COMPARISON OF TURBULENT NONPREMIXED COMBUSTION MODELS FOR MODELLING A BLUFF BODY FLAME

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Abstract Three combustion models are compared for predicting a bluff body syngas flame. The combustion models are the flame sheet, eddy break-up and laminar flamelet model. Comparison of predicted results with experimental data shows that the laminar flamelet model provides better prediction for temperature than the other two models.

Keywords: Combustion, Bluff-body, Flamelet

INTRODUCTION

The accurate prediction of combustion in practical systems has attracted attention of many researchers over the last few decades because of its potential impact on development of improved combustion equipment. Better thermal efficiency and lower pollution emission are two of the benefits that can be obtained from the development of advanced combustion models. Over the years several combustion models that account for the interaction of turbulence and chemistry have been developed and applied to a number of flames ranging from simple jet flames to complex combustion chambers. Nonpremixed combustion models that are currently available are conserved scalar based flame sheet model [Jones and Whitelaw, 1982], eddy break-up up and eddy dissipation model [Magnussen and Hjertager, 1976; Gran and Magnussen, 1996], laminar flamelet model [Peters, 1984, 1986], conditional moment closure (CMC) model [Bilger, 1993] and probability density function (pdf) transport model [Pope, 1985, 1990]. The pdf transport model is theoretically the most accurate and is capable of handling the reaction rate term without any modelling assumption. However, the model is very resource-intensive and the application of the model for industrial calculations is still not wide spread. The CMC model is a newer model and currently gaining some success in jet flames [Bilger, 2000]. However, the model is still under development and its successful application in practical situations is yet to be assessed. The flame sheet and eddy break-up models are currently the viable option for industrial applications and these models have been incorporated in a number of commercial CFD codes including FLUENT and CFX. Though the laminar flamelet model is not yet available in commercial CFD codes, Coelho and Peters [2001a, 2001b] have reported successful incorporation of the laminar flamelet model into a commercial CFD code through the user subroutine for simulating an industrial combustor.

A comparative study of the flame sheet, eddy breakup and laminar flamelet model is reported here. The configuration selected is a bluff body combustor [Correa and Gulati, 1992]. The bluff body combustor is a suitable compromise as a model problem because the combustor with its recirculation zone has some complexity of industrial furnace while retaining simple and well-defined inlet and boundary conditions.

MATHEMATICAL MODELS

The numerical model of turbulent combustion is formulated from the Favre-averaged Navier-Stokes equation together with turbulence and combustion models. Farve-averaged Navier-Stokes equation can be expressed in Cartesian tensor notation as:

$$\frac{\partial \bar{\rho}\tilde{u}_j}{\partial x_j} = 0 \qquad (1)$$

$$\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{u}_i\right) = -\frac{\partial P}{\partial x_i} + \mu_{eff}\frac{\partial}{\partial x_j}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) \qquad (2)$$

where μ_{eff} is effective viscosity given by $\mu_{eff} = \mu + \mu_t$

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The eddy viscosity μ_t is given by

$$\mu_t = \bar{\rho} C_\mu \frac{\tilde{k}^2}{\tilde{\varepsilon}}$$

In the present study, the standard $k-\varepsilon$ turbulence model has been used. The equation used to model turbulence kinetic energy, k is of the form:

$$\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{k}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_k}\frac{\partial \tilde{k}}{\partial x_j}\right) + G - \varepsilon \tag{4}$$

where G is turbulence production due to strain and is given by:

$$G = \mu_t\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)\frac{\partial \tilde{u}_i}{\partial x_j}$$

The transports equation for the dissipation of turbulent kinetic energy ε is of the form:

$$\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{\varepsilon}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial \tilde{\varepsilon}}{\partial x_j}\right) + C_{\varepsilon 1}\frac{\tilde{\varepsilon}}{\tilde{k}}G - C_{\varepsilon 2}\bar{\rho}\frac{\tilde{\varepsilon}^2}{\tilde{k}} \tag{5}$$

The model constants C_μ, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, σ_k, σ_ε have the values 0.09, 1.44, 1.92, 1.3 and 1.0 respectively.

The combustion models assessed in the present study are described below.

THE FLAME SHEET MODEL

The flame sheet model assumes that chemical reaction takes place in a single irreversible step at a thin flame sheet. The flame sheet is located at the stoichiometric mixture fraction. Outside the flame sheet, inert mixing between the reactants and products take place. In the flame sheet model, the mass fractions of fuel and oxidant are given by [Jones and Whitelaw, 1982; Kuo, 1986]:

$$m_{fu} = \int_0^1 \max\left(\frac{Z - Z_{st}}{1 - Z_{st}}, 0\right) P(Z)dZ \tag{6}$$

and

$$m_{ox} = \int_0^1 \max\left(1 - \frac{Z}{Z_{st}}, 0\right) P(Z)dZ \tag{7}$$

where Z_{st} is stoichiometric mixture fraction defined by

$$Z_{st} = \frac{m_{ox,A}}{s m_{fu,F} + m_{ox,A}} \tag{8}$$

the subscripts A and F refers to air and fuel stream respectively, s is stoichiometric mass of oxygen.

The mass fraction of products is obtained via

$$m_{pr} = 1 - m_{fu} - m_{ox} \tag{9}$$

The temperature is obtained from

$$H(T) = \int_0^1 \left(\int_{T_{ref}}^{T} c_P(T,Z)dT + H_{fu}m_{fu}(Z)\right)P(Z)dZ \tag{10}$$

where the specific heat capacity of the mixture, $c_P(T,Z)$ is obtained from JANAF table [Prothero, 1969] and H_{fu} is the heating value of fuel. The density is then obtained from the ideal gas law:

$$\rho = \int_0^1 \frac{P}{RT(Z)\sum_1^n \frac{m_i}{W_i}} P(Z)dZ \tag{11}$$

In above formulae $P(Z)$ is a probability density function and is assumed as a beta function. The $P(Z)$ is constructed from transport equations of mean mixture fraction, $\tilde{Z}$ and mixture fraction variance, $\tilde{Z}''^2$:

$$\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{Z}\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \tilde{Z}}{\partial x_j}\right) \tag{12}$$

$$\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{Z}''^2\right) = \frac{\partial}{\partial x_j}\left(\frac{\mu_t}{\sigma_t}\frac{\partial \tilde{Z}''^2}{\partial x_j}\right) + C_{g1}\mu_t\left(\frac{\partial \tilde{Z}''^2}{\partial x_j}\right)^2 - C_{g2}\frac{\tilde{\varepsilon}}{\tilde{k}}\bar{\rho}\tilde{Z}''^2 \tag{13}$$

where $\sigma_t = 0.7$ and the constants $C_{g1} = 2.8$ and $C_{g2} = 2.0$.

EDDY BREAK-UP (EBU) MODEL

The eddy break-up combustion model assumes the rate of chemical reaction as proportional to the rate of dissipation of eddies containing different reactants [Magnussen and Hjertager, 1976]. In the eddy break-up model, the rate of fuel burning is given by the expression:

$$R_{fu} = \frac{\tilde{\varepsilon}}{\tilde{k}}\min\left(Am_{fu}, A\frac{m_{ox}}{s}, B\frac{m_{pr}}{1+s}\right) \tag{14}$$

where A and B are constants with values 4.0 and 2.0 respectively; s is stoichiometric mass of oxygen. Transport equations for mass fraction of fuel, oxygen and product are solved with source term calculated from equation (14). Density is then obtained from the universal gas law.

THE LAMINAR FLAMELET MODEL

The laminar flamelet model views the turbulent flame as an ensemble of laminar flamelet structures, which are corrugated by the action of turbulent fluctuations [Peters, 1984, 1986]. The laminar flamelet modelling of turbulent combustion is a two-step process. In the first

step, a laminar flamelet library is calculated by solving governing equations for a counterflow diffusion flame. A detailed chemical reaction mechanism and a realistic transport properties can be prescribed for calculating the flamelet library as the flow is laminar. In the second step, the flamelet profiles are used as input data to a CFD code which calculates the mean scalar variables in a turbulent combustion as described below.

The flamelet profiles specify temperature, density and species concentrations by the mixture fraction and the scalar dissipation rate. For turbulent flames, the mean scalar variables are computed from the laminar flamelet relation of the mixture fraction and the scalar dissipation rate by integrating over a joint probability density function as

$$\tilde{\phi} = \int_0^\infty \int_0^1 \phi(Z,\chi) P(Z,\chi) dZ d\chi \qquad (15)$$

The assumption of statistical independence leads to $P(Z,\chi) = P(Z)P(\chi)$ [Peters, 1984]. The probability density function $P(Z)$ is assumed as a beta distribution and $P(\chi)$ as log-normal distribution [Peters, 1984]. In the CFD code, transport equations are solved for the mean mixture fraction $\tilde{Z}$ and mixture fraction variance $\tilde{Z}^{"2}$. The mean and variance of the mixture fraction completely describe the beta function. The mean value of the scalar dissipation rate can be modelled as

$$\tilde{\chi} = C_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \tilde{Z}^{"2} \qquad (16)$$

where $\tilde{k}$ and $\tilde{\varepsilon}$ are the mean turbulence kinetic energy and energy dissipation rate respectively and C_χ is a constant set equal to 2.0 [Peters, 1984]. The standard deviation for the log-normal distribution of the scalar dissipation rate is set equal to $\sigma_\chi^2 = 2.0$ [Peters, 1984].

NUMERICAL DETAILS

An in-house finite-volume CFD code is used to assess the combustion models. Central differencing has been employed to discretise all diffusive flux terms of the governing equations. The hybrid scheme has been used to treat the convection terms of all equations. Pressure coupling has been dealt with the SIMPLE algorithm [Patankar, 1980] in the solution procedure.

Calculations are carried out with grid arrangement employing 97 (axial) X 87 (radial) non-uniform grids. Grid refinement using 122 (axial) X 87 (radial) did not produce significant change in results and therefore, it was concluded that the spatial discretisation error was small enough to allow the underlying mathematical models to be evaluated using 97x87 grids. The grid lines were concentrated in the high shear region behind the bluff body.

There are some uncertainties in the specification of inlet conditions as experimental inlet data are not available. The velocity at the inlet is considered to be uniform according to Correa and Gulati [1992]. The inlet turbulence parameters are specified as

$$k_{in} = iU_{in}^2$$

$$\varepsilon_{in} = \frac{C_\mu^{1/4} k_{in}^{3/2}}{\lambda R}$$

where i is the turbulence intensity and λ is the length scale. In the present study, $i = 0.01$ and $\lambda = 0.07$ are used. Sensitivity study of the turbulence intensity and the length scale has not been carried out. However, Correa and Gulati [1992] mentioned that the effect of inlet conditions was negligible for this flame as the turbulence generated in the shear layer rapidly overwhelmed the inlet level.

The laminar flamelet library was calculated employing a full reaction mechanism of Warnatz [Peters, 1993] using a laminar flame and flamelet code RUN-1DL [Rogg, 1995]. The reaction mechanism was consisted of 24 reaction steps involving 12 species (CO, O_2, CO_2, H_2O, H_2O_2, HO_2, H, OH, O, H_2, HCO, N_2).

RESULTS AND DISCUSSION

The experiment of Correa and Gulati [1992] on a bluff body stabilised flame is used to assess the combustion models. The schematic drawing of the bluff body combustor is shown in Fig. 1. The fuel jet is located at the centre of a 15 cm X 15 cm square wind tunnel. The diameter of the fuel jet is 3.18 mm and the diameter of the bluff body is 38.1 mm. The syngas fuel consisted of 27.5% CO, 32.3% H_2 and 40.2% N_2 by volume. The fuel and air jet velocities were 80.0 m/s and 6.5 m/s respectively. Temperature was 300 K for both streams.

COMPARISON WITH PREVIOUS STUDIES

The results of the laminar flamelet model calculation are compared with the predictions of Correa and Gulati [1992] and Gran and Magnussen [1996]. Correa and Gulati [1992] used a partial equilibrium model for combustion and the $k-\varepsilon$ model for turbulence. Gran and Magnussen [1996] used the eddy dissipation combustion model and the $k-\varepsilon$ turbulence model. The axial mixture fraction profiles calculated in the present study and calculated by Correa and Gulati [1992] and Gran and Magnussen [1996] are shown in Fig. 2. The figure also shows the axial mixture fraction obtained by using a modified value of the constant $C_{\varepsilon 1}$. The present study with the standard $k-\varepsilon$ model underpredicts the mixture fraction profile, but is in good agreement with all previous studies. This discrepancy in the calculations was attributed to the turbulence modelling [Gran nad Magnussen, 1996; Correaand Gulati, 1992]. It is a well-known fact that the standard $k-\varepsilon$ model over estimate the spreading rate of the jet.

The turbulence model group of the International Workshop on Measurement and Computation of Turbulence Nonpremixed Flames (TNF) [TNF, 1996] has recommended the use of the $k-\varepsilon$ model with $C_{\varepsilon 1}=1.60$ for bluff body flames. This modification remarkably improves the prediction as shown in the figure.

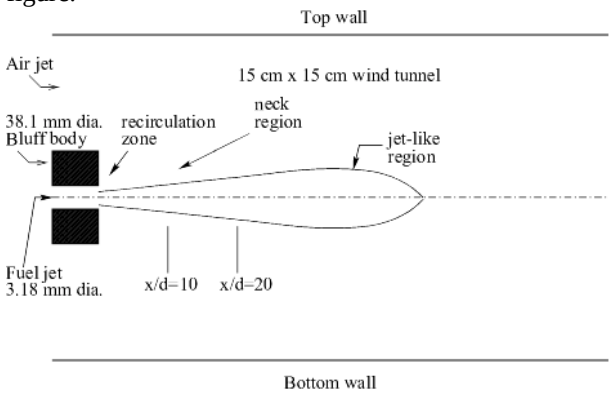

Fig. 1: Schematic drawing of the bluff body combustor

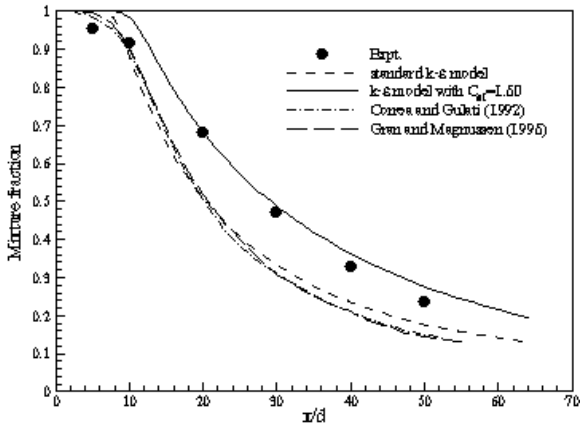

Fig. 2 Profiles of mixture fraction along the centreline showing comparison with previous studies

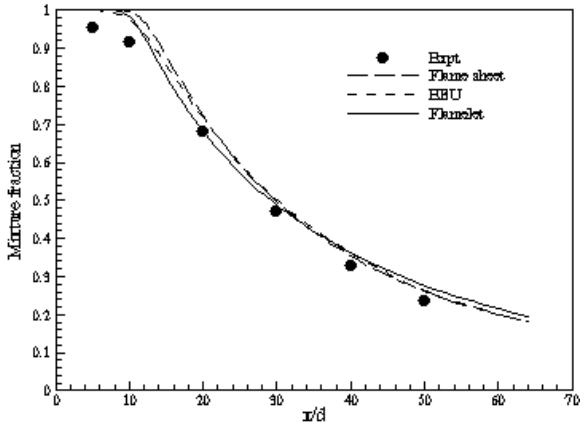

Fig. 3 Axial mixture fraction profiles

COMPARISON OF COMBUSTION MODELS

Comparison of axial mixture fraction profiles is shown in Fig. 3. The mixture fraction values are overpredicted upto x/d=10 by all the combustion models. This overprediction may be caused by the uncertainties about the inlet conditions. The flamelet model gives good prediction between x/d=10 and x/d=20 and then overpredicts further downstream. Other models overpredict the mixture fraction though slightly after x/d=10.

The radial mixture fraction profiles at two axial locations x/d=10 and x/d=20 are shown in Fig. 4. There is very small difference among the calculations of different combustion models and the agreement with the experimental data is good.

High-quality agreement of the mixture fraction profiles sets the stage for a meaningful evaluation of the combustion models for the prediction of temperature and species concentrations. Radial temperature profiles are shown in Fig. 5. The eddy dissipation model overpredicts the peak temperature by 400 K and the flame sheet model by approximately 200 K. The laminar flamelet model produces a very good agreement with the measurements. The peak experimental temperature is approximately 1600 K, which is several hundred below the equilibrium temperature of 2161 K. This clearly indicates that the flame does not reach the chemical equilibrium condition at these locations. The flamelet model incorporates the non-equilibrium effect and as a result produces a much better agreement of peak temperature. Fig. 6 and 7 show the radial profiles of mass fraction of H_2 and CO. The agreement is reasonably good by all the combustion models. All the combustion models underpredict the peak value of H_2O as shown in Fig. 8. Calculated speed vectors and temperature contours are shown in Fig. 9.

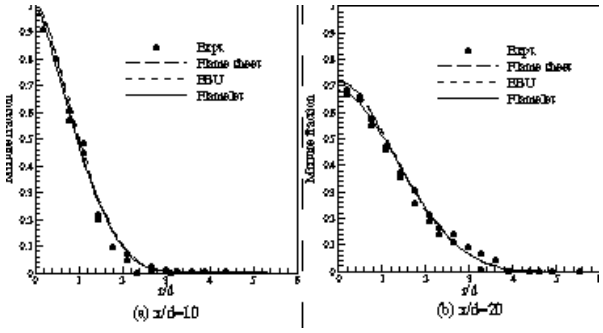

Fig. 4 Radial mixture fraction profiles

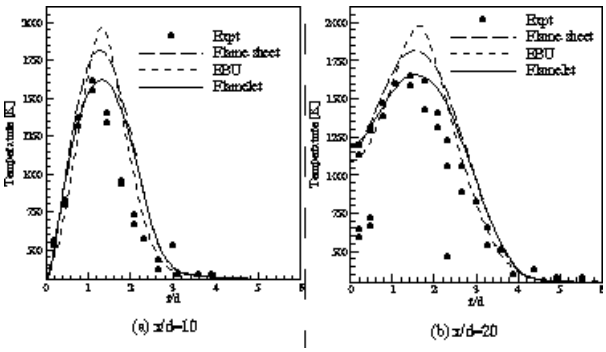

Fig. 5 Radial temperature profiles

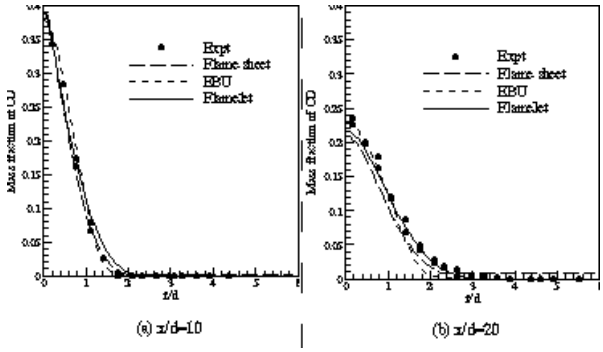

Fig. 6 Radial profiles of mass fraction of CO

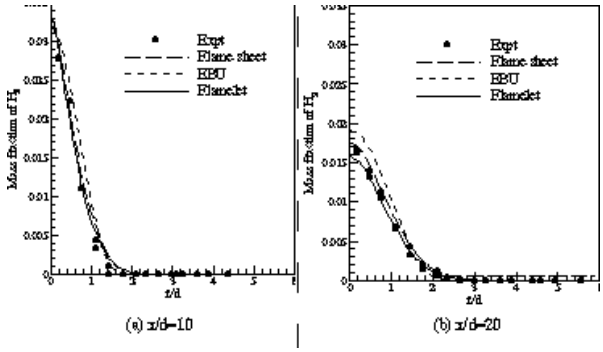

Fig. 7 Radial profiles of mass fraction of H_2

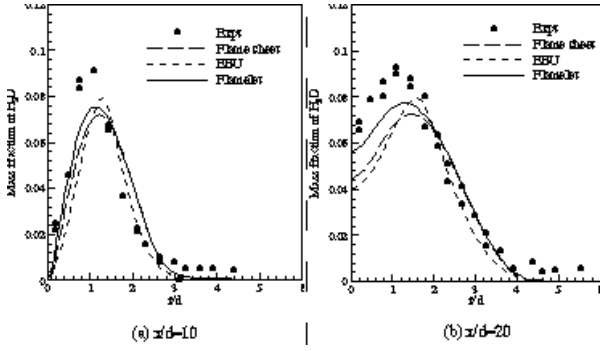

Fig. 8 Radial profiles of mass fraction of H_2O

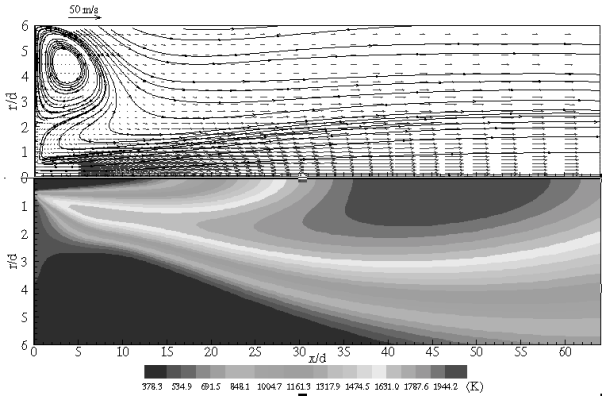

Fig. 9 Velocity vectors and temperature contours

CONCLUSIONS

Three combustion models widely used in combustion modelling are compared for a bluff body syngas flame. Though the flame sheet, eddy breakup and laminar flamelet models produce similar results for mass fraction of CO, H_2 and H_2O significant difference is observed for temperature prediction. Temperature is the most important property of a flame and it is therefore vital to reproduce temperature. Only the laminar flamelet model reproduced the temperature profile accurately.

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