used at different scalar dissipation rate below an assigned quenching limit. At X/D=50 and beyond, the mean scalar dissipation rate is so small, even at the centreline, that the SFM only gives a minute reduction in temperature. The accuracy of the SFM is therefore limited. This suggests that a different approach may be required to compute a flame with local extinction.



Figure 3: Radial profiles of mean temperature at X/D=30 and 50, using stretched and unstretched laminar flamelet models.

CONCLUSION

In this paper the applicability of a range of turbulence models have been investigated, and some model adjustments and developments have been proposed and tested. An attempt has been made to extend the earlier non-reacting flow studies at UMIST to improve the ε equation by making c_{ε^2} sensitive to the anisotropy invariants and adding an extra source term. This modification gives, overall, excellent flame predictions.

The present computational study has demonstrated that the standard SMC can capture the increased velocity induced by combustion and give good predictions of turbulent stresses, compared to the linear gradient transport approach. However, the standard turbulence models normally fail to produce the correct flow behaviour in the intense reaction region. By using a model which accounts for the anisotropy of the turbulence, the present computations have demonstrated that improved predictions of the spread of the jet flames and the flow properties at the outer edge of the flames can be obtained. The full cubic SMC (for both stresses and fluxes) produces the best overall agreement with the experimental data. It overcomes the deficiency of the standard SMC without excessively increasing the computing resources.

An attempt has been made in the present combustion modelling to address the local extinction feature found in the Sydney-Sandia M-Flame. A stretched laminar flamelet model has been adopted. The predictions of the temperature field are improved but are still far from reality, indicating that a more sophisticated modelling approach is required.

ACKNOWLEDGMENTS

The financial support of EPSRC is gratefully acknowledged.

REFERENCES

Chan, W.T., Ph.D. Thesis, UMIST (2000). Chan, W.T., and Zhang, Y., Engineering Turbulence Modelling and Experiments 4, pp. 821-830 (1999). Craft, T.J., and Launder, B.E., Int. J. Heat and Fluid Flow, vol. 17: 245-254 (1996). Craft, T.J., Launder, B.E., and Suga, K., Int. J. Heat and Fluid Flow, vol. 17: 108-115 (1996). Huang, P.G., and Leschziner M.A., Report TFD/83/9(R), Dept. of Mech. Eng., UMIST (1983). Jones, W.P., and Launder, B.E., Int. J. Heat Mass Transfer, vol. 15: 301-313 (1972). Jones, W.P., and Musonge, P., Proc. 4th Turbulent Shear Flow Symp., Karlsruhe, pp. 17.18-17.24 (1983). Launder, B.E., Int. J. Heat and Fluid Flow, vol. 10, No.4: 282-300 (1989). Launder, B.E., and Sharma, B.I., Lett. Heat Mass Transfer, vol. 1:131-138 (1974). Leonard, B.P., Comp. Maths. Appl. Mech. Eng., vol. 19: 59-98 (1979). Liew, S.K., Bray, K.N.C., and Moss, J.B., Combustion and Flame, vol. 56: 199-213 (1984). Lindstedt, R.P., and Vaos, E.M., Combustion and Flame, vol. 116: 461-485 (1999). Masri, A.R., and Pope, S.B., Combustion and Flame, vol. 71: 245-266 (1988). Masri, A.R., Bilger, R.W., and Dibble, R.W., Combustion and Flame, vol. 81: 13-29 (1990). Monin, A.S., Izv. Atm. Oceanic Phys., vol. 1: 45 (1965). Naot, D., Shavit, A., and Wolfshtein, M., Israel J. Tech., vol. 8: 259 (1970). Owen, R.G., Ph.D. Thesis, Pennsylvania State University (1973). Patankar, S.V., McGraw-Hill, New York (1980). Peeters, T.W.J., Ph.D. Thesis, Technische Universiteit Delft (1995). Rogg, B., Report CUED/A-THERMO/TR39, Cambridge University (1993). Rotta, J.C., Z. Phys., vol. 129:547-572 (1951). Shin, T.H., and Lumley, J.L., Report. FDA-85-3, Cornell University (1985).

Smooke, M.D., and Giovangigli, V., *Lecture Notes in Physics*, vol. 384: 1-47 (1991). Stroomer, P., Ph.D. Thesis, *Technische Universiteit Delft* (1995). Tsuji, H., *Progress in Energy and Combustion Science*, vol. 8: 93-119 (1982). Vries, J.De., Ph.D. Thesis, *Technische Universiteit Delft* (1994).