Numerical Simulation of CO Concentration on Flame Propagation in the Vicinity of the Wall -Validity of Non-Adiabatic FGM Approach-

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ABSTRACT

To design a gas turbine combustor for low emissions, carbon monoxide (CO) generated near the cooled wall is one of the important indexes. However, the measuring of CO concentration is difficult in experiments in actual conditions of high pressure and temperature. In this study, in order to take the heat loss effect on the cooled wall into account, a non-adiabatic flamelet generated manifolds (NA-FGM) approach, which can account for the change of gas composition due to the heat loss, is applied to two-dimensional numerical simulations of premixed flame near the cooled wall and the effect of equivalence ratio variation on the CO concentration is investigated. The results show that the CO concentrations predicted for the equivalence ratio of 1.0 using the NA-FGM approach are in good agreements with those using the detailed reaction approach, and that the NA-FGM approach can adequately catch the tendency of CO generation in the vicinity of the wall with heat loss.

NOMENCLATURE

- \( \zeta \) Progress variable
- \( C_p \) Isopiestic specific heat
- \( D_h \) Thermal diffusivity
- \( D_y \) Diffusion coefficient (\( D_y = \lambda/\rho C_p \))
- \( h \) Enthalpy
- \( p \) Pressure
- \( q_{\text{loss}} \) Source term of heat loss
- \( R \) Gas constant
- \( S_L \) Laminar flame velocity
- \( T \) Temperature
- \( u \) Velocity vector
- \( V_k \) Diffusion velocity of chemical species \( k \)
- \( W_k \) Molecular weight
- \( Y_k \) Mass fraction of chemical species \( k \)
- \( Z \) Mixture fraction

- \( \omega_c \) Generation rate of progress variable
- \( \omega_k \) Chemical reaction rate of chemical species \( k \)

- \( k \) Chemical species

INTRODUCTION

Aim of a recent gas turbine development is to reduce air pollution emissions (CO, NOx, etc.) with low environmental load. In this developed combustor, premixed combustion is applied to reduce NOx emissions. For premixed combustion fields, CO emission is one of the important issues to solve at a partial load for an industrial gas turbine [1, 2]. CO emission is mainly generated at the flame front, actually reaction zone, in the combustion chamber. When CO emission is formed in the vicinity of the wall, unburned fuel and CO are prone to flow out downstream. Therefore the prediction of CO emission in the vicinity of the wall is important in order to design a low emission combustor. However the measurement of CO is difficult at actual gas turbine conditions in high temperature and pressure fields.

Computational fluid dynamics (CFD) is a powerful tool to investigate the detailed distributions of various chemical species and temperature under the complicated combustion fields. CFD has been used to support to engineers in predicting the property of flame dynamics during the combustor design process [3-9]. Prediction of CO emission with high accuracies is required consideration of the detailed reaction mechanism in general. Because this detailed reaction approach needs to pay much expensive computational cost, a number of combustion models have been proposed. Conventionally, the G equation model [10, 11] is used to calculate premixed combustion; however this model does not calculate CO concentration accurately because it calculates unburned and burned gas compositions in the equilibrium conditions. Recently, the flamelet generated manifolds (FGM) approach [12] has been used for premixed combustion, because this model considers the detailed reaction mechanism by database called flamelet library. However, the database of the conventional FGM approach does not include the effect of heat loss. The FGM approach taking heat loss effect into account is called the non-adiabatic FGM (NA-FGM) approach. Some researches have attempted to develop efficient NA-FGM approaches [12-15]. Fiorina et al. [13] and Proch and Kempf [14] have suggested the way to take the heat loss effect into account to the database and verify its applicability to the steady burner flame. Fiorina et al. [15] have performed three-dimensional large-eddy simulations and showed the improvement in the accuracy of the flame height. There are some research employing NA-FGM approach, however, most of their studies targeted on the steady turbulent flame, and the...
applicability to propagating turbulent flame is not well investigated.

In this study, the validity of the NA-FGM approach to predict the CO concentration in the vicinity of the wall with heat loss is examined by comparing with those employing the detailed reaction approach, and the effect of equivalence ratio variation on the CO concentration is investigated using the NA-FGM approach.

TURBULENT COMBUSTION MODELS

Detailed reaction approach

The governing equations for the detailed reaction approach can be written as:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{1}
\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot \tau \tag{2}
\]

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h u) = \frac{\partial}{\partial t} \left( \rho \left( \frac{\partial Y_k}{\partial t} \right) \right) + \nabla \cdot (\rho Y_k V_k) + \rho \omega_k \tag{3}
\]

\[
\frac{\partial Y_k}{\partial t} + \nabla \cdot (\rho Y_k u) = -\nabla \cdot (\rho Y_k V_k) + \rho \omega_k \tag{4}
\]

\[
p = \rho R \sum_k \frac{Y_k}{W_k} \tag{5}
\]

where \( \rho \) is the density, \( u \) is velocity vector, \( p \) is pressure, \( \tau \) is shear stress tensor, \( h \) is enthalpy, \( h_k \) is enthalpy of chemical species \( k \), \( D_h \) is thermal diffusivity, \( Y_k \) is mass fraction of chemical species \( k \), \( V_k \) is diffusion velocity of chemical species \( k \), \( \omega_k \) is chemical reaction rate of chemical species \( k \), \( T \) is temperature, \( R \) is gas constant and \( W_k \) is molecular weight of chemical species \( k \).

Flamelet Generated Manifolds approach

The governing equations for the FGM approach can be written as:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \tag{6}
\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot \tau \tag{7}
\]

\[
\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h u) = \frac{\partial}{\partial t} \left( \rho \left( \frac{\partial Y_k}{\partial t} \right) \right) + \nabla \cdot (\rho Y_k V_k) + \rho \omega_k \tag{8}
\]

\[
\frac{\partial Y_k}{\partial t} + \nabla \cdot (\rho Y_k u) = -\nabla \cdot (\rho Y_k V_k) + \rho \omega_k \tag{9}
\]

\[
\frac{\partial Y_k}{\partial t} + \nabla \cdot (\rho C \dot{Y}_k) = -\nabla \cdot (\rho C \nabla T) + \rho \dot{\omega}_C \tag{10}
\]

where \( \dot{\omega}_C \) is generation rate of progress variable, \( C \) is the progress variable defined as mass fraction of burned gas (H₂O, H₂, CO₂ and CO), \( D_C \) is diffusion coefficient \( (D_C = \lambda / \rho C_p) \), \( \lambda \) is thermal conductivity and \( C_p \) is isopiestic specific heat.

This model needs a database called a flamelet library, which is obtained by the calculation of laminar flow flame under various conditions and generated by the calculation of a one dimensional laminar premixed flame. The governing equations for generating the flamelet library can be written as:

\[
\frac{\partial (\rho u)}{\partial x} = 0 \tag{11}
\]

\[
\rho u \frac{\partial Y_k}{\partial x} = \rho \dot{j_k} + \dot{m}_k \tag{12}
\]

\[
\rho u C_p \frac{\partial \theta}{\partial x} = \rho \left( \frac{\partial \theta}{\partial x} \right) - \sum_k C_p h_k \frac{\partial \theta}{\partial x} - \sum_k h_k \dot{m}_k \tag{13}
\]

This library was generated by the calculation of a one dimensional laminar premixed flame. This library was calculated by the detailed elementary reaction calculation with the FlameMaster code [16] in combination with GRIMech-3.0 [17]. This database provides all filtered scalar quantities as a function of the filtered mixture fraction \( Z \) and filtered progress variable \( C \).

Figure 1 shows an example of flamelet library for the FGM approach.

Non-Adiabatic Flamelet Generated Manifolds approach

In general, flamelet library for the FGM approach is not considered with heat loss. However, flame is generated in vicinity of the cooling wall for gas turbine combustor. Therefore, we applied a NA-FGM approach [14] due to include the effect of the heat loss.

Flamelet library considered the effect of the heat loss is calculated by the eq. (11), (12) and the following equation (14).

\[
\rho u C_p \frac{\partial \theta}{\partial x} = \rho \left( \frac{\partial \theta}{\partial x} \right) - \sum_k C_p h_k \frac{\partial \theta}{\partial x} - \sum_k h_k \dot{m}_k + \dot{q}_{loss} \tag{14}
\]

\[
\dot{q}_{loss} = \alpha \sum_k \dot{m}_k h_k \tag{15}
\]

where \( \dot{q}_{loss} \) is the source term of heat loss and \( \alpha \) is adjustment parameter. In this study, adjustment parameters from 0.0 to 0.4 were calculated every 0.05. The adjustment parameter is based on the maximum value of predicted heat loss. The maximum value of predicted heat loss was calculated by enthalpy of burnt gas at wall temperature. Figure 2 shows an example of flamelet library for the NA-FGM approach. Flamelet library for NA-FGM approach is defined three variable (mixture fraction \( Z \), progress variable \( C \) and difference of enthalpy \( \Delta h \)) in order to output some physical quantity. Difference of enthalpy \( \Delta h \) can be written as:

\[
\Delta h = h_0 - h \tag{16}
\]

where \( h_0 \) is enthalpy without heat loss, \( h \) is enthalpy obtained by eq. (8).
DESCRIPTIONS OF CALCULATION SETUP

In this study, two-dimensional premixed flame propagation near the cooled wall was adopted as verification object. Figure 3 shows the diagram of premixed turbulent combustion regimes [18]. According to this diagram, corrugated flamelets, thin reaction zones regime, and broken reaction zones regime are mainly recognized as a combustion configuration of the gas turbine combustor. This object can set thin reaction zones regime as calculation conditions for each equivalence ratio.

![Diagram of premixed turbulent combustion regimes](image)

The schematic diagram of the calculation domain is shown in figure 4. These calculations were conducted under atmospheric pressure in two-dimensional combustion field. Calculation domain is two-dimensions rectangular ($40.96 \text{ mm} \times 5.12 \text{ mm}$). The $x$ coordinate means a direction parallel to long side and the $y$ coordinate means a direction vertical to long side. Computational grids are divided into same range (20 µm) as staggered grid. 2048 grids are set at $x$ direction and 256 grids are set at $y$ direction. The boundary at $x$ direction is outlet. At the outlet boundary, the pressure in two-dimensional combustion field. Calculation domain.

The Laminar flame velocity $S_L$ was calculated by the detailed elementary reaction calculation with the FlameMaster code [16]. The laminar flame thickness $\delta_L$ is calculated by equation (17). These parameters are calculated at 700K. Lewis number is assumed 1 in case of the NA-FGM approach. Reynolds number is approximately 50 for each equivalence ratio.

$$\delta_L = \frac{L}{\text{Re} \cdot \text{Pr}}$$  

In this study, inhouse-code FK3 is used [20-23]. The spatial derivative of convective term in the momentum equation is approximated with a fourth-order central difference scheme, and a WENO scheme [24] is used to evaluate the scalar gradients. A third-order accurate SSP Runge–Kutta method [25] is adopted in time integration. Combustion behavior was calculated for 0.01 sec using CRAY: XE6 at the ACCMS, Kyoto University, with 1024 cores and 62.5 h of wall clock time in case of detailed reaction approach, and with 256 cores and 33.5 h of wall clock time in case of NA-FGM approach. CFL-number of all cases is less than 0.15. Time-step is 0.1 µsec.

RESULTS AND DISCUSSION

Validation of NA-FGM approach

Figures 6 and 7 show the instantaneous distribution of temperature, enthalpy, CO mass fraction at 800 µsec. The equivalence ratio of these results was set as stoichiometric ratio. The results using the detailed reaction approach are shown in figure 6. The results using the NA-FGM approach are shown in figure 7. In this study, high temperature region, which is more than 1500 K, is defined as flame.

Flame front structure is complicated by the effect of turbulence intensity for thin reaction zones regime. Flame reached the wall is propagating along the wall. After 800 µsec, maximum temperature 2291 K for the detailed reaction approach is similar with 2307 K for the NA-FGM approach. However, the NA-FGM approach underestimates flame reaching time at the part of calculation domain (a). This reason is that flamelet library does not consider flame stretch and unsteady flame phenomenon.

There is a difference of enthalpy for the detailed reaction approach between burned gas and unburnt gas on the line (b). The distribution of enthalpy on this line does not agree well with the results of detailed reaction approach. However, the NA-FGM approach can reproduce the decrease in

| Equivalence ratio $\phi$ [-] | Initial pressure [atm] | Initial temperature [K] | CFD approach | Detailed reaction | NA-FGM |
|-----------------------------|------------------------|-------------------------|--------------|-------------------|--------|
| 0.8                         | 1.0                    | 700                     | Done         | Done              | Done   |
| 1.0                         | 1.0                    | 700                     | Done         | Done              | Done   |
| 1.2                         | 1.0                    | 700                     | Done         | Done              | Done   |

![Initial turbulence fields (artificial)](image)

Fig. 5 Initial turbulence fields (artificial)

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|-----------------------------|------------------------|-------------------------|--------------|-------------------|--------|
| 0.8                         | 1.0                    | 700                     | Done         | Done              | Done   |
| 1.0                         | 1.0                    | 700                     | Done         | Done              | Done   |
| 1.2                         | 1.0                    | 700                     | Done         | Done              | Done   |
enthalpy near the flame reaching wall. From these points on, we confirmed the NA-FGM approach is effective for predicting the phenomenon in the vicinity of the wall.

Figure 6 Instantaneous distributions of temperature, enthalpy and CO mass fraction by detailed reaction approach at \( \phi = 1.0 \). Figure 7 Instantaneous distributions of temperature, enthalpy and CO mass fraction by the NA-FGM approach at \( \phi = 1.0 \).

Figure 8 shows the schematic diagram of point Ⅰ, point Ⅱ, line A-A' and line B-B'. The results at point Ⅰ for NA-FGM approach are captured the trends of temperature and CO mass fraction when time is passing. On the other hand, at point Ⅱ, the results of the NA-FGM approach need to be shifted for 300µsec due to overestimating flame propagation rate as shown figures 6 and 7. By shifting time, both of the result is match well as shown (c).

Figure 11 shows the instantaneous distribution of CO mass fraction on lines A-A' and B-B'. The distribution of CO mass fraction for the NA-FGM approach was compared with the results of the detailed reaction approach. On line A-A', the results using the NA-FGM approach are in good agreement with the detailed reaction approach. On the other hand, the NA-FGM approach cannot reproduce the distribution of CO mass fraction at the point (d) on line B-B'. This is caused that the turbulent flow affected to flame propagation velocity. In this study, the initial turbulent flow field is set. The flame in case of not considering turbulence flow simultaneously adheres to the upper (A-A') and lower (B-B') wall surfaces. By considering the turbulent flow, the flame propagation velocity in the upward direction and the downward direction are different as shown Fig.9 and 10. There was no significant difference in temperature and CO mass fraction between detailed reaction and NA-FGM at the upper wall (A-A) where the arrival time was fast. This is because the reaction is sufficiently advanced. On the lower wall (B-B) where the arrival time is slow, the reaction shows good agreement with the detailed reaction at the position where the reaction has progressed sufficiently (x=2–10 mm). However, the difference becomes large at the position where the flame has not arrived (x = -10–2 mm). This feature is indicated for other scalars as well as for CO.

Figure 12 shows the comparisons of the time series of maximum heat flux between detailed reaction approach and the NA-FGM approach on each wall. Since the wall heat flux affect the lifetime of the combustor, it is significance to investigate the predictability of the maximum wall heat flux. In figure 12, for the case of the NA-FGM approach, although the timing when the wall heat flux starts to increase is faster than the detailed reaction approach, the maximum wall heat flux value is approximately same as the detailed reaction approach.
Fig. 10 Time series data of temperature and CO mass fraction at point II

Fig. 11 Comparison of CO mass fraction between detailed reaction approach and the NA-FGM approach at \( \phi = 1.0 \) on lines A-A' and B-B'.

Fig. 12 Comparisons of time series data of maximum wall heat flux on the wall between detailed reaction approach and the NA-FGM approach at \( \phi = 1.0 \).

Effect of equivalence ratio on CO concentration

Figures 13, 14 and 15 show the time series of temperature, enthalpy and CO mass fraction distributions at each equivalence ratio. Figure 16 shows the time series of CO\(_2\) mass fraction distributions at \( \phi = 1.0 \). Figure 17 shows the schematic diagram of point III. Figure 18 shows the time series of CO mass fraction at point III obtained by the NA-FGM approach. Flame propagation rate at \( \phi = 1.0 \) is fastest in this study by the difference of laminar flame velocity. Flame propagation rate at \( \phi = 0.8 \) is 17% slower than that at \( \phi = 1.0 \). Flame propagation rate at \( \phi = 1.2 \) is 10% slower than that at \( \phi = 1.0 \). There is a little difference of enthalpy distribution at all equivalence ratio, and maximum value was changed by the quantity of heat loss at each equivalence ratio. This feature is also obtained for CO mass fraction. For lower equivalence ratio, CO mass fraction generated at flame front and flame zones is lower than higher equivalence ratio. Moreover, CO is prone to oxidize near the cooled wall. This is because CO oxidation, an exothermic reaction, is activated by decreasing temperature due to the heat loss. This is also evident from the increase in CO\(_2\) as shown figure 15.

Figure 19 shows the time series of CO rate of change by heat loss at point III obtained by the NA-FGM approach. 0 msec means flame reaching time to the wall. CO rate of change by the heat loss is calculated the following equation (18).

\[
\Delta Y_{CO} = \frac{Y_{CO, NA-FGM}}{Y_{CO, h=0}}
\]

where \( Y_{CO, NA-FGM} \) is CO mass fraction obtained by the NA-FGM approach, \( Y_{CO, h=0} \) is CO mass fraction obtained at \( \Delta h = 0 \) by the NA-FGM approach.

\( \Delta Y_{CO} \) peaks immediately after flame reached the wall. Then \( \Delta Y_{CO} \) is decreasing gradually as time goes by. The rate of \( \Delta Y_{CO} \) at \( \phi = 0.8 \) is slower until 0.4 msec. However, the rates of \( \Delta Y_{CO} \) at \( \phi = 1.0 \) and 1.2 are slower than that at \( \phi = 0.8 \) after 0.4 msec. This is because the fuel is lean \( \phi = 0.8 \) and oxygen is sufficiently present.
Fig. 13 Time series of temperature distributions at $\phi = 0.8$, 1.0 and 1.2 by NA-FGM approach

Fig. 14 Time series of enthalpy distributions at $\phi = 0.8$, 1.0 and 1.2 by NA-FGM approach
CONCLUSIONS

We applied two-dimensional numerical simulations employing a NA-FGM approach to consider the effect of the heat loss in the vicinity of the wall and examined the validity of the NA-FGM approach to predict the CO concentration by comparing with those employing a detailed reaction approach. Then we investigated the influence of the equivalence ratio on the CO generation in vicinity of the wall. The main results obtained are summarized as follows:

1) The NA-FGM approach can predict the progress of CO generation in the vicinity of the wall and maximum wall heat flux accurately for turbulent lean premixed combustion.

2) The CO concentration in the vicinity of the wall predicted using the NA-FGM approach tends to decrease due to the effect of heat loss through the cooled wall at each equivalence ratios. The effect of the heat loss plays an important role in prediction of CO generation near the wall for turbulent premixed combustion.

In conclusion, these results suggest that the NA-FGM approach is quite effective for the CO prediction for turbulent premixed combustion.

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