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Modification of Arrhenius Model for Numerical Modelling of Turbulent Flames

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ABSTRACT

For finite rate modeling of reactions, two major models are Arrhenius model and Eddy-dissipation model. Arrhenius model is used to simulate laminar flames and Eddy-dissipation for turbulence reactions. Arrhenius model is inaccurate for simulation of turbulent combustion because of ignoring turbulent fluctuations. In the present study, the Arrhenius model has been modified using a sine function to calculate the effect of temperature fluctuations on reaction rate. Simulation of combustion has been done by Sprint CFD code for the prediction of temperature distribution, rate of reaction and CO mass fraction. Comparison of results of modified Arrhenius model with the eddy-dissipation model and Experimental data show that the modified Arrhenius model has good agreement with the eddy-dissipation model and has a qualitative trend same as experimental data.
Keywords: Eddy-dissipation, Fluctuation, Reaction rate, Sine function

1. INTRODUCTION

Combustion plays an important role in many industrial applications because it is the main source of producing power and energy. Also from an environmental point of view, emission of pollutants due to combustion causes significant health problems [1-3]. Therefore, study of combustion is an important issue for many investigators. Since experimental investigation of combustion is expensive, numerical simulation has been used for decades. Numerical methods have become powerful tools to simulate complex combustion processes and to understand the physics involved [4].

For simulation of combustion, Arrhenius model, the eddy-dissipation model, and the PDF model are widely used in CFD. The PDF model could be able to simulate detailed finite-rate kinetics. However, it needs a large computer memory and computation time. Therefore, the model is used only for simple flows [5]. One of the most practical models is the eddy-dissipation model, because it is easy to implement and its results are acceptable for premixed and non-premixed flames [6]. In the eddy-dissipation model, every reaction is the same and the model only takes into account the turbulent rate. Therefore, the model should be used only for one-step global reaction and it cannot predict radical species. Multi-step chemical mechanisms are based on Arrhenius rates, and the Arrhenius model computes rate of reaction using Arrhenius expressions. The Arrhenius model is exact for laminar flames, but is inaccurate for turbulent flames, because this model ignores turbulent fluctuations that are effective on rate of reaction, temperature, and concentration of pollutants [7].

Shang et al. [8] investigated Effects of gas temperature fluctuation on the instantaneous char reaction of pulverized coal particle. Their results show that the gas temperature fluctuation leads to both faster char reaction and particles size reduction. In the other research[9], they show that the particle instantaneous temperature with the gas temperature fluctuation is different from that without the gas temperature fluctuation. Temperature fluctuations have a significant role in NO formation. The recent study indicates that thermal NOx production doubles for every 90 K temperature increase when the temperature is about 2200 K. Zhang and Zhang [10] studied effects of gas temperature fluctuation on the NO release from coal particle during char combustion. Their results represent that NO formation during the char combustion is further increased by the increase in the fluctuation amplitude of the gas temperature. Also, their investigations on Instantaneous de-volatilization of coal particles in a hot gas show that the particles lose their mass at a higher rate with the gas temperature fluctuation than without the gas temperature fluctuation [11]. Therefore, the Arrhenius model needs some corrections for turbulent flames.

Our aim in this paper is the modification of the Arrhenius model for simulation of turbulent combustion flames. For this purpose, effects of temperature fluctuations are considered by using a time-varying function. Also, to investigate the accuracy of the modified model, Temperature distribution of this model compares with eddy-dissipation model and experimental data. The results show that the modified Arrhenius model has good agreement with eddy-dissipation model.

2. Mathematical modeling

The mathematical modeling is the based on work of reference [12]. In this section, only numerical combustion modeling will be determined, because this is the main work of the present study.

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Combustion modeling

The energy addition due to combustion is determined in consideration of two-step, irreversible, global reaction following finite rate chemistry as:

$$C_{16}H_{34}+24.5(O_2+3.76N_2)\rightarrow 16CO+17H_2O+92.12N_2 \quad (1)$$

$$CO + 0.5O_2 \rightarrow CO_2 \quad (2)$$

The Arrhenius model and the eddy-dissipation model are used for combustion modeling. Rate of reaction in the eddy-dissipation model is controlled by turbulent mixing and is determined as followed[13]:

$$R_j = \rho A \frac{\varepsilon}{k} \min[\ S_F m_F , m_{O_2}\ ] \quad (3)$$

The Arrhenius model computes rate of reaction using Arrhenius expressions. Rate of reaction is described at the mean temperature and obtained using following the equation:

$$R(\overline{T}) = A\exp(\frac{-E}{R\overline{T}})C_F{}^{\alpha} C_{O_2}{}^{\beta} \quad (4)$$

In this paper, Temperature fluctuates with time around some mean represented by the form [14]:

$$\frac{T}{\overline{T}} = 1 + a_n f(t) \quad (5)$$

Where a_n is the amplitude of the fluctuation and *f(t)* is some time-varying function in which:

$$-1 \le f(t) \le 1 \quad \text{and} \quad \overline{T} = \frac{1}{\tau}\int_0^{\tau} T dt \quad (6)$$

T(t) can be considered to be composed of $\overline{T} + T'(t)$ where *T'* is the fluctuating component around the mean. Instantaneous rate of reaction is:

$$R(T) = A\exp(\frac{-E}{RT})C_F{}^{\alpha} C_{O_2}{}^{\beta} \quad (7)$$

Dividing the two expressions (4) and (7), one obtains:

$$\frac{R(T)}{R(\overline{T})} = \exp\{(\frac{E}{R\overline{T}})[1-(\frac{\overline{T}}{T})]\} \quad (8)$$

Obviously, then, for small fluctuations:

$$1-(\frac{\overline{T}}{T}) = \left[\frac{a_n f(t)}{[1+a_n f(t)]}\right] \approx a_n f(t) \quad (9)$$

The expression for the mean rate is written as:

$$\frac{\overline{R(T)}}{R(\overline{T})} = \frac{1}{\tau}\int_0^{\tau}\frac{R(T)}{R(\overline{T})}dt = \frac{1}{\tau}\int_0^{\tau}\exp(\frac{E}{R\overline{T}}a_n f(t))dt = \quad (10)$$

$$\frac{1}{\tau}\int_0^{\tau}[1+\frac{E}{R\overline{T}}a_n f(t) + \frac{1}{2}(\frac{E}{R\overline{T}}a_n f(t))^2 + ...]\,dt$$

But recall:

$$\int_0^{\tau} f(t)dt = 0 \quad (11)$$

If the fluctuations are considered sinusoidal, then [14]:

$$R(T) = R(\overline{T})[1+\frac{1}{4}(\frac{E}{R\overline{T}}a_n)^2] \quad (12)$$

3. Numerical Procedure

Sprint CFD code, that is an early version of Fluent [15], was used to simulate the processes inside the furnace [16]. The gas conservation equations were solved using a control-volume based computational procedure. The power law scheme was used to discretize the convective terms. The flow field pressure linked equations were solved by the SIMPLE algorithm. The set of algebraic equations were solved sequentially with the line-by-line method which is the combination of Gauss-Seidel method and the tridiagonal-matrix algorithm. The convergence criterion was determined by the requirement that the maximum value of the normalized residuals of any equation must be less than 1×10^{-5}. A numerical mesh of 100×36 grid nodes was used after several experiments, which showed that further refinement in either direction did not change the result

(maximum difference in velocity and other scalar functions in the carrier phase) by more than 2%. The grid spacing in axial and radial directions were changed smoothly to minimize the deterioration of the formal accuracy of the discretization scheme due to variable grid spacing and in such a way higher concentration of nodes occur near the inlet.

4. RESULTS AND DISCUSSION

Numerical simulations are performed for a cylindrical combustor with the internal diameter 20 cm and length 250 cm. Figure 1 shows furnace schematic plane. The furnace boundary conditions are given in table 1. The fuel spray is considered to consist of a finite size range, with the size distribution specified by the Rosin–Rammler function.

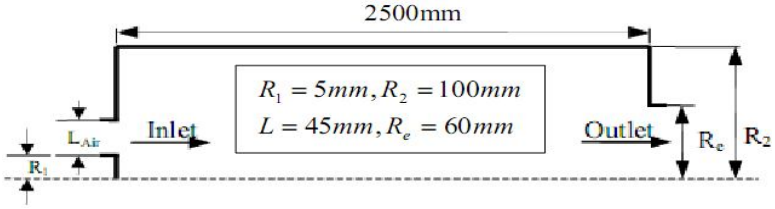

Figure 1. Schematic of the combustor

Table1- Boundary conditions

Velocity of Inlet Air(m/s)	3.45
Swirl Number of Inlet Air	0.25
Fuel Mass Flow(Kg/s)	$5.0*10^{-4}$
Equivalence Ratio	0.44
Minimum diameter of fuel droplets	[10-50] µm
Maximum diameter of fuel droplets	[60-120] µm
Inlet Air Temperature(K)	600
Chamber Wall Temperature(K)	1300
Fuel Spray Temperature(K)	333

To establish the accuracy of the present study, a comparison of the axial temperature distribution between numerical modeling result and experimental data under a similar condition is presented in Figure 2. It is observed that numerical results are in good qualitative agreement with the experimental data trend [17]. Also, this CFD code has been validated in the previous works [4, 12, 16].

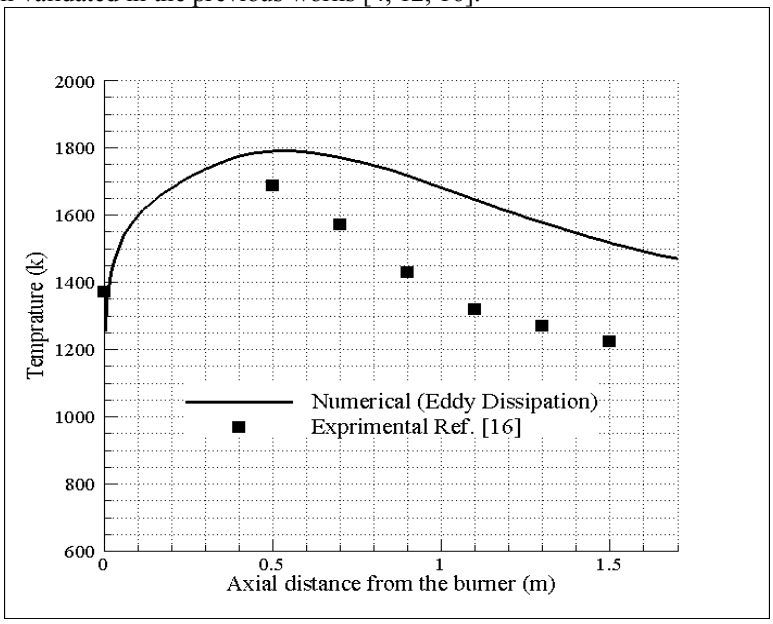

Figure 2. The comparison of axial temperature distribution between numerical result and experimental data

Figures 3 represent contour of O_2 reaction rate for three models. It is seen that oxygen and fuel burn as soon as they enter the combustor for the eddy- dissipation model. Also, the modified Arrhenius model can predict this behavior very close to the eddy-dissipation model result. However, reactants burn slowly for the Arrhenius model. The reason is the Arrhenius model ignores turbulent fluctuations that its maximum is in the jet outlet.

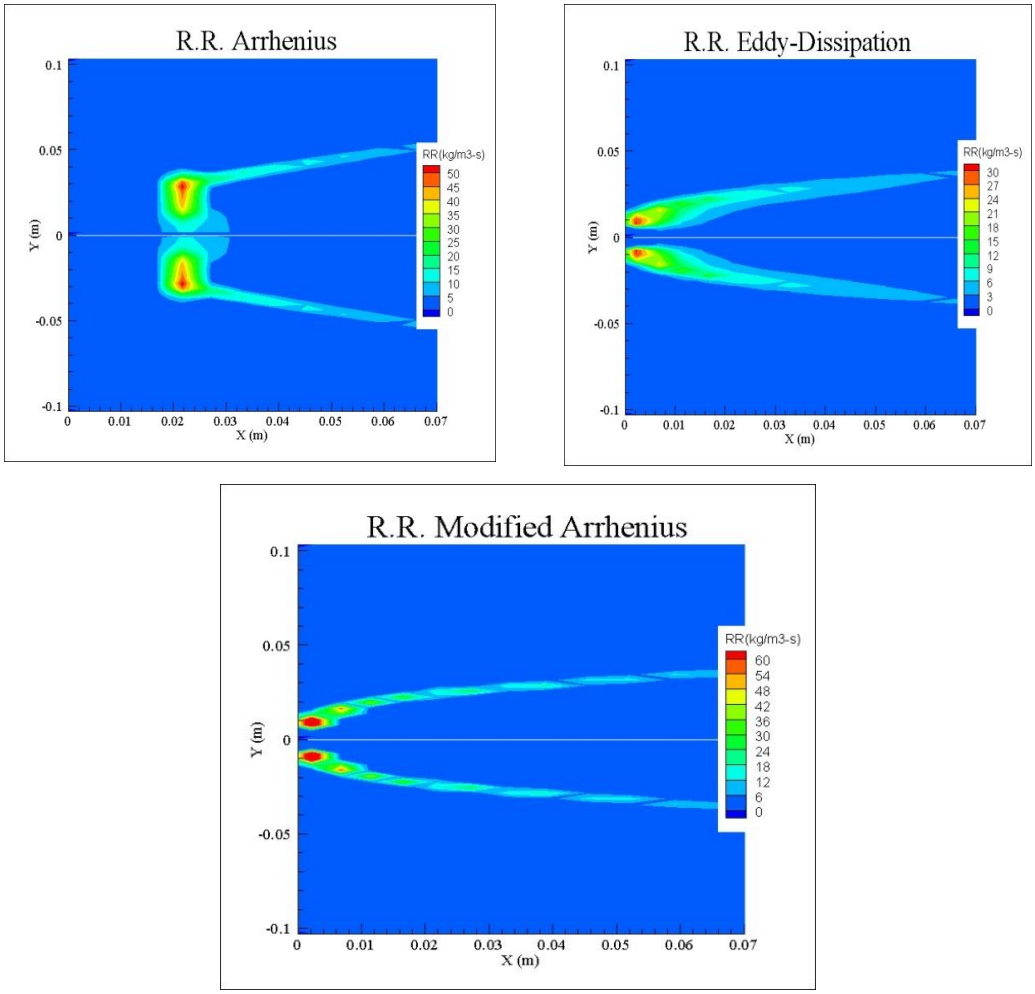

Figure 3. The comparison contour of O_2 reaction rate at the inlet

Figure 4 compares the predictions of radial temperature distribution for the Arrhenius model, the modified Arrhenius model, and the eddy-dissipation model at the inlet. The results show that trend and behavior of the modified Arrhenius model is the same as the eddy-dissipation model. However, the behavior of the Arrhenius model is very different from the eddy-dissipation model.

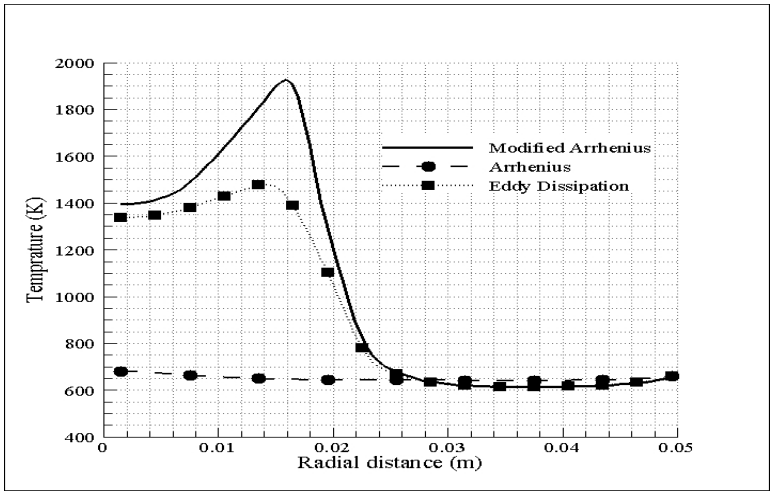

Figure 4. The comparison of radial temperature distribution at the inlet

Figure 5 demonstrates the effect of the inlet turbulence kinetic energy on computed maximum temperature inside the combustor for the Arrhenius model, the modified Arrhenius model and the eddy-dissipation model. In this figure, it is observed that the modified Arrhenius model results have been affected by turbulence kinetic energy. Also, these results have a qualitative trend same as the eddy-dissipation model. The turbulence kinetic energy has a significant effect on temperature because of it causes enhancement of the mixing rate and therefore a better combustion. Never can the Arrhenius model predict the effect of turbulence kinetic energy on combustion.

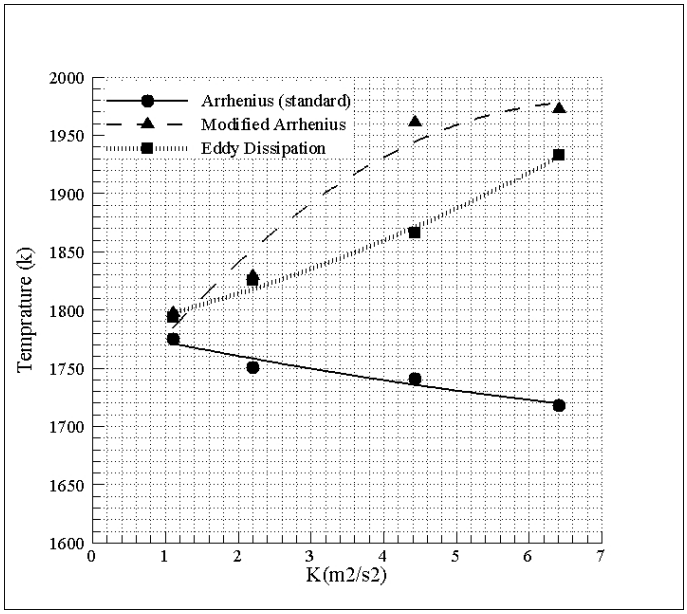

Figure 5. Effect of the turbulence kinetic energy on maximum temperature inside the combustor

A comparison of the axial temperature distribution between the modified Arrhenius model and the eddy-dissipation model is presented in Figure 6. It can be seen that the modified Arrhenius model has good agreement with the eddy-dissipation model.

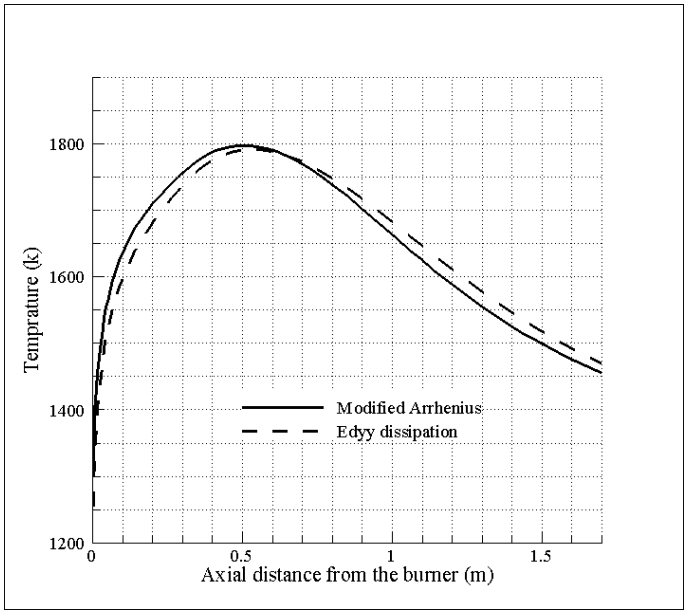

Figure 6. The comparison of prediction of axial temperature distribution

Figure 7 displays the effect of equivalence ratio on the output temperature and CO mass fraction for the modified Arrhenius model and the eddy-dissipation model. It can be seen that by increasing equivalence ratio temperature reaches a peak and then decreases for both models. Also, CO mass fraction decreases to a minimum and then increases for the modified Arrhenius model. However, CO mass fraction is the first constant and then increases for the eddy-dissipation model. This incoherence can be attributed to this reason that the model cannot predict radicals such as CO mass fraction.

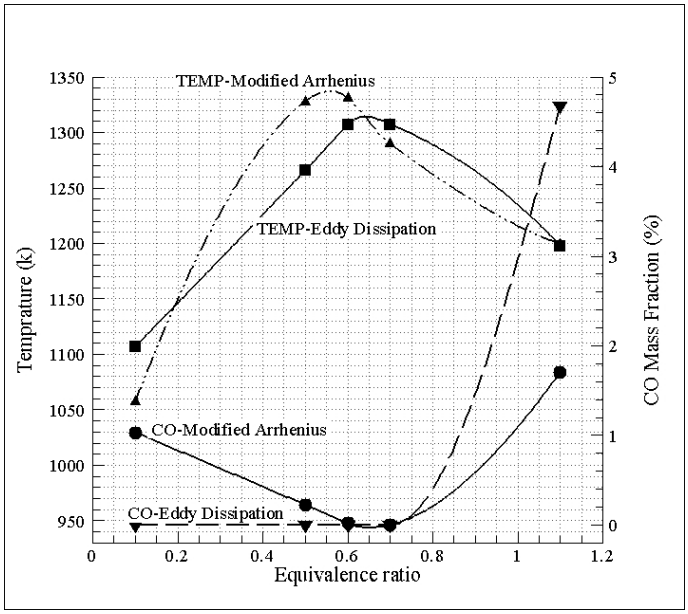

Figure 7 The comparison of output temperature and CO mass fraction under different equivalence ratios

5. Conclusion

In this paper, effects of turbulent fluctuations are considered by using a time-varying function for Arrhenius model. The Sprint CFD code is used to predict temperature distribution and CO mass fraction. The results of modified Arrhenius model are compared with eddy-dissipation model and Experimental data. The following conclusions are taken from the analysis of the results:

- The temperature fluctuations have the significant role in the rate of reaction.
- The modified Arrhenius model has good agreement with the eddy-dissipation model and has a qualitative trend same as the experimental data.
- The modified Arrhenius model is better than the eddy-dissipation model in predicting the mass fraction of carbon monoxide.

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