Prediction of CO emissions in turbulent super lean premixed combustion under pressurized conditions using an LES/non-adiabatic FGM approach

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ABSTRACT

A large eddy simulation (LES) employing a non-adiabatic flamelet generated manifolds (NA-FGM) approach, which can account for the effects of heat loss, is applied to CH₄-air super lean premixed combustion fields generated by an axisymmetric jet burner with cooled walls under pressurized conditions. In addition, the validity in predicting the CO emissions is examined. The NA-FGM approach captures the trends of CO emissions well during the experiments, in which the CO emissions increase with a decreasing equivalence ratio. It is shown that the increase in CO emissions for low equivalence ratios is not due to the increase in the CO production, but to the slow rate of CO consumption, which keeps the CO concentration high downstream. The results suggest that capturing such a sensitive reduction of CO consumption rate by heat loss is important for accurately predicting the CO emissions in developing a low-emissions gas turbine combustor at low load.

NOMENCLATURE

C	Progress variable [-]
C_p	Isobaric specific heat [J/kg/K]
D_h	Thermal diffusivity [m ² /s]
D_γ	Diffusion coefficient ($D_\gamma = \lambda/\rho C_p$) [m ² /s]
h_k	Enthalpy of species k [J/kg]
j_k	Mass diffusion flux of species k [kg/m ² s]
$\dot{m}_k$	Mass production rate of species k [kg/m ³ s]
P	Pressure [Pa]
$\dot{q}_{loss}$	Source term of heat loss [W/m ³]
T	Temperature [K]
u	Velocity vector [m/s]
Y_k	Mass fraction of chemical species k [-]
Z	Mixture fraction [-]

Greeks

α	Adjustment parameter
λ	Thermal conductivity
ϕ	Equivalence ratio [-]
μ	Viscosity [Pa·s]
ρ	Density [kg/m ³]
τ	Shear stress tensor
$\dot{\omega}_C$	Generation rate of progress variable+
$\dot{\omega}_k$	Chemical reaction rate of chemical species k

Subscripts

f	Fuel
k	Chemical species
st	Stoichiometric air-to-fuel ratio
$wall$	Wall

INTRODUCTION

In the development of gas turbine combustors, to prevent air pollution, it is important to reduce the NO_x and CO emissions generated by the combustion of hydrocarbon fuels. To control the NO_x emissions, it is effective to reduce the local flame temperature by decreasing the equivalence ratio. By contrast, if the equivalence ratio is decreased to achieve such a lean premixed combustion, the flame combustibility decreases; therefore, there is a possibility that CO is discharged in large quantities [e.g. 1, 2]. In addition, owing to the recent increase in renewable energy power generation, it is necessary to utilize the gas turbine for the purpose of supplementing an unstable power supply. It is therefore important to develop combustors capable of low emissions and stable combustion at low loads, unlike in a conventional combustor, which should operate stably at maximum load.

A low-emissions combustor was developed through combustion tests conducted in a high-pressure test rig at Mitsubishi Heavy Industries, Ltd. The results suggest that the CO generation/consumption in a gas turbine combustor occurs near a cooled wall with heat loss. However, the effect has not been sufficiently examined, mainly because it is difficult to understand the CO generation/consumption behavior near such a wall, namely the effect of quenching due to heat loss through the cooled wall on the CO consumption rate, because there are few measuring devices applicable in a high-pressure environment.

Computational fluid dynamics (CFD) employing both turbulent combustion models and turbulence models is expected to be a powerful tool for understanding high-pressure combustion behavior, for which measurements are difficult as mentioned above. In particular, a large-eddy simulation (LES), which models an eddy smaller than the cell size, has gained increasing application in recent years, because the application of an LES to complex reacting flows has been realistic with advancements in the supercomputing performance [e.g. 2-8]. As the turbulent combustion model, the flamelet approach [9], which utilizes the flame characteristics in the database (i.e., the flamelet library), is effective in terms of computational costs and is widely used instead of directly solving the Arrhenius equations when considering the detailed chemical reaction mechanisms. In general, the flamelet approach includes two types depending on the targeted flame characteristics, namely, a non-premixed (diffusion) flame and a premixed flame. For

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instance, the flamelet progress variable (FPV) approach [10] and flamelet generated manifolds (FGM) approach [11] are the representative flamelet methods developed for non-premixed and premixed flames, respectively. Regarding the CO prediction using the LES with flamelet approach, Vreman et al. [12] applied LESs of Sandia Flame D and Flame F using both non-premixed and premixed flamelet approaches and investigated the validity by comparing them with the experiment results. However, they did not consider the heat loss effect on the walls. By contrast, Donini et al. [13] applied the FGM approach by considering the heat loss effect to a premixed flame and examined the heat loss effect on CO emissions. However, no comparisons were made with the experiments. To take the heat loss effect into account in the flamelet approach, a non-adiabatic procedure [14] has been introduced in some previous studies for both non-premixed and premixed flames [15-19]. However, to assess the validity, comparisons with the experiment results are essential because of procedural complications.

The purpose of this study is, therefore, to apply an LES by employing a non-adiabatic FGM approach (referred to as “NA-FGM approach”, hereafter), which can consider the effect of heat loss on the chemical species composition [14-17], to CH₄-air super lean premixed flames for equivalence ratios of $\phi = 0.43, 0.45$ and 0.50 under pressurized conditions with heat loss through a cooled wall, and to examine the validity to predict the CO emissions based on a comparison with the experiment results. In addition, the effects of heat loss and equivalence ratio on CO emissions were investigated in detail.

NUMERICAL METHODS

Flamelet Generated Manifolds (FGM) approach

The governing equations for the FGM approach [11] can be written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (1)$$

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla P + \nabla \cdot \tau \quad (2)$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h u) = \nabla \cdot (\rho D_h \nabla h) \quad (3)$$

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho Z u) = \nabla \cdot (\rho D_Z \nabla Z) \quad (4)$$

$$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho C u) = \nabla \cdot (\rho D_C \nabla C) + \rho \dot{\omega}_C \quad (5)$$

where ρ is the density, u is the velocity vector, P is the pressure, τ is the shear stress tensor, h is the enthalpy, D_h is the thermal diffusivity, $\dot{\omega}_C$ is the generation reaction rate of progress variable C , C is the progress variable defined as the mass fraction of burned gas (H₂O, H₂, CO₂ and CO), D_γ is the diffusion coefficient ($D_\gamma = \lambda / \rho C_p$), λ is the thermal conductivity, and C_p is the specific isopiestic heat. This model requires a database called a flamelet library, which is generated using calculations involving a one-dimensional laminar premixed flame under various conditions, using the following governing equations:

$$\frac{\partial (\rho u)}{\partial x} = 0 \quad (6)$$

$$\rho u \frac{\partial Y_k}{\partial x} = -\frac{\partial j_k}{\partial x} + \dot{m}_k \quad (7)$$

$$\rho u C_p \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left(\lambda \frac{dT}{dx} \right) - \sum_k C_p j_k \frac{\partial T}{\partial x} - \sum_k h_k \dot{m}_k \quad (8)$$

Thus, this library is obtained through detailed elementary reaction calculations. This database provides all filtered scalar quantities as

functions of the filtered mixture fraction Z and filtered progress variable C .

Non-Adiabatic procedure

In general, a premixed flame is generated within the vicinity of the cooled wall in gas turbine combustors. Therefore, we apply the NA-FGM approach [14] to include the effect of heat loss. The flamelet library, using the effect of the considered heat loss [16], is calculated using equations (6), (7) and (9).

$$\rho u C_p \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) - \sum_k C_p j_k \frac{\partial T}{\partial x} - \sum_k h_k \dot{m}_k + \dot{q}_{loss} \quad (9)$$

$$\dot{q}_{loss} = \alpha \sum_k h_k \dot{m}_k \quad (10)$$

where $\dot{q}_{loss}$ is the source term of heat loss and α 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. Flamelet library for NA-FGM approach is defined three variables (mixture fraction Z , progress variable C and difference of enthalpy Δh) in order to output some physical quantity. Difference of enthalpy Δh can be written as:

$$\Delta h = h_0 - h \quad (11)$$

where h_0 is enthalpy without heat loss, h is enthalpy obtained by eq. (3).

DESCRIPTIONS OF CALCULATION SETUP

In this study, a turbulent lean premixed combustion in the thin reaction zones regime, which is a combustion configuration of a gas turbine combustor in a turbulent premixed flame diagram as designed by Peters [20], was adopted as the object of verification. A schematic diagram of the calculation domain for the Paul Scherrer Institute burner [21, 22] is shown in Figure 1. The feature of this combustion test rig can be applied between the atmospheric pressure and high pressure (2.0 MPa). Moreover, corrugated flamelets, the thin reaction zones regime, and the broken reaction zones regime in the diagram of a turbulent premixed flame can be set as the experimental conditions. This rig is composed of a cooling casing, turbulence grid, fuel header, combustion chamber and exhaust pipe. The combustion air was preheated to 823 K using an electrical heater. After mixing air and fuel in the mixing section, high-pressure air and fuel formed in the fuel header flow into the combustion chamber (inner diameter $D = 75$ mm) through the turbulence grid (inner diameter $d = 25$ mm, hole diameter $d_g = 3$ mm and blockage ratio $bg = 65$ %). The fuel reacts with the combustion air and a premixed flame then forms in the combustion chamber. The flue gases flow into the exhaust pipe. The axial direction from the upstream to the downstream of the burner indicates x , the height direction from the center of the combustion chamber indicates y , and the depth direction of the combustion chamber indicates z . Here, $x = 0$ mm is the inlet position from the fuel header to the combustion chamber, and $y = 0$ mm and $z = 0$ mm are the center axis of the combustion chamber in the figure. The velocity in the combustion chamber was measured indirectly using particle image velocimetry (PIV). CO emissions at $x = 300$ mm were measured using sampling probe. Full details of the tests are available in the literature [21, 22], the data of which were taken for validation. Figure 2 shows a schematic diagram of the computational grids. The computational region was divided into approximately 24 million cells. The control volume size close to the burner and in the reaction zone was approximately 0.01 mm, which was considered sufficient for the LES. The combustion chamber inner wall was set to be isothermal (300 K). The inner wall temperature was validated by comparing the calculation results with the experimental results at the outlet of the combustion

chamber. At the outlet boundary, the Neumann boundary condition is imposed for pressure, with free outflow conditions being imposed for the other variables.

Figure 1 Schematic diagram of combustion test rig [21, 22].

Figure 2 Schematic diagrams of computational grids.

Table 1 lists the calculation conditions. The bulk inlet velocity U_0 was 40 m/s. The fuel temperature was 293 K (non-reacting flow) or 673 K (reacting flow). The pressure at the chamber outlet was 1 bar (non-reacting flow) or 5 bar (reacting flow). The equivalence ratios were 0.43-0.50. Here, CH_4 was used as the fuel. Calculations (reacting flow) were carried out for Cases 2-4 (LES/NA-FGM approach) to confirm the sensitivity for CO emissions. The consideration of heat loss in the flamelet library was excluded for Cases 5-7 (LES/A-FGM approach) to confirm the sensitivity of the heat loss effect.

Table 1 Calculation conditions.

Case	P (bar)	ϕ (-)	T_f (K)	T_{wall} (K)	U_0 (m/s)	Reaction	Consideration of heat loss
1	1.0	-	293	293	40	Off	Off
2	5.0	0.43	673	300	40	On	On
3	5.0	0.45	673	300	40	On	On
4	5.0	0.50	673	300	40	On	On
5	5.0	0.43	673	300	40	On	Off
6	5.0	0.45	673	300	40	On	Off
7	5.0	0.50	673	300	40	On	Off

The governing equations are solved using an unstructured LES solver, i.e., FrontFlow/Red (FFR) extended by some research institutes, including Kyoto University, and referred to as FFR-Comb [e.g. 5-8, 15, 17]. The combustion field is treated as incompressible in a low Mach number approximation. The NA-FGM approach was previously implemented in the LES solver. The flamelet library is obtained through detailed elementary reaction calculations using the FlameMaster code [23]. The detailed reaction mechanism was applied to GRI-Mech 3.0, considering 53 species and 325 reaction steps [24]. A dynamic sub-grid scale model is applied as the turbulence model [25]. A first-order Euler implicit method was used for time advancement, and the time step was set to 1×10^{-6} s, which is based on a Courant-Friedrichs-Lewy (CFL) number of less than 1. The spatial derivative of the convective term in the momentum equation is approximated using a second-order central difference scheme of 95 % and a first-order upwind of 5 %. The turbulent Schmidt number and turbulent Prandtl number are set to 0.4. The statistics were collected for each case over three flow-through times, and all

simulations were calculated for 10 ms using a CRAY: XE6 at the ACCMS, Kyoto University, with 544 cores and 40 h of wall clock time.

RESULTS AND DISCUSSION

Non-reacting flow

To assess the prediction accuracy of the velocity, a non-reacting flow (Case 1) was first applied using the calculation conditions given in Table 1. Figure 3 shows the distributions of the instantaneous, time-averaged and RMS streamwise velocities on the x - y plane for Case 1. It accelerates within the vicinity of the turbulence grid, which becomes a turbulent flow generator, and the variation value near the burner inlet ($x = 0$ mm) is high in region (A). The premixed fuel jet is gradually damped from the upstream of the $\phi 25$ mm burner to the $\phi 75$ mm combustion chamber, and the potential core disappeared at approximately $x = 100$ mm. The recirculation zone near the wall in region (B) was generated owing to the sudden expansion of the diameter from $\phi 25$ to $\phi 75$ mm. The velocity variation becomes large in shear layers where the velocity gradient is caused by the sudden expansion of the end of the potential core at point (C) or the inner diameter of the combustor is large at point (D). Figures 4 and 5 show comparisons of the centerline profiles of the time-averaged and RMS streamwise velocities, and comparisons of the radial direction profiles of the time-averaged streamwise velocity at $x = 25$ mm and 175 mm between the LES (Case 1) and experiment [26], respectively. The values of the time-averaged and RMS streamwise velocities are normalized by an inlet bulk velocity of 40 m/s. The jet accelerated by the turbulence grid flows into the combustion chamber at above 40 m/s. After that, the potential core of the flow gradually decays from approximately $x = 100$ to 300 mm. The calculation results overestimate the RMS values at approximately $x = 0$ mm. There is a possibility of underestimating the damping of turbulence fluctuations owing to the low-order difference scheme or the problem of a lattice resolution near the turbulence grid. However, good agreement with the experimental results is confirmed $x = 50$ mm downstream of the velocity field, which is important for a flame formation. The calculation results reproduce the tendency of the experimental results from the viewpoint of predicting the flame behavior.

Figure 3 Distributions of instantaneous, time-averaged and RMS streamwise velocity on the x - y plane for Case 1.

Figure 4 Comparisons of centerline profiles of time-averaged and RMS streamwise velocity between LES (Case 1) and experiment [26].

Figure 5 Comparisons of radial direction profiles of time-averaged streamwise velocity at $x = 25$ mm and 175 mm between LES (Case 1) and experiment [26].

Reacting flow

Effect of equivalence ratios on flame length

Figures 6 shows the instantaneous iso-surfaces of progress variable $C = 0.1$, indicating flame fronts with the generation reaction rate of progress variable $\dot{\omega}_C$. Figures 7 the instantaneous distributions of temperature (top), enthalpy (middle), and progress variable (bottom) on the x - y plane for equivalence ratios of $\phi = 0.43, 0.45$, and 0.50 predicted by LES/NA-FGM (Cases 2, 3 and 4, respectively). According to Figures 6 and 7, the flame front structure is complicated by the effect of the turbulence eddy, and the flame is stably maintained in the outer recirculation zone. The burnt high-temperature gas is returned to the combustion chamber inlet by the outer recirculation flow (marked as (E) in Figure 7) as shown in Figure 3 (B), thereby maintaining the flame. The outer recirculation zone has much higher temperatures than the central zone in the core flow (marked as (F) in Figure 7). However, the temperature in this zone (E) is lower than the downstream, which is due to the lost heat of the burnt gas through the cooled wall at point (G) in Figure 7. Moreover, the value of heat loss increases with an increase in the equivalence ratio. Despite the occurrence of heat loss through the wall, the progress variable near region (H) did not greatly decrease. In this burner, there is a high possibility that the flame length does not change even if the effect of heat loss on the chemical reaction is ignored. Hence, the flame length was evaluated by comparing the centerline profiles of the progression variables. Figure 8 shows comparisons of the centerline profiles of the time-averaged normalized progress variable for equivalence ratios of $\phi = 0.43, 0.45$ and 0.50 , as predicted by LES/NA-FGM (Cases 2, 3 and 4) and LES/A-FGM (Cases 5, 6 and 7). The time-averaged progress variable is normalized by the maximum value of each case. The flame length during super lean combustion is an important factor of the prediction of CO emissions and the blow-off limit. Here, the flame length is defined as from $x = 0$ mm to the position at the normalized progress variable of 0.5. The flame lengths of LES/NA-FGM were 163.43 mm for $\phi = 0.43$, 155.11 mm for $\phi = 0.45$, and 133.68 mm for $\phi = 0.50$. The flame lengths of LES/A-FGM were 169.65 mm for $\phi = 0.43$, 159.07 mm for $\phi = 0.45$, and 125.85 mm for $\phi = 0.50$. The unburnt zones, where the progress variable is defined as equal to zero, expands in the streamwise direction as the equivalence ratio decreases, as shown in Figure 8. As a result, the flame length is validated to increase with a decrease in the equivalence ratio. This is because the lower the equivalence ratio is, the lower the flame propagation rate. In this study, the effect of the equivalence ratio on the flame length was

larger than that of the heat loss. Moreover, the difference in flame length between the flamelet library with heat loss and that without heat loss is significantly small.

Although the flame length of LES/NA-FGM for $\phi = 0.50$ (133.68 mm) is in good agreement with the experimental results (140 mm), the effect of the decrease in the equivalence ratio on the extension of the flame length is small for lower equivalence ratio conditions, and the difference in the flame length between $\phi = 0.45$ and $\phi = 0.43$ is significantly small. Therefore, it is necessary to improve the prediction accuracy of the flame length under the condition of $\phi = 0.43$, which is near the blow-off limit. To improve the prediction accuracy of the flame length, a flame stretch effect can be introduced into the NA-FGM approach. The thin reaction zones regime targeted in this study has three effects: the flame stretch effect, the diffusion enhancement effect of the preheated regime owing to the turbulent flow vortex, and the increasing rate of the flame surface area. The decrease in the flame propagation rate is caused by the flame stretch effect. Previous studies [3] have suggested that introducing a flame stretch effect [27] into the combustion model improves the prediction accuracy of the flame length, particularly under lower equivalence ratio conditions. Further consideration is needed to yield any findings regarding the introduction of the flame stretch effect into the NA-FGM approach to improve the prediction accuracy of the flame length.

Figure 6 Instantaneous iso-surfaces of progress variable with the generation reaction rate of progress variable $\dot{\omega}_C$ for equivalence ratios of $\phi = 0.43, 0.45$ and 0.50 predicted using LES/NA-FGM (Cases 2, 3 and 4, respectively).

Figure 7 Instantaneous distributions of temperature (top), enthalpy (middle), and progress variable (bottom) on the x - y plane for equivalence ratios of $\phi = 0.43, 0.45$ and 0.50 , predicted using LES/NA-FGM (Cases 2, 3 and 4, respectively).

Figure 8 Comparisons of centerline profiles of time-averaged normalized progress variable for equivalence ratios of $\phi = 0.43$, 0.45 and 0.50, predicted using LES/NA-FGM (Cases 2, 3 and 4) and LES/A-FGM (Cases 5, 6 and 7).

Effect of heat loss through the cooled wall on CO emissions

Figures 9 and 10 show a comparison of the time-averaged CO and NO emissions on the centerline at $x = 300$ mm among LES/NA-FGM (Cases 2, 3 and 4), LES/A-FGM (Cases 5, 6 and 7) and experiment [21], respectively. The experimental results show that the CO emissions increase, and the NO emissions decrease for leaner equivalence ratio conditions. The CO emissions of the experiments are approximately 28.0 ppm for $\phi = 0.43$, 5.8 ppm for $\phi = 0.45$, and 1.1 ppm for $\phi = 0.50$. The NO emissions of experiments are approximately 0.5 ppm for $\phi = 0.43$, 0.7 ppm for $\phi = 0.45$, and 1.2 ppm for $\phi = 0.50$. The trends of the CO and NO emissions obtained by LES/NA-FGM show good agreement with the experimental results. By contrast, in the case of LES/A-FGM, although the NO emissions are in good agreement with the experimental results, CO emissions for richer equivalence ratio is overestimated and CO emissions for leaner equivalence ratio is underestimated. Furthermore, we evaluated the factors leading to the high prediction accuracy of CO by LES/NA-FGM. Figures 11-13 show a comparison of the centerline profiles of the time-averaged CO volume fraction between LES/NA-FGM (Cases 2, 3 and 4) and LES/A-FGM (Cases 5, 6 and 7) for $\phi = 0.43$, 0.45 and 0.50. The CO volume fraction between the LES/A-FGM and LES/NA-FGM peaks at approximately $x = 100$ mm in the streamwise direction. It was found that the CO generation rate was almost the same regardless of the heat loss. By contrast, the CO consumption rate for LES/NA-FGM is slower than that for LES/A-FGM according to the distribution of the CO volume fraction at $x = 100$ mm downstream in the streamwise direction. Moreover, the CO emissions of LES/A-FGM under richer equivalence ratio conditions are high because the CO of the equilibrium composition without a heat loss is extracted from the flamelet library at $x = 300$ mm, as shown in Figure 11. The CO volume fraction at $x = 220$ mm downstream in the case of LES/A-FGM was found to be maintained for Case 5. By contrast, the CO volume fraction at $x = 300$ mm of the leaner equivalence ratios ($\phi = 0.43$ and 0.45) did not reach equilibrium even in the LES/A-FGM. This tendency is considered to cause an underestimation of the CO emissions owing to the faster CO consumption rate of the LES/A-FGM. These findings suggest that the difference in CO emissions downstream is caused by the CO consumption rate. Figure 14 shows a comparison of the CO generation and consumption rates for each equivalence ratio. The peak of the CO generation and consumption rates under richer conditions is higher than that under leaner conditions. Therefore, the calculation results confirmed that the high CO concentration region for the leaner conditions tends to be maintained until $x = 300$ mm because the CO consumption rate is lower.

Figure 9 Comparison of time-averaged CO emissions on the centerline at $x = 300$ mm among LES/NA-FGM (Cases 2, 3 and 4), LES/A-FGM (Cases 5, 6 and 7) and experiment [21].

Figure 10 Comparison of time-averaged NO emissions on the centerline at $x = 300$ mm among LES/NA-FGM (Cases 2, 3 and 4), LES/A-FGM (Cases 5, 6 and 7) and experiment [21].

Figure 11 Comparison of centerline profiles of time-averaged CO volume fraction for $\phi = 0.50$ between LES/NA-FGM (Case 2) and LES/A-FGM (Cases 5).

Figure 12 Comparison of centerline profiles of time-averaged CO volume fraction for $\phi = 0.45$ between LES/NA-FGM (Case 3) and LES/A-FGM (Cases 6).

Figure 13 Comparison of centerline profiles of time-averaged CO volume fraction for $\phi = 0.43$ between LES/NA-FGM (Case 4) and LES/A-FGM (Cases 7).

Figure 14 Comparison of CO generation/consumption rates in the flamelet library for $\Delta h = 1021181$.

Figures 15-17 show comparisons of the time-averaged distributions of the source term of the progress variable (top), CO mass fraction (middle) and OH mass fraction (bottom) on the x - y plane for each equivalence ratio between LES/NA-FGM (Cases 2, 3 and 4) and LES/A-FGM (Cases 5, 6 and 7). First, the effect of heat loss on the total reaction is evaluated according to the distribution of the production rate of the progress variable. The reaction of LES/NA-FGM is activated downstream of the burner (marked as (I), (J), and (K) in Figures 15-17, respectively). By contrast, the reaction by LES/A-FGM occurs rapidly near the burner (marked as (L), (M), and (N) in Figures 15-17, respectively). Under the condition of an equivalence ratio of 0.43, the reaction is activated 50 mm downstream of the burner. In particular, this tendency is more apparent under leaner premixed combustion conditions. It is considered that the slow reaction made it easier for CO to remain downstream. The CO generation position is then evaluated. The thickness of the high CO mass fraction layer expands by decreasing the equivalence ratio (marked as (O), (P), and (Q) in Figures 15-17, respectively). These results imply that this is one of the factors of large CO emissions at lower equivalence ratios. In addition, it is considered that the CO consumption rate is a more important factor for increasing the CO emissions. Here, the prediction accuracy of OH radicals is important because the OH radical is dominant for the CO consumption reaction as shown in equation (12).

There is a difference in the OH radical distribution between LES/A-FGM and LES/NA-FGM. When the heat loss through the cooled wall is not considered (LES/A-FGM), the OH mass fraction is asymptotic to the equilibrium value. By contrast, the OH radical by LES/NA-FGM is consumed downstream, and the OH mass fraction gradually decreases (marked as (R), (S), and (T) in Figures 15-17, respectively). This difference greatly affects the CO consumption rate. In addition, Figure 18 shows a comparison of the production rates of the CO mass fraction in the flamelet library for $\phi = 0.43$. As the reaction proceeds, the order of CO generation and consumption does not change owing to the effect of heat loss. Although the CO generation rate becomes lower owing to the effect of heat loss, it was less susceptible to the effect of heat loss through the cooled wall because CO was generated on the unburnt fuel side (the center side of the combustion chamber) as shown in Figures 15-17. By contrast, the CO consumed near the cooled wall was strongly affected by heat loss, and the CO consumption rate decreased with increasing heat loss, as shown in Figure 18. Hence, the difference in the CO consumption rate between LES/A-FGM and LES/NA-FGM is caused by heat loss through the cooled wall. As described in previous section, the flame length does not change between LES/A-FGM and LES/NA-FGM for the same equivalence

ratio. Therefore, the change in CO emissions is caused by the decrease in the CO consumption rate owing to heat loss.

Figure 15 Comparison of the time-averaged distributions of source term of progress variable (top), CO mass fraction (middle) and OH mass fraction (bottom) on the x - y plane for $\phi = 0.43$ between LES/NA-FGM (Case 2) and LES/A-FGM (Case 5).

Figure 16 Comparison of the time-averaged distributions of source term of progress variable (top), CO mass fraction (middle) and OH mass fraction (bottom) on the x - y plane for $\phi = 0.45$ between LES/NA-FGM (Case 3) and LES/A-FGM (Case 6).

Figure 17 Comparison of the time-averaged distributions of source term of progress variable (top), CO mass fraction (middle) and OH mass fraction (bottom) on the x - y plane for $\phi = 0.50$ between LES/NA-FGM (Case 4) and LES/A-FGM (Case 7).

Figure 18 Comparison of production rates of CO mass fraction in the flamelet library for $\phi = 0.43$ between each heat loss $\Delta h (= h_0 - h)$.

CONCLUSIONS

In this study, LES employing a NA-FGM approach, which can account for the effects of heat loss, was applied to CH₄-air super lean premixed combustion fields generated by an axisymmetric jet burner with a cooled wall under pressurized conditions, and the validity to predict the CO emissions was examined through a comparison with the results using the conventional FGM approach and the experiments. In addition, the effects of heat loss and equivalence ratio ($\phi = 0.43$ -0.5) on the CO emissions were investigated in detail.

It was found that the NA-FGM approach improved the prediction accuracies of not only the flame behavior but also the CO emissions compared to the conventional FGM approach, which inherently neglects the heat loss effect. The tendency of the flame length for the lowest equivalence ratio of $\phi = 0.43$, which corresponds to the blow-off limit, was well produced despite the difficulty in predicting a slight reaction at the flame holding point near the combustor inlet. The NA-FGM approach captured well the trend of CO emissions during experiments in which the CO emissions increased with a decrease in the equivalence ratio. This success could be achieved by considering the effects of heat loss on the chemical reactions, such as CO and OH radicals. It was also suggested that the cause of the increase in the CO emissions for low equivalence ratios was not due to the increase in the CO production, but to the slow consumption rate of CO, which kept the CO concentration high downstream.

In conclusion, these results suggested that capturing such a sensitive reduction of the CO consumption rate by heat loss is quite important for an accurate prediction of the total CO emissions in developing a cutting-edge low emissions gas turbine combustor at low load, and for its design tool, the LES employing the NA-FGM approach is strongly recommended.

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