Numerical Investigation of Turbulent Combustion Flow in Industrial Combustor with Flamelet Approach

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Abstract
In this paper, an industrial gas-turbine combustor was numerically investigated by applying large-eddy simulation for turbulent model and 2-scalar flamelet approach for combustion model. In the combustion model, the structures of premixed and non-premixed flame are expressed by conservative scalar and levelset function respectively. These two concepts are coupled for partial premixed combustion field. Flow field properties inside the flame (temperature, density, laminar flame speed) are determined by “flamelet data”. The flamelet data is mainly divided in “premixed-like flamelet data” and “diffusion-like flamelet data” in this study. The premixed-like flamelet data is based on chemical equilibrium assumption and is evaluated by 0-dimensional chemical reaction calculation. On the other hand, the diffusion-like flamelet data is based on laminar flamelet assumption and is evaluated by 1-dimensional counter flow combustion calculation. In this study, for the diffusion-like combustion field in the industrial combustor, diffusion-like flamelet data was newly applied. The predicted gas temperature showed a little higher value than the temperature calculated by using the premixed-like flamelet data. However, the predicted temperatures underestimated measured one. Therefore, in this case, it was cleared that difference of flamelet data is insignificant for improving analysis accuracy.

Key words: flamelet data, flamelet approach, LES, partial premixed combustion, diffusion-like combustion field

1. Introduction
In development of gas-turbine combustor, Dry Low Emission (DLE) combustion is one of the effective methods to achieve reduction in NOx (nitric oxide and nitrogen dioxide etc) emission and high heat efficiency in a gas-turbine system. In the DLE combustor, lean premixed combustion is used to exclude local high temperature region and make temperature distribution in the combustor uniform. Therefore it is important for development of the DLE combustor to investigate instantaneous flow field properties in local regions of the combustor. A Computational fluid dynamics (CFD) technique, in particular, large-eddy simulation (LES), enables us to obtain abundant about instantaneous combustion field properties. Thus, CFD has become an effective tool for development of DLE combustors. However, because in an actual combustor, premixed and non-premixed combustions often simultaneously appear and the flow field in the combustor is generally turbulent. From view of this point, introduction of many physical models is needed to numerically reproduce turbulent combustion field in the actual combustor. Therefore, the models used in the simulation are needed to be sufficiently validated.

In the previous research, Takahashi et al (2014) [1] numerically investigated combustion field in the DLE combustor for 160MW class gas-turbine produced by Toshiba Corporation (shown in Fig.1) by LES and flamelet...
approach. In the flamelet approach, structure inside the flame is considered as laminar flame, and flow field properties inside the flame (temperature, density, and laminar flame speed) is determined by flamelet data. In the research, the flamelet data based on assumption of chemical equilibrium model and was made by calculating 0-dimentional equilibrium solution. In other words, this flamelet data was based on close to premixed combustion calculation. The 160MW DLE combustor has two premixed burners (called "Fpp" and "Fm") and one diffusion burner (called "Fpd"). In the research, numerical simulations were conducted for several cases changing fuel balance for the three burners. In the result for the case increasing fuel in Fpd (Case A), gas temperature in an exit duct of the DLE combustor was underpredicted compared with the measured temperature. In the other hand, prediction of the temperature for the case increasing fuel in Fm (Case B) showed good agreement with the measured one for the Case B. The study concluded that the flamelet data based on the chemical equilibrium assumption was appropriate to the Case B (premixed-like combustion field), while the chemical assumption was not suitable for the Case A (diffusion-like combustion field).

In the present research, we make flamelet data for diffusion-like flame of the Case A based on assumption of laminar flamelet. Moreover we validate the flamelet model for the case A with gas temperature near the exit comparing with the measured one.

2. Flow-Field modeling
2.1 Governing Equation

In this research, we applied LES as a turbulent model under a low Mach number approximation. In the idea of LES, large eddies (grid scale) are calculated directly, small eddies (sub grid scale) which are considered to be universal are approximated by modeling. Governing equations must be spatially filtered for applying LES. Filtered continuity equation and momentum conservation laws which consists of the Navier-Stokes equation are respectively given by

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho \hat{u}_i}{\partial x_j} = 0, 
\]

\[
\frac{\partial \rho \hat{u}_i}{\partial t} + \frac{\partial \rho \hat{u}_i \hat{u}_j}{\partial x_j} = \frac{\partial \hat{p}}{\partial x_i} + \frac{\partial g}{\partial x_j} \left[ \mu \left( \frac{\partial \hat{u}_i}{\partial x_j} + \frac{\partial \hat{u}_j}{\partial x_i} \right) - \tau_{ij}^{SGS} \right],
\]

where \( \tau_{ij}^{SGS} \) means sub-grid scale (SGS) turbulent stress, and is represented by the standard Smagorinsky model [2]:

\[
\tau_{ij}^{SGS} = -2\mu^{SGS} \hat{S}_{ij},
\]

\[
\mu_{ij}^{SGS} = \hat{\rho}(Cs\Delta)^2 \sqrt{\hat{S}_{ij}\hat{S}_{ij}}
\]

where \( \Delta \) is the spatial filter width. In this research, the Smagorinsky constant, Cs, is assumed to 0.15. The strain

![Figure 1: Overview of Toshiba DLE combustor.](image_url)
tensor, $\tilde{S}_{ij}$, is calculated as follows:

$$\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)$$  \hspace{1cm} (5)$$

In the flamelet approach, equations of combustion field are composed of an improved $G$-equation which is proposed by Liu and Oshima [3] modifying the original flamelet approach [4, 5] and a conservation of scalar ($\xi$-equation). The scalar $\xi$ is defined by a mixture fraction of fuel and oxidant species which can be calculated by

$$\xi(x_i, t) = \frac{Y_{oxi} - Y(x_i, t)}{Y_{oxi} - Y_{fuel}},$$  \hspace{1cm} (6)$$

where $Y$ represents mass fraction. A partially-premixed flame is expressed by a combination of both the scalar function. The scalar transport equation of $\xi$ is expressed as follows:

$$\frac{\partial \rho \tilde{\xi}}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{\xi}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu SGS}{Sc} \frac{\partial \tilde{\xi}}{\partial x_j} \right) - \left[ \rho \left( \tilde{u}_i \tilde{\xi} - \tilde{u}_j \tilde{\xi} \right) \right].$$  \hspace{1cm} (7)$$

$$\tilde{\rho} \left( \tilde{u}_i \tilde{\xi} - \tilde{u}_j \tilde{\xi} \right) = \left( \frac{\mu SGS}{Sc SGS} \frac{\partial \tilde{\xi}}{\partial x_j} \right).$$  \hspace{1cm} (8)$$

where $Sc$ is the Schmidt number. Note that the second term on the right-hand side of Eq8 is modeled by the gradient diffusion assumption for the effect of SGS fluctuation. On the other hand, the $G$-equation is given by

$$\frac{\partial \rho \tilde{G}}{\partial t} + \frac{\partial \rho \tilde{u}_i \tilde{G}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu SGS}{\sigma_g} \tilde{G} \right) \frac{\lambda}{C_p} \frac{\partial \tilde{G}}{\partial x_j} + 2\tilde{\rho}_{u} S_{T} \tilde{G} \left[ \frac{\partial \tilde{G}}{\partial x_j} \right],$$  \hspace{1cm} (9)$$

where $\lambda$, $C_p$, $\rho_u$, and $S_T$ are the thermal conductivity, the specific heat at constant pressure, the density of unburnt gas, and the turbulent flame speed, respectively. The above equation actually describes propagation of flame surface. Thus, the variables $G$ is a level-set function and also means non-dimensional temperature. This flamelet approach is based on an assumption that the inner structure of turbulent flame is basically the same to that in a laminar flame. The levelset function $G$ indicates the partially-premixed flame between the unburnt ($G = 0$) and burnt ($G = 1$) states.

Turbulent flame speed, $S_T$, that is significant variable to feature flame structure in combustion field, is obtained by Daniele’s formulation [6] which is given by

$$\frac{S_T}{S_L} = \max \left\{ a \left( \frac{u'}{S_L} \right)^{0.63} \left( \frac{L_T}{\sigma_L} \right)^{-0.37} \left( \frac{p}{p_R} \right)^{0.63} \left( \frac{T_0}{T_R} \right)^{-0.63}, \alpha_{max} \right\},$$  \hspace{1cm} (10)$$

where $u'$ is the turbulence intensity, and

$$\left( \frac{L_T}{\sigma_L} \right) = b \left( \frac{p}{p_R} \right)^{0.66}, \hspace{0.5cm} a = 337.45, \hspace{0.5cm} b = 8.3, \hspace{0.5cm} p_R = 0.1MPa, \hspace{0.5cm} T_R = 1K.$$  

It is report in Ref. [6] that the turbulence flame speed has a limit value depending on pressure. In the present model, the limiter, $\alpha_{max}$, is evaluated as the following expression:
A laminar flame speed, $S_L$, becomes a variable dependent on the local mixture fraction, which is estimated by the solution of the laminar premixed flame in the same manner as for the other physical variables. The local temperature and density between the unburnt and burnt states are given by the linear coupling of $G$. These variables are given by

$$\tilde{T} = (1 - \tilde{G})T_u(\tilde{\xi}) + \tilde{G}T_b(\tilde{\xi}),$$  \hspace{1cm} (12)

$$\tilde{\rho} = \frac{\rho_u(\tilde{\xi})\rho_b(\tilde{\xi})}{(1 - \tilde{G})\rho_u(\tilde{\xi}) + \tilde{G}\rho_b(\tilde{\xi})} \hspace{1cm} (13)$$

The local laminar flame speed, the local density and the local temperature at burnt state are determined by reference to “flamelet data”.

### 2.2 Flamelet data

In this study, flamelet data was evaluated by the chemical reaction analysis using detail chemical reaction calculation software “CHEMKIN-PRO Release 15112” [7] with elemental chemical reaction “GRI-MECH 3.0” [8]. We made two flamelet data, which were respectively premixed like flamelet data based on the chemical equilibrium assumption and diffusion-like flamelet data based on the laminar flamelet assumption. Local temperature and local
density are obtained by the flamelet data with the scalar $\xi$. For convenience of calculation, the data are approximated by polynomial equations.

In the chemical equilibrium assumption, it is assumed that a time scale of combustion reaction is much smaller than that of mixture between fuel and oxidant, and consequently each chemical species locally reach chemical equilibrium at the moment when they mix. In this idea, the premixed-like flamelet data is evaluated by the 0-dimensional chemical reaction calculation. Here, the local temperature is adiabatic flame temperature with each scalar $\xi$ ($0 \leq \xi \leq 1$).

On the other hand, in the laminar flamelet assumption, it is assumed that speed of combustion reaction is not sufficiently fast comparing with diffusion speed of chemical species. Therefore, the combustion status is thought to be diffusion combustion. In this assumption, the diffusion-like flamelet data is evaluated by 1-dimensional counter flow combustion calculation. In this calculation, on the central axis connected by center of the fuel nozzle and one of the oxidant nozzle, a local scalar $\xi$, local temperature and local density with each coordinate are calculated.

The flamelet data which determines local laminar flame speed is common, and is calculated by 1-dimensional premixed combustion calculation. Because, mole fraction, pressure, and temperature of unburnt mixture gas are needed in evaluating laminar flame speed, the values are the same between the two models. The flamelet data are shown in Fig.2.

### 2.3 Numerical Implementation

The present simulations are performed with a software “Frontflow/Red ver. 3.1” [9] for the multi-physics simulation solver developed and distributed by Hokkaido University. The numerical scheme is discretized based on the finite volume for unstructured grid systems. For advection and viscous terms of the governing equations, the second-order central difference scheme is applied. However, momentum equations of velocity field are blended by first-order up wind scheme of 5% to suppress numerical oscillation. Spatial gradient of flow field variables at cell center are estimated by the Gauss method. For the time integrations, the Crank-Nicolson implicit scheme is adopted. Time step is set to $5 \times 10^{-7}$s. Poisson equation to correct pressure are solved by the ICCG method. Typical iteration number of the pressure correction equation is approximately 1,500 in this calculation. For massive parallel computation, MPI technique with domain partition approach is adopted.
2.4 Computation Geometry

For the DLE combustor, we fully use tetrahedral unstructured grid which is often applied to actual design and generally takes less human effort in the grid generation than hexahedral and/or combined grids. The combustor geometry including the main premixed burner, the pilot premixed burners, the pilot diffusion burners and cooling slits and holes on the side wall is solved by fine resolutions mesh of 45,483,350 tetrahedral elements and 7,742,288 nodes. Figure 3 shows $x$-$y$ plane ($z = 0 \text{ mm}$) and $x$-$z$ plane ($y = 0 \text{ mm}$) of the computational grids with outlines of boundaries. To resolve turbulent fluctuation finely, grids in the combustion region are concentrated while those in the exit duct part are relatively coarse.

Boundary groups of the analytical object are composed of inlet, outlet, and wall boundaries shown in Figs. 4(a) and 4(b). Moreover, the inlet boundary is categorized by the three parts: premixed inlet (fuel and air), diffusion inlet (pure fuel and pure air), and cooling air. Mass flow rate and temperature of air, fuel, and premixed gas at inlet boundaries are given. Fuel or air inflows through the ports of pilot diffusion burners (“Fpd” and “Apd”). Cooling air inflows through the slits and holes on the side wall. On the other hand, premixed gas flows through the main premixed burner (“Fm” and “Am”) and pilot premixed burner (“Fpp” and “App”). Pressure at the inlet boundary is determined by extrapolation from an interior point (neighboring cell of the inlet boundary) in the computational domain. At outlet, static pressure is fixed and outflow condition without reverse flow is imposed for the velocity field. No-slip condition is imposed for the velocity at all walls. There is no pressure gradient in the wall direction. In addition, the levelset function ($G$) and mixture fraction ($\xi$) are determined by the Neumann condition at the walls.

2.5 Calculation Conditions

In this simulation, we target “Case A” described above. In Case A, rich fuel inflows through the fuel inlet of the pilot diffusion burner, so that combustion field in the DLE combustor reproduces diffusion-like flames. Table 1 shows mass flow rate of fuel conditions at the three fuel inlets (Fpd, Fm, and Fpp). Table 2 shows the calculation conditions. Note that the typical fuel composition used in DLE combustor is methane of 89.6% (volume fraction), ethane of 5.6%, propane of 3.4%, and other higher alkanes.

The present simulation is mainly performed by 768 cores of computing system “HITACHI HA8000-tc/HT210” of Research Institute for Information Technology, Kyushu University. In typical case of this work, 1,000 time steps of combustion flow simulation on the 7.7 million nodes (and 45 million elements) spend approximately 1.2 hours by 768 cores of HITACHI HA8000-tc/HT210.
3 Results and Discussion

3.1 Comparison on measurement section

Gas temperature near the exit of the DLE combustor were measured with thermocouples. Measurement positions (“TC1”, “TC2”, “TC3”, “TC4”, and “TC5”) are described shown in Fig. 5. Comparison of time averaged temperatures by experiment, CFD approaches with diffusion-like and premixed-like flamelet data is shown in Fig. 6. The green plots in Fig.6(a)-8(a) are measurement points. Computed temperature by using the diffusion-like flamelet data based on the laminar flamelet assumption is approximately 50K higher than that calculated by using the premixed-like flamelet data based on the chemical equilibrium assumption. However, the temperatures simulated by using the diffusion-like flamelet data underestimate the measured ones. Therefore, prediction of temperature is not improved in the case using the diffusion-like flamelet data. Time averaged scalar $G$ and $\xi$ profiles are shown in Figs. 7, 8 respectively. Predicted scalar $G$ by using the diffusion-like flamelet data is totally lower than that by the premixed-like flamelet data. On the other hand, for predicted $\xi$, there is little difference between two models. Figure 9 shows both of flamelet data in range where the predicted $\xi$ is found in Fig.8. In the range of $\xi$, temperature of burnt gas calculated by the laminar flamelet assumption is approximately 100K higher than that calculated by the chemical equilibrium assumption. From the above, predicted scalar $G$, $\xi$, and temperature of flamelet data in the two assumption result in difference of temperature shown in Fig.5.

<table>
<thead>
<tr>
<th></th>
<th>Fpd</th>
<th>Fpp</th>
<th>Fm</th>
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<td>Fuel/Air ratio (kg/kg)</td>
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<td>Air temperature (K)</td>
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<td>Total pressure (MPa)</td>
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</tbody>
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Figure 5: Measuring position of gas temperature

(a) Calculated distribution (above: diffusion, below: premixed).
(b) Calculation and measurement profile.

Figure 6: Comparisons of measured and calculated by two flamelet data gas temperature profile at exit.
3.2 Ignition on the main premixed burner

According to the previous research [1], it seemed that no ignition sufficiently occurs downstream of the third duct of the main premixed burner for the case A simulated by using premixed-like flamelet data. This was because of low turbulent flame speed with decrease in laminar flame speed which is caused by lean mixture fraction in the main premixed burners. The problem of ignition resulted in underestimation of the gas temperature on the measurement section. We therefore examine the simulation result by using the two flamelet data near the third duct. Time averaged
scalar $G$ profile on $x$-$y$ plane is shown in Fig.10. Near each duct of main premixed burner, there does not appear remarkable difference of scalar $G$ between the results by two flamelet data. In addition, in both results, fuel inflowing through the second duct and the third duct seems not to be burning. However, in the whole region, scalar $G$ calculated by using the diffusion-like flamelet data is a little lower than one calculated by using the other flamelet data. From the above, although the two flamelet data affects the prediction of scalar $G$, it is thought that changing flamelet data makes no difference in prediction of ignition at the third burner of main premixed burner.

Time averaged distribution of mixture fraction is shown in Fig.11. Instantaneous distribution of laminar flame speed ($S_L$) and local turbulent flame speed ($S^* = 2S_T\tilde{G}$) on $x$-$y$ plane are shown in Fig.12 and Fig.13, respectively. Note that the two physical values are multiplied by density of unburnt gas, therefore, they are actually distributed as mass flux. There is no difference in the calculated mixture fraction between the two cases, and mixture fraction near the third duct is lower than that near the other ducts. It seems that the calculated laminar flame speed by using the diffusion-like flamelet data is lower than that by using the other in region between the pilot burner and the second duct. However, it is thought that time averaged laminar flame speed has little difference, because mixture fraction in each case is not different in the region, and the flamelet data is the same between each assumption. Turbulent flame speed calculated by Daniele’s model basically follows to laminar flame speed, so that difference of local turbulent speed between the cases is similar with that of laminar flame speed. Therefore, it is thought that no ignition in the case of using diffusion-like flamelet data is the same with that in the case of using premixed-like flamelet data.

![Figure 10: Time averaged $G$ distribution on $x$-$y$ plane.](image)

(a) Result of diffusion-like flamelet data.  
(b) Result of premixed-like flamelet data.

![Figure 11: Time averaged mixture fraction distribution on $x$-$y$ plane.](image)

(c) Result of diffusion-like flamelet data.  
(d) Result of premixed-like flamelet data.
4 Conclusions

Turbulent combustion fields in the dry low emission (DLE) combustor for 160MW class gas-turbine developed by Toshiba corporation were numerically simulated by large-eddy simulation (LES) as a turbulent model and 2-scalar flamelet approach as a combustion model. In this study, the diffusion-like flamelet data which determines temperature and density for mixture fraction calculated by a conservative scalar equation was newly made by the laminar flamelet assumption and used for the diffusion-like combustion field under lean fuel condition, instead of the premixed-like flamelet data by the chemical equilibrium assumption. The temperature calculated by using the diffusion-like flamelet data near the exit duct was a little higher than prediction by using premixed-like one. However, compared with measured temperature, calculated one by diffusion-like flamelet data was also underestimated. In addition, ignition at the third duct of the main premixed burner was inaccurately predicted in results by using both flamelet data. Therefore, it was clarified that difference of flamelet data have a slight influence on improving analysis accuracy in this diffusion-like combustion field. On the other hand, in the previous research [1] under the premixed-like combustion, it was reported that ignition at the third duct of main premixed burner was kept. It was suggested that turbulent flame speed was correctly predicted in the previous calculation. Therefore, factor improving analysis accuracy is expected to be turbulent flame speed model. It is thought that inaccurate prediction of turbulent flame speed makes the ignition not occur. Therefore, it is concluded that fundamental validation of turbulent flame speed model under diffusion-like combustion field is needed.
Acknowledgment

Christian Schwieder (Brandenburgische Technische Universität, BTU Cottbus) made a great contribution to the present study. Here, we express gratitude to him. The computation was mainly carried out using the computer facilities at the Research Institute for Information Technology, Kyushu University.

Reference


