Large-eddy simulation of a three-feed non-premixed flame for an oxy-fuel gas turbine burner

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ABSTRACT

The development of turbulent combustion models for a three-feed non-premixed flame is essential for the research of gas-turbine in the oxy-fuel integrated coal gasification combined cycle (IGCC) system. The quasi-two-dimensional flamelet models are considered effective and accurate substitutes for the two-dimensional flamelet model, however, there are still many aspects worth further investigations in terms of each dimension in the flamelet library. The considerations of heat loss, the presumed probability density function (PDF), and the resolution of the diluent fraction in large-eddy simulation (LES) should be attached importance to. In this paper, heat loss, diluent fraction PDF, and resolution of the diluent fraction have been investigated. It has been shown that the current heat loss model in the flamelet equation can correctly interpret the reactions which are facilitated by high temperature. The beta-PDF used for diluent fraction results in a lower temperature in the flame zone than that of the delta-PDF as the diluent fraction fluctuation used for diluent fraction results in a lower temperature in the flame zone. Watanabe et al. [8] viewed the fuel gas emanated in the coal combustion process as two separate flow streams and connected the two fuel streams by premixing them with varied proportions. A series of one-dimensional flamelet libraries are generated and integrated. Both DNS [8] and LES [9,10] results show reliable predictions although there is still room to improve. Perry and Mueller [11] also used the same model for LES and significant improvements over the one-dimensional FPV model have been achieved. With a diluted stream injected as the third stream, Yu et al. [12,13] have compared three multi-mixture-fraction based flamelet models and applied them by both DNS and LES, concluding that as the mixture fraction for the third stream is not too large the three models are equivalent, while as it is quite large (> 0.8) the scalar dissipation rates play important roles for each model.

INTRODUCTION

CO₂ emission becomes a significant issue nowadays, and a power plant is considered as the main resource of it. Many technologies are used to address this problem, however, the CO₂ capture and storage (CCS) or utilization (CCU) technologies in the power plant will reduce the thermal efficiency. Central Research Institute of Electric Power Industry (CRIEPI) in Japan proposed a concept namely Oxy-fuel IGCC [1,2], in which CO₂ is circulated and injected into both gasifier and gas turbine. When focused on the concept, Ihme et al. [6,7] introduced a parameter called oxidizer split to extend the single-mixture-fraction flamelet progress variable (FPV) approach for the configuration with three mixture fractions. It is pointed out that in the limit of weak interaction and negligible scalar dissipation rate concerning the oxidizer split, this model is equivalent to the two-dimensional flamelet model. Another approximation of the two-dimensional flamelet model is to connect the interaction of the three streams by gradually premixing two of the three streams, and thus reduce the system into a series of two-feed sub-systems. Watanabe et al. [8] viewed the fuel gas emanated in the coal combustion process as two separate flow streams and connected the two fuel streams by premixing them with varied proportions. A series of one-dimensional flamelet libraries are generated and integrated. Both DNS [8] and LES [9,10] results show reliable predictions although there is still room to improve. Perry and Mueller [11] also used the same model for LES and significant improvements over the one-dimensional FPV model have been achieved. With a diluted stream injected as the third stream, Yu et al. [12,13] have compared three multi-mixture-fraction based flamelet models and applied them by both DNS and LES, concluding that as the mixture fraction for the third stream is not too large the three models are equivalent, while as it is quite large (> 0.8) the scalar dissipation rates play important roles for each model.

Due to the nature of the multi-mixture-fraction-based models, more dimensions should be taken into accounts compared to that of the one-mixture-fraction-based models, especially for LES applications. In this paper, one of the models in the literature [12,13] has been chosen to investigate the effect of the heat loss and the diluent fraction PDF, and the resolution of the diluent fraction has also been considered.

QUASI-TWO-DIMENSIONAL FLAMELET MODEL

In the current work, one of the models in literature [12,13] is used in which the diluent is premixed with the oxidizer stream with...
Varied ratios. It is considered that the diluent stream mixes homogeneously with the oxidizer stream if the ratio increment is infinitesimal. And by gradually increasing the proportion of the diluent stream from zero to unity, a series of one-dimensional flamelet libraries can be established. If the increment of the proportion is small enough, the integration of the single libraries can be considered an approximation of the non-premixing process between the diluent and the oxidizer. Specifically, define the mixture fraction of the diluent stream as \( Z_i \), and it can be derived if the fuel stream mixture fraction \( Z_f \) and oxidizer stream mixture fraction \( Z_o \) are known since the three mixture fractions always add up to unity. Since only one mixture fraction is involved when solving the flamelet equations for an individual library, and the second mixture fraction was considered in the post process, we name the model quasi-two-dimensional flamelet model. To clarify the quantity of the third stream, a parameter named diluent fraction is defined as \( W \). In the one-dimensional flamelet library, the mixture fraction of the fuel side (only fuel stream in the current model) is defined by \( Z_i \). Supposing the mass of the fuel stream is \( m_f \), and the mass of the oxidizer stream is \( m_o \). The mass of the diluent part put in the oxidizer side is denoted by \( m_i \). Then according to its definition, the diluent fraction can be deduced as below.

\[
W = \frac{m_i}{m_f + m_i} = \frac{Z_i}{1 - Z_i} \tag{1}
\]

The mixture fraction on the fuel side can be derived as follow.

\[
Z^* = \frac{m_i}{m_f + m_i + m_o} = Z_i \tag{2}
\]

The FPV library without any consideration of heat loss based on the above model can be expressed as below from the DNS point of view.

\[
\Phi = \Phi(Z^*, W, C) \tag{3}
\]

Here, \( C \) is the progress variable and it is defined by the sum of the four species mass fraction \( C = Y_{CO2} + Y_{H2O} + Y_{CO} + Y_{H2} \) in this work.

In the LES study, the probability density function (PDF) distribution for the tracking parameters should be taken into account in the library, and also, the filtered mean and variance values in the flow field have to be figured out. It can be confirmed that the fuel side mixture fraction \( Z^* \) is the continuity parameter in the flamelet equations, while the diluent fraction \( W \) is discretized and integrated in the library. In this work, two kinds of PDF combinations have been considered: (1) Beta-PDF for \( Z^* \) combined with a Delta-PDF for \( W \), and (2) two-independent Beta-PDFs for both parameters.

As it can be observed from Eq. (1) there is a nonlinear correlation between \( Z_i, Z_f, \) and \( W \). Although it is possible to derive a transport equation for the filtered mean and variance of \( W \) here, a straightforward model and its detail are given as below. The sum of the three mixture fractions is always equal to unity and each mixture fraction is falling into the range of \([0, 1]\). By using the Maclaurin Series, the nonlinear correlation can be converted as below.

\[
\frac{Z_i}{1 - Z_i} = Z_i + Z_i Z_f + Z_i Z_f^2 + ... + Z_i (Z_f)^n + ... \tag{4}
\]

The mean value for \( W \) then resorts to the right-hand side terms, and to describe the mean values the correlations below which can be readily derived by the nature of the Favre filtering are indispensable.

\[
\bar{Z}_i Z_i = \bar{Z}_i \bar{Z}_i + Z_i Z_i^* \tag{5}
\]

\[
\bar{Z}_i Z_i^* = (Z_i^2 - \bar{Z}_i^2 - Z_i^*^2)/2 \tag{6}
\]

Then we can expand the right-hand side terms in Eq. (5) as Eqs. (8-10).

\[
\bar{Z}_i Z_i = \bar{Z}_i \bar{Z}_i + Z_i Z_i^* \tag{8}
\]

\[
\bar{Z}_i Z_i^* = (Z_i \bar{Z}_i) Z_i^* - \bar{Z}_i Z_i + (Z_i Z_i^*) \bar{Z}_i \approx \bar{Z}_i Z_i \tag{9}
\]

\[
Z_i Z_i^* = (Z_i \bar{Z}_i) Z_i^* - \bar{Z}_i Z_i + (Z_i Z_i^*) \bar{Z}_i \approx \bar{Z}_i Z_i (\bar{Z}_i)^2 \tag{10}
\]

As shown in Eqs. (8-10), to avoid the loss of generality, it is natural to approximate the \( n \)th term by omitting the quite small terms as below.

\[
\bar{Z}_i Z_i^* \approx \bar{Z}_i Z_i (\bar{Z}_i)^{n-1} \tag{11}
\]

By placing these approximate results back to Eq. (5) the filtered value of \( W \) can be expressed as below.

\[
\frac{Z_i}{1 - Z_i} = Z_i + Z_i Z_f^* \sum_{n=0}^{\infty} Z_i^* = \bar{Z}_i + Z_i Z_f^* / (1 - Z_i^*)
\]

\[
= \bar{Z}_i / (1 - \bar{Z}_i^*) + 0.5 \times (\bar{Z}_i^2 - \bar{Z}_i^3) / (1 - Z_i^*) \tag{12}
\]

As for the variance of \( Z_i^* \), since the fluctuations of the mixture fraction products are considered quite small, it is reasonable to use a truncate result to realize the approximation based on Eq. (4).

\[
\left( \frac{Z_i}{1 - Z_i} \right)^* = Z_i^* + (Z_i Z_i^*) \tag{13}
\]

The second term in Eq. (13) can be written by the mean and variance values as

\[
(Z_i Z_i^*)^* = Z_i^* Z_i^* = Z_i^* Z_i^* - \bar{Z}_i Z_i^* - \bar{Z}_i Z_i^* \tag{14}
\]

Do the filter operation for the square of Eq. (14), and ignore the quite small terms, then the variance of \( Z_i^* \) can be derived.

\[
\frac{Z_i^{*2}}{1 - Z_i^2} = (1 + Z_i^*) (1 + Z_i^* - Z_i^*) Z_i^{*2} + \bar{Z}_i (1 + \bar{Z}_i) Z_i^{*2} - \bar{Z}_i (1 + Z_i - Z_i^*) Z_i^{*2} \tag{15}
\]

In the above equations, to approximate the mean and variance for \( W \), mean values and the variances for three mixture fractions are necessary. The mean values can be obtained by solving conserved transport equations. The variances are modeled by the scaling law [14] as shown in Eq. (16), where the \( \langle \rangle \) is the filtered width, \( \rho \) is the density, and \( C_{Zi} \) can be derived by a dynamic procedure [15].

\[
\rho \bar{Z}_i^{*2} = C_{Zi} \rho \Delta \bar{Z}_i^{1/2} \tag{16}
\]

Also, considering the heat loss through the wall, the above flamelet model can be supplemented by introducing another parameter \( h^2 \) [9,16,17] which is the normalized total enthalpy. It is
assumed that the heat loss is proportional to the temperature source term in the flamelet equation. The steady flamelet equation can be modified by adding a parameter $a$ as shown in Eq. (17). By increasing $a$ from zero, the heat loss can be specified. As $a$ evolves larger, the heat generated in the source term cannot maintain the flame, and extinction will take place. In the present work, the maximum $a$ is set to be 0.6. Based on the result from Eq. (17), the normalized total enthalpy is formulated by Eq. (18).

$$h^* = \frac{h_{\text{max}} - h}{h_{\text{max}} - h_{\text{min}}}$$  \hspace{1cm} (18)

In the above two equations, $c_p$ is the specific heat capacity for constant pressure for the mixture, while $c_{\alpha,a}$ is that for species $k$. $M$ is the molecular weight of the mixture, $T$ is temperature, $Y_{ik}$ is the mass fraction of species $k$. $\chi$ is the scalar dissipation rate, $h_{\text{total}}$ is the specific total enthalpy for species $k$, and $\omega_{\alpha,a}$ is the corresponding reaction rate. $h$ is the total enthalpy which is obtained from the transport equation. $h_{\text{min}}$ is the total enthalpy obtained from the adiabatic library, while $h_{\text{max}}$ is that mapped from the maximum heat loss library. When solving the transport equation, the boundary of the total enthalpy $h$ will be determined by the adiabatic flamelet library, while $h_{\text{max}}$ is used to map from the maximum heat loss library. In this study, LES tests are performed. The filtered conservation equations of mass, momentum, and total enthalpy are solved and presented in Eqs. (22), (23), and (24).

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \quad \hspace{1cm} (22)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ 2\rho \left( \delta_{ij} - \frac{1}{3} \delta_{ij} \right) \right] \frac{\partial T}{\partial x_i} - \frac{\partial (\rho h)}{\partial x_i} + Q_{\text{vol}} \quad \hspace{1cm} (23)$$

$$\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho u_i h)}{\partial x_i} = - \frac{\partial p}{\partial x_i} \frac{\partial h}{\partial x_i} - \frac{\partial (\rho h)}{\partial x_i} + J_{\text{vol}} + Q_{\text{vol}} \quad \hspace{1cm} (24)$$

Also, the tracking parameters such as the mixture fractions and the progress variable are solved as given in Eqs. (25), (26), and (27).

$$\frac{\partial (\rho \tilde{Z}_i)}{\partial t} + \frac{\partial (\rho \tilde{u} \tilde{Z}_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{p}\tilde{D}_{\tilde{z}_i} \frac{\partial \tilde{Z}_i}{\partial x_i} \right) - \frac{\partial J_{\text{vol}}^{\tilde{z}_i}}{\partial x_i} \quad \hspace{1cm} (25)$$

$$\frac{\partial (\rho \tilde{Z}_i)}{\partial t} + \frac{\partial (\rho \tilde{u} \tilde{Z}_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{p}\tilde{D}_{\tilde{z}_i} \frac{\partial \tilde{Z}_i}{\partial x_i} \right) - \frac{\partial J_{\text{vol}}^{\tilde{z}_i}}{\partial x_i} \quad \hspace{1cm} (26)$$

$$\frac{\partial (\rho \tilde{C}_i)}{\partial t} + \frac{\partial (\rho \tilde{u} \tilde{C}_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{p}\tilde{D}_{\tilde{c}_i} \frac{\partial \tilde{C}_i}{\partial x_i} \right) - \frac{\partial J_{\text{vol}}^{\tilde{c}_i}}{\partial x_i} + \tilde{\omega}_i \quad \hspace{1cm} (27)$$

In the above equations, the tilde and overbar denote Favre filtering and spatial filtering. $u$ is the velocity component. $\nu$ is the source term of the progress variable. $D_{\nu}$, $D_{\omega}$, and $D_{\chi}$ are the diffusion coefficients that are derived based on the unity Lewis number. $p$ is the static pressure. $\mu$ is the molecular viscosity. $\delta$ is the Kronecker symbol, and $S_{ij}$ is the strain rate tensor and given by Eq. (28).

$$S_{ij} = 0.5 \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad \hspace{1cm} (28)$$

The sub-grid stress tensor expressed as Eq. (29) is modeled by a Smagorinsky model and the dynamic procedure [15].

$$\tau_{ij}^{\text{SGS}} = \rho \theta \delta_{ij} - \rho \tilde{u}_i \tilde{u}_j \quad \hspace{1cm} (29)$$

$J_0$, $J_{z1}$, $J_{z2}$, and $J_{C}$ are the residual subgrid fluxes that are...
modeled by the well-known gradient transport assumption [18-19] as shown in Eq. (30), in which $S_c$ is set as 0.4 [21]. $\mu_t$ is modeled by Eq. (31), and $C_t$ is also given by the dynamic procedure [15].

$$J^e_p = \widetilde{\rho u} \cdot \vec{q} - \widetilde{\rho \vec{u}} \cdot \vec{q} = \frac{\mu_t}{C_t} \left( \delta_{ij} \right)$$  \hspace{1cm} (30)

$$\mu_t = C_t \delta_{ij}$$ \hspace{0.5cm} (31)

$Q_{rad}$ is the source term of the radiative heat transfer and is modeled by the discrete ordinate method [22] coupled with the weighted sum of the gray gases (WSGG) gas model [23]. For the radiation, the temperature on the wall is estimated by that of the nearest inner cell.

**COMPUTATIONAL DETAILS**

In the current work, the burner configuration is based on the experiments performed by the Central Research Institute of Electric Power Industry (CRIEPI) in Japan [13,24,25]. The sketch of the computational domain is shown in Fig. 1. The fuel and oxidizer are injected alternately from the innermost swirl nozzles, while the rest of the nozzles are used to introduce the diluent stream. Very fine mesh is arranged near the nozzles, where the minimum local filtered width is less than 100 μm and a total of 8.2 million cells is used for the whole domain. In the experiments, the gas samples and temperature measurements were obtained along the marked red lines in the radial direction (0 mm > r > 30 mm) where the distances from the burner outlet are $x$ = 120 mm, $x$ = 260 mm, and $x$ = 400 mm.

The boundary conditions used in the experiment and flamelet libraries can be found in Table 2, where mole fraction ($X$) is used to show the compositions of each stream. In the running condition, the surrounding pressure is 1.0 atm. Also, an overall heat transfer coefficient of 80.0 W/(m²•K) was estimated from the experiment heat loss condition.

The present three cases are calculated by unstructured finite volume code FFR-Comb (NuFD/FrontFlowRed), which has been extended by our group. Spatial derivatives were discretized by the second-order formulations. 576 cores of Fujitsu PRIMERGY CX2550/CX2560 M4 at Kyushu University have been used for each case. 750,000 steps have been computed with a constant time step of $5 \times 10^{-7}$ s.

**RESULTS AND DISCUSSION**

In this section, time-averaged variables such as $\{\tilde{T}\}$, $\{\tilde{X}_O_2\}$, $\{\tilde{X}_C_O_2\}$, and $\{\tilde{X}_C_O\}$ are used to make comparisons between experiments, Case A, Case B, and Case C. The species mole fractions are obtained from the dry gas samples.

Fig. 2 shows the comparisons in terms of temperature and $O_2$ mole fraction, and Fig. 3 illustrates the comparisons for mole fraction of both $C_O_2$ and $C_O$.

![Fig. 2 Comparisons between results from the experiment, Case A, Case B, and Case C for time-averaged temperature (left) and $O_2$ mole fraction (right) in dry mixture samples at three streamwise locations x (top to bottom): 120 mm, 260 mm, and 400 mm.](image1)

![Fig. 3 Comparisons between results from the experiment, Case A, Case B, and Case C for time-averaged mole fraction of $C_O_2$ (left) and $C_O$ (right) in dry mixture samples at three streamwise locations x (top to bottom): 120 mm, 260 mm, and 400 mm.](image2)

It can be seen that the temperature predictions are almost the same for the three cases. As for the non-adiabatic cases Case B and Case C, the prediction is almost overlapped, owning to the negligible variance for the diluent fraction. Temperature predicted by Case A is not the direct mapping results but obtained from the total enthalpy and mapping species, whereas temperature predicted by Case B and Case C is directly looked up from the non-adiabatic libraries. For adiabatic and non-adiabatic cases, the total enthalpies in the flow field are solved by the same transport equation and will not be altered by species distribution, however, the differences in terms of the thermophysical variables and velocity filed will give different total enthalpies although the differences are slight. In
addition, the mapped species for Case A are only obtained from an adiabatic library, while for Case B and Case C the heat loss has been taken into accounts. Considering both the enthalpy and species, it is reasonable to have different temperature predictions for adiabatic and non-adiabatic cases. In the $x = 400$ mm curve, due to the achieved maximum $h_n$, the temperature predicted by non-adiabatic cases is lower than the adiabatic case. Although the temperature deviation is not apparent, the difference for the major species is relatively large between adiabatic and non-adiabatic cases according to Fig. 2. This is because the species in Case A are frozen in an adiabatic library, while in Case B and Case C the heat loss influence has been considered. It can be observed that the concentrations of reactants in Case A are higher than those of Case B and Case C. The non-adiabatic model in this work in Eq. (17) shows that the heat loss is increased as the temperature evolves higher. In the high-temperature area, it is reasonable to consider that the reactions are also severe, thus the reactants assumption is increased. As temperature prediction is almost the same, then for the non-adiabatic cases the temperature without considering heat loss would be higher, therefore, more products and fewer reactants have remained. To some extent, the adiabatic condition consequently suppresses the reactions which are facilitated by high temperature.

To further examine this analysis, comparisons are made for the adiabatic and non-adiabatic libraries for the mass fraction of reactant species CO and product species CO$_2$ as shown in Fig. 4. The ranges have been narrowed to distinguish the difference. It can be observed that especially around a mixture fraction of 0.2, more products and fewer reactants are computed by the non-adiabatic flamelet ((c) and (d)) on the condition of the identical tracking parameters. This trend is consistent with that in literature [17] in which the non-adiabatic case indeed predicted more H$_2$O although comparisons for other major species are missed.

As for the two non-adiabatic cases Case B and Case C, the difference lies in the PDF used for the diluent fraction $W$. The mixing between the diluent and other streams according to the burner configuration in Fig. 1 makes the fluctuation of $W$ non-zero, while the absence of $W$ variance in the library equals a zero $W$ fluctuation and thus obtains a higher temperature. The nature of the present burner makes the three streams mix quite well as soon as they are injected, therefore, the fluctuation of the diluent fraction is quite small for most of the grid cells even in the flame zone which results in a small difference. Although the two independent beta-PDFs have been implemented for $Z$ and $W$, the resolution is coarse. In this context, the Dirichlet joint PDF [26] for two mixture fractions would be a better candidate and it will be implemented in future work.

The PDF implemented for the tracking parameters is associated with the dimensions as well as the resolutions. Here based on the tracking parameters obtained from Case B at $x = 5$ mm, four libraries listed in Table 1(b) are used to test different resolutions of the mean variables with the variances are ignored. Case F is considered as a reference, and the results are shown in Fig. 6.

It can be observed that the resolution in Table 1(a) can basically represent the results in a fine-grids library. However, as for some cases, as the stoichiometric mixture fraction ($Z_{1,st}$) is quite small, which means the large gradients are focused on the small mixture fraction space, then more grids are needed. A strategy is to use non-
uniformed grids for a single library, however, as the Z_{i,\alpha} is varied in the single libraries of the current model, for every single library, identical grid distribution is required for a specific dimension to do the integration, then the balance of the PDF and resolutions should be taken into consideration. It is also observed that as 11 grid points are set for the diluent fraction, the interpolation error tends to occur, especially for temperature and mass fraction of O_2. The third stream is only premixed with O_2 in this work by coupling with W, and in this context, the O_2 mass fraction is quite sensitive to W. Fig. 7 shows the distribution of W in the same locations as Fig. 6 shows, the dash lines and two ends such as 0.0 and 1.0 are the grids in the library. The parts of the curve located between the grids have to be interpolated when mapping the library. When W is distributed close to some grid point that is stored in the library, such as r < 7 mm, the prediction is expected consistent with the fine-grid library. It is important to ensure enough grids for the diluent fraction as a large gradient takes place where the linear interpolation usually gives inaccurate results for coarse resolution.

**CONCLUSIONS**

In this work, LESs have been tested by coupling a quasi-two-dimensional flamelet model. The influence of the heat loss consideration on the current model has been discussed. The absence of the heat loss consideration will suppress the reactions which are facilitated by high temperature. Different PDFs for the diluent fraction will result in different mapping data in the flame zone as its fluctuation is not zero, however, the consideration of the variance requires more dimensions in the LES library and will decrease the library resolution. For the quasi-two-dimensional flamelet model application, it is also very important to ensure a fine resolution for W.

**ACKNOWLEDGEMENTS**

This work is partially supported by MEXT as “Program for Promoting Researches on the Supper-computer Fugaku” (Digital Twins of Real World’s Clean Energy Systems with Integrated Utilization of Supper-simulation and AI) and used computational resources of ITO computer provided by the RIKEN Center for Computational Science (Project ID: hp200123). This work is also partially supported by the HPCI System Research Project (Project ID: hp170315).

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