International Communications in Heat and Mass Transfer 38 (2011) 363–367

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Implementation of the eddy dissipation model of turbulent non-premixed combustion in OpenFOAM ☆

Hassan I. Kassem [a,*], Khalid M. Saqr [a], Hossam. S. Aly [b], Mohsin M. Sies [a], Mazlan Abdul Wahid [a,*]

[a] High-Speed Reacting Flow Laboratory, Faculty of Mechanical Engineering Universiti Teknologi Malaysia, 81310 Skudai, Johor, Malaysia
[b] Department of Aeronautical Engineering, Faculty of Mechanical Engineering Universiti Teknologi Malaysia, 81310 Skudai, Johor, Malaysia

ARTICLE INFO

Available online 16 December 2010

Keywords:
EDM
OpenFOAM
Turbulent
Combustion
Fluent
EBU
Jet flame

ABSTRACT

This work discusses the implementation of eddy dissipation model in OpenFOAM CFD toolbox. The code was validated in modeling of confined non-premixed Methane jet flame. The model predictions were extensively compared against published experimental results as well as ANSYS Fluent® predictions. The differences between the implemented model in OpenFOAM and Fluent were demonstrated.

1. Introduction

1.1. Background

Combustion is, indeed, an interdisciplinary topic. It combines the most sophisticated phenomena of fluid dynamics and chemical reactions. Turbulent combustion interaction is one of the most complicated products of this combination. Studying the effect of turbulence, which is a classical unsolved physical phenomenon, on chemical reaction is challenging in many aspects. The main challenge is comprehending the complex effects of a macro level phenomenon (turbulence) on a molecular lever phenomenon (chemical reaction) [1,2]. Such complexity has led the researchers to develop various physical models. Eddy dissipation model (EDM) is one of those models which is based on eddy brake up model. It assumes that the reaction is mixing controlled (i.e. mixed fuel and oxidizer are burnt). The computational cost of EDM is very attractive to many industrial fields where huge computational resources are not available for detailed chemical kinetics, which is simply not required in many engineering problems. Also EDM is a very good research tool for investigating the effects of turbulence on chemical reaction directly. Thus, EDM has been implemented in many widely used commercial CFD codes like Fluent® and CFX®.

1.2. The eddy dissipation model

Eddy break-up model is one of D.B. Spalding's contributions [3]. Spalding concluded from his experimental work that the chemical kinetics has a minor effect on turbulent combustion compared to the aerodynamics of flow field [3–7]. The turbulent combustion reaction rate in EBU is the rate by which large eddies break into small eddies, which create sufficient interface area for molecular mixing. Spatially speaking, this interface area is where combustion takes place. Based on the same concept the eddy dissipation model was developed with minor changes in constants and the representation of species concentrations [8]. The mixing controlled combustion models have numerous privileges in modeling many engineering applications which are highly turbulent flow and the effect of chemical kinetics can be neglected without affecting the overall predicted temperature. Some of these privileges can be concluded from a brief review of the recent relevant literature. Recently Achim et al. [9] modeled a full scale coal fire tube boiler using EDM for gas phase combustion. This case was modeled for design and optimization purposes which show the capitalists of EDM as powerful engineering tool. Eddy break-up model is also suitable for fire simulations; Huang et al. [10] compared it against two other combustion models. Saqr et al. studied the effect of free stream turbulence on jet flames and NOx and soot formation [11,12] which is not possible by other combustion models. They have also modeled whirling flames which is very challenging for any turbulence combustion model [13]. Chatterjee et al. [14] have used the EDM to investigate the effect of inlet air swirl and fuel injection angle on the flow and combustion phenomena of a typical diffusion-controlled spray combustion process in a can-type gas turbine combust. They have easily integrated the EDM with a two-phase

☆ Communicated by W.J. Minkowycz.

* Corresponding authors.
E-mail addresses: Hassan.kassem@gmail.com (H.I. Kassem), mazlan@fkm.utm.my (M.A. Wahid).

0735-1933/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.icheatmasstransfer.2010.12.012

Eulerian–Lagrangian formulation of the fuel spray and evaporation. Gassoumi et al. [15] have also used the EDM to conduct a numerical study of the swirl effect on a coaxial jet combustor flame including radiative heat transfer. Other examples of using the EDM to model turbulent combustion in industrial systems can be found in [16–20].

1.3. OpenFOAM CFD toolbox

OpenFOAM has attracted much attention recently because it is an open source code designed for continuum mechanics applications specially CFD applications. It is a C++ toolbox based on object oriented programming [21]. This makes OpenFOAM sustainable in terms of reuse and development by many users all around the world, in contrast to the single block programming codes which are very hard to develop or even understand. OpenFOAM is released under the GPL [22,23]. OpenFOAM gives a flexible framework which combines all the required tools for solving any CFD problem. This framework consists of enormous groups of libraries for different mathematical, numerical and physical models. Linking the mathematical/numerical tools with the physical models in a main C++ function produces different solvers and utilities. There are many recent contributions in implementing different solvers and physical models in OpenFOAM [24–28]. OpenFOAM, undoubtedly, opens new horizons for CFD community for efficient models devolving, allowing the industrial sectors to be updated with all new models without any delay for waiting the new models to be implemented in the commercial CFD codes.

Motivated by the importance of the eddy dissipation model as an engineering tool and the capabilities of OpenFOAM, we decided to implement the EDM in OpenFOAM. Until the present moment, an EDM implementation in OpenFOAM has not been reported in open literature. This article reveals the implementation of the eddy dissipation model of Magnussen [8] in OpenFOAM. The newly developed OpenFOAM solver comprising the EDM is validated against the experimental results of Brookes and Moss [29]. Then the results are briefly compared with similar case predictions by ANSYS Fluent®, which use the Magnussen's eddy dissipation version with some modifications [8,30].

2. The EdmFoam1.4 solver

EdmFoam1.4 is the newly developed OpenFOAM solver which includes the EDM for modeling turbulent combustion. The new solver is based on rhoReactingFoam solver in OpenFOAM, which is a variant of one of the OpenFOAM basic solvers called the reactingFoam. The main difference between rhoReactingFoam and reactingFoam is that the thermo-physical properties are calculated based on density instead of compressibility [22,23]. Both are unsteady uncoupled solvers. The pressure–velocity coupling is based on unsteady PISO algorithm. The combustion model in the both solvers is Chalmers PaSR model [31]. Such model calculates the reaction rate based on turbulence and chemical time scales. The reactingFoam solver was used recently by Marzouk et al. [32] for comparing eight finite-rate chemistry kinetics for CO/H2 combustion.

EdmFoam1.4 uses the same framework of the latter two solvers, but the turbulent combustion reaction rate is calculated based on eddy break-up model in Magnussen formula [8]. Thus the governing equations of the rhoReactingFoam solver were used with changing the source terms in species transport equation and sensible enthalpy equations. Also the chemical kinetics solver which calculates the chemistry time scale in the original solvers was disabled to reduce the required computational resources, and because it is not required in EdmFoam1.4. However, the solver is still under development to optimize the code performance. The solver is available upon request from the authors. Also it will be available soon for direct download from HiRef website [33]. In order to develop the new EdmFoam1.4 solver, we have used the OpenFOAM repository version 1.6.x which was recently released as version 1.7.

3. Governing equations of the EdmFoam1.4 solver

The conservation equations for turbulent combustion flow and standard kepsilon turbulence model are as the following [2,32];

Continuity equation

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla.\left(\overline{\rho}\widetilde{\vec{U}}\right) = 0 \tag{1}$$

Momentum equations

$$\frac{\partial\left(\overline{\rho}\widetilde{\vec{U}}\right)}{\partial t} + \nabla.\left(\overline{\rho}\widetilde{\vec{U}}\widetilde{\vec{U}}\right) = -\nabla\overline{\rho} + \nabla.\left(\overline{\overline{\tau}}_{eff}\right) + \overline{\rho}\vec{g} \tag{2}$$

Sensible enthalpy equation

$$\frac{\partial\left(\overline{\rho}\widetilde{h_s}\right)}{\partial t} + \nabla.\left(\overline{\rho}\widetilde{\vec{U}}\widetilde{h_s}\right) = \nabla.\left(\alpha_{eff}\nabla\widetilde{h_s}\right) + \frac{\partial\overline{\rho}}{\partial t}\dot{\omega}_T \tag{3}$$

Species transport equation

$$\frac{\partial\left(\overline{\rho}\widetilde{Y_i}\right)}{\partial t} + \nabla.\left(\overline{\rho}\widetilde{\vec{U}}\widetilde{Y_i}\right) = \nabla.\left(\mu_{eff}\nabla\widetilde{Y_i}\right) + \frac{\partial\overline{\rho}}{\partial t}\dot{\omega}_i \tag{4}$$

where U is the velocity vector, P is the pressure, ρ is the flow density, h_s is the sensible enthalpy, Y is the mass fraction, $\sum_{i=1}^{n} Y_i = 1$, $\sum_{i=1}^{n}\omega_i = 0$ and $\dot{\omega}_T = -\sum_{i}^{n} = 1 - \Delta h_{fi}^0\omega_i . - \Delta h_{fi}^0$ is the enthalpy of formation of specie (i) at the standard reference temperature 298.15 K.

The bar denotes a time averaged value and tilde denotes a Favre-averaged value, such as

$$\tilde{\varphi} \equiv \frac{\overline{\rho\varphi}}{\overline{\rho}} \tag{5}$$

The effective stress tensor in Eq. (2), τ_{eff} represents the summation of viscous and turbulent stresses. Also the effective thermal flux in Eq. (3), α_{eff} and the species flux in Eq. (4), μ_{eff} are calculated as the summation of the viscous and turbulent fluxes. The solver assumes that laminar and turbulent Prandtl number, Schmidt number and Lewis number for each species are unity. Therefore the effective thermal flux and species flux are calculated as the following;

$$\alpha_{eff} = \alpha + \mu_t \tag{6}$$

$$\mu_{eff} = \mu + \mu_t \tag{7}$$

$$\mu_t = C_\mu\overline{\rho}\frac{\tilde{k}^2}{\tilde{\varepsilon}} \tag{8}$$

where α is the dynamic thermal diffusivity, μ is the dynamic viscosity and μ_t is the turbulent viscosity. $\tilde{k}$ and $\tilde{\varepsilon}$ are the Favre-averaged turbulent kinetic energy per unit mass and its dissipation, respectively. Their transport equations as per standard kepsilon model are

$$\frac{\partial\left(\overline{\rho}\tilde{k}\right)}{\partial t} + \nabla.\left(\overline{\rho}\widetilde{\vec{U}}\tilde{k}\right) = P + \nabla.\left(\left[\mu + \frac{\mu_t}{\sigma_k}\right]\nabla\tilde{k}\right) - \overline{\rho}\tilde{\varepsilon} \tag{9}$$

$$\frac{\partial(\overline{\rho}\tilde{\varepsilon})}{\partial t} + \nabla.\left(\overline{\rho}\widetilde{\vec{U}}\tilde{\varepsilon}\right) = \nabla.\left(\left[\mu + \frac{\mu_t}{\sigma_k}\right]\nabla\tilde{\varepsilon}\right) + \frac{\tilde{\varepsilon}}{\tilde{k}}(C_{\varepsilon 1}P - C_{\varepsilon 2}\overline{\rho}\tilde{\varepsilon}) \tag{10}$$

where P is the production rate of $\left(\overline{\rho}\tilde{k}\right)$;

$$P = 2\mu_t\left(\widetilde{\overline{\overline{S}}} : \widetilde{\overline{\overline{S}}} - \frac{1}{3}\left[\nabla.\widetilde{\vec{U}}\right]^2\right) - \frac{2}{3}\overline{\rho}\tilde{k}\left(\nabla.\widetilde{\vec{U}}\right) \tag{11}$$

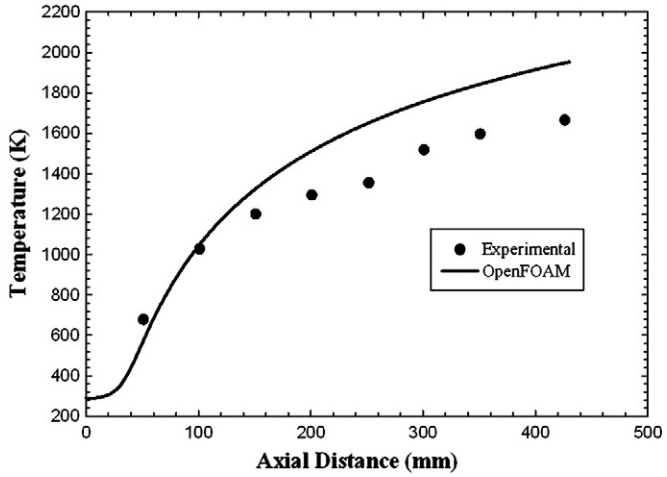

Fig. 1. Mean temperature at centerline.

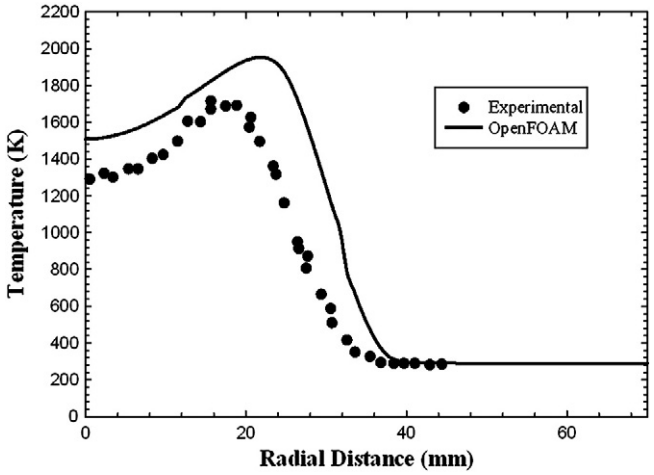

Fig. 3. Mean temperature at x = 200 mm.

$$\tilde{\bar{S}} = \frac{1}{2}\left(\nabla\tilde{U} + \nabla\tilde{U}^{T}\right) \tag{12}$$

The constants are $C_{\mu}=0.09$, $\sigma_k=1$, $\sigma_{\varepsilon}=1.3$, $C_{\varepsilon 1}=1.44$ and $C_{\varepsilon 2}=1.92$.

The above equations are closed except the species transport Eq. (4). The source term, ω_i is the reaction rate. Here comes the role of turbulent combustion modeling, where the eddy dissipation model was implemented.

$$\dot{\omega}_{fuel} = -A\overline{\rho}\frac{\varepsilon}{k}\, min\left(\widetilde{Y_{fuel}}, \frac{\widetilde{Y_{ox}}}{S}\right) \tag{13}$$

where A = 4 is a model constant and S is stoichiometric required oxygen in kilograms to burn one kilogram of the fuel.

4. Numerical model

The experimental setup as reported by Brookes and Moss [29] of the confined non-premixed flame has a combustor length of 1000 mm and a diameter of 155 mm. The fuel nozzle diameter is 4.07 mm with coaxial air inlet. The computational domain was assumed to be three dimensions axisymmetric; therefore the computational domain dimensions are 1000mm × 77.5 mm with wedge angle of 2°. The computational domain was discretized to 105,000 quadrilateral grid cells. The air and fuel velocity were 0.5 m/s and 20 m/s respectively with 5% free stream turbulence intensity for both fuel and air inlets.

As mentioned above, the EdmFoam1.4 solver is based on unsteady PISO algorithm with two pressure correctors and two momentum correctors per time step and convergence criteria for residuals 10^{-6}. The time step was selected to be 10^{-5} s with corresponding Courant (CFL) number of approximately 0.5. The discretization scheme for the unsteady term is implicit Euler scheme which is first order bounded [23]. Normalize Variable Diagram (NVD) schemes were used for the convective terms. The second order central difference schemes were used for diffusion terms and mass fluxes at face centers from cell values. The flow reached the steady state conditions after approximately 2 s. All results are reported after 2.5 s to ensure that the reacting flow has totally reached the steady state conditions. The convergence criterion for checking the steady state conditions is comparing the instantaneous temperature profiles at the flame centerline and different radial temperature profiles.

5. Results and discussion

5.1. Temperature at centerline

Fig. 1 shows the mean temperature values at the flame centerline. The axial temperature shows very good qualitative and quantitative agreement against the experimental measurements. There is minor

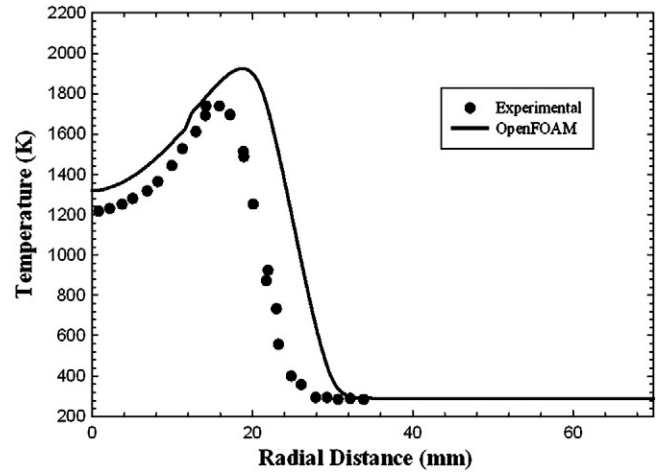

Fig. 2. Mean temperature at x = 150 mm.

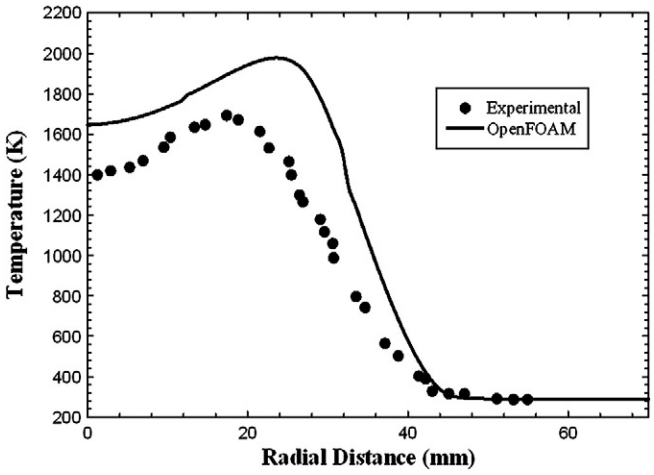

Fig. 4. Mean temperature at x = 250 mm.

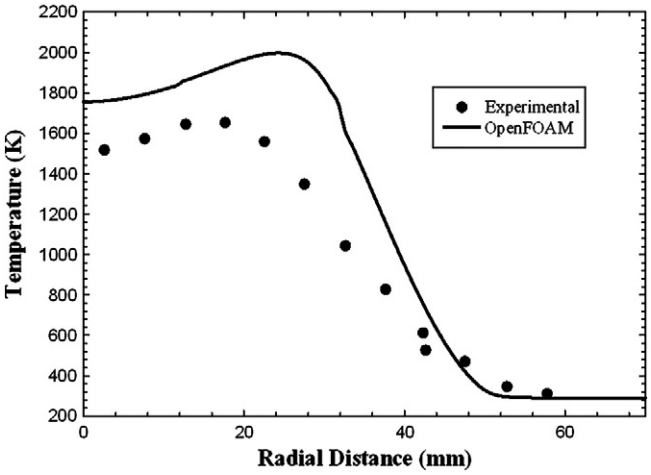

Fig. 5. Mean temperature at x = 300 mm.

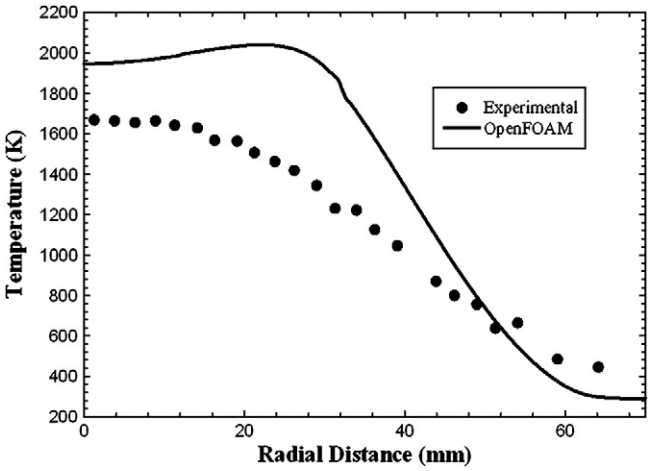

Fig. 7. Mean temperature at x = 425 mm.

gap in the quantitative results in the first 200 mm of the flame and it is growing gradually after that. For more investigation, the radial temperature profiles will be compared at different axial distances.

5.2. Radial temperature profiles

Figs. 2–7 show the radial temperature profiles at six different axial distances. They also show a very good agreement with the experimental data. Also as mentioned in the previous section that the gap between the quantitative increases as the axial distance increases especially after 200 mm. However the radial profiles show that the differences are not only on values but also in trends. Fig. 7 shows the most diversity in trend as expected from the previous results. These minor differences are most likely due to the performance of standard kepsilon model in free shear flows.

5.3. ANSYS-Fluent results

The aim of this section is to introduce a preliminary comparison between OpenFOAM results and ANSYS Fluent® results for the same case discussed above. This is meant for verifying the newly developed solver, EdmFoam1.4, against one of the most used commercial CFD codes. Fig. 8 shows this comparison for the axial temperature profile. It is clear from Fig. 8 that Fluent over predicted the temperature with a sudden drop by the end of the curve. This drop is an indicator of the flame tip. In the matter of fact, the experimental results show that the visible flame length is around 600 mm [29]. Quantitatively speaking, OpenFOAM predicted flame length is 660 mm while Fluent® predicted such length at approximately 407 mm (the flame length is calculated as the axial distance between the fuel inlet and the location of the maximum temperature on the flame).

This difference between EdmFoam1.4 and Fluent® in calculating the flame length is due to two main reasons. Firstly, Fluent calculates the reaction rate as the minimum value of three expressions of the products concentrations [30], although the original paper [8] of the EDM uses the products concentration equation for premixed flames only. Secondly, the EDM model implemented in Fluent® can be ignited by high temperature source not only by initializing the solution with value for products concentrations which shows that the Fluent® implementation of the EDM taking into account the value of the Arrhenius reaction rate. However, this inclusion of the Arrhenius reaction rate in the EDM of Fluent® is not revealed to its users, not even in the user manual of the software. Perhaps the EDM implementation of Fluent® can yield seemingly accurate results in some cases. However, it is difficult to claim that such results reflect, solely, the turbulence combustion interaction as described by the eddy dissipation model of Magnussen [8].

6. Conclusion

The eddy dissipation model was implemented successfully in OpenFOAM through the new EdmFoam1.4 solver. The model was

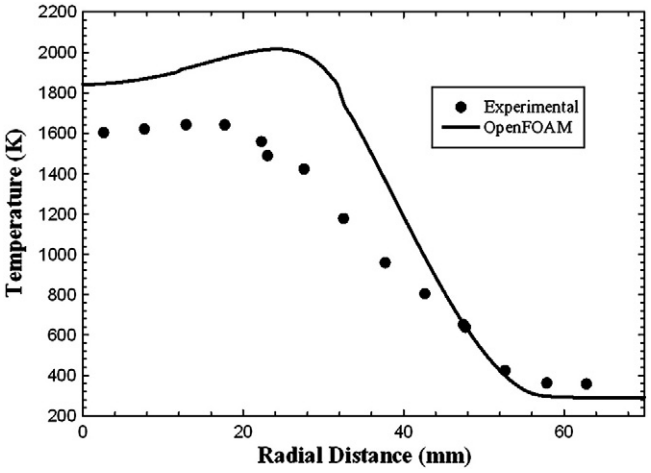

Fig. 6. Mean temperature at x = 350 mm.

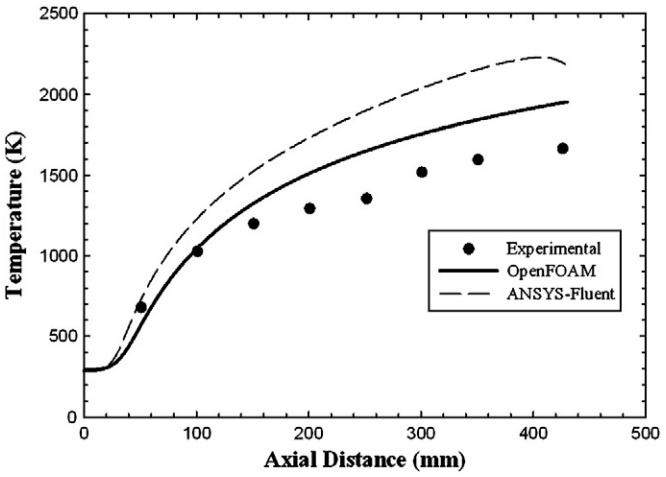

Fig. 8. Mean temperature at centerline.

used for modeling confined co-flowing non-premixed jet flame. The results showed very good agreement in both qualitative and quantitative aspects. The mean temperature at centerline was compared with Fluent® predictions. Fluent showed over predictions in temperature values and under prediction in flame length. It is highly recommended to investigate Fluent® modifications and its effect on results for different cases. Many future validation cases for the new solver with different flame configurations will be done to investigate the solver performance and model capabilities.

Acknowledgements

This work has been funded by the Ministry of Higher Education of Malaysia (MOHE) under grant FRGS-VOT 78587. The authors would like to thank Dr. Chris Greenshields, the head of OpenFOAM training for his motivational OpenFOAM training course and for his continuing support for the OpenFOAM community.

References

[1] N. Peters, Turbulent Combustion, Cambridge University Press, UK, 2000.
[2] T. Poinsot, D. Veynante, Theoretical and Numerical Combustion, Edwards Publishing. PA, USA, 2001.
[3] V. Artemov, S.B. Beale, G. de Vahl Davis, M.P. Escudier, N. Fueyo, B.E. Launder, E. Leonardi, M.R. Malin, W.J. Minkowycz, S.V. Patankar, A. Pollard, W. Rodi, A. Runchal, S.P. Vanka, A tribute to D.B. Spalding and his contributions in science and engineering, International Journal of Heat and Mass Transfer 52 (17–18) (2009) 3884–3905.
[4] E.E. Khalil, D.B. Spalding, J.H. Whitelaw, The calculation of local flow properties in two-dimensional furnaces, International Journal of Heat and Mass Transfer 18 (6) (1975) 775–791.
[5] D.B. Spalding, Mixing and chemical reaction in steady confined turbulent flames, Symposium (International) on Combustion 13 (1) (1971) 649–657.
[6] D.B. Spalding, Development of the Eddy-Break-Up Model of Turbulent Combustion, 1976, pp. 1657–1663.
[7] D.B. Spalding, Development of the eddy-break-up model of turbulent combustion, Symposium (International) on Combustion 16 (1) (1977) 1657–1663.
[8] B.F. Magnussen, B.H. Hjertager, On mathematical modeling of turbulent combustion with special emphasis on soot formation and combustion, Symposium (International) on Combustion 16 (1) (1977) 719–729.
[9] D. Achim, J. Naser, Y.S. Morsi, S. Pascoe, Numerical investigation of full scale coal combustion model of tangentially fired boiler with the effect of mill ducting, Heat and Mass Transfer/Waerme- und Stoffuebertragung 46 (1) (2009) 1–13.
[10] Y.L. Huang, H.R. Shiu, S.H. Chang, W.F. Wu, S.L. Chen, Comparison of combustion models in cleanroom fire, Journal of Mechanics 24 (3) (2008) 267–275.
[11] K.M. Saqr, H.S. Aly, M.M. Sies, M.A. Wahid, Effect of free stream turbulence on NOx and Soot formation in turbulent diffusion CH4-air flames, International Communications in Heat and Mass Transfer 37 (6) (2010) 611–617.
[12] K.M. Saqr, M.M. Sies, M.A. Wahid, Numerical investigation of the turbulence combustion interaction in non-premixed CH_4/air flames, International Journal of Applied Mathematics and Mechanics 5 (8) (2009) 69–79.
[13] K.M. Saqr, M.M. Sies, H.M. Ujir, M.A. Wahid, Whirling flames for fuel economy and low NOx combustion in: Proceedings of the 10th Asian International Conference on Fluid Machinery, American Institute of Physics, KL, Malaysia, 2009, pp. 225–235.
[14] D. Chatterjee, A. Datta, A.K. Ghosh, S.K. Som, Effects of inlet air swirl and spray cone angle on combustion and emission performance of a liquid fuel spray in a gas turbine combustor, Journal of the Institution of Engineers (India): Aerospace Engineering Journal 85 (2) (2004) 41–46.
[15] T. Gassoumi, K. Guedri, R. Said, Numerical study of the swirl effect on a coaxial jet combustor flame including radiative heat transfer, Numerical Heat Transfer; Part A: Applications 56 (11) (2009) 897–913.
[16] H.C. Cho, Y.K. Lee, Reactor performance with primary/secondary swirl intensity and direction in coal gasification process, International Journal of Energy Research 25 (13) (2001) 1151–1163.
[17] K. Majidi, CFD modeling of non-premixed combustion in a gas turbine combustor, in: U.S. Rohatgi, D. Mewes, J. Betaille, I. Rhodes (Eds.), American Society of Mechanical Engineers, Fluids Engineering Division (Publication) FED, Montreal, Que., 2002, pp. 971–977.
[18] J. Ha, Z. Zhu, Computation of turbulent reactive flows in industrial burners, Applied Mathematical Modelling 22 (12) (1998) 1059–1070.
[19] M. Naitoh, F. Kasahara, R. Kubota, I. Ohshima, Analysis on pipe rupture of steam condensation line at Hamaoka-1, (II): hydrogen combustion and pipe deformation, Journal of Nuclear Science and Technology 40 (12) (2003) 1041–1051.
[20] Z.M. Liu, H.Z. Hao, Y.M. Jin, H.M. Liu, C.F. Ma, Influence of finite chemistry reaction rate model on high temperature air combustion, Beijing Gongye Daxue Xuebao / Journal of Beijing University of Technology 33 (4) (2007) 413–418.
[21] H.G.W.a.G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, COMPUTERS IN PHYSICS 12 (6) (1998).
[22] in, www.openfoam.com.
[23] OpenFOAM, OpenFOAM user guide, 2010.
[24] F. Brusiani, G.M. Bianchi, T. Lucchini, G. D'Errico, Implementation of a finite-element based mesh motion technique in an open source CFD code, in: Proceedings of the Spring Technical Conference of the ASME Internal Combustion Engine Division, Milwaukee, WI, 2009, pp. 611–624.
[25] J. Fradera, L. Batet, E. Mas De Les Valls, L. Sedano, Numeric implementation of two-phase tritium transport models for natural helium nucleated bubbles in lead–lithium. Implications for HCLL breeding blanket channels, Proceedings—Symposium on Fusion Engineering, 2009., San Diego, CA.
[26] W. Mitianieca, Combustion of CNG in charged spark ignition engines, AIP Conference Proceedings, Czestochowa, 2009, pp. 98–113.
[27] H. Weller, Predicting mesh density for adaptive modelling of the global atmosphere, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 367 (1907) (2009) 4523–4542.
[28] L.F.L.R. Silva, R.B. Damian, P.L.C. Lage, Implementation and analysis of numerical solution of the population balance equation in CFD packages, Computers & Chemical Engineering 32 (12) (2008) 2933–2945.
[29] S.J. Brookes, J.B. Moss, Measurements of soot and thermal radiation from confined turbulent jet diffusion flames of methane, Combustion and Flame 116 (1999) 49–61.
[30] ANSYS Fluent theory and user guide.
[31] J. Chomiak, A. Karlsson, Flame Liftoff in Diesel Sprays, Twenty-sixth Symposium (International) on Combustion/The Combustion Institute, 1996, pp. 2557–2564.
[32] O.A. Marzouk, D. Huckaby, A comparative study of eight finite-rate chemistry kinetics for CO/H2 combustion, Engineering applications of computational fluid mechanics 4 (3) (2010) 331–356.
[33] HiREF, http://www.fkm.utm.my/hiref/.