

Kashan - IRAN Feb. 2012



STUDY OF A TURBULENT NON-PREMIXED METHANE-AIR REACTING FLAME IN A BURNER USING FLAME HOLDER

S. Abdolmehi Hashemi^{*}, Najmeh Hajialigol^{*,§} and Kiumars Mazaheri^{**} ^{*} Department of Mechanical Engineering, University of Kashan ^{**} Department of Mechanical Engineering, Tarbiat Modares University of Tehran

[§]Najmeh.Hajialigol@Gmail.com

ABSTRACT: Beta Probability Density Function (β -PDF) model is applied to investigate the turbulent nonpremixed combustion flow, including species concentrations and temperature, in a burner. Gaseous methane (CH₄) is injected at the centre of the burner inlet. Air is supplied through the surrounding of this fuel inlet. The governing equations are solved by a finite volume approach and are discretized with the second order upwind scheme. The Realizable k- ϵ turbulence model is applied to model turbulence. The Discrete Ordinate radiation heat transfer method is also used. The values of the species mole fraction, temperature and density, which are the functions of the mixture fraction, are determined by integration over a β -PDF. In this study wall as a flame holder is used to stabilize the flame.

Keywords: Flame holder, Turbulence model, PDF model, Numerical simulation

INTRODUCTION

The problem of flame stabilization is an important issue for designing of burners. Flames are frequently stabilized within a refractory passageway, referred to as a burner tile, in industrial burners. Flame stabilization techniques such as bluff-body and swirl vanes have been brought into practical use. Stabilization occurs by creating a recirculation zone, the simplest being the wake behind a bluff-body. Tankin et al. [1] studied the bluff-body effect on the bluff-body stabilized flame combustor and concluded that central jet having higher momentum than air jet, penetrates through recirculation zone and affects its size. Swirl combustion has been widely used in various industrial combustors because of its promising performance of mixing and flame holding [2, 3].

Employing an appropriate turbulence model is a main task in a flow with turbulent nature. Standard k- ε eddy viscosity model (Ske), which is a complete and simple model, is widely used in various turbulence computational fluid dynamics problems such as in near-wall turbulent flows [4-7] and in rotating turbulent flows [8]. It is shown that Ske turbulence model can relatively predict the flow and temperature distributions for a reacting flow [9]. However, this model is not appropriate for flows with a high mean shear rate or a massive separation. Hence, for dominating these defects, the Realizable turbulence model (Rke) was introduced with a new formulation for the turbulent viscosity.

Numerous experimental and numerical researches have been carried out on the turbulent combustion of non-premixed flames. Ellzey et al. [10] simulated an axisymmetric confined diffusion flame formed between a H_2 - N_2 jet and compared their results with an analytical solution. They showed that if diffusion coefficients and densities are variable, small radial velocities are induced and



Kashan - IRAN Feb. 2012



the flame interface is somewhat deformed. The PDF model with a fast chemistry assumption can be employed to consider the reaction–turbulence interactions. There are three assumed forms of the PDF which used in the modeling of turbulent reacting flows: the double δ function, the clipped Gaussian function and the β function with two average methods: the Favre and the Reynolds methods [11]. Among them, the β -PDF that proposed and validated by Hannon et al. [12], shows comparatively better results for a turbulent reacting flow. Repp et al. [13] compared two models for turbulence-chemistry interaction, including a Monte Carlo and a presumed β -PDF in a confined diffusion flame. They showed that both PDF models present a similar accuracy level of prediction of mean quantities. Despite the fact that the presumed β -PDF model carries out using reasonable computational efforts, the Monte Carlo PDF causes well capturing turbulence-chemistry interaction in low Damkohler numbers such as the local extinction. Cao et al. [14] applied a joint PDF method for a lifted turbulent jet flame with H₂/N₂ fuel. They showed this method can be captured some flame parameters such as velocity, mixture fraction and species concentration very well.

This study uses a wall around the exit of fuel and air as a flame holder. About our knowledge, no experimental and numerical study has been carried out on this problem. To begin this study base on numerical method and on the other hand, a validated numerical simulation can be employed investigators in this paper have set about to an experimental setup at the first step. Aim of this paper is to investigate the turbulent non-premixed combustion, including species concentrations and temperature by using β -PDF and FLUENT commercial software [15]. Finite volume method as well as k- ϵ turbulence and DO radiation models are used to solve the governing equations

EXPERIMENTAL SETUP

Fig. 1 shows the experimental setup that is used. It is consisted of air and fuel supply systems, burner, thermocouples, control PC and a single wall flame holder. The air supply system is consisted of a tank of air, a flow control valve and a calibrated rotameter. The fuel is natural gas. Inlet air and fuel temperatures were at 300 K. The fuel and air are injected from two independent ways and are mixed in the burner. The wall that is shown in the Fig. 1 has a flame holder role. Data for temperature field is obtained with thermocouples. LABVIEW software in control PC shows the data of temperature field in the digital signal.



Figure1. Experimental setup



Kashan - IRAN Feb. 2012



GOVERNING EQUATIONS

Conservative equations for a steady state reacting flow are used here. A generalized equation includes overall mass, momentum, energy and chemical species concentration equation can be written as [16]:

$$\sum_{i} \frac{\partial}{\partial x_{i}} (\rho V_{i} \phi) = \sum_{i} \frac{\partial}{\partial x_{i}} (\Gamma_{\phi} \frac{\partial \phi}{\partial x_{i}}) + S_{\phi}$$
(1)

where quantity Φ dictates the special equation. For $\Phi=1$, velocity component, h and y_i it yields conservation equation of mass, momentum, energy and species mass fraction. S_{Φ} is the source term in the conservation equations.

TURBULENCE MODEL

The realizable k- ε turbulence model [17] is applied in this study. In comparison with the standard k- ε , this model hinders the negation of values of the normal Reynolds stresses by employing a new turbulent eddy viscosity formulation. It also utilizes a new transport equation for dissipation rate, which hires different sink and source terms. Because of some disadvantages of the standard k- ε turbulence model, some researchers proposed the realizable model for diffusion flames [18, 19]. Further details of the realizable k- ε turbulence model can be found in [17].

Turbulence intensity is expressed as:

$$I = \frac{V'}{V_{avr}} = \sqrt{\frac{\frac{2}{3}k}{u^2 + v^2}}$$
(2)

TURBULENCE-COMBUSTION INTERACTIONS

Because of the fluctuating characteristics of the turbulent mixing process, the probability density function is a skilled method for the cases including combustion process and turbulent flow. In this study, we employ the presumed PDF model with assumption of the fast chemistry. In this model, the PDF is defined in terms of two parameters: the mean and its variance of scalar quantity. Due to better results for the turbulent reacting flow with comparison to the other PDF model, the β -PDF model [12] is used to calculate the thermodynamic properties. In the presumed β -PDF model, the mixture fraction, *f*, is defined in terms of mass fraction of

specie i, Y*i*: $Y_i - Y_i$ or

$$f = \frac{Y_{i,ox}}{Y_{i,f} - Y_{i,ox}}$$
(3)

where the subscripts f and ox denote the fuel and oxidant stream, respectively.

The transport equations of mean mixture fraction, \overline{f} and its variance, $\overline{f'}^2$, are:

$$\frac{\partial}{\partial t}(\rho \bar{f}) + \frac{\partial}{\partial x_{j}}(\rho u_{j} \bar{f}) = \frac{\partial}{\partial x_{j}}(\frac{\mu_{t}}{\sigma_{t}}\frac{\partial \bar{f}}{\partial x_{j}})$$
(4)





Kashan - IRAN Feb. 2012

$$\frac{\partial}{\partial t}(\rho \overline{f'}^{2}) + \frac{\partial}{\partial x_{j}}(\rho u_{j} \overline{f'}^{2}) = \frac{\partial}{\partial x_{j}}(\frac{\mu_{t}}{\sigma_{t}} \frac{\partial \overline{f'}^{2}}{\partial x_{j}}) + C_{g} \mu_{t}(\frac{\partial \overline{f}}{\partial x_{j}}) - C_{d} \rho \frac{\varepsilon}{k} \overline{f'}^{2}$$
(5)

where the constant values of σ_t , C_g and C_d are 0.85, 2.86 and 2.0, respectively. The relation between the obtained time-averaged values from the above equations and the instantaneous mixture fraction is made by a PDF. This function is written as p(f), which is the probability that the fluid spends in the state f. The method applies the mean values of species concentration and temperature. The mean species mass fraction and temperature, $\overline{\phi_i}$, is calculated from:

$$\overline{\phi_i} = \int_0^1 p(f) \phi_i(f) df$$
(6)
Where $p(f) = \frac{f^{\alpha - 1} (1 - f)^{\beta - 1}}{\int f^{\alpha - 1} (1 - f)^{\beta - 1} df}$

 α and β are defined as follow:

$$\alpha = \bar{f} \left[\frac{\bar{f}(1-\bar{f})}{\bar{f'}^2} - 1 \right]$$
(7)

$$\beta = (1 - \bar{f}) \left[\frac{\bar{f}(1 - \bar{f})}{\bar{f'}^2} - 1 \right]$$
(8)

For the non-adiabatic case, the mean enthalpy transport equation is described as:

$$\frac{\partial}{\partial t}(\rho \,\overline{h}) + \nabla .(\rho \,\overline{v} \,\overline{h}) = \nabla .(\frac{k_t}{c_p} \nabla \,\overline{h}) + S_h \tag{9}$$

where S_h is a source term because of radiation heat transfer to the wall boundaries. Chemical equilibrium is used for determining product mole fractions.

RADIATION HEAT TRANSFER MODELING

The radiation model may play a crucial role in the heat transfer to the surrounding walls in a combustor [20, 21]. The radiation heat transfer equation (RTE) for an absorbing, emitting and scattering medium at position r and direction s is [22]:

$$\frac{dI(r,s)}{ds} = -(a + \sigma_s)I(r,s) + an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \times \int_0^{4\pi} I(r,s')\Phi(s,s')d\Omega'$$
(10)

Here *r*, *s*, *s*, *a*, *n*, σ_s , σ , *I*, *T*, Φ and Ω' denote position vector, direction vector, scattering direction vector, path length, absorption coefficient, refractive index, scattering coefficient, Stefan-Boltzman constant (= 5.672×10^{-8} W/m²k⁴), total radiation intensity, local temperature, phase function and solid angle, consecutively.

The discrete ordinate method (DOM) [23] is an appropriate model to simulate radiation heat transfer for the most applicable cases. It has been demonstrated that the model is a skillful and accurate method for PDF modeling of reacting flow [24]. Further information about this method can be found in [23].



Kashan - IRAN Feb. 2012



(12)

GEOMETRY AND BOUNDARY CONDITIONS

Fig. 2 shows axisymmetric geometry of the existing burner model. According to the experimental setup, the radius of fuel inlet (R_f) and the radius of air inlet (R_a) of the coaxial burner are 0.003m and 0.011m, the length (L_h) and radius of flame holder (R_h) are 0.1m and 0.0315m respectively and 0<z<0.5m. The velocity of fuel and air are 5.9 m/s and 6.8 m/s respectively. The fuel that is used is 100% methane.

The inlet air turbulence kinetic energy and its dissipation rate are expressed as [16]:

$$k = \frac{3}{2} (U_{ref} I)^2 \qquad \varepsilon = 0.16 \frac{k^{1.5}}{\ell}$$
(11)

In which I, L, U_{ref} are defined as turbulence intensity, characteristic length and inlet velocity respectively. ℓ is predicted by [16]:

 $\ell=0.07L$

The flow leaves the burner with absolute pressure of 1bar. The wall of the burner is adiabatic.



Figure2. Burner configuration.

NUMERICAL PROCEDURE

The conservation equations for mass, momentum, energy, species as well as fuel combustion, kinetic energy turbulence and its dissipation rate are discretized using the Finite Volume Method [16] and a second order upwind scheme. The SIMPLE algorithm is used to indicate the velocity and pressure coupling.

The criterion of convergence of the solution is that the maximum value of the normalized residual of energy equation and the other transport equations must be less than 10^{-6} and 10^{-4} respectively. In order to prevent the divergence of the non-linear equations, appropriate under relaxation factors are employed. The grid is denser near the annular inlet zone due to the mixing and reaction process. In the present study, it is found that the grid size of 35600 cells for the geometry ensures a grid independent solution.

MODEL VALIDATION

In order to validate the numerical model, the present solution is compared with the experimental data. Fig. 3 represents the comparison among numerical results and experimental data along the centreline of the burner (r=0 and 0 < z < 0.5m). as it is shown the numerical results are in a good agreement with the experimental data.



Kashan - IRAN Feb. 2012





Figure3. Axial distribution of temperature at r=0: comparison among numerical results and experimental data.

RESULTS AND DISCUSSIONS

Fig. 4 shows predicted temperature distributions. The maximum value of temperature in this case is 1522 K. This figure shows that the flame temperature at the centre of the burner increases along the axial direction and drops gradually to the downstream from $z \sim 0.43$ m.



Figure4. Temperature distributions [K]

Recirculation zones which are filled with hot gases and serve as a heat source is illustrated in Fig. 5. Between these recirculation zones and the surrounding flow, there exists a turbulent exchange by which the unburned gases are supplied continuously with the energy necessary for ignition. This holds both for the initial flame in the immediate neighborhood of the flame holder and for the main flame spreading from the recirculation zone.



Figure 5. Recirculation zone

In Fig. 6 the temperature of 1400K at a mixture fraction (*f*) of 0 corresponds to that of the air stream, whereas the temperature of 298K at f = 1 is that of the methane. At the stoichiometric condition (f_{stoich}), which is at about 0.09, the oxygen and fuel stream curves meet together and







react, see in Fig. 6 (c), as a result a maximum temperature of 1806K is achieved at this location of f. The corresponding density at stoichiometric shows a minimum value. The concentrations of CO₂ and H₂O have their maximum close to the stoichiometric condition, whereas CO has the maximum value under the fuel rich conditions.



Figure 6. Flame results showing the dependence of the (a) temperature, (b) density and (c)-(d) species mole fractions on the mixture fraction.

Fig. 7 reveals the computationally predicted temperatures along the centerline. The corresponding mean density results are also presented in this figure. In Fig. 7, the predicted mean axial temperature on the centreline initially starts with the fuel temperature at the inlet. As the combustion takes place, the flame temperature increases and achieves a maximum value of 1806K at about z = 0.364m. The flame temperature then drops gradually to the downstream with a value of about 1390K. The mean density decreases from the inlet as the temperature rises and becomes minimum at the point where the temperature is maximum. The density then rises very slowly towards the downstream of the burner, which is consistent with the falling temperature.





Figure7. Mean temperature and density results along the centerline of the burner.

It might be interesting to see how the results presented above are linked with the mixture fraction and its variance, given the fact that they are a function of these two variables. These results are presented in Fig. 8. The mixture fraction decreases from the upstream to the downstream. The magnitude of the variance of the mixture fraction behaves a rapid decay at the upstream and then slowly decay to the downstream.



Figure8. Profiles of the mixture fraction and its variance along the axial direction.



In Fig 9 (a), (b) shows the predicted species mean mole fractions along the axial direction. The centreline mean mole fraction of CH_4 in Fig. 9(a) decays, which is consistent with the decay of the mixture fraction profile seen in Fig. 8. Results of the mole fraction of O_2 increases continuously towards the downstream, a result that is consistent with the simulated mixture fraction decay (Fig. 8) and the flamelet data shown in Fig. 6. The locations of peaks of the combustion products CO, H_2O and CO_2 are at about z=0.24, 0.38, 0.42m respectively.



Figure9. Mean mole fraction of the combustion species at the centerline.

CONCLUSION

Investigation on the turbulent non-premixed combustion, including species concentrations and temperature by using β -PDF and FLUENT commercial software is the goal of this paper. The governing equations are solved by a finite volume approach and are discretized with the second order upwind scheme. The results shows that at f_{stoich} , place witch the oxygen and fuel stream curves meet together and react, maximum value of temperature and minimum value of the density occurred. The manner of CH₄ mole fraction curve is similar to mean mixture fraction along the centerline.

REFERENCES

- [1] Tankin, R. S., Roquemore, W. M., Chiu, H. H., Lottes, S. A., [1986], A study of a bluffbody combustor using laser sheet lighting, *Exp Fluids*, Vol. 4, pp. 205–13.
- [2] Lefebvre, A.W., [1983], Gas Turbine Combustion, Hemisphere, New York.
- [3] Huang, Y., Yang, V., [2005], Proc. Combust. Inst, 30.
- [4] Jones, W. P. and Launder, B. E., [1973], The calculations of low-Reynolds number phenomena with a two-equation model of turbulence, *Int. J. Heat Mass Transfer*, Vol. 16, pp. 1119-1130.
- [5] Chien, K. Y., [1982], Predictions of channel and boundary layer flow with a low-Reynolds-number turbulence model, *AIAA J.*, Vol. 20, pp 33-38.







- [6] Yang, Z., and Shih, T. H., [1993], A new time scale based k-ε model for near wall turbulence, *AIAA J*, Vol. 31, pp. 1191-1198.
- [7] Shih, T. H. and Lumley, J. L., Kolmogorov behavior of near wall turbulence and its application in turbulence modeling, NASA TM 105663.
- [8] Bardina, J., Ferziger, J. H. and Reynolds, W. C., [1983], Improved turbulence models based on large eddy simulation of homogeneous, incompressible, turbulent flows. Rept. No. TF-19, Stanford University, Stanford, CA.
- [9] Nisbet, J., Davidson, L. and Olsson, E., [1992], Analysis of two fast-chimistry combustion models and turbulence modeling in variable density flow, *comput. fluid dyn*, Vol. 1, pp. 557-563.
- [10] Ellzey, J. L., Laskey, K.J., and Oran, E.S., [1991], A study of confined diffusion flames, *Comb. Flame*, Vol. 84, pp. 249-264.
- [11] Poinsot, T. and Veynante, D., [2001], Theoretical and numerical combustion, Philadelphia, PA: R.T. Edwards, Inc.
- [12] Hannon, J., Hearn, S., Marshall, L. and Zhou, W., [1998], Assessment of CFD approaches to predicting fast chemical reactions, in: Annual AICH meeting, chemical and biological reactors session, Miami Beach, FL, November, pp. 15-20.
- [13] Repp, S., Sadiki, A., Schneider, C., Hinz, A., Landenfeld, T. and Janicka J., [2002], Prediction of swirling confined diffusion flame with a Monte Carlo and a presumed PDF model, *Int. J. Heat Mass Transfer*, Vol. 45, pp. 1271-1285.
- [14] Cao, R. R., Pope, S. B., and Masri A.R., [2005], Turbulent lifted flames in a vitiated coflow investigated using joint PDF calculations, *Comb. Flame*, Vol. 142, pp. 438-453.
- [15] FLUENT User's Manual, Version 6.3.26, 2006.
- [16] Versteeg, H. K. Malalasekera, W. [1995], *An introduction to computational fluid dynamics: the finite volume method*. Addison Wesley-Longman.
- [17] Shi, T. H., Lion, W. W., Shabbir, A., Yang, Z., Zhu, J. A., [1995], new k-ε eddyviscosity model for high Reynolds numerical turbulent flows-model development and validation, *Comput Fluids*, Vol. 24, pp. 227–238.
- [18] Hashemi, S. A, Fattahi, A., Sheikhzadeh, G. A., Mehrabian, M. A., [2011], Investigation of the effect of air turbulence intensity on NO_x emission in non-premixed hydrogen and hydrogen-hydrocarbon composite fuel combustion, *Int J Hydrogen Energ*, Vol. 36, pp. 10159-169.
- [19] Poinsot, T., Veynante, D., [2001], Theoretical and numerical combustion, Philadelphia PA: R.T. Edwards, Inc.
- [20] Chen, J. Y., and Chang, W. C., [1996], Flamelet and PDF modeling of CO and NOx emissions from a turbulent, methane hydrogen jet nonpremixed flame, *Symposium (International) on Combustion*, Vol. 26, pp. 2207-2214.
- [21] Naik, S. V., Laurendeau, N. M, Cooke, J. A., and Smooke, M. D., [2003], Quantitative laser-saturated fluorescence measurements of nitric oxide in counter-flow diffusion flames under sooting oxy-fuel conditions, *Combust. Flame*, Vol. 134, pp. 425-431.
- [22] Modest, MF., [2003], *Radiative heat transfer*, Academic Press.
- [23] Fiveland, WA., [1984], Discrete-ordinate solution of radiative transport equation for rectangular enclosure, *J. Heat Mass Transfer*, Vol. 40, pp. 699–706.



Kashan - IRAN Feb. 2012



[24] Bazdidi-Tehrani, F.and Zeinivand, H., [2010], Presumed PDF modeling of reactive two-phase flow in a three dimensional jet-stabilized model combustor, *J. Energ. Conv. Manag.*, Vol. 51, pp. 225-234.