Further development of the modified Eddy Dissipation Model

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Abstract. The eddy dissipation model (EDM) has been used extensively in turbulent combustion modelling because of its simplicity, good convergence, and reasonable accuracy. A modified EDM model was developed to improve the accuracy of the model a few years ago. In the application for the jet flame and the opposed jet flame, it demonstrates very good accuracy. However, in the application for the bluff body diffusion flames, its accuracy is not good enough. In the current study, it is found out that the existence of wall of these flames influences the simulation accuracy. In the region near the wall, the ratio of turbulence dissipation rate to turbulent kinetic energy is too large and causing too high combustion reaction rate which is not realistic. By adding a limit to this ratio, the reaction rate near wall will be reasonable. The further developed modified version of EDM model gives very good prediction accuracy for the jet flow and the bluff body flow. With this near wall treatment, the modified EDM model will show good performance for internal combustion and free jet combustion.

1. Introduction

In the field of energy and power, combustion is a basic energy conversion method and has been widely used in various engineering practices. The complexity of turbulent combustion has led many scholars to carry out various researches on it. It is of great significance to establish a reasonable turbulent combustion model for CFD simulation of turbulent flames and its applications in engineering practices. The Eddy Dissipation Model (EDM) has been widely used in CFD simulation of turbulent non-premixed flames due to its simplicity and good accuracy.

The eddy dissipation model is based on the following three assumptions: (1) the combustion reaction rate is fast; (2) the fuel consumption rate of the turbulent diffusion flame depends only on the turbulent mixing rate of fuel and oxygen; (3) the fuel consumption rate is inversely proportional to turbulent time scale (kinetic energy divided by turbulent dissipation rate). Based on the above three assumptions, Magnussen and Hjertager [1] give the equations for the reaction rates:

\[ f + o = (1 + S) p \]  

\[ R = \rho \frac{\varepsilon}{k} A \cdot \min[Y_f, \frac{Y_o}{S}, B \cdot \frac{Y_o}{(1 + S)}] \]

Where \( f \) is fuel; \( o \) is oxidant; \( p \) is product; \( S \) is stoichiometric mass ratio of oxidant to fuel; \( \rho \) is density;
\( \varepsilon \) is turbulent dissipation rate; \( k \) is turbulent kinetic energy; \( Y \) is mass fraction; \( A=4 \) and \( B = 0.5 \). \( A \) is used for the simulation of diffusion flames and \( B \) is used for premixed flames. The EDM model has been applied to CFD commercial software such as Fluent, STAR-CD, CFX because of its reasonable assumptions, fast calculation and good convergence. The EDM model has been widely used in many scenarios including gas turbine combustion [2-4].

Wang [5] used the EDM model to simulate 7 round jet flames and 4 opposed jet flames. With \( A = 4 \), the simulated temperature field was significantly different from the experimental data. It is pointed out that each flame has an optimal \( A \) value and the optimal \( A \) value has certain correlation with the turbulent Reynolds number in the reaction zone (the larger the Reynolds number, the smaller the \( A \) value). The modified EDM model was proposed:

\[
R = \rho A_{\text{local}} \frac{\varepsilon}{k} [Y f \left( \frac{Y}{S} \right)] \quad (3)
\]

\[
A_{\text{local}} = 145 / \text{Re}_{\varepsilon,\text{local}}^{0.9} \quad (4)
\]

\[
\text{Re}_{\varepsilon,\text{local}} = 0.164 \frac{\rho k^2}{\mu \varepsilon} \quad (5)
\]

Where \( \mu \) is the dynamic viscosity. \( A \) is a variable related to the local Reynolds number. The modified EDM model predicts very good temperature field for 7 round jet flames and 4 opposed jet flames. Wang [6] tested the modified EDM model with three non-premixed bluff body flames and five non-premixed swirling flames. The result is not very good. For the bluff body flame, the combustion rate near the wall is over estimated. This might be the main cause of the inaccuracy for the application in the bluff body flame. For the swirling flames, the flow field is hard to be calculated accurately with regular two-equation turbulence model, the failure in flow field calculation might be the main cause for the application in the swirling flame. Also the over estimation of the near wall reaction rate might contribute a little.

This paper will further improve the modified EDM model. The model is mainly improved in the following aspects.

(1) The transport properties such as viscosity, conductivity, and mass diffusivity in the reference [5] are constants. This treatment is suitable for strong turbulent flow where turbulent mixing is dominating. But it is not suitable for weak turbulent combustion. In this paper, the transport properties such as viscosity, mass diffusivity and thermal conductivity are set as functions of temperature, and the mixing rules are used for mixture. The usage of these real properties will make the model suitable for both strong and weak turbulent combustion.

(2) When using the EDM model to simulate the combustion reaction, the dissociation of combustion products such as \( \text{H}_2\text{O} \) and \( \text{CO}_2 \), etc. is not considered, resulting in a calculated flame temperature higher than the actual value. The model proposed by Wang [5-6] corrects this by increasing the specific heat of the combustion product. This is ok for subsonic flow where the correct specific heat and molecular weight are not important. However, the accurate value of these are crucial for the supersonic combustion. Using the dissociation reactions such as \( 2\text{H}+\text{M}=\text{H}_2+\text{M} \), \( \text{H}+\text{OH}+\text{M}=\text{H}_2\text{O}+\text{M} \), \( \text{H}+\text{O}+\text{M}=\text{OH}+\text{M} \), \( \text{CO}+\text{O}(\text{+M})=\text{CO}_2(\text{+M}) \) will solve the problem and make the model applicable for both subsonic flow and supersonic flow.

(3) In the vicinity of the wall surface, since the value of the kinetic energy \( k \) becomes very small, the value of \( \varepsilon/k \) is very large, so that the combustion reaction rate near the wall surface is very large, which is not true in reality. The value of \( \varepsilon/k \) should be limited to a suitable value so that the reaction rate near wall is more realistic.
Wang [6] could not establish a general turbulent combustion model for the swirling flames, which is most likely caused by inaccurate calculation of the flow field of swirling flames. In this paper, the swirling flames are removed and we will try to establish a general turbulent combustion model.

In this paper, six jet flames and three bluff body flames are selected from the experimental database of Sandia Lab [7] and Sydney Lab [8]. The fuel jet nozzle diameter, the fuel composition, and the jet velocity are shown in Table 1.

For the bluff flame (Fig.1), the blunt body surface is ceramic insulation surface, its diameter is D=50mm, and the air outlet is 150mm*150mm. The air velocity is 40 m/s and the fuel is a mixture of 50%CH₄ and 50%H₂.

![Figure 1. Schematic diagram of turbulent non-premixed bluff body flame [8]](image)

The detailed parameters of the turbulent non-premixed jet flame and bluff body flame are shown in Table 1:

| Burner | Nozzle diameter (mm) | Fuel velocity (m/s) | Fuel Composition | Coflow air velocity (m/s) |
|--------|----------------------|---------------------|------------------|---------------------------|
| 1 Jet  | 3.75                 | 296                 | 100%H₂           | 1                         |
| 2 Jet  | 3.75                 | 294                 | 80%H₂, 20%HE     | 1                         |
| 3 Jet  | 4.58                 | 76                  | 30%H₂, 40%CO, 30%N₂ | 0.75                      |
| 4 Jet  | 7.72                 | 45                  | 30%H₂, 40%CO, 30%N₂ | 0.75                      |
| 5 Jet  | 8                    | 63.2                | 22.1%CH₄, 33.2%H₂, 44.7%N₂ | 0.3                       |
| 6 Jet  | 8                    | 42.2                | 22.1%CH₄, 33.2%H₂, 44.7%N₂ | 0.3                       |
| 7 Bluff| 3.6                  | 118                 | 50%H₂, 50%CH₄    | 40                        |
2. CFD settings

The commercial CFD software STAR-CCM+ is used for numerical simulation. The K-Epsilon low RE model is chosen for turbulence modeling. When simulating jet flames, the K-Epsilon model overpredicts the turbulent dissipation [9], resulting in shorter flame height. By adjusting the model parameter $C_{t1}$ of the turbulent dissipation equation [10], the turbulent dissipation can be reduced, and the calculated flame height is guaranteed to be consistent with the experiment (the calculated axial temperature peak position coincides with the experimental position). The K-Epsilon turbulence model parameter $C_{t1}$ of the flame 1~9 is set to 1.5, 1.5, 1.565, 1.555, 1.58, 1.54, 1.56, 1.56, 1.56 respectively.

The boundary conditions such as fuel composition, fuel velocity, and co-flow air velocity is set according to experimental data [7-8]. Because the turbulence parameters of the combustion zone are mainly generated by the shear flow of the jet flow and the co-flow, the turbulence parameters of the fuel nozzle outlet have little effect on the simulation results. The turbulent boundary conditions of the nozzle have been varied to check this insensitivity. The turbulence parameters of the nozzle outlet are established according to the available experimental data. Some experimental conditions are not specified. The turbulence intensity of 5% and the turbulence length 50% nozzle diameter are used. The species transport properties are calculated with polynomial functions of temperature. The mass fraction average value is calculated for mixture. The normal NASA format is used for species specific heat.

The following reversible dissociation reactions are used: $2H^+M = H_2+M$, $H+OH+M = H_2O+M$, $H+O+M = OH+M$, $CO+O(+M) = CO_2(+M)$. In order to limit the reaction rate near wall, the value of $\varepsilon/k$ is limited to less than 10000s$^{-1}$.

For the turbulent combustion of $H_2$, $CO$ and $CH_4$, one-step chemical reactions are used: $H_2 + 0.5O_2 = H_2O$, $CO + 0.5O_2 = CO_2$, $CH_4 + 2O_2 = CO_2 + 2H_2O$. Considering the influence of high temperature flame radiation, a volumetric heat source is set using field function.

$$q_v = -4\sigma K_p (T_h^4 - T_\infty^4)$$

(6)

$$K_p = P_{CO_2}K_{CO_2} + P_{CO}K_{CO} + P_{H_2O}K_{H_2O}$$

(7)

$T_\infty$ is the ambient temperature, $\sigma$ is the Stephen-Boltzmann constant, $K_p$ is the Planck absorption coefficient of the mixture, and $P_i$ and $K_i$ are the partial pressure and Planck absorption coefficient of the components $i$. $K_i$ is a function of temperature [11].

Because geometry and physics are axisymmetric, the circumferential direction is not simulated. The calculation domain is fan-shaped in the circumferential direction, and one layer grid is arranged in the circumferential direction. Its two sides are set as symmetry planes. The simulation domain guarantees at least 2 times of the flame height in the axial direction and at least 1.5 times of air outlet diameter in the radial direction. The quality of the grid affects the simulation result, the convergence and the simulation time. Taking the flame 1 case as an example, the number of meshes is 66878, except that the mesh next to the central axis is a prismatic mesh, and the rest are hexagonal meshes. Through the grid density test, the mesh independence is guaranteed. The grid distribution is not uniformly distributed, with more grids placed near the fuel nozzle outlet and fewer grids in the areas axially and radially away from the center.
3. Results and discussion

The modified eddy dissipation model is proposed as,

\[ R = \rho A_{local} W \cdot \left[ Y, \frac{Y}{5} \right], \quad W = \min \left( \frac{e}{k}, 10000 \right) \]  

(8)

\[ A_{local} = \frac{35}{Re_{r,local}^{0.9}} \]  

(9)

\[ Re_{r,local} = 0.164 \frac{\rho k^2}{\mu \varepsilon} \]  

(10)

The \( \mu \) here is a variable connected with temperature. Six non-premixed jet flames were calculated and three non-premixed bluff body flames were calculated by the modified EDM model. The simulation results are compared with the experimental data. Due to the space limitation, this paper presents the comparison of the axial temperature for flames 1–6, the comparison of the radial temperature for flame 4, the comparison of the radial temperature for flames 7–9.

Figure 2. Axial temperature comparison of flame 1, experimental data source from Sandia National Laboratory (www.sandia.gov/TNF/)
**Figure 3.** Axial temperature comparison of Flame 2, experimental data source from Sandia National Laboratory (www.sandia.gov/TNF/)

**Figure 4.** Axial temperature comparison of Flame 3, experimental data source from Sandia National Laboratory (www.sandia.gov/TNF/)

**Figure 5.** Axial temperature comparison of Flame 4, experimental data source from Sandia National Laboratory (www.sandia.gov/TNF/)
Figure 6. Radial (154.4 mm above nozzle exit) temperature comparison of flame 4, experimental data source from Sandia National Laboratories (www.sandia.gov/TNF/)

Figure 7. Radial (231.6 mm above nozzle exit) temperature comparison of flame 4, experimental data source from Sandia National Laboratories (www.sandia.gov/TNF/)

Figure 8. Radial (308.8 mm above nozzle exit) temperature comparison of flame 4, experimental data source from Sandia National Laboratories (www.sandia.gov/TNF/)
**Figure 9.** Radial (386mm above nozzle exit) temperature comparison of flame 4, experimental data source from Sandia National Laboratories (www.sandia.gov/TNF/)

**Figure 10.** Radial (463.2mm above nozzle exit) temperature comparison of flame 4, experimental data source from Sandia National Laboratories (www.sandia.gov/TNF/)

**Figure 11.** Axial temperature comparison of Flame 5, experimental data source from Sandia National Laboratory (www.sandia.gov/TNF/)
Figure 12. Axial temperature comparison of flame 6, experimental data source from Sandia National Laboratory (www.sandia.gov/TNF/)

Figure 13. Radial (120 mm above nozzle exit) temperature comparison of flame 7, experimental point data source [8]

Figure 14. Radial (13 mm above nozzle exit) temperature comparison of flame 8, experimental point data source [8]
Figure 15. Radial (65 mm above nozzle exit) temperature comparison of Flame 7, experimental point data source [8]

From the above comparison (Figure 2–15), it can be seen that the newly modified EDM model predicts the round jet flame and the bluff body flames pretty well.

4. Conclusion

The modified EDM model is further developed. The main modification are using the accurate transport properties to extend it applicability for low turbulence flow, using the dissociation reactions to extend its applicability to supersonic flow, using the limitation of $\varepsilon/k$ to give more real near wall reaction rate. Six round jet flames and three bluff body flames are simulated and the result are compared well with the experimental data.

References

[1] Magnussen B and Hjertager B 1977 On Mathematical Modelling of Turbulent Combustion With Special Emphasis on Soot Formation and Combust J. Symposium on Combustion. 16(1):719-729.
[2] Gabler H, Yetter R, Glassman I 1998 Asymmetric whirl combustion-A new approach for non-premixed low NO (x) gas turbine combustor design C(34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit. 3530)
[3] Mongia H 2013 Recent Progress in Comprehensive Modeling of Gas Turbine Combustion (AIAA Aerospace Sciences Meeting & Exhibit)
[4] Gobbato P, Masi M, Toffolo A 2011 Numerical simulation of a hydrogen fuelled gas turbine combustor J. International Journal of Hydrogen Energy. 36(13):7993-8002.
[5] Wang P Y 2015 The model constant A of the eddy dissipation model J. Prog Comput Fluid Dyn. 16(2).
[6] Li Q, Yang H, Wang P Y 2015 Accuracy improvement of the modified EDM model for non-premixed turbulent combustion in gas turbine J. Case Studies in Thermal Engineering. 6:69-76.
[7] Sandia National Lab (International Workshop on Measurement and Computation of Turbulent Non-Premixed Flames:http://www.ca.sandia.gov/TNF/abstract.html)
[8] AR Masri (Flame database:www.sydney.edu.au/engineering/aeromech/thermofluids/database.html)
[9] Pope S 1978 An explanation of the turbulent round-jet/plane-jet anomaly J. AIAA journal. 16(3): 279-281
[10] Morse A 1980 Axisymmetric free shear flows with and without swirl J
[11] Ju Y, Guo H, Liu F 1999 Effects of the Lewis number and radiative heat loss on the bifurcation and extinction of CH4/O2-N2-He flames J. Journal of Fluid Mechanics. 379:165-190.